

The Book of Statistical Proofs

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Chapter I

General Theorems

1 Probability theory

1.1 Random experiments

1.1.1 Random experiment

Definition: A random experiment is any repeatable procedure that results in one (\rightarrow I/1.2.2) out of a well-defined set of possible outcomes.

- The set of possible outcomes is called sample space (\rightarrow I/1.1.2).
- A set of zero or more outcomes is called a random event (\rightarrow I/1.2.1).
- A function that maps from events to probabilities is called a probability function (\rightarrow I/1.5.1).

Together, sample space (\rightarrow I/1.1.2), event space (\rightarrow I/1.1.3) and probability function (\rightarrow I/1.1.4) characterize a random experiment.

Sources:

- Wikipedia (2020): “Experiment (probability theory)”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-11-19; URL: [https://en.wikipedia.org/wiki/Experiment_\(probability_theory\)](https://en.wikipedia.org/wiki/Experiment_(probability_theory)).

1.1.2 Sample space

Definition: Given a random experiment (\rightarrow I/1.1.1), the set of all possible outcomes from this experiment is called the sample space of the experiment. A sample space is usually denoted as Ω and specified using set notation.

Sources:

- Wikipedia (2021): “Sample space”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-11-26; URL: https://en.wikipedia.org/wiki/Sample_space.

1.1.3 Event space

Definition: Given a random experiment (\rightarrow I/1.1.1), an event space \mathcal{E} is any set of events, where an event (\rightarrow I/1.2.1) is any set of zero or more elements from the sample space (\rightarrow I/1.1.2) Ω of this experiment.

Sources:

- Wikipedia (2021): “Event (probability theory)”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-11-26; URL: [https://en.wikipedia.org/wiki/Event_\(probability_theory\)](https://en.wikipedia.org/wiki/Event_(probability_theory)).

1.1.4 Probability space

Definition: Given a random experiment (\rightarrow I/1.1.1), a probability space (Ω, \mathcal{E}, P) is a triple consisting of

- the sample space (\rightarrow I/1.1.2) Ω , i.e. the set of all possible outcomes from this experiment;
- an event space (\rightarrow I/1.1.3) $\mathcal{E} \subseteq 2^\Omega$, i.e. a set of subsets from the sample space, called events (\rightarrow I/1.2.1);
- a probability measure $P : \mathcal{E} \rightarrow [0, 1]$, i.e. a function mapping from the event space (\rightarrow I/1.1.3) to the real numbers, observing the axioms of probability (\rightarrow I/1.4.1).

Sources:

- Wikipedia (2021): “Probability space”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-11-26; URL: https://en.wikipedia.org/wiki/Probability_space#Definition.

1.1.5 Measured data

Definition: Data, also “measured data”, are any set of one or more random variables (\rightarrow I/1.2.2) – discrete or continuous (\rightarrow I/1.2.6), univariate or multivariate (\rightarrow I/1.2.7) – that have been observed, measured or collected in the course of a random experiment (\rightarrow I/1.1.1).

The random variables that are part of data have probability distributions (\rightarrow I/1.5.1). Assumptions for these probability distributions are made with generative models (\rightarrow I/5.1.1). Generative models can form the basis for statistical tests (\rightarrow I/4.3.1) checking statistical hypotheses (\rightarrow I/4.2.1).

1.1.6 Statistical sample

Definition: Let X be a random variable (\rightarrow I/1.2.2) or a set of random variables (\rightarrow I/1.2.2). Then, a sample, also “statistical sample”, is a set of realizations of this random variable, obtained via observation and measurement (\rightarrow I/1.1.5) within random experiments (\rightarrow I/1.1.1):

$$x = \{x_1, \dots, x_n\} . \quad (1)$$

Sources:

- Elliott, Graham (2024): “Sampling”; in: *Understanding Statistics*, retrieved on 2024-11-15; URL: <https://econweb.ucsd.edu/~gelliott/Chapter5.html>.

1.1.7 Sample size

Definition: Let $x = \{x_1, \dots, x_n\}$ be a statistical sample (\rightarrow I/1.1.6) from a random variable (\rightarrow I/1.2.2) or a set of random variables (\rightarrow I/1.2.2) X . Then, the number of elements n in this sample is called the “sample size”.

Sources:

- Wikipedia (2024): “Sampling (statistics)”; in: *Wikipedia, the free encyclopedia*, retrieved on 2024-11-22; URL: [https://en.wikipedia.org/wiki/Sampling_\(statistics\)](https://en.wikipedia.org/wiki/Sampling_(statistics)).

1.1.8 Sample statistic

Definition: A statistic, also “sample statistic”, is any quantity calculated from the data points (\rightarrow I/1.1.5) in a sample (\rightarrow I/1.1.6) that is used for statistical purposes.

Examples include statistics used to estimate the parameters (\rightarrow I/1.5.7) of a probability distribution (\rightarrow I/1.5.1) and test statistics (\rightarrow I/4.3.5) to evaluate statistical hypotheses (\rightarrow I/4.2.1).

Sources:

- Wikipedia (2024): “Statistic”; in: *Wikipedia, the free encyclopedia*, retrieved on 2024-10-04; URL: <https://en.wikipedia.org/wiki/Statistic>.

1.1.9 Descriptive vs. inferential

Definition: A statistic (\rightarrow I/1.1.8) may be called

- a descriptive statistic, if it quantitatively describes or summarizes a statistical sample (\rightarrow I/1.1.6) or estimates (\rightarrow I/3.1.1) aspects of the probability distribution (\rightarrow I/1.5.1) from which the sample is drawn, e.g. sample mean (\rightarrow I/1.12.2);
- an inferential statistic, if its sampling distribution (\rightarrow I/1.5.6) under the null hypothesis (\rightarrow I/4.3.2) can be used for testing hypotheses (\rightarrow I/4.3.1) about parameters (\rightarrow I/1.5.7) of the distribution (\rightarrow I/1.5.1) from which the sample is drawn, e.g. F-statistic (\rightarrow IV/1.3.1).

Sources:

- Wikipedia (2025): “Descriptive statistics”; in: *Wikipedia, the free encyclopedia*, retrieved on 2025-04-04; URL: https://en.wikipedia.org/wiki/Descriptive_statistics.
- Wikipedia (2025): “Statistical inference”; in: *Wikipedia, the free encyclopedia*, retrieved on 2025-04-04; URL: https://en.wikipedia.org/wiki/Statistical_inference.

1.2 Random variables

1.2.1 Random event

Definition: A random event E is the outcome of a random experiment (\rightarrow I/1.1.1) which can be described by a statement that is either true or false.

- If the statement is true, the event is said to take place, denoted as E .
- If the statement is false, the complement of E occurs, denoted as \overline{E} .

In other words, a random event is a random variable (\rightarrow I/1.2.2) with two possible values (true and false, or 1 and 0). A random experiment (\rightarrow I/1.1.1) with two possible outcomes is called a Bernoulli trial (\rightarrow II/1.2.1).

Sources:

- Wikipedia (2020): “Event (probability theory)”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-11-19; URL: [https://en.wikipedia.org/wiki/Event_\(probability_theory\)](https://en.wikipedia.org/wiki/Event_(probability_theory)).

1.2.2 Random variable

Definition: A random variable may be understood

- informally, as a real number $X \in \mathbb{R}$ whose value is the outcome of a random experiment (\rightarrow I/1.1.1);
- formally, as a measurable function X defined on a probability space (\rightarrow I/1.1.4) (Ω, \mathcal{E}, P) that maps from a sample space (\rightarrow I/1.1.2) Ω to the real numbers \mathbb{R} using an event space (\rightarrow I/1.1.3) \mathcal{E} and a probability function (\rightarrow I/1.5.1) P ;
- more broadly, as any random quantity X such as a random event (\rightarrow I/1.2.1), a random scalar (\rightarrow I/1.2.2), a random vector (\rightarrow I/1.2.3) or a random matrix (\rightarrow I/1.2.4).

Sources:

- Wikipedia (2020): “Random variable”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-05-27; URL: https://en.wikipedia.org/wiki/Random_variable#Definition.

1.2.3 Random vector

Definition: A random vector, also called “multivariate random variable”, is an n -dimensional column vector $X \in \mathbb{R}^{n \times 1}$ whose entries are random variables (\rightarrow I/1.2.2).

Sources:

- Wikipedia (2020): “Multivariate random variable”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-05-27; URL: https://en.wikipedia.org/wiki/Multivariate_random_variable.

1.2.4 Random matrix

Definition: A random matrix, also called “matrix-valued random variable”, is an $n \times p$ matrix $X \in \mathbb{R}^{n \times p}$ whose entries are random variables (\rightarrow I/1.2.2). Equivalently, a random matrix is an $n \times p$ matrix whose columns are n -dimensional random vectors (\rightarrow I/1.2.3).

Sources:

- Wikipedia (2020): “Random matrix”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-05-27; URL: https://en.wikipedia.org/wiki/Random_matrix.

1.2.5 Constant

Definition: A constant is a quantity which does not change and thus always has the same value. From a statistical perspective, a constant is a random variable (\rightarrow I/1.2.2) which is equal to its expected value (\rightarrow I/1.12.1)

$$X = E(X) \quad (1)$$

or equivalently, whose variance is zero (\rightarrow I/1.13.6)

$$\text{Var}(X) = 0. \quad (2)$$

Sources:

- ProofWiki (2020): “Definition: Constant”; in: *ProofWiki*, retrieved on 2020-09-09; URL: <https://proofwiki.org/wiki/Definition:Constant#Definition>.

1.2.6 Discrete vs. continuous

Definition: Let X be a random variable (\rightarrow I/1.2.2) with possible outcomes \mathcal{X} . Then,

- X is called a discrete random variable, if \mathcal{X} is either a finite set or a countably infinite set; in this case, X can be described by a probability mass function (\rightarrow I/1.6.1);
- X is called a continuous random variable, if \mathcal{X} is an uncountably infinite set; if it is absolutely continuous, X can be described by a probability density function (\rightarrow I/1.7.1).

Sources:

- Wikipedia (2020): “Random variable”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-10-29; URL: https://en.wikipedia.org/wiki/Random_variable#Standard_case.

1.2.7 Univariate vs. multivariate

Definition: Let X be a random variable (\rightarrow I/1.2.2) with possible outcomes \mathcal{X} . Then,

- X is called a two-valued random variable or random event (\rightarrow I/1.2.1), if \mathcal{X} has exactly two elements, e.g. $\mathcal{X} = \{E, \bar{E}\}$ or $\mathcal{X} = \{\text{true}, \text{false}\}$ or $\mathcal{X} = \{1, 0\}$;
- X is called a univariate random variable or random scalar (\rightarrow I/1.2.2), if \mathcal{X} is one-dimensional, i.e. (a subset of) the real numbers \mathbb{R} ;
- X is called a multivariate random variable or random vector (\rightarrow I/1.2.3), if \mathcal{X} is multi-dimensional, e.g. (a subset of) the n -dimensional Euclidean space \mathbb{R}^n ;
- X is called a matrix-valued random variable or random matrix (\rightarrow I/1.2.4), if \mathcal{X} is (a subset of) the set of $n \times p$ real matrices $\mathbb{R}^{n \times p}$.

Sources:

- Wikipedia (2020): “Multivariate random variable”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-11-06; URL: https://en.wikipedia.org/wiki/Multivariate_random_variable.

1.2.8 independent and identically distributed

Definition: Let X_i for $i = 1, \dots, n$ be random variables (\rightarrow I/1.2.2). Then, X_1, \dots, X_n are called independent and identically distributed (i.i.d.), if (i) they are statistically independent (\rightarrow I/1.3.6) and (ii) they follow the same probability distribution (\rightarrow I/1.5.1) \mathcal{D} with the same parameters θ :

$$X_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{D}(\theta), \quad i = 1, \dots, n. \quad (1)$$

Often, especially in linear regression models, error terms (\rightarrow III/1.5.1) are independent and identically distributed according to a normal distribution (\rightarrow II/3.2.1) with mean zero and unknown variance:

$$\varepsilon_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2), \quad i = 1, \dots, n. \quad (2)$$

Sources:

- Wikipedia (2024): “Independent and identically distributed random variables”; in: *Wikipedia, the free encyclopedia*, retrieved on 2024-08-08; URL: https://en.wikipedia.org/wiki/Independent_and_identically_distributed_random_variables#Introduction.

1.3 Probability

1.3.1 Probability

Definition: Let E be a statement about an arbitrary event such as the outcome of a random experiment (\rightarrow I/1.1.1). Then, $p(E)$ is called the probability of E and may be interpreted as

- (objectivist interpretation of probability:) some physical state of affairs, e.g. the relative frequency of occurrence of E , when repeating the experiment (“Frequentist probability”); or
- (subjectivist interpretation of probability:) a degree of belief in E , e.g. the price at which someone would buy or sell a bet that pays 1 unit of utility if E and 0 if not E (“Bayesian probability”).

Sources:

- Wikipedia (2020): “Probability”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-05-10; URL: <https://en.wikipedia.org/wiki/Probability#Interpretations>.

1.3.2 Joint probability

Definition: Let A and B be two arbitrary statements about random variables (\rightarrow I/1.2.2), such as statements about the presence or absence of an event or about the value of a scalar, vector or matrix. Then, $p(A, B)$ is called the joint probability of A and B and is defined as the probability (\rightarrow I/1.3.1) that A and B are both true.

Sources:

- Wikipedia (2020): “Joint probability distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-05-10; URL: https://en.wikipedia.org/wiki/Joint_probability_distribution.
- Jason Browlee (2019): “A Gentle Introduction to Joint, Marginal, and Conditional Probability”; in: *Machine Learning Mastery*, retrieved on 2021-08-01; URL: <https://machinelearningmastery.com/joint-marginal-and-conditional-probability-for-machine-learning/>.

1.3.3 Marginal probability

Definition: (law of marginal probability, also called “sum rule”) Let A and X be two arbitrary statements about random variables (\rightarrow I/1.2.2), such as statements about the presence or absence of an event or about the value of a scalar, vector or matrix. Furthermore, assume a joint probability (\rightarrow I/1.3.2) distribution $p(A, X)$. Then, $p(A)$ is called the marginal probability of A and, 1) if X is a discrete (\rightarrow I/1.2.6) random variable (\rightarrow I/1.2.2) with domain \mathcal{X} , is given by

$$p(A) = \sum_{x \in \mathcal{X}} p(A, x) ; \quad (1)$$

2) if X is a continuous (\rightarrow I/1.2.6) random variable (\rightarrow I/1.2.2) with domain \mathcal{X} , is given by

$$p(A) = \int_{\mathcal{X}} p(A, x) dx . \quad (2)$$

The law of marginal probability can be motivated from the law of total probability (\rightarrow I/1.4.11) which follows from the Kolmogorov axioms of probability (\rightarrow I/1.4.1).

Sources:

- Wikipedia (2020): “Marginal distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-05-10; URL: https://en.wikipedia.org/wiki/Marginal_distribution#Definition.
- Jason Browlee (2019): “A Gentle Introduction to Joint, Marginal, and Conditional Probability”; in: *Machine Learning Mastery*, retrieved on 2021-08-01; URL: <https://machinelearningmastery.com/joint-marginal-and-conditional-probability-for-machine-learning/>.

1.3.4 Conditional probability

Definition: (law of conditional probability, also called “product rule”) Let A and B be two arbitrary statements about random variables (\rightarrow I/1.2.2), such as statements about the presence or absence of an event or about the value of a scalar, vector or matrix. Furthermore, assume a joint probability (\rightarrow I/1.3.2) distribution $p(A, B)$. Then, $p(A|B)$ is called the conditional probability that A is true, given that B is true, and is given by

$$p(A|B) = \frac{p(A, B)}{p(B)} \quad (1)$$

where $p(B)$ is the marginal probability (\rightarrow I/1.3.3) of B .

Sources:

- Wikipedia (2020): “Conditional probability”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-05-10; URL: https://en.wikipedia.org/wiki/Conditional_probability#Definition.
- Jason Browlee (2019): “A Gentle Introduction to Joint, Marginal, and Conditional Probability”; in: *Machine Learning Mastery*, retrieved on 2021-08-01; URL: <https://machinelearningmastery.com/joint-marginal-and-conditional-probability-for-machine-learning/>.

1.3.5 Exceedance probability

Definition: Let $X = \{X_1, \dots, X_n\}$ be a set of n random variables (\rightarrow I/1.2.2) which the joint probability distribution (\rightarrow I/1.5.2) $p(X) = p(X_1, \dots, X_n)$. Then, the exceedance probability for random variable X_i is the probability (\rightarrow I/1.3.1) that X_i is larger than all other random variables X_j , $j \neq i$:

$$\begin{aligned} \varphi(X_i) &= \Pr(\forall j \in \{1, \dots, n | j \neq i\} : X_i > X_j) \\ &= \Pr\left(\bigwedge_{j \neq i} X_i > X_j\right) \\ &= \Pr(X_i = \max(\{X_1, \dots, X_n\})) \\ &= \int_{X_i = \max(X)} p(X) dX . \end{aligned} \tag{1}$$

Sources:

- Stephan KE, Penny WD, Daunizeau J, Moran RJ, Friston KJ (2009): “Bayesian model selection for group studies”; in: *NeuroImage*, vol. 46, pp. 1004–1017, eq. 16; URL: <https://www.sciencedirect.com/science/article/abs/pii/S1053811909002638>; DOI: 10.1016/j.neuroimage.2009.03.025.
- Soch J, Allefeld C (2016): “Exceedance Probabilities for the Dirichlet Distribution”; in: *arXiv stat.AP*, 1611.01439; URL: <https://arxiv.org/abs/1611.01439>.

1.3.6 Statistical independence

Definition: Generally speaking, random variables (\rightarrow I/1.2.2) are statistically independent, if their joint probability (\rightarrow I/1.3.2) can be expressed in terms of their marginal probabilities (\rightarrow I/1.3.3).

1) A set of discrete random variables (\rightarrow I/1.2.2) X_1, \dots, X_n with possible values $\mathcal{X}_1, \dots, \mathcal{X}_n$ is called statistically independent, if

$$p(X_1 = x_1, \dots, X_n = x_n) = \prod_{i=1}^n p(X_i = x_i) \quad \text{for all } x_i \in \mathcal{X}_i, i = 1, \dots, n \tag{1}$$

where $p(x_1, \dots, x_n)$ are the joint probabilities (\rightarrow I/1.3.2) of X_1, \dots, X_n and $p(x_i)$ are the marginal probabilities (\rightarrow I/1.3.3) of X_i .

2) A set of continuous random variables (\rightarrow I/1.2.2) X_1, \dots, X_n defined on the domains $\mathcal{X}_1, \dots, \mathcal{X}_n$ is called statistically independent, if

$$F_{X_1, \dots, X_n}(x_1, \dots, x_n) = \prod_{i=1}^n F_{X_i}(x_i) \quad \text{for all } x_i \in \mathcal{X}_i, i = 1, \dots, n \quad (2)$$

or equivalently, if the probability densities (\rightarrow I/1.7.1) exist, if

$$f_{X_1, \dots, X_n}(x_1, \dots, x_n) = \prod_{i=1}^n f_{X_i}(x_i) \quad \text{for all } x_i \in \mathcal{X}_i, i = 1, \dots, n \quad (3)$$

where F are the joint (\rightarrow I/1.5.2) or marginal (\rightarrow I/1.5.3) cumulative distribution functions (\rightarrow I/1.8.1) and f are the respective probability density functions (\rightarrow I/1.7.1).

Sources:

- Wikipedia (2020): “Independence (probability theory)”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-06-06; URL: [https://en.wikipedia.org/wiki/Independence_\(probability_theory\)#Definition](https://en.wikipedia.org/wiki/Independence_(probability_theory)#Definition).

1.3.7 Conditional independence

Definition: Generally speaking, random variables (\rightarrow I/1.2.2) are conditionally independent given another random variable, if they are statistically independent (\rightarrow I/1.3.6) in their conditional probability distributions (\rightarrow I/1.5.4) given this random variable.

1) A set of discrete random variables (\rightarrow I/1.2.6) X_1, \dots, X_n with possible values $\mathcal{X}_1, \dots, \mathcal{X}_n$ is called conditionally independent given the random variable Y with possible values \mathcal{Y} , if

$$p(X_1 = x_1, \dots, X_n = x_n | Y = y) = \prod_{i=1}^n p(X_i = x_i | Y = y) \quad \text{for all } x_i \in \mathcal{X}_i \quad \text{and all } y \in \mathcal{Y} \quad (1)$$

where $p(x_1, \dots, x_n | y)$ are the joint (conditional) probabilities (\rightarrow I/1.3.2) of X_1, \dots, X_n given Y and $p(x_i | y)$ are the marginal (conditional) probabilities (\rightarrow I/1.3.3) of X_i given Y .

2) A set of continuous random variables (\rightarrow I/1.2.6) X_1, \dots, X_n with possible values $\mathcal{X}_1, \dots, \mathcal{X}_n$ is called conditionally independent given the random variable Y with possible values \mathcal{Y} , if

$$F_{X_1, \dots, X_n | Y=y}(x_1, \dots, x_n) = \prod_{i=1}^n F_{X_i | Y=y}(x_i) \quad \text{for all } x_i \in \mathcal{X}_i \quad \text{and all } y \in \mathcal{Y} \quad (2)$$

or equivalently, if the probability densities (\rightarrow I/1.7.1) exist, if

$$f_{X_1, \dots, X_n | Y=y}(x_1, \dots, x_n) = \prod_{i=1}^n f_{X_i | Y=y}(x_i) \quad \text{for all } x_i \in \mathcal{X}_i \quad \text{and all } y \in \mathcal{Y} \quad (3)$$

where F are the joint (conditional) (\rightarrow I/1.5.2) or marginal (conditional) (\rightarrow I/1.5.3) cumulative distribution functions (\rightarrow I/1.8.1) and f are the respective probability density functions (\rightarrow I/1.7.1).

Sources:

- Wikipedia (2020): “Conditional independence”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-11-19; URL: https://en.wikipedia.org/wiki/Conditional_independence#Conditional_independence_of_random_variables.

1.3.8 Self-independence

Theorem: Let E be a random event (\rightarrow I/1.2.1). Then, E is independent of itself (\rightarrow I/1.3.6), if and only if its probability (\rightarrow I/1.3.1) is zero or one:

$$E \text{ self-independent} \Leftrightarrow p(E) = 0 \quad \text{or} \quad p(E) = 1 . \quad (1)$$

Proof: According to the definition of statistical independence (\rightarrow I/1.3.6), it must hold that:

$$\begin{aligned} p(E, E) &= p(E) \cdot p(E) \\ p(E) &= (p(E))^2 . \end{aligned} \quad (2)$$

For $0 \leq p(E) \leq 1$, this is only fulfilled, if

$$p(E) = 0 \quad \text{or} \quad p(E) = 1 . \quad (3)$$

Both is possible, since the lower bound of probability is zero (\rightarrow I/1.4.1) and the upper bound of probability is one (\rightarrow I/1.4.7). ■

Sources:

- Wikipedia (2024): “Independence (probability theory)”; in: *Wikipedia, the free encyclopedia*, retrieved on 2024-09-20; URL: [https://en.wikipedia.org/wiki/Independence_\(probability_theory\)#Self-independence](https://en.wikipedia.org/wiki/Independence_(probability_theory)#Self-independence).
- Soch, Joram (2023): “Suppose A is an event. Can A be independent of itself?”; in: *X*, Aug 7, 2023, 03:59 PM; URL: <https://x.com/JoramSoch/status/1688550557034651648>.

1.3.9 Probability under independence

Theorem: Let A and B be two statements about random variables (\rightarrow I/1.2.2). Then, if A and B are independent (\rightarrow I/1.3.6), marginal (\rightarrow I/1.3.3) and conditional (\rightarrow I/1.3.4) probabilities are equal:

$$\begin{aligned} p(A) &= p(A|B) \\ p(B) &= p(B|A) . \end{aligned} \quad (1)$$

Proof: If A and B are independent (\rightarrow I/1.3.6), then the joint probability (\rightarrow I/1.3.2) is equal to the product of the marginal probabilities (\rightarrow I/1.3.3):

$$p(A, B) = p(A) \cdot p(B) . \quad (2)$$

The law of conditional probability (\rightarrow I/1.3.4) states that

$$p(A|B) = \frac{p(A, B)}{p(B)} . \quad (3)$$

Combining (2) and (3), we have:

$$p(A|B) = \frac{p(A) \cdot p(B)}{p(B)} = p(A) . \quad (4)$$

Equivalently, we can write:

$$p(B|A) \stackrel{(3)}{=} \frac{p(A, B)}{p(A)} \stackrel{(2)}{=} \frac{p(A) \cdot p(B)}{p(A)} = p(B) . \quad (5)$$

■

Sources:

- Wikipedia (2021): “Independence (probability theory)”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-07-23; URL: [https://en.wikipedia.org/wiki/Independence_\(probability_theory\)#Definition](https://en.wikipedia.org/wiki/Independence_(probability_theory)#Definition).

1.3.10 Mutual exclusivity

Definition: Generally speaking, random events (\rightarrow I/1.2.1) are mutually exclusive, if they cannot occur together, such that their intersection is equal to the empty set (\rightarrow I/1.4.4).

More precisely, a set of statements A_1, \dots, A_n is called mutually exclusive, if

$$p(A_1, \dots, A_n) = 0 \quad (1)$$

where $p(A_1, \dots, A_n)$ is the joint probability (\rightarrow I/1.3.2) of the statements A_1, \dots, A_n .

Sources:

- Wikipedia (2021): “Mutual exclusivity”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-07-23; URL: https://en.wikipedia.org/wiki/Mutual_exclusivity#Probability.

1.3.11 Probability under exclusivity

Theorem: Let A and B be two statements about random variables (\rightarrow I/1.2.2). Then, if A and B are mutually exclusive (\rightarrow I/1.3.10), the probability (\rightarrow I/1.3.1) of their disjunction is equal to the sum of the marginal probabilities (\rightarrow I/1.3.3):

$$p(A \vee B) = p(A) + p(B) . \quad (1)$$

Proof: If A and B are mutually exclusive (\rightarrow I/1.3.10), then their joint probability (\rightarrow I/1.3.2) is zero:

$$p(A, B) = 0 . \quad (2)$$

The addition law of probability states that

$$p(A \cup B) = p(A) + p(B) - p(A \cap B) \quad (3)$$

which, in logical rather than set-theoretic expression, becomes

$$p(A \vee B) = p(A) + p(B) - p(A, B) . \quad (4)$$

Because the union of mutually exclusive events is the empty set (\rightarrow I/1.3.10) and the probability of the empty set is zero (\rightarrow I/1.4.4), the joint probability (\rightarrow I/1.3.2) term cancels out:

$$p(A \vee B) = p(A) + p(B) - p(A, B) \stackrel{(2)}{=} p(A) + p(B) . \quad (5)$$

■

Sources:

- Wikipedia (2021): “Mutual exclusivity”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-07-23; URL: https://en.wikipedia.org/wiki/Mutual_exclusivity#Probability.

1.4 Probability axioms

1.4.1 Axioms of probability

Definition: Let there be a sample space (\rightarrow I/1.1.2) Ω , an event space (\rightarrow I/1.1.3) \mathcal{E} and a probability measure P , such that $p(E)$ is the probability (\rightarrow I/1.3.1) of some event (\rightarrow I/1.2.1) $E \in \mathcal{E}$. Then, we introduce three axioms of probability:

- First axiom: The probability of an event is a non-negative real number:

$$p(E) \in \mathbb{R}, p(E) \geq 0, \text{ for all } E \in \mathcal{E} . \quad (1)$$

- Second axiom: The probability that at least one elementary event in the sample space will occur is one:

$$p(\Omega) = 1 . \quad (2)$$

- Third axiom: The probability of any countable sequence of disjoint (i.e. mutually exclusive (\rightarrow I/1.3.10)) events E_1, E_2, E_3, \dots is equal to the sum of the probabilities of the individual events:

$$p\left(\bigcup_{i=1}^{\infty} E_i\right) = \sum_{i=1}^{\infty} p(E_i) . \quad (3)$$

Sources:

- A.N. Kolmogorov (1950): “Elementary Theory of Probability”; in: *Foundations of the Theory of Probability*, p. 2; URL: <https://archive.org/details/foundationsofthe00kolm/page/2/mode/2up>.
- Alan Stuart & J. Keith Ord (1994): “Probability and Statistical Inference”; in: *Kendall’s Advanced Theory of Statistics, Vol. 1: Distribution Theory*, ch. 8.6, p. 288, eqs. 8.2-8.4; URL: <https://www.wiley.com/en-us/Kendall%27s+Advanced+Theory+of+Statistics%2C+3+Volumes%2C+Set%2C+6th+Edition-p-9780470669549>.
- Wikipedia (2021): “Probability axioms”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-07-30; URL: https://en.wikipedia.org/wiki/Probability_axioms#Axioms.

1.4.2 Monotonicity of probability

Theorem: Probability (\rightarrow I/1.3.1) is monotonic, i.e. if A is a subset of or equal to B , then the probability of A is smaller than or equal to B :

$$A \subseteq B \quad \Rightarrow \quad p(A) \leq p(B) . \quad (1)$$

Proof: Set $E_1 = A$, $E_2 = B \setminus A$ and $E_i = \emptyset$ for $i \geq 3$. Then, the sets E_i are pairwise disjoint and $E_1 \cup E_2 \cup \dots = B$, because $A \subseteq B$. Thus, from the third axiom of probability (\rightarrow I/1.4.1), we have:

$$p(B) = p(A) + p(B \setminus A) + \sum_{i=3}^{\infty} p(E_i) . \quad (2)$$

Since, by the first axiom of probability (\rightarrow I/1.4.1), the right-hand side is a series of non-negative numbers converging to $p(B)$ on the left-hand side, it follows that

$$p(A) \leq p(B) . \quad (3)$$

Sources:

- A.N. Kolmogorov (1950): “Elementary Theory of Probability”; in: *Foundations of the Theory of Probability*, p. 6; URL: <https://archive.org/details/foundationsofthe00kolm/page/6/mode/2up>.
- Alan Stuart & J. Keith Ord (1994): “Probability and Statistical Inference”; in: *Kendall’s Advanced Theory of Statistics, Vol. 1: Distribution Theory*, pp. 288-289; URL: <https://www.wiley.com/en-us/Kendall%27s+Advanced+Theory+of+Statistics%2C+3+Volumes%2C+Set%2C+6th+Edition-p-9>
- Wikipedia (2021): “Probability axioms”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-07-30; URL: https://en.wikipedia.org/wiki/Probability_axioms#Monotonicity.

1.4.3 Monotonicity of probability

Theorem: Probability (\rightarrow I/1.3.1) is monotonic, i.e. if A is a subset of or equal to B , then the probability of A is smaller than or equal to B :

$$A \subseteq B \quad \Rightarrow \quad p(A) \leq p(B) . \quad (1)$$

Proof: When $A \subseteq B$, then B is equal to the union of A and the intersection of B with the complement (\rightarrow I/1.4.6) of A :

$$B = A \cup (B \cap \overline{A}) . \quad (2)$$

Moreover, the intersection of A and the intersection of B with the complement of A is equal to the empty set:

$$A \cap (B \cap \overline{A}) = \emptyset . \quad (3)$$

Thus, the third axiom of probability (\rightarrow I/1.4.1) implies:

$$\begin{aligned} p(B) &= p(A) + p(B \cap \overline{A}) \\ p(A) &= p(B) - p(B \cap \overline{A}) . \end{aligned} \quad (4)$$

Since $p(B \cap \overline{A}) \geq 0$ by the first axiom of probability (\rightarrow I/1.4.1), it must hold that $p(A) \leq p(B)$.

Sources:

- Ostwald, Dirk (2023): “Elementare Wahrscheinlichkeiten”; in: *Wahrscheinlichkeitstheorie und Frequentistische Inferenz*, Einheit (2), Folien 8-10; URL: https://www.ipsy.ovgu.de/ipsy_media/Methodenlehre+I/Wintersemester+2324/Wahrscheinlichkeitstheorie+und+Frequentistische+Inferenz/2_Elementare_Wahrscheinlichkeiten.pdf.

1.4.4 Probability of the empty set

Theorem: The probability (\rightarrow I/1.3.1) of the empty set is zero:

$$p(\emptyset) = 0 . \quad (1)$$

Proof: Let A and B be two events fulfilling $A \subseteq B$. Set $E_1 = A$, $E_2 = B \setminus A$ and $E_i = \emptyset$ for $i \geq 3$. Then, the sets E_i are pairwise disjoint and $E_1 \cup E_2 \cup \dots = B$. Thus, from the third axiom of probability (\rightarrow I/1.4.1), we have:

$$p(B) = p(A) + p(B \setminus A) + \sum_{i=3}^{\infty} p(E_i) . \quad (2)$$

Assume that the probability of the empty set is not zero, i.e. $p(\emptyset) > 0$. Then, the right-hand side of (2) would be infinite. However, by the first axiom of probability (\rightarrow I/1.4.1), the left-hand side must be finite. This is a contradiction. Therefore, $p(\emptyset) = 0$. ■

Sources:

- A.N. Kolmogorov (1950): “Elementary Theory of Probability”; in: *Foundations of the Theory of Probability*, p. 6, eq. 3; URL: <https://archive.org/details/foundationsofthe00kolm/page/6/mode/2up>.
- Alan Stuart & J. Keith Ord (1994): “Probability and Statistical Inference”; in: *Kendall’s Advanced Theory of Statistics, Vol. 1: Distribution Theory*, ch. 8.6, p. 288, eq. (b); URL: <https://www.wiley.com/en-us/Kendall%27s+Advanced+Theory+of+Statistics%2C+3+Volumes%2C+Set%2C+6th+Edition-p-9780470669549>.
- Wikipedia (2021): “Probability axioms”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-07-30; URL: https://en.wikipedia.org/wiki/Probability_axioms#The_probability_of_the_empty_set.

1.4.5 Probability of the empty set

Theorem: The probability (\rightarrow I/1.3.1) of the empty set is zero:

$$p(\emptyset) = 0 . \quad (1)$$

Proof: Let $E_i = \emptyset$ for $i = 1, 2, \dots$. Then, $E_i \cap E_j = \emptyset \cap \emptyset = \emptyset$ for $i, j \geq 1$ and $\bigcup_{i=1}^{\infty} E_i = \bigcup_{i=1}^{\infty} \emptyset = \emptyset$. Thus, E_1, E_2, \dots is a countable sequence of disjoint events so that, with the third axiom of probability (\rightarrow I/1.4.1), it holds that:

$$\begin{aligned} p\left(\bigcup_{i=1}^{\infty} E_i\right) &= \sum_{i=1}^{\infty} p(E_i) \\ p(\emptyset) &= \sum_{i=1}^{\infty} p(\emptyset) . \end{aligned} \quad (2)$$

Since, by the first axiom of probability (\rightarrow I/1.4.1), probabilities are non-negative, i.e. $p(\emptyset) \geq 0$, we are searching for a non-negative number which, when added to itself infinitely, is equal to itself. The only such number is zero, i.e. $p(\emptyset) = 0$.

**Sources:**

- Ostwald, Dirk (2023): “Wahrscheinlichkeitsräume”; in: *Wahrscheinlichkeitstheorie und Frequentistische Inferenz*, Einheit (1), Folie 19; URL: https://www.ipsy.ovgu.de/ipsy_media/Methodenlehre+I/Wintersemester+2324/Wahrscheinlichkeitstheorie+und+Frequentistische+Inferenz/1_Wahrscheinlichkeitsraeume.pdf.

1.4.6 Probability of the complement

Theorem: The probability (\rightarrow I/1.3.1) of a complement of a set is one minus the probability of this set:

$$p(\bar{A}) = 1 - p(A) \quad (1)$$

where $\bar{A} = \Omega \setminus A$ and Ω is the sample space (\rightarrow I/1.1.2).

Proof: Since A and \bar{A} are mutually exclusive (\rightarrow I/1.3.10) and $A \cup \bar{A} = \Omega$, the third axiom of probability (\rightarrow I/1.4.1) implies:

$$\begin{aligned} p(A \cup \bar{A}) &= p(A) + p(\bar{A}) \\ p(\Omega) &= p(A) + p(\bar{A}) \\ p(\bar{A}) &= p(\Omega) - p(A) . \end{aligned} \quad (2)$$

The second axiom of probability (\rightarrow I/1.4.1) states that $p(\Omega) = 1$, such that we obtain:

$$p(\bar{A}) = 1 - p(A) . \quad (3)$$

**Sources:**

- A.N. Kolmogorov (1950): “Elementary Theory of Probability”; in: *Foundations of the Theory of Probability*, p. 6, eq. 2; URL: <https://archive.org/details/foundationsofthe00kolm/page/6/mode/2up>.
- Alan Stuart & J. Keith Ord (1994): “Probability and Statistical Inference”; in: *Kendall’s Advanced Theory of Statistics, Vol. 1: Distribution Theory*, ch. 8.6, p. 288, eq. (c); URL: <https://www.wiley.com/en-us/Kendall%27s+Advanced+Theory+of+Statistics%2C+3+Volumes%2C+Set%2C+6th+Edition-p-9780470669549>.
- Wikipedia (2021): “Probability axioms”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-07-30; URL: https://en.wikipedia.org/wiki/Probability_axioms#The_complement_rule.

1.4.7 Range of probability

Theorem: The probability (\rightarrow I/1.3.1) of an event is bounded between 0 and 1:

$$0 \leq p(E) \leq 1 . \quad (1)$$

Proof: From the first axiom of probability (\rightarrow I/1.4.1), we have:

$$p(E) \geq 0 . \quad (2)$$

By combining the first axiom of probability (\rightarrow I/1.4.1) and the probability of the complement (\rightarrow I/1.4.6), we obtain:

$$\begin{aligned} 1 - p(E) = p(\overline{E}) &\geq 0 \\ 1 - p(E) &\geq 0 \\ p(E) &\leq 1 . \end{aligned} \tag{3}$$

Together, (2) and (3) imply that

$$0 \leq p(E) \leq 1 . \tag{4}$$

■

Sources:

- A.N. Kolmogorov (1950): “Elementary Theory of Probability”; in: *Foundations of the Theory of Probability*, p. 6; URL: <https://archive.org/details/foundationsofthe00kolm/page/6/mode/2up>.
- Alan Stuart & J. Keith Ord (1994): “Probability and Statistical Inference”; in: *Kendall’s Advanced Theory of Statistics, Vol. 1: Distribution Theory*, pp. 288-289; URL: <https://www.wiley.com/en-us/Kendall%27s+Advanced+Theory+of+Statistics%2C+3+Volumes%2C+Set%2C+6th+Edition-p-9>
- Wikipedia (2021): “Probability axioms”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-07-30; URL: https://en.wikipedia.org/wiki/Probability_axioms#The_numeric_bound.

1.4.8 Addition law of probability

Theorem: The probability (\rightarrow I/1.3.1) of the union of A and B is the sum of the probabilities of A and B minus the probability of the intersection of A and B :

$$p(A \cup B) = p(A) + p(B) - p(A \cap B) . \tag{1}$$

Proof: Let $E_1 = A$ and $E_2 = B \setminus A$, such that $E_1 \cup E_2 = A \cup B$. Then, by the third axiom of probability (\rightarrow I/1.4.1), we have:

$$\begin{aligned} p(A \cup B) &= p(A) + p(B \setminus A) \\ p(A \cup B) &= p(A) + p(B \setminus [A \cap B]) . \end{aligned} \tag{2}$$

Then, let $E_1 = B \setminus [A \cap B]$ and $E_2 = A \cap B$, such that $E_1 \cup E_2 = B$. Again, from the third axiom of probability (\rightarrow I/1.4.1), we obtain:

$$\begin{aligned} p(B) &= p(B \setminus [A \cap B]) + p(A \cap B) \\ p(B \setminus [A \cap B]) &= p(B) - p(A \cap B) . \end{aligned} \tag{3}$$

Plugging (3) into (2), we finally get:

$$p(A \cup B) = p(A) + p(B) - p(A \cap B) . \tag{4}$$

■

Sources:

- A.N. Kolmogorov (1950): “Elementary Theory of Probability”; in: *Foundations of the Theory of Probability*, p. 2; URL: <https://archive.org/details/foundationsofthe00kolm/page/2/mode/2up>.
- Alan Stuart & J. Keith Ord (1994): “Probability and Statistical Inference”; in: *Kendall’s Advanced Theory of Statistics, Vol. 1: Distribution Theory*, ch. 8.6, p. 288, eq. (a); URL: <https://www.wiley.com/en-us/Kendall%27s+Advanced+Theory+of+Statistics%2C+3+Volumes%2C+Set%2C+6th+Edition-p-9780470669549>.
- Wikipedia (2021): “Probability axioms”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-07-30; URL: https://en.wikipedia.org/wiki/Probability_axioms#Further_consequences.

1.4.9 Bonferroni’s inequality

Theorem: The probability (\rightarrow I/1.3.1) of the intersection of A and B is larger than or equal to the sum of the probabilities of A and B minus one:

$$p(A \cap B) \geq p(A) + p(B) - 1 . \quad (1)$$

Proof: The addition law of probability (\rightarrow I/1.4.8) states that, for two events (\rightarrow I/1.2.1) A and B , it holds true that

$$p(A \cup B) = p(A) + p(B) - p(A \cap B) . \quad (2)$$

Rearranging for $p(A \cap B)$, we have:

$$p(A \cap B) = p(A) + p(B) - p(A \cup B) . \quad (3)$$

The range of probability (\rightarrow I/1.4.7) is

$$0 \leq p(E) \leq 1 . \quad (4)$$

Thus, $p(A \cup B)$ is at most one. (This is the case, if A and B are collectively exhaustive (\rightarrow I/1.4.12) and their union is thus equal to the sample space (\rightarrow I/1.4.1) Ω .) With this, we are able to derive a lower bound for $p(A \cap B)$, as given by the theorem:

$$p(A \cap B) \geq p(A) + p(B) - 1 . \quad (5)$$

■

Sources:

- Probability Fact (2021): “Bonferroni’s inequality”; in: X , retrieved on 2025-01-10; URL: <https://x.com/ProbFact/status/1462828945968189443>.
- Wikipedia (2025): “Boole’s inequality”; in: *Wikipedia, the free encyclopedia*, retrieved on 2025-01-10; URL: https://en.wikipedia.org/wiki/Boole%27s_inequality#Bonferroni_inequalities.

1.4.10 Boole’s inequality

Theorem: The probability (\rightarrow I/1.3.1) of any countable sequence of events (\rightarrow I/1.2.1) A_1, A_2, A_3, \dots is smaller than or equal to the sum of the probabilities of the individual events (\rightarrow I/1.4.1):

$$p\left(\bigcup_{i=1}^{\infty} A_i\right) \leq \sum_{i=1}^{\infty} p(A_i) . \quad (1)$$

Proof: The addition law of probability (\rightarrow I/1.4.8) states that, for two events (\rightarrow I/1.2.1) A and B , we have:

$$p(A \cup B) = p(A) + p(B) - p(A \cap B) . \quad (2)$$

We will prove the statement by induction, i.e. observe that it holds for $n = 1$ event and show that, if it holds for n events, it also holds for $n + 1$ events. For $n = 1$, it is obviously true that:

$$p(A_1) \leq p(A_1) . \quad (3)$$

We shall suppose that statement (1) holds for A_1, \dots, A_n :

$$p\left(\bigcup_{i=1}^n A_i\right) \leq \sum_{i=1}^n p(A_i) . \quad (4)$$

Using (2), for A_1, \dots, A_n, A_{n+1} , we then have:

$$p\left(\bigcup_{i=1}^{n+1} A_i\right) = p\left(\bigcup_{i=1}^n A_i \cup A_{n+1}\right) = p\left(\bigcup_{i=1}^n A_i\right) + p(A_{n+1}) - p\left(\bigcup_{i=1}^n A_i \cap A_{n+1}\right) . \quad (5)$$

Since, by the first axiom of probability (\rightarrow I/1.4.1), any probability is positive

$$p\left(\bigcup_{i=1}^n A_i \cap A_{n+1}\right) \geq 0 , \quad (6)$$

it follows from (5) that

$$p\left(\bigcup_{i=1}^{n+1} A_i\right) \leq p\left(\bigcup_{i=1}^n A_i\right) + p(A_{n+1}) \quad (7)$$

and using (4), we get

$$p\left(\bigcup_{i=1}^{n+1} A_i\right) \leq \sum_{i=1}^n p(A_i) + p(A_{n+1}) , \quad (8)$$

such that

$$p\left(\bigcup_{i=1}^{n+1} A_i\right) \leq \sum_{i=1}^{n+1} p(A_i) . \quad (9)$$

Together, (3) and the transition from (4) to (9), prove the theorem. ■

Sources:

- Wikipedia (2025): “Boole’s inequality”; in: *Wikipedia, the free encyclopedia*, retrieved on 2025-01-10; URL: https://en.wikipedia.org/wiki/Boole%27s_inequality#Proof_using_induction.

1.4.11 Law of total probability

Theorem: Let A be a subset of sample space (\rightarrow I/1.1.2) Ω and let B_1, \dots, B_n be finite or countably infinite partition of Ω , such that $B_i \cap B_j = \emptyset$ for all $i \neq j$ and $\cup_i B_i = \Omega$. Then, the probability (\rightarrow I/1.3.1) of the event A is

$$p(A) = \sum_i p(A \cap B_i) . \quad (1)$$

Proof: Because all B_i are disjoint, sets $(A \cap B_i)$ are also disjoint:

$$B_i \cap B_j = \emptyset \quad \Rightarrow \quad (A \cap B_i) \cap (A \cap B_j) = A \cap (B_i \cap B_j) = A \cap \emptyset = \emptyset . \quad (2)$$

Because the B_i are exhaustive, the sets $(A \cap B_i)$ are also exhaustive:

$$\cup_i B_i = \Omega \quad \Rightarrow \quad \cup_i (A \cap B_i) = A \cap (\cup_i B_i) = A \cap \Omega = A . \quad (3)$$

Thus, the third axiom of probability (\rightarrow I/1.4.1) implies that

$$p(A) = \sum_i p(A \cap B_i) . \quad (4)$$

■

Sources:

- Alan Stuart & J. Keith Ord (1994): “Probability and Statistical Inference”; in: *Kendall’s Advanced Theory of Statistics, Vol. 1: Distribution Theory*, p. 288, eq. (d); p. 289, eq. 8.7; URL: <https://www.wiley.com/en-us/Kendall%27s+Advanced+Theory+of+Statistics%2C+3+Volumes%2C+Set%2C+6th+Edition-p-9780470669549>.
- Wikipedia (2021): “Law of total probability”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-08-08; URL: https://en.wikipedia.org/wiki/Law_of_total_probability#Statement.

1.4.12 Probability of exhaustive events

Theorem: Let B_1, \dots, B_n be mutually exclusive (\rightarrow I/1.3.10) and collectively exhaustive subsets of a sample space (\rightarrow I/1.1.2) Ω . Then, their total probability (\rightarrow I/1.4.11) is one:

$$\sum_i p(B_i) = 1 . \quad (1)$$

Proof: Because all B_i are mutually exclusive, we have:

$$B_i \cap B_j = \emptyset \quad \text{for all } i \neq j . \quad (2)$$

Because the B_i are collectively exhaustive, we have:

$$\cup_i B_i = \Omega . \quad (3)$$

Thus, the third axiom of probability (\rightarrow I/1.4.1) implies that

$$\sum_i p(B_i) = p(\Omega) . \quad (4)$$

and the second axiom of probability (\rightarrow I/1.4.1) implies that

$$\sum_i p(B_i) = 1 . \quad (5)$$

■

Sources:

- Alan Stuart & J. Keith Ord (1994): “Probability and Statistical Inference”; in: *Kendall’s Advanced Theory of Statistics, Vol. 1: Distribution Theory*, pp. 288-289; URL: <https://www.wiley.com/en-us/Kendall%27s+Advanced+Theory+of+Statistics%2C+3+Volumes%2C+Set%2C+6th+Edition-p-9>
- Wikipedia (2021): “Probability axioms”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-08-08; URL: https://en.wikipedia.org/wiki/Probability_axioms#Axioms.

1.4.13 Probability of exhaustive events

Theorem: Let B_1, \dots, B_n be mutually exclusive (\rightarrow I/1.3.10) and collectively exhaustive subsets of a sample space (\rightarrow I/1.1.2) Ω . Then, their total probability (\rightarrow I/1.4.11) is one:

$$\sum_i p(B_i) = 1 . \quad (1)$$

Proof: The addition law of probability (\rightarrow I/1.4.8) states that for two events (\rightarrow I/1.2.1) A and B , the probability (\rightarrow I/1.3.1) of at least one of them occurring is:

$$p(A \cup B) = p(A) + p(B) - p(A \cap B) . \quad (2)$$

Recursively applying this law to the events B_1, \dots, B_n , we have:

$$\begin{aligned} p(B_1 \cup \dots \cup B_n) &= p(B_1) + p(B_2 \cup \dots \cup B_n) - p(B_1 \cap [B_2 \cup \dots \cup B_n]) \\ &= p(B_1) + p(B_2) + p(B_3 \cup \dots \cup B_n) - p(B_2 \cap [B_3 \cup \dots \cup B_n]) - p(B_1 \cap [B_2 \cup \dots \cup B_n]) \\ &\vdots \\ &= p(B_1) + \dots + p(B_n) - p(B_1 \cap [B_2 \cup \dots \cup B_n]) - \dots - p(B_{n-1} \cap B_n) \\ p(\cup_i^n B_i) &= \sum_i^n p(B_i) - \sum_i^{n-1} p(B_i \cap [\cup_{j=i+1}^n B_j]) \\ &= \sum_i^n p(B_i) - \sum_i^{n-1} p(\cup_{j=i+1}^n [B_i \cap B_j]) . \end{aligned} \quad (3)$$

Because all B_i are mutually exclusive, we have:

$$B_i \cap B_j = \emptyset \quad \text{for all } i \neq j . \quad (4)$$

Since the probability of the empty set is zero (\rightarrow I/1.4.4), this means that the second sum on the right-hand side of (3) disappears:

$$p(\cup_i^n B_i) = \sum_i^n p(B_i) . \quad (5)$$

Because the B_i are collectively exhaustive, we have:

$$\cup_i B_i = \Omega . \quad (6)$$

Since the probability of the sample space is one (\rightarrow I/1.4.1), this means that the left-hand side of (5) becomes equal to one:

$$1 = \sum_i^n p(B_i) . \quad (7)$$

This proves the statement in (1). ■

Sources:

- Alan Stuart & J. Keith Ord (1994): “Probability and Statistical Inference”; in: *Kendall’s Advanced Theory of Statistics, Vol. 1: Distribution Theory*, pp. 288-289; URL: <https://www.wiley.com/en-us/Kendall%27s+Advanced+Theory+of+Statistics%2C+3+Volumes%2C+Set%2C+6th+Edition-p-9>
- Wikipedia (2022): “Probability axioms”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-03-27; URL: https://en.wikipedia.org/wiki/Probability_axioms#Consequences.

1.5 Probability distributions

1.5.1 Probability distribution

Definition: Let X be a random variable (\rightarrow I/1.2.2) with the set of possible outcomes \mathcal{X} . Then, a probability distribution of X is a mathematical function that gives the probabilities (\rightarrow I/1.3.1) of occurrence of all possible outcomes $x \in \mathcal{X}$ of this random variable.

Sources:

- Wikipedia (2020): “Probability distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-05-17; URL: https://en.wikipedia.org/wiki/Probability_distribution.

1.5.2 Joint distribution

Definition: Let X and Y be random variables (\rightarrow I/1.2.2) with sets of possible outcomes \mathcal{X} and \mathcal{Y} . Then, a joint distribution of X and Y is a probability distribution (\rightarrow I/1.5.1) that specifies the probability of the event that $X = x$ and $Y = y$ for each possible combination of $x \in \mathcal{X}$ and $y \in \mathcal{Y}$.

- The joint distribution of two scalar random variables (\rightarrow I/1.2.2) is called a bivariate distribution.
- The joint distribution of a random vector (\rightarrow I/1.2.3) is called a multivariate distribution.
- The joint distribution of a random matrix (\rightarrow I/1.2.4) is called a matrix-variate distribution.

Sources:

- Wikipedia (2020): “Joint probability distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-05-17; URL: https://en.wikipedia.org/wiki/Joint_probability_distribution.

1.5.3 Marginal distribution

Definition: Let X and Y be random variables (\rightarrow I/1.2.2) with sets of possible outcomes \mathcal{X} and \mathcal{Y} . Then, the marginal distribution of X is a probability distribution (\rightarrow I/1.5.1) that specifies the probability of the event that $X = x$ irrespective of the value of Y for each possible value $x \in \mathcal{X}$. The marginal distribution can be obtained from the joint distribution (\rightarrow I/1.5.2) of X and Y using the law of marginal probability (\rightarrow I/1.3.3).

Sources:

- Wikipedia (2020): “Marginal distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-05-17; URL: https://en.wikipedia.org/wiki/Marginal_distribution.

1.5.4 Conditional distribution

Definition: Let X and Y be random variables (\rightarrow I/1.2.2) with sets of possible outcomes \mathcal{X} and \mathcal{Y} . Then, the conditional distribution of X given that Y is a probability distribution (\rightarrow I/1.5.1) that specifies the probability of the event that $X = x$ given that $Y = y$ for each possible combination of $x \in \mathcal{X}$ and $y \in \mathcal{Y}$. The conditional distribution of X can be obtained from the joint distribution (\rightarrow I/1.5.2) of X and Y and the marginal distribution (\rightarrow I/1.5.3) of Y using the law of conditional probability (\rightarrow I/1.3.4).

Sources:

- Wikipedia (2020): “Conditional probability distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-05-17; URL: https://en.wikipedia.org/wiki/Conditional_probability_distribution.

1.5.5 Unimodal vs. multimodal distribution

Definition: Let X be a continuous (\rightarrow I/1.2.6) random variable (\rightarrow I/1.2.2) with some probability distribution (\rightarrow I/1.5.1) P characterized by probability density function (\rightarrow I/1.7.1) $f_X(x)$. Then,

- P is called a unimodal probability distribution, if $f_X(x)$ has exactly one local maximum;
- P is called a bimodal probability distribution, if $f_X(x)$ has exactly two local maxima;
- P is called a trimodal probability distribution, if $f_X(x)$ has exactly three local maxima;
- P is called a multimodal probability distribution, if $f_X(x)$ has more than one local maximum.

Note that this definition of multimodality differs from the strict definition of the mode (\rightarrow I/1.18.3) in which only the global maximum of $f_X(x)$ would be considered the single mode (\rightarrow I/1.18.3).

Sources:

- Weisstein, Eric W. (2024): “Mode”; in: *Wolfram MathWorld*, retrieved on 2024-10-25; URL: <https://mathworld.wolfram.com/Mode.html>.
- Wikipedia (2024): “Unimodality”; in: *Wikipedia, the free encyclopedia*, retrieved on 2024-10-25; URL: https://en.wikipedia.org/wiki/Unimodality#Unimodal_probability_distribution.

1.5.6 Sampling distribution

Definition: Let there be a random sample (\rightarrow I/1.1.6) with finite sample size (\rightarrow I/1.1.7). Then, the probability distribution (\rightarrow I/1.5.1) of a given statistic (\rightarrow I/1.1.8) computed from this sample, e.g. a test statistic (\rightarrow I/4.3.5), is called a sampling distribution.

Sources:

- Wikipedia (2021): “Sampling distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-03-31; URL: https://en.wikipedia.org/wiki/Sampling_distribution.

1.5.7 Statistical parameter

Definition: A parameter, also “statistical parameter”, is any fixed quantity, i.e. constant (\rightarrow I/1.2.5) scalar, vector or matrix, that describes a parametrized probability distribution (\rightarrow I/1.5.1) by influencing its probability mass function (\rightarrow I/1.6.1) or probability density function (\rightarrow I/1.7.1).

Examples of parameters include the mean and variance parameters of a normal distribution (\rightarrow II/3.2.1), covariance parameters in a multivariate (\rightarrow II/4.1.1) or matrix (\rightarrow II/5.1.1)-normal distribution, shape and rate parameters of the gamma distribution (\rightarrow II/3.4.1) or the vector of category probabilities in a multinomial distribution (\rightarrow II/2.2.1).

Sources:

- Wikipedia (2024): “Statistical parameter”; in: *Wikipedia, the free encyclopedia*, retrieved on 2024-09-27; URL: https://en.wikipedia.org/wiki/Statistical_parameter#Parameterised_distributions.

1.5.8 Location parameter

Definition: Let $\mathcal{D}(\mu, \lambda)$ denote a family of probability distributions (\rightarrow I/1.5.1) with statistical parameters (\rightarrow I/1.5.7) μ and λ . Then, the parameter μ is referred to as a “location parameter”, if and only if the following holds: When a random variable (\rightarrow I/1.2.2) X is following the probability distribution $\mathcal{D}(\mu, \lambda)$, then the random variable $Y = X - \mu$ is following the probability distribution $\mathcal{D}(0, \lambda)$.

$$X \sim \mathcal{D}(\mu^*, \lambda^*) \quad \Rightarrow \quad Y = X - \mu^* \sim \mathcal{D}(0, \lambda^*) . \quad (1)$$

This implies an identity of the cumulative distribution functions (\rightarrow I/1.8.1):

$$\begin{aligned} F_Y(y) &= F_X(y + \mu^*) \\ F_{\mathcal{D}}(y; 0, \lambda^*) &= F_{\mathcal{D}}(y + \mu^*; \mu^*, \lambda^*) . \end{aligned} \quad (2)$$

The parameter (\rightarrow I/1.5.7) μ can be scalar-, vector- or matrix-valued for random variables (\rightarrow I/1.2.2), vectors (\rightarrow I/1.2.3) or matrices (\rightarrow I/1.2.4) X .

Sources:

- Wikipedia (2025): “Location–scale family”; in: *Wikipedia, the free encyclopedia*, retrieved on 2025-03-14; URL: https://en.wikipedia.org/wiki/Location%E2%80%93scale_family.
- Wikipedia (2025): “Location parameter”; in: *Wikipedia, the free encyclopedia*, retrieved on 2025-03-14; URL: https://en.wikipedia.org/wiki/Location_parameter#Definition.

1.5.9 Scale parameter

Definition: Let $\mathcal{D}(\lambda, \sigma)$ denote a family of probability distributions (\rightarrow I/1.5.1) with statistical parameters (\rightarrow I/1.5.7) λ and σ . Then, the parameter σ is referred to as a “scale parameter”, if and only if the following holds: When a random variable (\rightarrow I/1.2.2) X is following the probability

distribution $\mathcal{D}(\lambda, \sigma)$, then the random variable $Y = X/\sigma$ is following the probability distribution $\mathcal{D}(\lambda, 1)$.

$$X \sim \mathcal{D}(\lambda^*, \sigma^*) \quad \Rightarrow \quad Y = \frac{X}{\sigma^*} \sim \mathcal{D}(\lambda^*, 1) . \quad (1)$$

This implies an identity of the cumulative distribution functions (\rightarrow I/1.8.1):

$$\begin{aligned} F_Y(y) &= F_X(\sigma^* y) \\ F_{\mathcal{D}}(y; \lambda^*, 1) &= F_{\mathcal{D}}(\sigma^* y; \lambda^*, \sigma^*) . \end{aligned} \quad (2)$$

The parameter (\rightarrow I/1.5.7) σ can be scalar for a random variable (\rightarrow I/1.2.2) X or matrix-valued for a random matrix (\rightarrow I/1.2.4) X .

Sources:

- Wikipedia (2025): “Location–scale family”; in: *Wikipedia, the free encyclopedia*, retrieved on 2025-03-14; URL: https://en.wikipedia.org/wiki/Location%E2%80%93scale_family.
- Wikipedia (2025): “Scale parameter”; in: *Wikipedia, the free encyclopedia*, retrieved on 2025-03-14; URL: https://en.wikipedia.org/wiki/Scale_parameter#Definition.

1.5.10 Rate parameter

Definition: Let $\mathcal{D}(\lambda, \rho)$ denote a family of probability distributions (\rightarrow I/1.5.1) with statistical parameters (\rightarrow I/1.5.7) λ and ρ . Then, the parameter ρ is referred to as a “rate parameter” or “inverse scale parameter”, if it is the reciprocal inverse of a scale parameter (\rightarrow I/1.5.9) with respect to this family of distributions.

$$\rho \text{ rate} \quad \Leftrightarrow \quad \sigma = 1/\rho \text{ scale} . \quad (1)$$

Sources:

- Wikipedia (2025): “Rate parameter”; in: *Wikipedia, the free encyclopedia*, retrieved on 2025-03-14; URL: https://en.wikipedia.org/wiki/Scale_parameter#Rate_parameter.

1.5.11 Shape parameter

Definition: Let $\mathcal{D}(\lambda, \chi)$ denote a family of probability distributions (\rightarrow I/1.5.1) with statistical parameters (\rightarrow I/1.5.7) λ and χ . Then, the parameter χ is referred to as a “shape parameter”, if it is neither a location parameter (\rightarrow I/1.5.8) nor a scale parameter (\rightarrow I/1.5.9) nor a function of these (such as a rate parameter (\rightarrow I/1.5.10)).

Sources:

- Wikipedia (2025): “Shape parameter”; in: *Wikipedia, the free encyclopedia*, retrieved on 2025-03-14; URL: https://en.wikipedia.org/wiki/Shape_parameter.

1.5.12 Degrees of freedom

Definition: Degrees of freedom can refer to

- a parameter (\rightarrow I/1.5.7) or parameters (\rightarrow I/1.5.7) of certain probability distributions (\rightarrow I/1.5.1), such as the chi-squared distribution (\rightarrow II/3.7.1), the t-distribution (\rightarrow II/3.3.1) or the F-distribution (\rightarrow II/3.8.1);
- the number of values in the final calculation of a statistic (\rightarrow I/1.1.8) that are free to vary, such as $n - 1$ for a sample variance (\rightarrow I/1.13.2) calculated from n data points (\rightarrow I/1.1.5).

Some statistics (\rightarrow I/1.1.8) have sampling distributions (\rightarrow I/1.5.6) whose parameters (\rightarrow I/1.5.7) (in the former sense) are equal to their degrees of freedom (in the latter sense). For example, a function of the sample variance follows a chi-squared distribution with $n - 1$ degrees of freedom (\rightarrow II/3.2.7).

Sources:

- Wikipedia (2024): “Degrees of freedom (statistics)”; in: *Wikipedia, the free encyclopedia*, retrieved on 2024-10-11; URL: [https://en.wikipedia.org/wiki/Degrees_of_freedom_\(statistics\)](https://en.wikipedia.org/wiki/Degrees_of_freedom_(statistics)).
- Animated Software (2024): “Degrees of Freedom”; in: *Glossary of Statistical Terms*, retrieved on 2024-10-11; URL: <https://www.animatedsoftware.com/statglos/sgdegree.htm>.

1.6 Probability mass function

1.6.1 Definition

Definition: Let X be a discrete (\rightarrow I/1.2.6) random variable (\rightarrow I/1.2.2) with possible outcomes \mathcal{X} . Then, $f_X(x) : \mathbb{R} \rightarrow [0, 1]$ is the probability mass function (PMF) of X , if

$$f_X(x) = 0 \tag{1}$$

for all $x \notin \mathcal{X}$,

$$\Pr(X = x) = f_X(x) \tag{2}$$

for all $x \in \mathcal{X}$ and

$$\sum_{x \in \mathcal{X}} f_X(x) = 1. \tag{3}$$

Sources:

- Wikipedia (2020): “Probability mass function”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-02-13; URL: https://en.wikipedia.org/wiki/Probability_mass_function.

1.6.2 Probability mass function of sum of independents

Theorem: Let X and Y be two independent (\rightarrow I/1.3.6) discrete (\rightarrow I/1.2.6) random variables (\rightarrow I/1.2.2) with possible values \mathcal{X} and \mathcal{Y} and let $Z = X + Y$. Then, the probability mass function (\rightarrow I/1.6.1) of Z is given by

$$\begin{aligned}
f_Z(z) &= \sum_{y \in \mathcal{Y}} f_X(z - y) f_Y(y) \\
\text{or } f_Z(z) &= \sum_{x \in \mathcal{X}} f_Y(z - x) f_X(x)
\end{aligned} \tag{1}$$

where $f_X(x)$, $f_Y(y)$ and $f_Z(z)$ are the probability mass functions (\rightarrow I/1.6.1) of X , Y and Z .

Proof: Using the definition of the probability mass function (\rightarrow I/1.6.1) and the expected value (\rightarrow I/1.12.1), the first equation can be derived as follows:

$$\begin{aligned}
f_Z(z) &= \Pr(Z = z) \\
&= \Pr(X + Y = z) \\
&= \Pr(X = z - Y) \\
&= \mathbb{E}[\Pr(X = z - Y | Y = y)] .
\end{aligned} \tag{2}$$

By construction, X and Y are independent (\rightarrow I/1.3.6), such that conditional probabilities are equal to marginal probabilities (\rightarrow I/1.3.9), i.e. $\Pr(X = z - Y | Y = y) = \Pr(X = z - Y)$ and we have:

$$\begin{aligned}
f_Z(z) &= \mathbb{E}[\Pr(X = z - Y)] \\
&= \mathbb{E}[f_X(z - Y)] \\
&= \sum_{y \in \mathcal{Y}} f_X(z - y) f_Y(y) .
\end{aligned} \tag{3}$$

The second equation can be derived by switching X and Y . ■

Sources:

- Taboga, Marco (2017): “Sums of independent random variables”; in: *Lectures on probability and mathematical statistics*, retrieved on 2021-08-30; URL: <https://www.statlect.com/fundamentals-of-probability/sums-of-independent-random-variables>.

1.6.3 Probability mass function of strictly increasing function

Theorem: Let X be a discrete (\rightarrow I/1.2.6) random variable (\rightarrow I/1.2.2) with possible outcomes \mathcal{X} and let $g(x)$ be a strictly increasing function on the support of X . Then, the probability mass function (\rightarrow I/1.6.1) of $Y = g(X)$ is given by

$$f_Y(y) = \begin{cases} f_X(g^{-1}(y)) , & \text{if } y \in \mathcal{Y} \\ 0 , & \text{if } y \notin \mathcal{Y} \end{cases} \tag{1}$$

where $g^{-1}(y)$ is the inverse function of $g(x)$ and \mathcal{Y} is the set of possible outcomes of Y :

$$\mathcal{Y} = \{y = g(x) : x \in \mathcal{X}\} . \tag{2}$$

Proof: Because a strictly increasing function is invertible, the probability mass function (\rightarrow I/1.6.1) of Y can be derived as follows:

$$\begin{aligned}
 f_Y(y) &= \Pr(Y = y) \\
 &= \Pr(g(X) = y) \\
 &= \Pr(X = g^{-1}(y)) \\
 &= f_X(g^{-1}(y)) .
 \end{aligned} \tag{3}$$

■

Sources:

- Taboga, Marco (2017): “Functions of random variables and their distribution”; in: *Lectures on probability and mathematical statistics*, retrieved on 2020-10-29; URL: <https://www.statlect.com/fundamentals-of-probability/functions-of-random-variables-and-their-distribution#hid3>.

1.6.4 Probability mass function of strictly decreasing function

Theorem: Let X be a discrete (\rightarrow I/1.2.6) random variable (\rightarrow I/1.2.2) with possible outcomes \mathcal{X} and let $g(x)$ be a strictly decreasing function on the support of X . Then, the probability mass function (\rightarrow I/1.6.1) of $Y = g(X)$ is given by

$$f_Y(y) = \begin{cases} f_X(g^{-1}(y)) , & \text{if } y \in \mathcal{Y} \\ 0 , & \text{if } y \notin \mathcal{Y} \end{cases} \tag{1}$$

where $g^{-1}(y)$ is the inverse function of $g(x)$ and \mathcal{Y} is the set of possible outcomes of Y :

$$\mathcal{Y} = \{y = g(x) : x \in \mathcal{X}\} . \tag{2}$$

Proof: Because a strictly decreasing function is invertible, the probability mass function (\rightarrow I/1.6.1) of Y can be derived as follows:

$$\begin{aligned}
 f_Y(y) &= \Pr(Y = y) \\
 &= \Pr(g(X) = y) \\
 &= \Pr(X = g^{-1}(y)) \\
 &= f_X(g^{-1}(y)) .
 \end{aligned} \tag{3}$$

■

Sources:

- Taboga, Marco (2017): “Functions of random variables and their distribution”; in: *Lectures on probability and mathematical statistics*, retrieved on 2020-11-06; URL: <https://www.statlect.com/fundamentals-of-probability/functions-of-random-variables-and-their-distribution#hid6>.

1.6.5 Probability mass function of invertible function

Theorem: Let X be an n -dimensional random vector (\rightarrow I/1.2.3) of discrete random variables (\rightarrow I/1.2.6) with possible outcomes \mathcal{X} and let $g : \mathbb{R}^n \rightarrow \mathbb{R}^n$ be an invertible function on the support of X . Then, the probability mass function (\rightarrow I/1.6.1) of $Y = g(X)$ is given by

$$f_Y(y) = \begin{cases} f_X(g^{-1}(y)) , & \text{if } y \in \mathcal{Y} \\ 0 , & \text{if } y \notin \mathcal{Y} \end{cases} \quad (1)$$

where $g^{-1}(y)$ is the inverse function of $g(x)$ and \mathcal{Y} is the set of possible outcomes of Y :

$$\mathcal{Y} = \{y = g(x) : x \in \mathcal{X}\} . \quad (2)$$

Proof: Because an invertible function is a one-to-one mapping, the probability mass function (\rightarrow I/1.6.1) of Y can be derived as follows:

$$\begin{aligned} f_Y(y) &= \Pr(Y = y) \\ &= \Pr(g(X) = y) \\ &= \Pr(X = g^{-1}(y)) \\ &= f_X(g^{-1}(y)) . \end{aligned} \quad (3)$$

■

Sources:

- Taboga, Marco (2017): “Functions of random vectors and their distribution”; in: *Lectures on probability and mathematical statistics*, retrieved on 2021-08-30; URL: <https://www.statlect.com/fundamentals-of-probability/functions-of-random-vectors>.

1.7 Probability density function

1.7.1 Definition

Definition: Let X be a continuous (\rightarrow I/1.2.6) random variable (\rightarrow I/1.2.2) with possible outcomes \mathcal{X} . Then, $f_X(x) : \mathbb{R} \rightarrow \mathbb{R}$ is the probability density function (PDF) of X , if

$$f_X(x) \geq 0 \quad (1)$$

for all $x \in \mathbb{R}$,

$$\Pr(X \in A) = \int_A f_X(x) dx \quad (2)$$

for any $A \subset \mathcal{X}$ and

$$\int_{\mathcal{X}} f_X(x) dx = 1 . \quad (3)$$

Sources:

- Wikipedia (2020): “Probability density function”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-02-13; URL: https://en.wikipedia.org/wiki/Probability_density_function.

1.7.2 Probability density function of sum of independents

Theorem: Let X and Y be two independent (\rightarrow I/1.3.6) continuous (\rightarrow I/1.2.6) random variables (\rightarrow I/1.2.2) with possible values \mathcal{X} and \mathcal{Y} and let $Z = X + Y$. Then, the probability density function (\rightarrow I/1.7.1) of Z is given by

$$\begin{aligned} f_Z(z) &= \int_{-\infty}^{+\infty} f_X(z-y)f_Y(y) \, dy \\ \text{or } f_Z(z) &= \int_{-\infty}^{+\infty} f_Y(z-x)f_X(x) \, dx \end{aligned} \quad (1)$$

where $f_X(x)$, $f_Y(y)$ and $f_Z(z)$ are the probability density functions (\rightarrow I/1.7.1) of X , Y and Z .

Proof: The cumulative distribution function of a sum of independent random variables (\rightarrow I/1.8.2) is

$$F_Z(z) = E[F_X(z-Y)] . \quad (2)$$

The probability density function is the first derivative of the cumulative distribution function (\rightarrow I/1.7.7), such that

$$\begin{aligned} f_Z(z) &= \frac{d}{dz} F_Z(z) \\ &= \frac{d}{dz} E[F_X(z-Y)] \\ &= E \left[\frac{d}{dz} F_X(z-Y) \right] \\ &= E[f_X(z-Y)] \\ &= \int_{-\infty}^{+\infty} f_X(z-y)f_Y(y) \, dy . \end{aligned} \quad (3)$$

The second equation can be derived by switching X and Y . ■

Sources:

- Taboga, Marco (2017): “Sums of independent random variables”; in: *Lectures on probability and mathematical statistics*, retrieved on 2021-08-30; URL: <https://www.statlect.com/fundamentals-of-probability/sums-of-independent-random-variables>.

1.7.3 Probability density function of strictly increasing function

Theorem: Let X be a continuous (\rightarrow I/1.2.6) random variable (\rightarrow I/1.2.2) with possible outcomes \mathcal{X} and let $g(x)$ be a strictly increasing function on the support of X . Then, the probability density function (\rightarrow I/1.7.1) of $Y = g(X)$ is given by

$$f_Y(y) = \begin{cases} f_X(g^{-1}(y)) \frac{dg^{-1}(y)}{dy} , & \text{if } y \in \mathcal{Y} \\ 0 , & \text{if } y \notin \mathcal{Y} \end{cases} \quad (1)$$

where $g^{-1}(y)$ is the inverse function of $g(x)$ and \mathcal{Y} is the set of possible outcomes of Y :

$$\mathcal{Y} = \{y = g(x) : x \in \mathcal{X}\} . \quad (2)$$

Proof: The cumulative distribution function of a strictly increasing function (\rightarrow I/1.8.3) is

$$F_Y(y) = \begin{cases} 0 , & \text{if } y < \min(\mathcal{Y}) \\ F_X(g^{-1}(y)) , & \text{if } y \in \mathcal{Y} \\ 1 , & \text{if } y > \max(\mathcal{Y}) \end{cases} \quad (3)$$

Because the probability density function is the first derivative of the cumulative distribution function (\rightarrow I/1.7.7)

$$f_X(x) = \frac{dF_X(x)}{dx} , \quad (4)$$

the probability density function (\rightarrow I/1.7.1) of Y can be derived as follows:

1) If y does not belong to the support of Y , $F_Y(y)$ is constant, such that

$$f_Y(y) = 0, \quad \text{if } y \notin \mathcal{Y} . \quad (5)$$

2) If y belongs to the support of Y , then $f_Y(y)$ can be derived using the chain rule:

$$\begin{aligned} f_Y(y) &\stackrel{(4)}{=} \frac{d}{dy} F_Y(y) \\ &\stackrel{(3)}{=} \frac{d}{dy} F_X(g^{-1}(y)) \\ &= f_X(g^{-1}(y)) \frac{dg^{-1}(y)}{dy} . \end{aligned} \quad (6)$$

Taking together (5) and (6), eventually proves (1). ■

Sources:

- Taboga, Marco (2017): “Functions of random variables and their distribution”; in: *Lectures on probability and mathematical statistics*, retrieved on 2020-10-29; URL: <https://www.statlect.com/fundamentals-of-probability/functions-of-random-variables-and-their-distribution#hid4>.

1.7.4 Probability density function of strictly decreasing function

Theorem: Let X be a continuous (\rightarrow I/1.2.6) random variable (\rightarrow I/1.2.2) with possible outcomes \mathcal{X} and let $g(x)$ be a strictly decreasing function on the support of X . Then, the probability density function (\rightarrow I/1.7.1) of $Y = g(X)$ is given by

$$f_Y(y) = \begin{cases} -f_X(g^{-1}(y)) \frac{dg^{-1}(y)}{dy} , & \text{if } y \in \mathcal{Y} \\ 0 , & \text{if } y \notin \mathcal{Y} \end{cases} \quad (1)$$

where $g^{-1}(y)$ is the inverse function of $g(x)$ and \mathcal{Y} is the set of possible outcomes of Y :

$$\mathcal{Y} = \{y = g(x) : x \in \mathcal{X}\} . \quad (2)$$

Proof: The cumulative distribution function of a strictly decreasing function (\rightarrow I/1.8.4) is

$$F_Y(y) = \begin{cases} 1, & \text{if } y > \max(\mathcal{Y}) \\ 1 - F_X(g^{-1}(y)) + \Pr(X = g^{-1}(y)), & \text{if } y \in \mathcal{Y} \\ 0, & \text{if } y < \min(\mathcal{Y}) \end{cases} \quad (3)$$

Note that for continuous random variables, the probability (\rightarrow I/1.7.1) of point events is

$$\Pr(X = a) = \int_a^a f_X(x) dx = 0 . \quad (4)$$

Because the probability density function is the first derivative of the cumulative distribution function (\rightarrow I/1.7.7)

$$f_X(x) = \frac{dF_X(x)}{dx} , \quad (5)$$

the probability density function (\rightarrow I/1.7.1) of Y can be derived as follows:

1) If y does not belong to the support of Y , $F_Y(y)$ is constant, such that

$$f_Y(y) = 0, \quad \text{if } y \notin \mathcal{Y} . \quad (6)$$

2) If y belongs to the support of Y , then $f_Y(y)$ can be derived using the chain rule:

$$\begin{aligned} f_Y(y) &\stackrel{(5)}{=} \frac{d}{dy} F_Y(y) \\ &\stackrel{(3)}{=} \frac{d}{dy} [1 - F_X(g^{-1}(y)) + \Pr(X = g^{-1}(y))] \\ &\stackrel{(4)}{=} \frac{d}{dy} [1 - F_X(g^{-1}(y))] \\ &= -\frac{d}{dy} F_X(g^{-1}(y)) \\ &= -f_X(g^{-1}(y)) \frac{dg^{-1}(y)}{dy} . \end{aligned} \quad (7)$$

Taking together (6) and (7), eventually proves (1). ■

Sources:

- Taboga, Marco (2017): “Functions of random variables and their distribution”; in: *Lectures on probability and mathematical statistics*, retrieved on 2020-11-06; URL: <https://www.statlect.com/fundamentals-of-probability/functions-of-random-variables-and-their-distribution#hid7>.

1.7.5 Probability density function of invertible function

Theorem: Let X be an n -dimensional random vector (\rightarrow I/1.2.3) of continuous random variables (\rightarrow I/1.2.6) with possible outcomes $\mathcal{X} \subseteq \mathbb{R}^n$ and let $g : \mathbb{R}^n \rightarrow \mathbb{R}^n$ be an invertible and differentiable function on the support of X . Then, the probability density function (\rightarrow I/1.7.1) of $Y = g(X)$ is given by

$$f_Y(y) = \begin{cases} f_X(g^{-1}(y)) |J_{g^{-1}}(y)|, & \text{if } y \in \mathcal{Y} \\ 0, & \text{if } y \notin \mathcal{Y} \end{cases}, \quad (1)$$

if the Jacobian determinant satisfies

$$|J_{g^{-1}}(y)| \neq 0 \quad \text{for all } y \in \mathcal{Y} \quad (2)$$

where $g^{-1}(y)$ is the inverse function of $g(x)$, $J_{g^{-1}}(y)$ is the Jacobian matrix of $g^{-1}(y)$

$$J_{g^{-1}}(y) = \begin{bmatrix} \frac{dx_1}{dy_1} & \cdots & \frac{dx_1}{dy_n} \\ \vdots & \ddots & \vdots \\ \frac{dx_n}{dy_1} & \cdots & \frac{dx_n}{dy_n} \end{bmatrix}, \quad (3)$$

$|J|$ is the determinant of J and \mathcal{Y} is the set of possible outcomes of Y :

$$\mathcal{Y} = \{y = g(x) : x \in \mathcal{X}\}. \quad (4)$$

Proof:

1) First, we obtain the cumulative distribution function (\rightarrow I/1.8.1) of $Y = g(X)$. The joint CDF (\rightarrow I/1.8.11) is given by

$$\begin{aligned} F_Y(y) &= \Pr(Y_1 \leq y_1, \dots, Y_n \leq y_n) \\ &= \Pr(g_1(X) \leq y_1, \dots, g_n(X) \leq y_n) \\ &= \int_{A(y)} f_X(x) dx \end{aligned} \quad (5)$$

where $A(y)$ is the following subset of the n -dimensional Euclidean space:

$$A(y) = \{x \in \mathbb{R}^n : g_j(x) \leq y_j \text{ for all } j = 1, \dots, n\} \quad (6)$$

and $g_j(X)$ is the function which returns the j -th element of Y , given a vector X .

2) Next, we substitute $x = g^{-1}(y)$ into the integral which gives us

$$\begin{aligned} F_Y(z) &= \int_{B(z)} f_X(g^{-1}(y)) dg^{-1}(y) \\ &= \int_{-\infty}^{z_n} \cdots \int_{-\infty}^{z_1} f_X(g^{-1}(y)) dg^{-1}(y). \end{aligned} \quad (7)$$

where we have modified the integration regime $B(z)$ which reads

$$B(z) = \{y \in \mathbb{R}^n : y \leq z_j \text{ for all } j = 1, \dots, n\} . \quad (8)$$

3) The formula for change of variables in multivariable calculus states that

$$y = f(x) \quad \Rightarrow \quad dy = |J_f(x)| dx . \quad (9)$$

Applied to equation (7), this yields

$$\begin{aligned} F_Y(z) &= \int_{-\infty}^{z_n} \dots \int_{-\infty}^{z_1} f_X(g^{-1}(y)) |J_{g^{-1}}(y)| dy \\ &= \int_{-\infty}^{z_n} \dots \int_{-\infty}^{z_1} f_X(g^{-1}(y)) |J_{g^{-1}}(y)| dy_1 \dots dy_n . \end{aligned} \quad (10)$$

4) Finally, we obtain the probability density function (\rightarrow I/1.7.1) of $Y = g(X)$. Because the PDF is the derivative of the CDF (\rightarrow I/1.7.7), we can differentiate the joint CDF to get

$$\begin{aligned} f_Y(z) &= \frac{d^n}{dz_1 \dots dz_n} F_Y(z) \\ &= \frac{d^n}{dz_1 \dots dz_n} \int_{-\infty}^{z_n} \dots \int_{-\infty}^{z_1} f_X(g^{-1}(y)) |J_{g^{-1}}(y)| dy_1 \dots dy_n \\ &= f_X(g^{-1}(z)) |J_{g^{-1}}(z)| \end{aligned} \quad (11)$$

which can also be written as

$$f_Y(y) = f_X(g^{-1}(y)) |J_{g^{-1}}(y)| . \quad (12)$$

■

Sources:

- Taboga, Marco (2017): “Functions of random vectors and their distribution”; in: *Lectures on probability and mathematical statistics*, retrieved on 2021-08-30; URL: <https://www.statlect.com/fundamentals-of-probability/functions-of-random-vectors>.
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1.7.6 Probability density function of linear transformation

Theorem: Let X be an n -dimensional random vector (\rightarrow I/1.2.3) of continuous random variables (\rightarrow I/1.2.6) with possible outcomes $\mathcal{X} \subseteq \mathbb{R}^n$ and let $Y = \Sigma X + \mu$ be a linear transformation of this random variable with constant (\rightarrow I/1.2.5) n -dimensional vector μ and constant (\rightarrow I/1.2.5) $n \times n$ matrix Σ . Then, the probability density function (\rightarrow I/1.7.1) of Y is

$$f_Y(y) = \begin{cases} \frac{1}{|\Sigma|} f_X(\Sigma^{-1}(y - \mu)) , & \text{if } y \in \mathcal{Y} \\ 0 , & \text{if } y \notin \mathcal{Y} \end{cases} \quad (1)$$

where $|\Sigma|$ is the determinant of Σ and \mathcal{Y} is the set of possible outcomes of Y :

$$\mathcal{Y} = \{y = \Sigma x + \mu : x \in \mathcal{X}\} . \quad (2)$$

Proof: Because the linear function $g(X) = \Sigma X + \mu$ is invertible and differentiable, we can determine the probability density function of an invertible function of a continuous random vector (\rightarrow I/1.7.5) using the relation

$$f_Y(y) = \begin{cases} f_X(g^{-1}(y)) |J_{g^{-1}}(y)| , & \text{if } y \in \mathcal{Y} \\ 0 , & \text{if } y \notin \mathcal{Y} \end{cases} . \quad (3)$$

The inverse function is

$$X = g^{-1}(Y) = \Sigma^{-1}(Y - \mu) = \Sigma^{-1}Y - \Sigma^{-1}\mu \quad (4)$$

and the Jacobian matrix is

$$J_{g^{-1}}(y) = \begin{bmatrix} \frac{dx_1}{dy_1} & \cdots & \frac{dx_1}{dy_n} \\ \vdots & \ddots & \vdots \\ \frac{dx_n}{dy_1} & \cdots & \frac{dx_n}{dy_n} \end{bmatrix} = \Sigma^{-1} . \quad (5)$$

Plugging (4) and (5) into (3) and applying the determinant property $|A^{-1}| = |A|^{-1}$, we obtain

$$f_Y(y) = \frac{1}{|\Sigma|} f_X(\Sigma^{-1}(y - \mu)) . \quad (6)$$

■

Sources:

- Taboga, Marco (2017): “Functions of random vectors and their distribution”; in: *Lectures on probability and mathematical statistics*, retrieved on 2021-08-30; URL: <https://www.statlect.com/fundamentals-of-probability/functions-of-random-vectors>.

1.7.7 Probability density function in terms of cumulative distribution function

Theorem: Let X be a continuous (\rightarrow I/1.2.6) random variable (\rightarrow I/1.2.2). Then, the probability distribution function (\rightarrow I/1.7.1) of X is the first derivative of the cumulative distribution function (\rightarrow I/1.8.1) of X :

$$f_X(x) = \frac{dF_X(x)}{dx} . \quad (1)$$

Proof: The cumulative distribution function in terms of the probability density function of a continuous random variable (\rightarrow I/1.8.6) is given by:

$$F_X(x) = \int_{-\infty}^x f_X(t) dt, \quad x \in \mathbb{R} . \quad (2)$$

Taking the derivative with respect to x , we have:

$$\frac{dF_X(x)}{dx} = \frac{d}{dx} \int_{-\infty}^x f_X(t) dt . \quad (3)$$

The fundamental theorem of calculus states that, if $f(x)$ is a continuous real-valued function defined on the interval $[a, b]$, then it holds that

$$F(x) = \int_a^x f(t) dt \quad \Rightarrow \quad F'(x) = f(x) \quad \text{for all } x \in (a, b) . \quad (4)$$

Applying (4) to (2), it follows that

$$F_X(x) = \int_{-\infty}^x f_X(t) dt \quad \Rightarrow \quad \frac{dF_X(x)}{dx} = f_X(x) \quad \text{for all } x \in \mathbb{R} . \quad (5)$$

■

Sources:

- Wikipedia (2020): “Fundamental theorem of calculus”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-11-12; URL: https://en.wikipedia.org/wiki/Fundamental_theorem_of_calculus#Formal_statements.

1.7.8 Joint probability density function

Definition: Let $X \in \mathbb{R}^n$ be a continuous (\rightarrow I/1.2.6) random vector (\rightarrow I/1.2.3). Then, a function $f_X(x) : \mathbb{R}^n \rightarrow \mathbb{R}$ is the joint (\rightarrow I/1.5.2) probability density function (\rightarrow I/1.7.1) of X , if

$$f_X(x) \geq 0 \quad (1)$$

for all $x \in \mathbb{R}^n$,

$$\Pr(X \in A) = \int_A f_X(x) dx \quad (2)$$

for any $A \subset \mathbb{R}^n$ and

$$\int_{\mathbb{R}^n} f_X(x) dx = 1 . \quad (3)$$

Sources:

- Wikipedia (2025): “Probability density function”; in: *Wikipedia, the free encyclopedia*, retrieved on 2025-02-06; URL: https://en.wikipedia.org/wiki/Probability_density_function#Densities_associated_with_multiple_variables.

1.8 Cumulative distribution function

1.8.1 Definition

Definition: The cumulative distribution function (CDF) of a random variable (\rightarrow I/1.2.2) X at a given value x is defined as the probability (\rightarrow I/1.3.1) that X is smaller than x :

$$F_X(x) = \Pr(X \leq x) . \quad (1)$$

1) If X is a discrete (\rightarrow I/1.2.6) random variable (\rightarrow I/1.2.2) with possible outcomes \mathcal{X} and the probability mass function (\rightarrow I/1.6.1) $f_X(x)$, then the cumulative distribution function is the function (\rightarrow I/1.8.5) $F_X(x) : \mathbb{R} \rightarrow [0, 1]$ with

$$F_X(x) = \sum_{\substack{t \in \mathcal{X} \\ t \leq x}} f_X(t) . \quad (2)$$

2) If X is a continuous (\rightarrow I/1.2.6) random variable (\rightarrow I/1.2.2) with possible outcomes \mathcal{X} and the probability density function (\rightarrow I/1.7.1) $f_X(x)$, then the cumulative distribution function is the function (\rightarrow I/1.8.6) $F_X(x) : \mathbb{R} \rightarrow [0, 1]$ with

$$F_X(x) = \int_{-\infty}^x f_X(t) dt . \quad (3)$$

Sources:

- Wikipedia (2020): “Cumulative distribution function”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-02-17; URL: https://en.wikipedia.org/wiki/Cumulative_distribution_function#Definition.

1.8.2 Cumulative distribution function of sum of independents

Theorem: Let X and Y be two independent (\rightarrow I/1.3.6) random variables (\rightarrow I/1.2.2) and let $Z = X + Y$. Then, the cumulative distribution function (\rightarrow I/1.8.1) of Z is given by

$$\begin{aligned} F_Z(z) &= \mathbb{E}[F_X(z - Y)] \\ \text{or } F_Z(z) &= \mathbb{E}[F_Y(z - X)] \end{aligned} \quad (1)$$

where $F_X(x)$, $F_Y(y)$ and $F_Z(z)$ are the cumulative distribution functions (\rightarrow I/1.8.1) of X , Y and Z and $\mathbb{E}[\cdot]$ denotes the expected value (\rightarrow I/1.12.1).

Proof: Using the definition of the cumulative distribution function (\rightarrow I/1.8.1), the first equation can be derived as follows:

$$\begin{aligned} F_Z(z) &= \Pr(Z \leq z) \\ &= \Pr(X + Y \leq z) \\ &= \Pr(X \leq z - Y) \\ &= \mathbb{E}[\Pr(X \leq z - Y | Y = y)] \\ &= \mathbb{E}[\Pr(X \leq z - Y)] \\ &= \mathbb{E}[F_X(z - Y)] . \end{aligned} \quad (2)$$

Note that the second-last transition is justified by the fact that X and Y are independent (\rightarrow I/1.3.6), such that conditional probabilities are equal to marginal probabilities (\rightarrow I/1.3.9). The second equation can be derived by switching X and Y . ■

Sources:

- Taboga, Marco (2017): “Sums of independent random variables”; in: *Lectures on probability and mathematical statistics*, retrieved on 2021-08-30; URL: <https://www.statlect.com/fundamentals-of-probability/sums-of-independent-random-variables>.

1.8.3 Cumulative distribution function of strictly increasing function

Theorem: Let X be a random variable (\rightarrow I/1.2.2) with possible outcomes \mathcal{X} and let $g(x)$ be a strictly increasing function on the support of X . Then, the cumulative distribution function (\rightarrow I/1.8.1) of $Y = g(X)$ is given by

$$F_Y(y) = \begin{cases} 0, & \text{if } y < \min(\mathcal{Y}) \\ F_X(g^{-1}(y)), & \text{if } y \in \mathcal{Y} \\ 1, & \text{if } y > \max(\mathcal{Y}) \end{cases} \quad (1)$$

where $g^{-1}(y)$ is the inverse function of $g(x)$ and \mathcal{Y} is the set of possible outcomes of Y :

$$\mathcal{Y} = \{y = g(x) : x \in \mathcal{X}\} . \quad (2)$$

Proof: The support of Y is determined by $g(x)$ and by the set of possible outcomes of X . Moreover, if $g(x)$ is strictly increasing, then $g^{-1}(y)$ is also strictly increasing. Therefore, the cumulative distribution function (\rightarrow I/1.8.1) of Y can be derived as follows:

1) If y is lower than the lowest value (\rightarrow I/1.20.1) Y can take, then $\Pr(Y \leq y) = 0$, so

$$F_Y(y) = 0, \quad \text{if } y < \min(\mathcal{Y}) . \quad (3)$$

2) If y belongs to the support of Y , then $F_Y(y)$ can be derived as follows:

$$\begin{aligned} F_Y(y) &= \Pr(Y \leq y) \\ &= \Pr(g(X) \leq y) \\ &= \Pr(X \leq g^{-1}(y)) \\ &= F_X(g^{-1}(y)) . \end{aligned} \quad (4)$$

3) If y is higher than the highest value (\rightarrow I/1.20.2) Y can take, then $\Pr(Y \leq y) = 1$, so

$$F_Y(y) = 1, \quad \text{if } y > \max(\mathcal{Y}) . \quad (5)$$

Taking together (3), (4), (5), eventually proves (1). ■

Sources:

- Taboga, Marco (2017): “Functions of random variables and their distribution”; in: *Lectures on probability and mathematical statistics*, retrieved on 2020-10-29; URL: <https://www.statlect.com/fundamentals-of-probability/functions-of-random-variables-and-their-distribution#hid2>.

1.8.4 Cumulative distribution function of strictly decreasing function

Theorem: Let X be a random variable (\rightarrow I/1.2.2) with possible outcomes \mathcal{X} and let $g(x)$ be a strictly decreasing function on the support of X . Then, the cumulative distribution function (\rightarrow I/1.8.1) of $Y = g(X)$ is given by

$$F_Y(y) = \begin{cases} 1, & \text{if } y > \max(\mathcal{Y}) \\ 1 - F_X(g^{-1}(y)) + \Pr(X = g^{-1}(y)), & \text{if } y \in \mathcal{Y} \\ 0, & \text{if } y < \min(\mathcal{Y}) \end{cases} \quad (1)$$

where $g^{-1}(y)$ is the inverse function of $g(x)$ and \mathcal{Y} is the set of possible outcomes of Y :

$$\mathcal{Y} = \{y = g(x) : x \in \mathcal{X}\} . \quad (2)$$

Proof: The support of Y is determined by $g(x)$ and by the set of possible outcomes of X . Moreover, if $g(x)$ is strictly decreasing, then $g^{-1}(y)$ is also strictly decreasing. Therefore, the cumulative distribution function (\rightarrow I/1.8.1) of Y can be derived as follows:

1) If y is higher than the highest value (\rightarrow I/1.20.2) Y can take, then $\Pr(Y \leq y) = 1$, so

$$F_Y(y) = 1, \quad \text{if } y > \max(\mathcal{Y}) . \quad (3)$$

2) If y belongs to the support of Y , then $F_Y(y)$ can be derived as follows:

$$\begin{aligned} F_Y(y) &= \Pr(Y \leq y) \\ &= 1 - \Pr(Y > y) \\ &= 1 - \Pr(g(X) > y) \\ &= 1 - \Pr(X < g^{-1}(y)) \\ &= 1 - \Pr(X < g^{-1}(y)) - \Pr(X = g^{-1}(y)) + \Pr(X = g^{-1}(y)) \\ &= 1 - [\Pr(X < g^{-1}(y)) + \Pr(X = g^{-1}(y))] + \Pr(X = g^{-1}(y)) \\ &= 1 - \Pr(X \leq g^{-1}(y)) + \Pr(X = g^{-1}(y)) \\ &= 1 - F_X(g^{-1}(y)) + \Pr(X = g^{-1}(y)) . \end{aligned} \quad (4)$$

3) If y is lower than the lowest value (\rightarrow I/1.20.1) Y can take, then $\Pr(Y \leq y) = 0$, so

$$F_Y(y) = 0, \quad \text{if } y < \min(\mathcal{Y}) . \quad (5)$$

Taking together (3), (4), (5), eventually proves (1). ■

Sources:

- Taboga, Marco (2017): “Functions of random variables and their distribution”; in: *Lectures on probability and mathematical statistics*, retrieved on 2020-11-06; URL: <https://www.statlect.com/fundamentals-of-probability/functions-of-random-variables-and-their-distribution#hid5>.

1.8.5 Cumulative distribution function of discrete random variable

Theorem: Let X be a discrete (\rightarrow I/1.2.6) random variable (\rightarrow I/1.2.2) with possible values \mathcal{X} and probability mass function (\rightarrow I/1.6.1) $f_X(x)$. Then, the cumulative distribution function (\rightarrow I/1.8.1) of X is

$$F_X(x) = \sum_{\substack{t \in \mathcal{X} \\ t \leq x}} f_X(t) . \quad (1)$$

Proof: The cumulative distribution function (\rightarrow I/1.8.1) of a random variable (\rightarrow I/1.2.2) X is defined as the probability that X is smaller than x :

$$F_X(x) = \Pr(X \leq x) . \quad (2)$$

The probability mass function (\rightarrow I/1.6.1) of a discrete (\rightarrow I/1.2.6) random variable (\rightarrow I/1.2.2) X returns the probability that X takes a particular value x :

$$f_X(x) = \Pr(X = x) . \quad (3)$$

Taking these two definitions together, we have:

$$\begin{aligned} F_X(x) &\stackrel{(2)}{=} \sum_{\substack{t \in \mathcal{X} \\ t \leq x}} \Pr(X = t) \\ &\stackrel{(3)}{=} \sum_{\substack{t \in \mathcal{X} \\ t \leq x}} f_X(t) . \end{aligned} \quad (4)$$

■

1.8.6 Cumulative distribution function of continuous random variable

Theorem: Let X be a continuous (\rightarrow I/1.2.6) random variable (\rightarrow I/1.2.2) with possible values \mathcal{X} and probability density function (\rightarrow I/1.7.1) $f_X(x)$. Then, the cumulative distribution function (\rightarrow I/1.8.1) of X is

$$F_X(x) = \int_{-\infty}^x f_X(t) dt . \quad (1)$$

Proof: The cumulative distribution function (\rightarrow I/1.8.1) of a random variable (\rightarrow I/1.2.2) X is defined as the probability that X is smaller than x :

$$F_X(x) = \Pr(X \leq x) . \quad (2)$$

The probability density function (\rightarrow I/1.7.1) of a continuous (\rightarrow I/1.2.6) random variable (\rightarrow I/1.2.2) X can be used to calculate the probability that X falls into a particular interval A :

$$\Pr(X \in A) = \int_A f_X(x) dx . \quad (3)$$

Taking these two definitions together, we have:

$$\begin{aligned}
F_X(x) &\stackrel{(2)}{=} \Pr(X \in (-\infty, x]) \\
&\stackrel{(3)}{=} \int_{-\infty}^x f_X(t) dt .
\end{aligned} \tag{4}$$

■

1.8.7 Exceedance probability based on cumulative distribution function

Theorem: Let X be a random variable (\rightarrow I/1.2.2) with possible values \mathcal{X} and cumulative distribution function (\rightarrow I/1.8.1) $F_X(x)$. Then, the exceedance probability (\rightarrow I/1.3.11) that X is larger than some value x is

$$\Pr(X > x) = 1 - F_X(x) . \tag{1}$$

Proof: Note that $\{X \mid X > x\}$ and $\{X \mid X \leq x\}$ are disjoint sets

$$\{X \mid X > x\} \cap \{X \mid X \leq x\} = \emptyset \tag{2}$$

and that they comprise the set of all outcomes, i.e. the sample space (\rightarrow I/1.1.2):

$$\{X \mid X > x\} \cup \{X \mid X \leq x\} = \mathcal{X} = \Omega . \tag{3}$$

Using the second axiom of probability (\rightarrow I/1.4.1), we have:

$$\begin{aligned}
p(\Omega) &= 1 \\
p(\{X \mid X > x\} \cup \{X \mid X \leq x\}) &= 1 .
\end{aligned} \tag{4}$$

Using the third axiom of probability (\rightarrow I/1.4.1), we get:

$$\begin{aligned}
p(\{X \mid X > x\}) + p(\{X \mid X \leq x\}) &= 1 \\
p(\{X \mid X > x\}) &= 1 - p(\{X \mid X \leq x\}) \\
\Pr(X > x) &= 1 - \Pr(X \leq x) .
\end{aligned} \tag{5}$$

Using the definition of the cumulative distribution function (\rightarrow I/1.8.1), we finally have:

$$\Pr(X > x) = 1 - F_X(x) . \tag{6}$$

■

Sources:

- Ostwald, Dirk (2023): “Zufallsvariablen”; in: *Wahrscheinlichkeitstheorie und Frequentistische Inferenz*, Einheit (3), Folie 34; URL: https://www.ipsy.ovgu.de/ipsy_media/Methodenlehre+I/Wintersemester2324/Wahrscheinlichkeitstheorie+und+Frequentistische+Inferenz/3_Zufallsvariablen.pdf.

1.8.8 Probability integral transform

Theorem: Let X be a continuous (\rightarrow I/1.2.6) random variable (\rightarrow I/1.2.2) with invertible (\rightarrow I/1.11.1) cumulative distribution function (\rightarrow I/1.8.1) $F_X(x)$. Then, the random variable (\rightarrow I/1.2.2)

$$Y = F_X(X) \quad (1)$$

has a standard uniform distribution (\rightarrow II/3.1.2).

Proof: The cumulative distribution function (\rightarrow I/1.8.1) of $Y = F_X(X)$ can be derived as

$$\begin{aligned} F_Y(y) &= \Pr(Y \leq y) \\ &= \Pr(F_X(X) \leq y) \\ &= \Pr(X \leq F_X^{-1}(y)) \\ &= F_X(F_X^{-1}(y)) \\ &= y \end{aligned} \quad (2)$$

which is the cumulative distribution function of a continuous uniform distribution (\rightarrow II/3.1.4) with $a = 0$ and $b = 1$, i.e. the cumulative distribution function (\rightarrow I/1.8.1) of the standard uniform distribution (\rightarrow II/3.1.2) $\mathcal{U}(0, 1)$. ■

Sources:

- Wikipedia (2021): “Probability integral transform”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-04-07; URL: https://en.wikipedia.org/wiki/Probability_integral_transform#Proof.

1.8.9 Inverse transformation method

Theorem: Let U be a continuous (\rightarrow I/1.2.6) random variable (\rightarrow I/1.2.2) having a standard uniform distribution (\rightarrow II/3.1.2). Then, the random variable (\rightarrow I/1.2.2)

$$X = F_X^{-1}(U) \quad (1)$$

has a probability distribution (\rightarrow I/1.5.1) characterized by the invertible (\rightarrow I/1.11.1) cumulative distribution function (\rightarrow I/1.8.1) $F_X(x)$.

Proof: With the cumulative distribution function of the continuous uniform distribution (\rightarrow II/3.1.4), the cumulative distribution function (\rightarrow I/1.8.1) of the standard uniform distribution (\rightarrow II/3.1.2) is

$$U \sim \mathcal{U}(0, 1) \quad \Rightarrow \quad F_U(u) = \Pr(U \leq u) = u. \quad (2)$$

Thus, the cumulative distribution function (\rightarrow I/1.8.1) of the transformation $X = F_X^{-1}(U)$ can be derived as

$$\begin{aligned} \Pr(X \leq x) &= \Pr(F_X^{-1}(U) \leq x) \\ &= \Pr(U \leq F_X(x)) \\ &= F_U(F_X(x)) \\ &= F_X(x). \end{aligned} \quad (3)$$

Sources:

- Wikipedia (2021): “Inverse transform sampling”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-04-07; URL: https://en.wikipedia.org/wiki/Inverse_transform_sampling#Proof_of_correctness.

1.8.10 Distributional transformation

Theorem: Let X and Y be two continuous (\rightarrow I/1.2.6) random variables (\rightarrow I/1.2.2) with cumulative distribution function (\rightarrow I/1.8.1) $F_X(x)$ and invertible cumulative distribution function (\rightarrow I/1.8.1) $F_Y(y)$. Then, the random variable (\rightarrow I/1.2.2)

$$\tilde{X} = F_Y^{-1}(F_X(X)) \quad (1)$$

has the same probability distribution (\rightarrow I/1.5.1) as Y .

Proof: The cumulative distribution function (\rightarrow I/1.8.1) of the transformation $\tilde{X} = F_Y^{-1}(F_X(X))$ can be derived as

$$\begin{aligned} F_{\tilde{X}}(y) &= \Pr(\tilde{X} \leq y) \\ &= \Pr(F_Y^{-1}(F_X(X)) \leq y) \\ &= \Pr(F_X(X) \leq F_Y(y)) \\ &= \Pr(X \leq F_X^{-1}(F_Y(y))) \\ &= F_X(F_X^{-1}(F_Y(y))) \\ &= F_Y(y) \end{aligned} \quad (2)$$

which shows that \tilde{X} and Y have the same cumulative distribution function (\rightarrow I/1.8.1) and are thus identically distributed (\rightarrow I/1.5.1).

Sources:

- Soch, Joram (2020): “Distributional Transformation Improves Decoding Accuracy When Predicting Chronological Age From Structural MRI”; in: *Frontiers in Psychiatry*, vol. 11, art. 604268; URL: <https://www.frontiersin.org/articles/10.3389/fpsy.2020.604268/full>; DOI: 10.3389/fpsy.2020.604268

1.8.11 Joint cumulative distribution function

Definition: Let $X \in \mathbb{R}^n$ be an n -dimensional random vector (\rightarrow I/1.2.3). Then, the joint (\rightarrow I/1.5.2) cumulative distribution function (\rightarrow I/1.8.1) of X is defined as the probability (\rightarrow I/1.3.1) that each entry X_i is smaller than a specific value x_i for $i = 1, \dots, n$:

$$F_X(x) = \Pr(X_1 \leq x_1, \dots, X_n \leq x_n) . \quad (1)$$

Sources:

- Wikipedia (2021): “Cumulative distribution function”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-04-07; URL: https://en.wikipedia.org/wiki/Cumulative_distribution_function#Definition_for_more_than_two_random_variables.

1.9 Moment-generating function

1.9.1 Definition

Definition:

1) The moment-generating function of a random variable (\rightarrow I/1.2.2) $X \in \mathbb{R}$ is

$$M_X(t) = \mathbb{E} [e^{tX}], \quad t \in \mathbb{R}. \quad (1)$$

2) The moment-generating function of a random vector (\rightarrow I/1.2.3) $X \in \mathbb{R}^n$ is

$$M_X(t) = \mathbb{E} [e^{t^T X}], \quad t \in \mathbb{R}^n. \quad (2)$$

Sources:

- Wikipedia (2020): “Moment-generating function”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-01-22; URL: https://en.wikipedia.org/wiki/Moment-generating_function#Definition.
- Taboga, Marco (2017): “Joint moment generating function”; in: *Lectures on probability and mathematical statistics*, retrieved on 2021-10-07; URL: <https://www.statlect.com/fundamentals-of-probability/joint-moment-generating-function>.

1.9.2 Moment-generating function of sum of independents

Theorem: Let X and Y be two independent (\rightarrow I/1.3.6) random variables (\rightarrow I/1.2.2) and let $Z = X + Y$. Then, the moment-generating function (\rightarrow I/1.9.1) of Z is given by

$$M_Z(t) = M_X(t) \cdot M_Y(t) \quad (1)$$

where $M_X(t)$, $M_Y(t)$ and $M_Z(t)$ are the moment-generating functions (\rightarrow I/1.9.1) of X , Y and Z .

Proof: The moment-generating function of a random variable (\rightarrow I/1.9.1) X is

$$M_X(t) = \mathbb{E} (\exp [tX]) \quad (2)$$

and therefore the moment-generating function of the sum Z is given by

$$\begin{aligned} M_Z(t) &= \mathbb{E} (\exp [tZ]) \\ &= \mathbb{E} (\exp [t(X + Y)]) \\ &= \mathbb{E} (\exp [tX] \cdot \exp [tY]) . \end{aligned} \quad (3)$$

Because the expected value is multiplicative for independent random variables (\rightarrow I/1.12.7), we have

$$\begin{aligned} M_Z(t) &= \mathbb{E} (\exp [tX]) \cdot \mathbb{E} (\exp [tY]) \\ &= M_X(t) \cdot M_Y(t) . \end{aligned} \quad (4)$$

■

Sources:

- Probability Fact (2021): “If X and Y are independent, the moment generating function (MGF)”; in: X , retrieved on 2024-11-08; URL: <https://x.com/ProbFact/status/1468264616706859016>.

1.9.3 Moment-generating function of arbitrary function

Theorem: Let X be a random variable (\rightarrow I/1.2.2) with the expected value (\rightarrow I/1.12.1) function $E_X[\cdot]$. Then, the moment-generating function (\rightarrow I/1.9.1) of $Y = g(X)$ is equal to

$$M_Y(t) = E_X [\exp(t g(X))] . \quad (1)$$

Proof: The moment-generating function (\rightarrow I/1.9.1) is defined as

$$M_Y(t) = E [\exp(t Y)] . \quad (2)$$

Due of the law of the unconscious statistician (\rightarrow I/1.12.9)

$$\begin{aligned} E[g(X)] &= \sum_{x \in \mathcal{X}} g(x) f_X(x) \\ E[g(X)] &= \int_{\mathcal{X}} g(x) f_X(x) dx , \end{aligned} \quad (3)$$

$Y = g(X)$ can simply be substituted into (2) to give

$$M_Y(t) = E_X [\exp(t g(X))] . \quad (4)$$

■

Sources:

- Taboga, Marco (2017): “Functions of random vectors and their distribution”; in: *Lectures on probability and mathematical statistics*, retrieved on 2021-09-22; URL: <https://www.statlect.com/fundamentals-of-probability/functions-of-random-vectors>.

1.9.4 Moment-generating function of linear transformation

Theorem: Let X be an n -dimensional random vector (\rightarrow I/1.2.3) with the moment-generating function (\rightarrow I/1.9.1) $M_X(t)$. Then, the moment-generating function of the linear transformation $Y = AX + b$ is given by

$$M_Y(t) = \exp [t^T b] \cdot M_X(At) \quad (1)$$

where A is an $m \times n$ matrix and b is an $m \times 1$ vector.

Proof: The moment-generating function of a random vector (\rightarrow I/1.9.1) X is

$$M_X(t) = E (\exp [t^T X]) \quad (2)$$

and therefore the moment-generating function of the random vector (\rightarrow I/1.2.3) Y is given by

$$\begin{aligned} M_Y(t) &= E (\exp [t^T (AX + b)]) \\ &= E (\exp [t^T AX] \cdot \exp [t^T b]) \\ &= \exp [t^T b] \cdot E (\exp [(At)^T X]) \\ &= \exp [t^T b] \cdot M_X(At) . \end{aligned} \quad (3)$$

**Sources:**

- ProofWiki (2020): “Moment Generating Function of Linear Transformation of Random Variable”; in: *ProofWiki*, retrieved on 2020-08-19; URL: https://proofwiki.org/wiki/Moment_Generating_Function_of_Linear_Transformation_of_Random_Variable.

1.9.5 Moment-generating function of linear combination

Theorem: Let X_1, \dots, X_n be n independent (\rightarrow I/1.3.6) random variables (\rightarrow I/1.2.2) with moment-generating functions (\rightarrow I/1.9.1) $M_{X_i}(t)$. Then, the moment-generating function of the linear combination $X = \sum_{i=1}^n a_i X_i$ is given by

$$M_X(t) = \prod_{i=1}^n M_{X_i}(a_i t) \quad (1)$$

where a_1, \dots, a_n are n real numbers.

Proof: The moment-generating function of a random variable (\rightarrow I/1.9.1) X_i is

$$M_{X_i}(t) = E(\exp[tX_i]) \quad (2)$$

and therefore the moment-generating function of the linear combination X is given by

$$\begin{aligned} M_X(t) &= E(\exp[tX]) \\ &= E\left(\exp\left[t \sum_{i=1}^n a_i X_i\right]\right) \\ &= E\left(\prod_{i=1}^n \exp[t a_i X_i]\right). \end{aligned} \quad (3)$$

Because the expected value is multiplicative for independent random variables (\rightarrow I/1.12.7), we have

$$\begin{aligned} M_X(t) &= \prod_{i=1}^n E(\exp[(a_i t)X_i]) \\ &= \prod_{i=1}^n M_{X_i}(a_i t). \end{aligned} \quad (4)$$

**Sources:**

- ProofWiki (2020): “Moment Generating Function of Linear Combination of Independent Random Variables”; in: *ProofWiki*, retrieved on 2020-08-19; URL: https://proofwiki.org/wiki/Moment_Generating_Function_of_Linear_Combination_of_Independent_Random_Variables.

1.10 Probability-generating function

1.10.1 Definition

Definition:

1) If X is a discrete (\rightarrow I/1.2.6) random variable (\rightarrow I/1.2.2) taking values in the non-negative integers $\{0, 1, \dots\}$, then the probability-generating function of X is defined as

$$G_X(z) = \sum_{x=0}^{\infty} f_X(x) z^x \quad (1)$$

where $z \in \mathbb{C}$ and $f_X(x)$ is the probability mass function (\rightarrow I/1.6.1) of X .

2) If X is a discrete (\rightarrow I/1.2.6) random vector (\rightarrow I/1.2.3) taking values in the n -dimensional integer lattice $x \in \{0, 1, \dots\}^n$, then the probability-generating function of X is defined as

$$G_X(z) = \sum_{x_1=0}^{\infty} \cdots \sum_{x_n=0}^{\infty} f_{X_1, \dots, X_n}(x_1, \dots, x_n) z_1^{x_1} \cdots z_n^{x_n} \quad (2)$$

where $z \in \mathbb{C}^n$ and $f_{X_1, \dots, X_n}(x_1, \dots, x_n)$ is the probability mass function (\rightarrow I/1.6.1) of X .

Sources:

- Wikipedia (2020): “Probability-generating function”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-05-31; URL: https://en.wikipedia.org/wiki/Probability-generating_function#Definition.

1.10.2 Probability-generating function in terms of expected value

Theorem: Let X be a discrete (\rightarrow I/1.2.6) random variable (\rightarrow I/1.2.2) whose set of possible values \mathcal{X} is a subset of the natural numbers \mathbb{N} . Then, the probability-generating function (\rightarrow I/1.10.1) of X can be expressed in terms of an expected value (\rightarrow I/1.12.1) of a function of X

$$G_X(z) = \mathbb{E} [z^X] \quad (1)$$

where $z \in \mathbb{C}$.

Proof: The law of the unconscious statistician (\rightarrow I/1.12.9) states that

$$\mathbb{E}[g(X)] = \sum_{x \in \mathcal{X}} g(x) f_X(x) \quad (2)$$

where $f_X(x)$ is the probability mass function (\rightarrow I/1.6.1) of X . Here, we have $g(X) = z^X$, such that

$$\mathbb{E} [z^X] = \sum_{x \in \mathcal{X}} z^x f_X(x) . \quad (3)$$

By the definition of X , this is equal to

$$\mathbb{E} [z^X] = \sum_{x=0}^{\infty} f_X(x) z^x . \quad (4)$$

The right-hand side is equal to the probability-generating function (\rightarrow I/1.10.1) of X :

$$\mathbb{E} [z^X] = G_X(z) . \quad (5)$$

**Sources:**

- ProofWiki (2022): “Probability Generating Function as Expectation”; in: *ProofWiki*, retrieved on 2022-10-11; URL: https://proofwiki.org/wiki/Probability_Generating_Function_as_Expectation.

1.10.3 Probability-generating function of zero

Theorem: Let X be a random variable (\rightarrow I/1.2.2) with probability-generating function (\rightarrow I/1.10.1) $G_X(z)$ and probability mass function (\rightarrow I/1.6.1) $f_X(x)$. Then, the value of the probability-generating function at zero is equal to the value of the probability mass function at zero:

$$G_X(0) = f_X(0) . \quad (1)$$

Proof: The probability-generating function (\rightarrow I/1.10.1) of X is defined as

$$G_X(z) = \sum_{x=0}^{\infty} f_X(x) z^x \quad (2)$$

where $f_X(x)$ is the probability mass function (\rightarrow I/1.6.1) of X . Setting $z = 0$, we obtain:

$$\begin{aligned} G_X(0) &= \sum_{x=0}^{\infty} f_X(x) \cdot 0^x \\ &= f_X(0) + 0^1 \cdot f_X(1) + 0^2 \cdot f_X(2) + \dots \\ &= f_X(0) + 0 + 0 + \dots \\ &= f_X(0) . \end{aligned} \quad (3)$$

**Sources:**

- ProofWiki (2022): “Probability Generating Function of Zero”; in: *ProofWiki*, retrieved on 2022-10-11; URL: https://proofwiki.org/wiki/Probability_Generating_Function_of_Zero.

1.10.4 Probability-generating function of one

Theorem: Let X be a random variable (\rightarrow I/1.2.2) with probability-generating function (\rightarrow I/1.10.1) $G_X(z)$ and set of possible values \mathcal{X} . Then, the value of the probability-generating function at one is equal to one:

$$G_X(1) = 1 . \quad (1)$$

Proof: The probability-generating function (\rightarrow I/1.10.1) of X is defined as

$$G_X(z) = \sum_{x=0}^{\infty} f_X(x) z^x \quad (2)$$

where $f_X(x)$ is the probability mass function (\rightarrow I/1.6.1) of X . Setting $z = 1$, we obtain:

$$\begin{aligned}
G_X(1) &= \sum_{x=0}^{\infty} f_X(x) \cdot 1^x \\
&= \sum_{x=0}^{\infty} f_X(x) \cdot 1 \\
&= \sum_{x=0}^{\infty} f_X(x) .
\end{aligned} \tag{3}$$

Because the probability mass function (\rightarrow I/1.6.1) sums up to one, this becomes:

$$\begin{aligned}
G_X(1) &= \sum_{x \in \mathcal{X}} f_X(x) \\
&= 1 .
\end{aligned} \tag{4}$$

■

Sources:

- ProofWiki (2022): “Probability Generating Function of One”; in: *ProofWiki*, retrieved on 2022-10-11; URL: https://proofwiki.org/wiki/Probability_Generating_Function_of_One.

1.11 Other probability functions

1.11.1 Quantile function

Definition: Let X be a random variable (\rightarrow I/1.2.2) with the cumulative distribution function (\rightarrow I/1.8.1) (CDF) $F_X(x)$. Then, the function $Q_X(p) : [0, 1] \rightarrow \mathbb{R}$ which is the inverse CDF is the quantile function (QF) of X . More precisely, the QF is the function that, for a given quantile $p \in [0, 1]$, returns the smallest x for which $F_X(x) = p$:

$$Q_X(p) = \min \{x \in \mathbb{R} \mid F_X(x) = p\} . \tag{1}$$

Sources:

- Wikipedia (2020): “Probability density function”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-02-17; URL: https://en.wikipedia.org/wiki/Quantile_function#Definition.

1.11.2 Quantile function in terms of cumulative distribution function

Theorem: Let X be a continuous (\rightarrow I/1.2.6) random variable (\rightarrow I/1.2.2) with the cumulative distribution function (\rightarrow I/1.8.1) $F_X(x)$. If the cumulative distribution function is strictly monotonically increasing, then the quantile function (\rightarrow I/1.11.1) is identical to the inverse of $F_X(x)$:

$$Q_X(p) = F_X^{-1}(x) . \tag{1}$$

Proof: The quantile function (\rightarrow I/1.11.1) $Q_X(p)$ is defined as the function that, for a given quantile $p \in [0, 1]$, returns the smallest x for which $F_X(x) = p$:

$$Q_X(p) = \min \{x \in \mathbb{R} \mid F_X(x) = p\} . \quad (2)$$

If $F_X(x)$ is continuous and strictly monotonically increasing, then there is exactly one x for which $F_X(x) = p$ and $F_X(x)$ is an invertible function, such that

$$Q_X(p) = F_X^{-1}(p) . \quad (3)$$

■

Sources:

- Wikipedia (2020): “Quantile function”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-11-12; URL: https://en.wikipedia.org/wiki/Quantile_function#Definition.

1.11.3 Characteristic function

Definition:

1) The characteristic function of a random variable (\rightarrow I/1.2.2) $X \in \mathbb{R}$ is

$$\varphi_X(t) = \mathbb{E} [e^{itX}] , \quad t \in \mathbb{R} . \quad (1)$$

2) The characteristic function of a random vector (\rightarrow I/1.2.3) $X \in \mathbb{R}^n$ is

$$\varphi_X(t) = \mathbb{E} [e^{it^T X}] , \quad t \in \mathbb{R}^n . \quad (2)$$

3) The characteristic function of a random matrix (\rightarrow I/1.2.4) $X \in \mathbb{R}^{n \times p}$ is

$$\varphi_X(t) = \mathbb{E} [e^{i \operatorname{tr}(t^T X)}] , \quad t \in \mathbb{R}^{n \times p} . \quad (3)$$

Sources:

- Wikipedia (2021): “Characteristic function (probability theory)”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-09-22; URL: [https://en.wikipedia.org/wiki/Characteristic_function_\(probability_theory\)#Definition](https://en.wikipedia.org/wiki/Characteristic_function_(probability_theory)#Definition).
- Taboga, Marco (2017): “Joint characteristic function”; in: *Lectures on probability and mathematical statistics*, retrieved on 2021-10-07; URL: <https://www.statlect.com/fundamentals-of-probability/joint-characteristic-function>.

1.11.4 Characteristic function of arbitrary function

Theorem: Let X be a random variable (\rightarrow I/1.2.2) with the expected value (\rightarrow I/1.12.1) function $\mathbb{E}_X[\cdot]$. Then, the characteristic function (\rightarrow I/1.11.3) of $Y = g(X)$ is equal to

$$\varphi_Y(t) = \mathbb{E}_X [\exp(it g(X))] . \quad (1)$$

Proof: The characteristic function (\rightarrow I/1.11.3) is defined as

$$\varphi_Y(t) = \mathbb{E} [\exp(it Y)] . \quad (2)$$

Due of the law of the unconscious statistician (\rightarrow I/1.12.9)

$$\begin{aligned} \mathbb{E}[g(X)] &= \sum_{x \in \mathcal{X}} g(x) f_X(x) \\ \mathbb{E}[g(X)] &= \int_{\mathcal{X}} g(x) f_X(x) \, dx, \end{aligned} \tag{3}$$

$Y = g(X)$ can simply be substituted into (2) to give

$$\varphi_Y(t) = \mathbb{E}_X [\exp(it g(X))] . \tag{4}$$

■

Sources:

- Taboga, Marco (2017): “Functions of random vectors and their distribution”; in: *Lectures on probability and mathematical statistics*, retrieved on 2021-09-22; URL: <https://www.statlect.com/fundamentals-of-probability/functions-of-random-vectors>.

1.11.5 Cumulant-generating function

Definition:

1) The cumulant-generating function of a random variable (\rightarrow I/1.2.2) $X \in \mathbb{R}$ is

$$K_X(t) = \log \mathbb{E} [e^{tX}] , \quad t \in \mathbb{R} . \tag{1}$$

2) The cumulant-generating function of a random vector (\rightarrow I/1.2.3) $X \in \mathbb{R}^n$ is

$$K_X(t) = \log \mathbb{E} [e^{t^T X}] , \quad t \in \mathbb{R}^n . \tag{2}$$

Sources:

- Wikipedia (2020): “Cumulant”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-05-31; URL: <https://en.wikipedia.org/wiki/Cumulant#Definition>.

1.12 Expected value

1.12.1 Definition

Definition:

1) The expected value (or, mean) of a discrete random variable (\rightarrow I/1.2.2) X with domain \mathcal{X} is

$$\mathbb{E}(X) = \sum_{x \in \mathcal{X}} x \cdot f_X(x) \tag{1}$$

where $f_X(x)$ is the probability mass function (\rightarrow I/1.6.1) of X .

2) The expected value (or, mean) of a continuous random variable (\rightarrow I/1.2.2) X with domain \mathcal{X} is

$$\mathbb{E}(X) = \int_{\mathcal{X}} x \cdot f_X(x) \, dx \tag{2}$$

where $f_X(x)$ is the probability density function (\rightarrow I/1.7.1) of X .

Sources:

- Wikipedia (2020): “Expected value”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-02-13; URL: https://en.wikipedia.org/wiki/Expected_value#Definition.

1.12.2 Sample mean

Definition: Let $x = \{x_1, \dots, x_n\}$ be a sample (\rightarrow I/1.1.6) from a random variable (\rightarrow I/1.2.2) X . Then, the sample mean of x is denoted as \bar{x} and is given by

$$\bar{x} = \frac{1}{n} \sum_{i=1}^n x_i . \quad (1)$$

Sources:

- Wikipedia (2021): “Sample mean and covariance”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-04-16; URL: https://en.wikipedia.org/wiki/Sample_mean_and_covariance#Definition_of_the_sample_mean.

1.12.3 Non-negative random variable

Theorem: Let X be a non-negative random variable (\rightarrow I/1.2.2). Then, the expected value (\rightarrow I/1.12.1) of X is

$$E(X) = \int_0^{\infty} (1 - F_X(x)) dx \quad (1)$$

where $F_X(x)$ is the cumulative distribution function (\rightarrow I/1.8.1) of X .

Proof: Because the cumulative distribution function gives the probability of a random variable being smaller than a given value (\rightarrow I/1.8.1),

$$F_X(x) = \Pr(X \leq x) , \quad (2)$$

we have (\rightarrow I/1.8.7)

$$1 - F_X(x) = \Pr(X > x) , \quad (3)$$

such that

$$\int_0^{\infty} (1 - F_X(x)) dx = \int_0^{\infty} \Pr(X > x) dx \quad (4)$$

which, using the probability density function (\rightarrow I/1.7.1) of X , can be rewritten as

$$\begin{aligned}
\int_0^\infty (1 - F_X(x)) \, dx &= \int_0^\infty \int_x^\infty f_X(z) \, dz \, dx \\
&= \int_0^\infty \int_0^z f_X(z) \, dx \, dz \\
&= \int_0^\infty f_X(z) \int_0^z 1 \, dx \, dz \\
&= \int_0^\infty [x]_0^z \cdot f_X(z) \, dz \\
&= \int_0^\infty z \cdot f_X(z) \, dz
\end{aligned} \tag{5}$$

and by applying the definition of the expected value (\rightarrow I/1.12.1), we see that

$$\int_0^\infty (1 - F_X(x)) \, dx = \int_0^\infty z \cdot f_X(z) \, dz = E(X) \tag{6}$$

which proves the identity given above. ■

Sources:

- Kemp, Graham (2014): “Expected value of a non-negative random variable”; in: *StackExchange Mathematics*, retrieved on 2020-05-18; URL: <https://math.stackexchange.com/questions/958472/expected-value-of-a-non-negative-random-variable>.

1.12.4 Non-negativity

Theorem: If a random variable (\rightarrow I/1.2.2) is strictly non-negative, its expected value (\rightarrow I/1.12.1) is also non-negative, i.e.

$$E(X) \geq 0, \quad \text{if } X \geq 0. \tag{1}$$

Proof:

1) If $X \geq 0$ is a discrete random variable, then, because the probability mass function (\rightarrow I/1.6.1) is always non-negative, all the addends in

$$E(X) = \sum_{x \in \mathcal{X}} x \cdot f_X(x) \tag{2}$$

are non-negative, thus the entire sum must be non-negative.

2) If $X \geq 0$ is a continuous random variable, then, because the probability density function (\rightarrow I/1.7.1) is always non-negative, the integrand in

$$E(X) = \int_{\mathcal{X}} x \cdot f_X(x) \, dx \tag{3}$$

is strictly non-negative, thus the term on the right-hand side is a Lebesgue integral, so that the result on the left-hand side must be non-negative.

**Sources:**

- Wikipedia (2020): “Expected value”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-02-13; URL: https://en.wikipedia.org/wiki/Expected_value#Basic_properties.

1.12.5 Linearity

Theorem: The expected value (\rightarrow I/1.12.1) is a linear operator, i.e.

$$\begin{aligned} E(X + Y) &= E(X) + E(Y) \\ E(a X) &= a E(X) \end{aligned} \quad (1)$$

for random variables (\rightarrow I/1.2.2) X and Y and a constant (\rightarrow I/1.2.5) a .

Proof:

1) If X and Y are discrete random variables (\rightarrow I/1.2.6), the expected value (\rightarrow I/1.12.1) is

$$E(X) = \sum_{x \in \mathcal{X}} x \cdot f_X(x) \quad (2)$$

and the law of marginal probability (\rightarrow I/1.3.3) states that

$$p(x) = \sum_{y \in \mathcal{Y}} p(x, y) . \quad (3)$$

Applying this, we have

$$\begin{aligned} E(X + Y) &= \sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} (x + y) \cdot f_{X,Y}(x, y) \\ &= \sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} x \cdot f_{X,Y}(x, y) + \sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} y \cdot f_{X,Y}(x, y) \\ &= \sum_{x \in \mathcal{X}} x \sum_{y \in \mathcal{Y}} f_{X,Y}(x, y) + \sum_{y \in \mathcal{Y}} y \sum_{x \in \mathcal{X}} f_{X,Y}(x, y) \\ &\stackrel{(3)}{=} \sum_{x \in \mathcal{X}} x \cdot f_X(x) + \sum_{y \in \mathcal{Y}} y \cdot f_Y(y) \\ &\stackrel{(2)}{=} E(X) + E(Y) \end{aligned} \quad (4)$$

as well as

$$\begin{aligned} E(a X) &= \sum_{x \in \mathcal{X}} a x \cdot f_X(x) \\ &= a \sum_{x \in \mathcal{X}} x \cdot f_X(x) \\ &\stackrel{(2)}{=} a E(X) . \end{aligned} \quad (5)$$

2) If X and Y are continuous random variables (\rightarrow I/1.2.6), the expected value (\rightarrow I/1.12.1) is

$$E(X) = \int_{\mathcal{X}} x \cdot f_X(x) \, dx \quad (6)$$

and the law of marginal probability (\rightarrow I/1.3.3) states that

$$p(x) = \int_{\mathcal{Y}} p(x, y) \, dy. \quad (7)$$

Applying this, we have

$$\begin{aligned} E(X + Y) &= \int_{\mathcal{X}} \int_{\mathcal{Y}} (x + y) \cdot f_{X,Y}(x, y) \, dy \, dx \\ &= \int_{\mathcal{X}} \int_{\mathcal{Y}} x \cdot f_{X,Y}(x, y) \, dy \, dx + \int_{\mathcal{X}} \int_{\mathcal{Y}} y \cdot f_{X,Y}(x, y) \, dy \, dx \\ &= \int_{\mathcal{X}} x \int_{\mathcal{Y}} f_{X,Y}(x, y) \, dy \, dx + \int_{\mathcal{Y}} y \int_{\mathcal{X}} f_{X,Y}(x, y) \, dx \, dy \\ &\stackrel{(7)}{=} \int_{\mathcal{X}} x \cdot f_X(x) \, dx + \int_{\mathcal{Y}} y \cdot f_Y(y) \, dy \\ &\stackrel{(6)}{=} E(X) + E(Y) \end{aligned} \quad (8)$$

as well as

$$\begin{aligned} E(aX) &= \int_{\mathcal{X}} a x \cdot f_X(x) \, dx \\ &= a \int_{\mathcal{X}} x \cdot f_X(x) \, dx \\ &\stackrel{(6)}{=} a E(X). \end{aligned} \quad (9)$$

Collectively, this shows that both requirements for linearity are fulfilled for the expected value (\rightarrow I/1.12.1), for discrete (\rightarrow I/1.2.6) as well as for continuous (\rightarrow I/1.2.6) random variables. The present derivation also holds for the expected value of random vectors (\rightarrow I/1.12.16) as well as for the expected value of random matrices (\rightarrow I/1.12.19). ■

Sources:

- Wikipedia (2020): “Expected value”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-02-13; URL: https://en.wikipedia.org/wiki/Expected_value#Basic_properties.
- Michael B, Kuldeep Guha Mazumder, Geoff Pilling et al. (2020): “Linearity of Expectation”; in: *brilliant.org*, retrieved on 2020-02-13; URL: <https://brilliant.org/wiki/linearity-of-expectation/>.

1.12.6 Monotonicity

Theorem: The expected value (\rightarrow I/1.12.1) is monotonic, i.e.

$$E(X) \leq E(Y), \quad \text{if } X \leq Y. \quad (1)$$

Proof: Let $Z = Y - X$. Due to the linearity of the expected value (\rightarrow I/1.12.5), we have

$$E(Z) = E(Y - X) = E(Y) - E(X) . \quad (2)$$

With the non-negativity property of the expected value (\rightarrow I/1.12.4), it also holds that

$$Z \geq 0 \quad \Rightarrow \quad E(Z) \geq 0 . \quad (3)$$

Together with (2), this yields

$$E(Y) - E(X) \geq 0 \quad (4)$$

and rearranging, we have

$$E(X) \leq E(Y) . \quad (5)$$

■

Sources:

- Wikipedia (2020): “Expected value”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-02-17; URL: https://en.wikipedia.org/wiki/Expected_value#Basic_properties.

1.12.7 (Non-)Multiplicativity

Theorem:

1) If two random variables (\rightarrow I/1.2.2) X and Y are independent (\rightarrow I/1.3.6), the expected value (\rightarrow I/1.12.1) is multiplicative, i.e.

$$E(XY) = E(X)E(Y) . \quad (1)$$

2) If two random variables (\rightarrow I/1.2.2) X and Y are dependent (\rightarrow I/1.3.6), the expected value (\rightarrow I/1.12.1) is not necessarily multiplicative, i.e. there exist X and Y such that

$$E(XY) \neq E(X)E(Y) . \quad (2)$$

Proof:

1) If X and Y are independent (\rightarrow I/1.3.6), it holds that

$$p(x, y) = p(x)p(y) \quad \text{for all } x \in \mathcal{X}, y \in \mathcal{Y} . \quad (3)$$

Applying this to the expected value for discrete random variables (\rightarrow I/1.12.1), we have

$$\begin{aligned} E(XY) &= \sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} (x \cdot y) \cdot f_{X,Y}(x, y) \\ &\stackrel{(3)}{=} \sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} (x \cdot y) \cdot (f_X(x) \cdot f_Y(y)) \\ &= \sum_{x \in \mathcal{X}} x \cdot f_X(x) \sum_{y \in \mathcal{Y}} y \cdot f_Y(y) \\ &= \sum_{x \in \mathcal{X}} x \cdot f_X(x) \cdot E(Y) \\ &= E(X)E(Y) . \end{aligned} \quad (4)$$

And applying it to the expected value for continuous random variables (\rightarrow I/1.12.1), we have

$$\begin{aligned}
 E(XY) &= \int_{\mathcal{X}} \int_{\mathcal{Y}} (x \cdot y) \cdot f_{X,Y}(x, y) \, dy \, dx \\
 &\stackrel{(3)}{=} \int_{\mathcal{X}} \int_{\mathcal{Y}} (x \cdot y) \cdot (f_X(x) \cdot f_Y(y)) \, dy \, dx \\
 &= \int_{\mathcal{X}} x \cdot f_X(x) \int_{\mathcal{Y}} y \cdot f_Y(y) \, dy \, dx \\
 &= \int_{\mathcal{X}} x \cdot f_X(x) \cdot E(Y) \, dx \\
 &= E(X) E(Y) .
 \end{aligned} \tag{5}$$

2) Let X and Y be Bernoulli random variables (\rightarrow II/1.2.1) with the following joint probability (\rightarrow I/1.3.2) mass function (\rightarrow I/1.6.1)

$$\begin{aligned}
 p(X = 0, Y = 0) &= 1/2 \\
 p(X = 0, Y = 1) &= 0 \\
 p(X = 1, Y = 0) &= 0 \\
 p(X = 1, Y = 1) &= 1/2
 \end{aligned} \tag{6}$$

and thus, the following marginal probabilities (\rightarrow I/1.3.3):

$$\begin{aligned}
 p(X = 0) &= p(X = 1) = 1/2 \\
 p(Y = 0) &= p(Y = 1) = 1/2 .
 \end{aligned} \tag{7}$$

Then, X and Y are dependent, because

$$p(X = 0, Y = 1) \stackrel{(6)}{=} 0 \neq \frac{1}{2} \cdot \frac{1}{2} \stackrel{(7)}{=} p(X = 0) p(Y = 1) , \tag{8}$$

and the expected value of their product is

$$\begin{aligned}
 E(XY) &= \sum_{x \in \{0,1\}} \sum_{y \in \{0,1\}} (x \cdot y) \cdot p(x, y) \\
 &= (1 \cdot 1) \cdot p(X = 1, Y = 1) \\
 &\stackrel{(6)}{=} \frac{1}{2}
 \end{aligned} \tag{9}$$

while the product of their expected values is

$$\begin{aligned}
 E(X) E(Y) &= \left(\sum_{x \in \{0,1\}} x \cdot p(x) \right) \cdot \left(\sum_{y \in \{0,1\}} y \cdot p(y) \right) \\
 &= (1 \cdot p(X = 1)) \cdot (1 \cdot p(Y = 1)) \\
 &\stackrel{(7)}{=} \frac{1}{4}
 \end{aligned} \tag{10}$$

and thus,

$$E(XY) \neq E(X)E(Y) . \quad (11)$$

■

Sources:

- Wikipedia (2020): “Expected value”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-02-17; URL: https://en.wikipedia.org/wiki/Expected_value#Basic_properties.

1.12.8 Law of total expectation

Theorem: (law of total expectation, also called “law of iterated expectations”) Let X be a random variable (\rightarrow I/1.2.2) with expected value (\rightarrow I/1.12.1) $E(X)$ and let Y be any random variable (\rightarrow I/1.13.1) defined on the same probability space (\rightarrow I/1.1.4). Then, the expected value (\rightarrow I/1.12.1) of the conditional expectation of X given Y is the same as the expected value (\rightarrow I/1.12.1) of X :

$$E(X) = E[E(X|Y)] . \quad (1)$$

Proof: Let X and Y be discrete random variables (\rightarrow I/1.2.6) with sets of possible outcomes \mathcal{X} and \mathcal{Y} . Then, the expectation of the conditional expectation can be rewritten as:

$$\begin{aligned} E[E(X|Y)] &= E \left[\sum_{x \in \mathcal{X}} x \cdot \Pr(X = x|Y) \right] \\ &= \sum_{y \in \mathcal{Y}} \left[\sum_{x \in \mathcal{X}} x \cdot \Pr(X = x|Y = y) \right] \cdot \Pr(Y = y) \\ &= \sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} x \cdot \Pr(X = x|Y = y) \cdot \Pr(Y = y) . \end{aligned} \quad (2)$$

Using the law of conditional probability (\rightarrow I/1.3.4), this becomes:

$$\begin{aligned} E[E(X|Y)] &= \sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} x \cdot \Pr(X = x, Y = y) \\ &= \sum_{x \in \mathcal{X}} x \sum_{y \in \mathcal{Y}} \Pr(X = x, Y = y) . \end{aligned} \quad (3)$$

Using the law of marginal probability (\rightarrow I/1.3.3), this becomes:

$$\begin{aligned} E[E(X|Y)] &= \sum_{x \in \mathcal{X}} x \cdot \Pr(X = x) \\ &= E(X) . \end{aligned} \quad (4)$$

■

Sources:

- Wikipedia (2021): “Law of total expectation”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-11-26; URL: https://en.wikipedia.org/wiki/Law_of_total_expectation#Proof_in_the_finite_and_countable_cases.

1.12.9 Law of the unconscious statistician

Theorem: Let X be a random variable (\rightarrow I/1.2.2) and let $Y = g(X)$ be a function of this random variable.

1) If X is a discrete random variable with possible outcomes \mathcal{X} and probability mass function (\rightarrow I/1.6.1) $f_X(x)$, the expected value (\rightarrow I/1.12.1) of $g(X)$ is

$$E[g(X)] = \sum_{x \in \mathcal{X}} g(x) f_X(x) . \quad (1)$$

2) If X is a continuous random variable with possible outcomes \mathcal{X} and probability density function (\rightarrow I/1.7.1) $f_X(x)$, the expected value (\rightarrow I/1.12.1) of $g(X)$ is

$$E[g(X)] = \int_{\mathcal{X}} g(x) f_X(x) dx . \quad (2)$$

Proof: Suppose that g is differentiable and that its inverse g^{-1} is monotonic.

1) The expected value (\rightarrow I/1.12.1) of $Y = g(X)$ is defined as

$$E[Y] = \sum_{y \in \mathcal{Y}} y f_Y(y) . \quad (3)$$

Writing the probability mass function $f_Y(y)$ in terms of $y = g(x)$, we have:

$$\begin{aligned} E[g(X)] &= \sum_{y \in \mathcal{Y}} y \Pr(g(x) = y) \\ &= \sum_{y \in \mathcal{Y}} y \Pr(x = g^{-1}(y)) \\ &= \sum_{y \in \mathcal{Y}} y \sum_{x=g^{-1}(y)} f_X(x) \\ &= \sum_{y \in \mathcal{Y}} \sum_{x=g^{-1}(y)} y f_X(x) \\ &= \sum_{y \in \mathcal{Y}} \sum_{x=g^{-1}(y)} g(x) f_X(x) . \end{aligned} \quad (4)$$

Finally, noting that “for all y , then for all $x = g^{-1}(y)$ ” is equivalent to “for all x ”, if g^{-1} is a monotonic function, we can conclude that

$$E[g(X)] = \sum_{x \in \mathcal{X}} g(x) f_X(x) . \quad (5)$$

2) Let $y = g(x)$. The derivative of an inverse function is

$$\frac{d}{dy}(g^{-1}(y)) = \frac{1}{g'(g^{-1}(y))} \quad (6)$$

Because $x = g^{-1}(y)$, this can be rearranged into

$$dx = \frac{1}{g'(g^{-1}(y))} dy \quad (7)$$

and substituting (7) into (2), we get

$$\int_{\mathcal{X}} g(x) f_X(x) dx = \int_{\mathcal{Y}} y f_X(g^{-1}(y)) \frac{1}{g'(g^{-1}(y))} dy . \quad (8)$$

Considering the cumulative distribution function (\rightarrow I/1.8.1) of Y , one can deduce:

$$\begin{aligned} F_Y(y) &= \Pr(Y \leq y) \\ &= \Pr(g(X) \leq y) \\ &= \Pr(X \leq g^{-1}(y)) \\ &= F_X(g^{-1}(y)) . \end{aligned} \quad (9)$$

Differentiating to get the probability density function (\rightarrow I/1.7.1) of Y , the result is:

$$\begin{aligned} f_Y(y) &= \frac{d}{dy} F_Y(y) \\ &\stackrel{(9)}{=} \frac{d}{dy} F_X(g^{-1}(y)) \\ &= f_X(g^{-1}(y)) \frac{d}{dy} (g^{-1}(y)) \\ &\stackrel{(6)}{=} f_X(g^{-1}(y)) \frac{1}{g'(g^{-1}(y))} . \end{aligned} \quad (10)$$

Finally, substituting (10) into (8), we have:

$$\int_{\mathcal{X}} g(x) f_X(x) dx = \int_{\mathcal{Y}} y f_Y(y) dy = E[Y] = E[g(X)] . \quad (11)$$

■

Sources:

- Wikipedia (2020): “Law of the unconscious statistician”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-07-22; URL: https://en.wikipedia.org/wiki/Law_of_the_unconscious_statistician#Proof.
- Taboga, Marco (2017): “Transformation theorem”; in: *Lectures on probability and mathematical statistics*, retrieved on 2021-09-22; URL: <https://www.statlect.com/glossary/transformation-theorem>.

1.12.10 Squared expectation of a product

Theorem: Let X and Y be two random variables (\rightarrow I/1.2.2) with expected values (\rightarrow I/1.12.1) $E(X)$ and $E(Y)$ and let $E(XY)$ exist and be finite. Then, the square of the expectation of the product of X and Y is less than or equal to the product of the expectation of the squares of X and Y :

$$[E(XY)]^2 \leq E(X^2) E(Y^2) . \quad (1)$$

Proof: Note that Y^2 is a non-negative random variable (\rightarrow I/1.2.2) whose expected value is also non-negative (\rightarrow I/1.12.4):

$$E(Y^2) \geq 0 . \quad (2)$$

1) First, consider the case that $E(Y^2) > 0$. Define a new random variable Z as

$$Z = X - Y \frac{E(XY)}{E(Y^2)} . \quad (3)$$

Once again, because Z^2 is always non-negative, we have the expected value:

$$E(Z^2) \geq 0 . \quad (4)$$

Thus, using the linearity of the expected value (\rightarrow I/1.12.5), we have

$$\begin{aligned} 0 &\leq E(Z^2) \\ &\leq E\left(\left(X - Y \frac{E(XY)}{E(Y^2)}\right)^2\right) \\ &\leq E\left(X^2 - 2XY \frac{E(XY)}{E(Y^2)} + Y^2 \frac{[E(XY)]^2}{[E(Y^2)]^2}\right) \\ &\leq E(X^2) - 2E(XY) \frac{E(XY)}{E(Y^2)} + E(Y^2) \frac{[E(XY)]^2}{[E(Y^2)]^2} \\ &\leq E(X^2) - 2 \frac{[E(XY)]^2}{E(Y^2)} + \frac{[E(XY)]^2}{E(Y^2)} \\ &\leq E(X^2) - \frac{[E(XY)]^2}{E(Y^2)} , \end{aligned} \quad (5)$$

giving

$$[E(XY)]^2 \leq E(X^2) E(Y^2) \quad (6)$$

as required.

2) Next, consider the case that $E(Y^2) = 0$. In this case, Y must be a constant (\rightarrow I/1.2.5) with mean (\rightarrow I/1.12.1) $E(Y) = 0$ and variance (\rightarrow I/1.13.1) $\text{Var}(Y) = 0$, thus we have

$$\Pr(Y = 0) = 1 . \quad (7)$$

This implies

$$\Pr(XY = 0) = 1 , \quad (8)$$

such that

$$E(XY) = 0 . \quad (9)$$

Thus, we can write

$$0 = [E(XY)]^2 = E(X^2) E(Y^2) = 0 , \quad (10)$$

giving

$$[E(XY)]^2 \leq E(X^2) E(Y^2) \quad (11)$$

as required.

**Sources:**

- ProofWiki (2022): “Square of Expectation of Product is Less Than or Equal to Product of Expectation of Squares”; in: *ProofWiki*, retrieved on 2022-10-11; URL: https://proofwiki.org/wiki/Square_of_Expectation_of_Product_is_Less_Than_or_Equal_to_Product_of_Expectation_of_Squares.

1.12.11 Jensen’s inequality

Theorem: Let X be a univariate (\rightarrow I/1.2.7) random variable (\rightarrow I/1.2.2) with probability mass function (\rightarrow I/1.6.1) (if discrete (\rightarrow I/1.2.6)) or probability density function (\rightarrow I/1.7.1) (if continuous (\rightarrow I/1.2.6)) $f_X(x)$ and let $g(x)$ be a convex function. Then, the function value, evaluated at the expected value (\rightarrow I/1.12.1) of X , is smaller than or equal to the expected value (\rightarrow I/1.12.1) of the function value, evaluated at X :

$$g(E[X]) \leq E[g(X)] . \quad (1)$$

Proof: A function $g(x)$ is said to be convex on the interval $[x_1, x_2]$, if every straight line connecting two points of the function’s graph lies above the function’s graph:

$$g(qx_1 + (1 - q)x_2) \leq qg(x_1) + (1 - q)g(x_2) \quad \text{for any } q \in [0, 1] . \quad (2)$$

This property can be extended to an arbitrary number of points x_i , $i = 1, \dots, n$, with $q_i \geq 0$, $i = 1, \dots, n$ and $\sum_{i=1}^n q_i = 1$, such that

$$g\left(\sum_{i=1}^n q_i x_i\right) \leq \sum_{i=1}^n q_i g(x_i) . \quad (3)$$

If $\{x_1, \dots, x_n\}$ is the set of possible values for a discrete random variable (\rightarrow I/1.2.6) X , then the q_i fulfill the definition of a probability mass function (\rightarrow I/1.6.1) $f_X(x_i) = q_i$. With the law of the unconscious statistician (\rightarrow I/1.12.9), it then follows that

$$g(E[X]) \leq E[g(X)] . \quad (4)$$

The above property can be further extended to a continuum of points $x \in \mathcal{X}$, with $q(x) \geq 0$ and $\int_{\mathcal{X}} q(x) dx = 1$, such that

$$g\left(\int_{\mathcal{X}} q(x)x dx\right) \leq \int_{\mathcal{X}} q(x)g(x) dx . \quad (5)$$

If \mathcal{X} is the set of possible values for a continuous random variable (\rightarrow I/1.2.6) X , then $q(x)$ fulfill the definition of a probability density function (\rightarrow I/1.7.1) $f_X(x) = q(x)$. With the law of the unconscious statistician (\rightarrow I/1.12.9), it then follows that

$$g(E[X]) \leq E[g(X)] . \quad (6)$$

This completes the proof.

**Sources:**

- Ostwald et al. (2014): “A tutorial on variational Bayes for latent linear stochastic time-series models”; in: *Journal of Mathematical Psychology*, vol. 60, pp. 1-19, App. A; URL: <https://www.sciencedirect.com/science/article/pii/S0022249614000352>; DOI: 10.1016/j.jmp.2014.04.0.

1.12.12 Markov’s inequality

Theorem: Let X be a non-negative (\rightarrow I/1.12.3) random variable (\rightarrow I/1.2.2) and let $a > 0$ be a positive real number. Then, the probability (\rightarrow I/1.3.1) that X is larger than or equal to a is smaller than or equal to the expected value (\rightarrow I/1.12.1) of X , divided by a :

$$\Pr(X \geq a) \leq \frac{E(X)}{a} . \quad (1)$$

Proof: Let us define an indicator variable that is one whenever X is larger than or equal to a :

$$I_{X \geq a} = \begin{cases} 0 , & \text{if } X < a \\ 1 , & \text{if } X \geq a . \end{cases} \quad (2)$$

It is clear that the following inequality holds:

$$a I_{X \geq a} \leq X . \quad (3)$$

Taking the expectation (\rightarrow I/1.12.1) on both sides, we have:

$$\begin{aligned} E(a I_{X \geq a}) &\leq E(X) \\ a E(I_{X \geq a}) &\leq E(X) \\ a [0 \cdot \Pr(I_{X \geq a} = 0) + 1 \cdot \Pr(I_{X \geq a} = 1)] &\leq E(X) \\ a \Pr(X \geq a) &\leq E(X) \\ \Pr(X \geq a) &\leq \frac{E(X)}{a} . \end{aligned} \quad (4)$$

■

Sources:

- Probability and Statistics (2023): “On Markov’s Inequality”; in: X , retrieved on 2025-01-10; URL: <https://x.com/probnstat/status/1713998688530370794>.
- Wikipedia (2025): “Markov’s inequality”; in: *Wikipedia, the free encyclopedia*, retrieved on 2025-01-10; URL: https://en.wikipedia.org/wiki/Markov%27s_inequality#Probability-theoretic_proof.

1.12.13 Chebyshev’s inequality

Theorem: Let X be a random variable (\rightarrow I/1.2.2) with finite expected value (\rightarrow I/1.12.1) μ and finite variance (\rightarrow I/1.13.1) σ^2 . Then, for any positive real number $k > 0$, the following inequality holds:

$$\Pr(|X - \mu| \geq k\sigma) \leq \frac{1}{k^2} . \quad (1)$$

Proof: Markov's inequality (\rightarrow I/1.12.12) states that, for any positive real number $a > 0$, the probability (\rightarrow I/1.3.1) that Y is larger than or equal to a is smaller than or equal to the expected value (\rightarrow I/1.12.1) of Y , divided by a :

$$\Pr(Y \geq a) \leq \frac{E(Y)}{a} . \quad (2)$$

The variance of a random variable (\rightarrow I/1.13.1) is defined as:

$$\sigma^2 = \text{Var}(X) = E[(X - \mu)^2] \quad \text{where} \quad \mu = E(X) . \quad (3)$$

Let $Y = (X - \mu)^2$ and $a = (k\sigma)^2$. Using Markov's inequality, we then have:

$$\begin{aligned} \Pr(|X - \mu| \geq k\sigma) &= \Pr((X - \mu)^2 \geq (k\sigma)^2) \\ &\stackrel{(2)}{\leq} \frac{E[(X - \mu)^2]}{(k\sigma)^2} \\ &\stackrel{(3)}{=} \frac{\sigma^2}{k^2\sigma^2} \\ &= \frac{1}{k^2} . \end{aligned} \quad (4)$$

■

Sources:

- Wikipedia (2025): “Chebyshev’s inequality”; in: *Wikipedia, the free encyclopedia*, retrieved on 2025-01-10; URL: https://en.wikipedia.org/wiki/Chebyshev%27s_inequality#Proof.

1.12.14 Weak law of large numbers

Theorem: Let X_1, \dots, X_n be independent and identically distributed (\rightarrow I/1.2.8) random variables (\rightarrow I/1.2.2) with expected value (\rightarrow I/1.12.1) $E(X_i) = \mu$ and finite variance (\rightarrow I/1.13.1) $\text{Var}(X_i) < \infty$ for $i = 1, \dots, n$. The sample mean (\rightarrow I/1.12.2) is defined as

$$\bar{X} = \frac{1}{n} \sum_{i=1}^n X_i . \quad (1)$$

Then, for any positive number $\epsilon > 0$, the probability that the absolute difference of the sample mean (\rightarrow I/1.12.2) from the expected value (\rightarrow I/1.12.1) μ is smaller than ϵ will approach one, as sample size (\rightarrow I/1.1.7) goes to infinity:

$$\lim_{n \rightarrow \infty} \Pr(|\bar{X} - \mu| < \epsilon) = 1 . \quad (2)$$

Proof: Since X_1, \dots, X_n are independent and identically distributed (\rightarrow I/1.2.8), they have the same mean, denoted as μ , and the same variance, denoted as σ^2 . Using the linearity of the expected value (\rightarrow I/1.12.5), the expected value of the sample mean becomes:

$$\begin{aligned}
E(\bar{X}) &= E\left(\frac{1}{n} \sum_{i=1}^n X_i\right) \\
&= \frac{1}{n} \sum_{i=1}^n E(X_i) \\
&= \frac{1}{n} n E(X_i) \\
&= \mu .
\end{aligned} \tag{3}$$

Moreover, with the scaling of the variance upon multiplication (\rightarrow I/1.13.8) and the additivity of the variance under independence (\rightarrow I/1.13.11), the variance of the sample mean becomes:

$$\begin{aligned}
\text{Var}(\bar{X}) &= \text{Var}\left(\frac{1}{n} \sum_{i=1}^n X_i\right) \\
&= \frac{1}{n^2} \text{Var}\left(\sum_{i=1}^n X_i\right) \\
&= \frac{1}{n^2} \sum_{i=1}^n \text{Var}(X_i) \\
&= \frac{1}{n^2} n \sigma^2 \\
&= \frac{\sigma^2}{n} .
\end{aligned} \tag{4}$$

Chebyshev's inequality (\rightarrow I/1.12.13) makes a statement about a random variable (\rightarrow I/1.2.2) X in relation to its mean μ and variance σ^2 for any positive number $k > 0$:

$$\Pr(|X - \mu| \geq k\sigma) \leq \frac{1}{k^2} . \tag{5}$$

Applying this inequality to the random variable \bar{X} , we have:

$$\begin{aligned}
\Pr(|\bar{X} - E(\bar{X})| \geq x) &\leq \frac{\text{Var}(\bar{X})}{x^2} \\
\Pr(|\bar{X} - \mu| \geq \epsilon) &\leq \frac{\sigma^2}{n\epsilon^2} .
\end{aligned} \tag{6}$$

Since the cumulative distribution function can be used to relate probabilities of inverse events (\rightarrow I/1.8.7), i.e. $\Pr(X \geq x) = 1 - \Pr(X < x)$, we have:

$$\begin{aligned}
1 - \Pr(|\bar{X} - \mu| < \epsilon) &\leq \frac{\sigma^2}{n\epsilon^2} \\
\Pr(|\bar{X} - \mu| < \epsilon) &\geq 1 - \frac{\sigma^2}{n\epsilon^2} .
\end{aligned} \tag{7}$$

Now taking the limit for $n \rightarrow \infty$ on both sides, while considering that ϵ and σ^2 are finite, gives:

$$\begin{aligned}
\lim_{n \rightarrow \infty} \Pr(|\bar{X} - \mu| < \epsilon) &\geq \lim_{n \rightarrow \infty} \left(1 - \frac{\sigma^2}{n\epsilon^2}\right) \\
&\geq 1 - \lim_{n \rightarrow \infty} \frac{\sigma^2/\epsilon^2}{n} \\
&\geq 1.
\end{aligned} \tag{8}$$

Since the upper limit of probability is one (\rightarrow I/1.4.7), this implies that:

$$\lim_{n \rightarrow \infty} \Pr(|\bar{X} - \mu| < \epsilon) = 1. \tag{9}$$

■

Sources:

- Ostwald, Dirk (2023): “Ungleichungen und Grenzwerte”; in: *Wahrscheinlichkeitstheorie und Frequentistische Inferenz*, Einheit (6), Folie 19-20; URL: https://www.ipsy.ovgu.de/ipsy_media/Methodenlehre+I/Wintersemester+2324/Wahrscheinlichkeitstheorie+und+Frequentistische+Inferenz/6_Ungleichungen_und_Grenzwerte.pdf.
- Wikipedia (2024): “Law of large numbers”; in: *Wikipedia, the free encyclopedia*, retrieved on 2024-09-13; URL: https://en.wikipedia.org/wiki/Law_of_large_numbers#Proof_of_the_weak_law.

1.12.15 Expected value minimizes squared error

Theorem: Let X_1, \dots, X_n be a collection of random variables (\rightarrow I/1.2.2) with common mean (\rightarrow I/1.12.1) $E(X_i) = \mu$, $i = 1, \dots, n$. Then, μ minimizes the mean squared error:

$$\mu = \arg \min_{a \in \mathbb{R}} E[(X_i - a)^2]. \tag{1}$$

Proof: Using the linearity of expectation (\rightarrow I/1.12.5), we can simplify the objective function:

$$E[(X_i - a)^2] = E[X_i^2 - 2aX_i + a^2] = a^2 - 2a\mu + E(X_i^2). \tag{2}$$

Setting the first derivative

$$\frac{d}{da} [a^2 - 2a\mu + E(X_i^2)] = 2a - 2\mu \tag{3}$$

to zero to perform a derivative test, we obtain:

$$2a - 2\mu = 0 \quad \Leftrightarrow \quad a = \mu. \tag{4}$$

The second derivative is equal to 2, which is greater than 0. Since $a = \mu$ is the sole critical point, we can conclude that this value is the unique global minimum. This completes the proof that the expected value minimizes the mean squared error.

■

Sources:

- Wikipedia (2024): “Derivative test”; in: *Wikipedia, the free encyclopedia*, retrieved on 2024-09-13; URL: https://en.wikipedia.org/wiki/Derivative_test.

1.12.16 Expected value of a random vector

Definition: Let X be an n -dimensional random vector (\rightarrow I/1.2.3). Then, the expected value (\rightarrow I/1.12.1) of X is an n -dimensional vector whose entries correspond to the expected values of the entries of the random vector:

$$E(X) = E \left(\begin{bmatrix} X_1 \\ \vdots \\ X_n \end{bmatrix} \right) = \begin{bmatrix} E(X_1) \\ \vdots \\ E(X_n) \end{bmatrix} . \quad (1)$$

Sources:

- Taboga, Marco (2017): “Expected value”; in: *Lectures on probability theory and mathematical statistics*, retrieved on 2021-07-08; URL: <https://www.statlect.com/fundamentals-of-probability/expected-value#hid12>.
- Wikipedia (2021): “Multivariate random variable”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-07-08; URL: https://en.wikipedia.org/wiki/Multivariate_random_variable#Expected_value.

1.12.17 Expectation of a quadratic form

Theorem: Let X be an n -dimensional random vector (\rightarrow I/1.2.3) with mean (\rightarrow I/1.12.1) μ and covariance (\rightarrow I/1.16.1) Σ and let A be a symmetric $n \times n$ matrix. Then, the expectation of the quadratic form $X^T A X$ is

$$E [X^T A X] = \mu^T A \mu + \text{tr}(A \Sigma) . \quad (1)$$

Proof: Note that $X^T A X$ is a 1×1 matrix. We can therefore write

$$E [X^T A X] = E [\text{tr} (X^T A X)] . \quad (2)$$

Using the trace property $\text{tr}(ABC) = \text{tr}(BCA)$, this becomes

$$E [X^T A X] = E [\text{tr} (A X X^T)] . \quad (3)$$

Because mean and trace are linear operators (\rightarrow I/1.12.20), we have

$$E [X^T A X] = \text{tr} (A E [X X^T]) . \quad (4)$$

Note that the covariance matrix can be partitioned into expected values (\rightarrow I/1.16.3)

$$\text{Cov}(X, X) = E(X X^T) - E(X)E(X)^T , \quad (5)$$

such that the expected value of the quadratic form becomes

$$E [X^T A X] = \text{tr} (A [\text{Cov}(X, X) + E(X)E(X)^T]) . \quad (6)$$

Finally, applying mean (\rightarrow I/1.12.1) and covariance (\rightarrow I/1.16.1) of X , we have

$$\begin{aligned}
E[X^T A X] &= \text{tr}(A[\Sigma + \mu\mu^T]) \\
&= \text{tr}(A\Sigma + A\mu\mu^T) \\
&= \text{tr}(A\Sigma) + \text{tr}(A\mu\mu^T) \\
&= \text{tr}(A\Sigma) + \text{tr}(\mu^T A \mu) \\
&= \mu^T A \mu + \text{tr}(A\Sigma) .
\end{aligned} \tag{7}$$

■

Sources:

- Kendrick, David (1981): “Expectation of a quadratic form”; in: *Stochastic Control for Economic Models*, pp. 170-171.
- Wikipedia (2020): “Multivariate random variable”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-07-13; URL: https://en.wikipedia.org/wiki/Multivariate_random_variable#Expectation_of_a_quadratic_form.
- Halvorsen, Kjetil B. (2012): “Expected value and variance of trace function”; in: *StackExchange Cross Validated*, retrieved on 2020-07-13; URL: <https://stats.stackexchange.com/questions/34477/expected-value-and-variance-of-trace-function>.
- Sarwate, Dilip (2013): “Expected Value of Quadratic Form”; in: *StackExchange Cross Validated*, retrieved on 2020-07-13; URL: <https://stats.stackexchange.com/questions/48066/expected-value-of-quadratic-form>.

1.12.18 Expectation of a bilinear form

Theorem: Let X be an n -dimensional random vector (\rightarrow I/1.2.3) with mean (\rightarrow I/1.12.1) μ_X and let Y be an m -dimensional random vector (\rightarrow I/1.2.3) with mean (\rightarrow I/1.12.1) μ_Y where X and Y can or cannot be of equal of size ($n = m$ or $n \neq m$). Further, let A be an $n \times m$ matrix and let Σ_{XY} be the cross-covariance matrix (\rightarrow I/1.16.9) of X and Y . Then, the expectation of the bilinear form $X^T A Y$ is

$$E[X^T A Y] = \mu_X^T A \mu_Y + \text{tr}(A^T \Sigma_{XY}) . \tag{1}$$

Proof: Note that $X^T A Y = Y^T A^T X$ is a 1×1 matrix. We can therefore write

$$E[X^T A Y] = E[\text{tr}(Y^T A^T X)] . \tag{2}$$

Using the trace property $\text{tr}(ABC) = \text{tr}(BCA)$, this becomes

$$E[X^T A Y] = E[\text{tr}(A^T X Y^T)] . \tag{3}$$

Because mean and trace are linear operators (\rightarrow I/1.12.20), we have

$$E[X^T A Y] = \text{tr}(A^T E[XY^T]) . \tag{4}$$

Note that the cross-covariance matrix can be partitioned into expected values (\rightarrow I/1.16.10)

$$\text{Cov}(X, Y) = E(XY^T) - E(X)E(Y)^T , \tag{5}$$

such that the expected value of the quadratic form becomes

$$E[X^T A Y] = \text{tr}(A[\text{Cov}(X, Y) + E(X)E(Y)^T]) . \tag{6}$$

Finally, applying the means (\rightarrow I/1.12.1) and cross-covariance (\rightarrow I/1.16.9) of X and Y , we have

$$\begin{aligned}
 E[X^T AY] &= \text{tr}(A^T [\Sigma_{XY} + \mu_X \mu_Y^T]) \\
 &= \text{tr}(A^T \Sigma_{XY} + A^T \mu_X \mu_Y^T) \\
 &= \text{tr}(A^T \Sigma_{XY}) + \text{tr}(A^T \mu_X \mu_Y^T) \\
 &= \text{tr}(A^T \Sigma_{XY}) + \text{tr}(\mu_Y^T A^T \mu_X) \\
 &= \text{tr}(A^T \Sigma_{XY}) + \text{tr}(\mu_X^T A \mu_Y) \\
 &= \mu_X^T A \mu_Y + \text{tr}(A^T \Sigma_{XY}) .
 \end{aligned} \tag{7}$$

■

1.12.19 Expected value of a random matrix

Definition: Let X be an $n \times p$ random matrix (\rightarrow I/1.2.4). Then, the expected value (\rightarrow I/1.12.1) of X is an $n \times p$ matrix whose entries correspond to the expected values of the entries of the random matrix:

$$E(X) = E \left(\begin{bmatrix} X_{11} & \dots & X_{1p} \\ \vdots & \ddots & \vdots \\ X_{n1} & \dots & X_{np} \end{bmatrix} \right) = \begin{bmatrix} E(X_{11}) & \dots & E(X_{1p}) \\ \vdots & \ddots & \vdots \\ E(X_{n1}) & \dots & E(X_{np}) \end{bmatrix} . \tag{1}$$

Sources:

- Taboga, Marco (2017): “Expected value”; in: *Lectures on probability theory and mathematical statistics*, retrieved on 2021-07-08; URL: <https://www.statlect.com/fundamentals-of-probability/expected-value#hid13>.

1.12.20 Expectation of a trace

Theorem: Let A be an $n \times n$ random matrix (\rightarrow I/1.2.4). Then, the expectation (\rightarrow I/1.12.1) of the trace of A is equal to the trace of the expectation (\rightarrow I/1.12.1) of A :

$$E[\text{tr}(A)] = \text{tr}(E[A]) . \tag{1}$$

Proof: The trace of an $n \times n$ matrix A is defined as:

$$\text{tr}(A) = \sum_{i=1}^n a_{ii} . \tag{2}$$

Using this definition of the trace, the linearity of the expected value (\rightarrow I/1.12.5) and the expected value of a random matrix (\rightarrow I/1.12.19), we have:

$$\begin{aligned}
\mathbb{E}[\text{tr}(A)] &= \mathbb{E} \left[\sum_{i=1}^n a_{ii} \right] \\
&= \sum_{i=1}^n \mathbb{E}[a_{ii}] \\
&= \text{tr} \left(\begin{bmatrix} \mathbb{E}[a_{11}] & \dots & \mathbb{E}[a_{1n}] \\ \vdots & \ddots & \vdots \\ \mathbb{E}[a_{n1}] & \dots & \mathbb{E}[a_{nn}] \end{bmatrix} \right) \\
&= \text{tr}(\mathbb{E}[A]) .
\end{aligned} \tag{3}$$

■

Sources:

- drerD (2018): “‘Trace trick’ for expectations of quadratic forms”; in: *StackExchange Mathematics*, retrieved on 2021-12-07; URL: <https://math.stackexchange.com/a/3004034/480910>.

1.13 Variance**1.13.1 Definition**

Definition: The variance of a random variable (\rightarrow I/1.2.2) X is defined as the expected value (\rightarrow I/1.12.1) of the squared deviation from its expected value (\rightarrow I/1.12.1):

$$\text{Var}(X) = \mathbb{E}[(X - \mathbb{E}(X))^2] . \tag{1}$$

Sources:

- Wikipedia (2020): “Variance”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-02-13; URL: <https://en.wikipedia.org/wiki/Variance#Definition>.

1.13.2 Sample variance

Definition: Let $x = \{x_1, \dots, x_n\}$ be a sample (\rightarrow I/1.1.6) from a random variable (\rightarrow I/1.2.2) X . Then, the sample variance of x is given by

$$\hat{\sigma}^2 = \frac{1}{n} \sum_{i=1}^n (x_i - \bar{x})^2 \tag{1}$$

and the unbiased sample variance of x is given by

$$s^2 = \frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x})^2 \tag{2}$$

where \bar{x} is the sample mean (\rightarrow I/1.12.2).

Sources:

- Wikipedia (2021): “Variance”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-04-16; URL: https://en.wikipedia.org/wiki/Variance#Sample_variance.

1.13.3 Pooled sample variance

Definition: Let $x_i = \{x_{i1}, \dots, x_{in_i}\}$ for $i = 1, \dots, k$ be samples (\rightarrow I/1.1.6) from a random variable (\rightarrow I/1.2.2) X whose expected value (\rightarrow I/1.12.1), but not variance (\rightarrow I/1.13.1) potentially depends on sample index i . Then, the pooled sample variance (\rightarrow I/1.13.2) of $x = \{x_1, \dots, x_k\}$ is given by

$$s_{1\dots k}^2 = \frac{1}{n - k} \sum_{i=1}^k \sum_{j=1}^{n_i} (x_{ij} - \bar{x}_i)^2 \quad (1)$$

where \bar{x}_i is the sample mean (\rightarrow I/1.12.2) of the i -th sample

$$\bar{x}_i = \frac{1}{n_i} \sum_{j=1}^{n_i} x_{ij} \quad (2)$$

and n is the total sample size (\rightarrow I/1.1.7):

$$n = \sum_{i=1}^k n_i. \quad (3)$$

Sources:

- Soch, Joram; Ostwald, Dirk (2024): “Einfaktorielle Varianzanalyse”; in: *Allgemeines Lineares Modell*, Einheit (10), Folien 27-29; URL: https://www.ipsy.ovgu.de/ipsy_media/Methodenlehre+I/Sommersemester+2024/Allgemeines+Lineares+Modell/10_Einfaktorielle_Varianzanalyse.pdf.
- Wikipedia (2025): “Pooled variance”; in: *Wikipedia, the free encyclopedia*, retrieved on 2025-01-10; URL: https://en.wikipedia.org/wiki/Pooled_variance#Definition_and_computation.

1.13.4 Partition into expected values

Theorem: Let X be a random variable (\rightarrow I/1.2.2). Then, the variance (\rightarrow I/1.13.1) of X is equal to the mean (\rightarrow I/1.12.1) of the square of X minus the square of the mean (\rightarrow I/1.12.1) of X :

$$\text{Var}(X) = E(X^2) - E(X)^2. \quad (1)$$

Proof: The variance (\rightarrow I/1.13.1) of X is defined as

$$\text{Var}(X) = E[(X - E[X])^2] \quad (2)$$

which, due to the linearity of the expected value (\rightarrow I/1.12.5), can be rewritten as

$$\begin{aligned} \text{Var}(X) &= E[(X - E[X])^2] \\ &= E[X^2 - 2X E(X) + E(X)^2] \\ &= E(X^2) - 2E(X)E(X) + E(X)^2 \\ &= E(X^2) - E(X)^2. \end{aligned} \quad (3)$$

**Sources:**

- Wikipedia (2020): “Variance”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-05-19; URL: <https://en.wikipedia.org/wiki/Variance#Definition>.

1.13.5 Non-negativity

Theorem: The variance (\rightarrow I/1.13.1) is always non-negative, i.e.

$$\text{Var}(X) \geq 0 . \quad (1)$$

Proof: The variance (\rightarrow I/1.13.1) of a random variable (\rightarrow I/1.2.2) is defined as

$$\text{Var}(X) = \text{E} [(X - \text{E}(X))^2] . \quad (2)$$

1) If X is a discrete random variable (\rightarrow I/1.2.2), then, because squares and probabilities are strictly non-negative, all the addends in

$$\text{Var}(X) = \sum_{x \in \mathcal{X}} (x - \text{E}(X))^2 \cdot f_X(x) \quad (3)$$

are also non-negative, thus the entire sum must be non-negative.

2) If X is a continuous random variable (\rightarrow I/1.2.2), then, because squares and probability densities are strictly non-negative, the integrand in

$$\text{Var}(X) = \int_{\mathcal{X}} (x - \text{E}(X))^2 \cdot f_X(x) \, dx \quad (4)$$

is always non-negative, thus the term on the right-hand side is a Lebesgue integral, so that the result on the left-hand side must be non-negative.

**Sources:**

- Wikipedia (2020): “Variance”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-06-06; URL: https://en.wikipedia.org/wiki/Variance#Basic_properties.

1.13.6 Variance of a constant

Theorem: The variance (\rightarrow I/1.13.1) of a constant (\rightarrow I/1.2.5) is zero

$$a = \text{const.} \quad \Rightarrow \quad \text{Var}(a) = 0 \quad (1)$$

and if the variance (\rightarrow I/1.13.1) of X is zero, then X is a constant (\rightarrow I/1.2.5)

$$\text{Var}(X) = 0 \quad \Rightarrow \quad X = \text{const.} \quad (2)$$

Proof:

1) A constant (\rightarrow I/1.2.5) is defined as a quantity that always has the same value. Thus, if understood as a random variable (\rightarrow I/1.2.2), the expected value (\rightarrow I/1.12.1) of a constant is equal to itself:

$$E(a) = a . \quad (3)$$

Plugged into the formula of the variance (\rightarrow I/1.13.1), we have

$$\begin{aligned} \text{Var}(a) &= E [(a - E(a))^2] \\ &= E [(a - a)^2] \\ &= E(0) . \end{aligned} \quad (4)$$

Applied to the formula of the expected value (\rightarrow I/1.12.1), this gives

$$E(0) = \sum_{x=0} x \cdot f_X(x) = 0 \cdot 1 = 0 . \quad (5)$$

Together, (4) and (5) imply (1).

2) The variance (\rightarrow I/1.13.1) is defined as

$$\text{Var}(X) = E [(X - E(X))^2] . \quad (6)$$

Because $(X - E(X))^2$ is strictly non-negative (\rightarrow I/1.12.4), the only way for the variance to become zero is, if the squared deviation is always zero:

$$(X - E(X))^2 = 0 . \quad (7)$$

This, in turn, requires that X is equal to its expected value (\rightarrow I/1.12.1)

$$X = E(X) \quad (8)$$

which can only be the case, if X always has the same value (\rightarrow I/1.2.5):

$$X = \text{const.} \quad (9)$$

■

Sources:

- Wikipedia (2020): “Variance”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-06-27; URL: https://en.wikipedia.org/wiki/Variance#Basic_properties.

1.13.7 Invariance under addition

Theorem: The variance (\rightarrow I/1.13.1) is invariant under addition of a constant (\rightarrow I/1.2.5):

$$\text{Var}(X + a) = \text{Var}(X) \quad (1)$$

Proof: The variance (\rightarrow I/1.13.1) is defined in terms of the expected value (\rightarrow I/1.12.1) as

$$\text{Var}(X) = E [(X - E(X))^2] . \quad (2)$$

Using this and the linearity of the expected value (\rightarrow I/1.12.5), we can derive (1) as follows:

$$\begin{aligned}
\text{Var}(X + a) &\stackrel{(2)}{=} \text{E} [((X + a) - \text{E}(X + a))^2] \\
&= \text{E} [(X + a - \text{E}(X) - a)^2] \\
&= \text{E} [(X - \text{E}(X))^2] \\
&\stackrel{(2)}{=} \text{Var}(X) .
\end{aligned} \tag{3}$$

■

Sources:

- Wikipedia (2020): “Variance”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-07-07; URL: https://en.wikipedia.org/wiki/Variance#Basic_properties.

1.13.8 Scaling upon multiplication

Theorem: The variance (\rightarrow I/1.13.1) scales upon multiplication with a constant (\rightarrow I/1.2.5):

$$\text{Var}(aX) = a^2 \text{Var}(X) \tag{1}$$

Proof: The variance (\rightarrow I/1.13.1) is defined in terms of the expected value (\rightarrow I/1.12.1) as

$$\text{Var}(X) = \text{E} [(X - \text{E}(X))^2] . \tag{2}$$

Using this and the linearity of the expected value (\rightarrow I/1.12.5), we can derive (1) as follows:

$$\begin{aligned}
\text{Var}(aX) &\stackrel{(2)}{=} \text{E} [((aX) - \text{E}(aX))^2] \\
&= \text{E} [(aX - a\text{E}(X))^2] \\
&= \text{E} [(a[X - \text{E}(X)])^2] \\
&= \text{E} [a^2(X - \text{E}(X))^2] \\
&= a^2 \text{E} [(X - \text{E}(X))^2] \\
&\stackrel{(2)}{=} a^2 \text{Var}(X) .
\end{aligned} \tag{3}$$

■

Sources:

- Wikipedia (2020): “Variance”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-07-07; URL: https://en.wikipedia.org/wiki/Variance#Basic_properties.

1.13.9 Variance of a sum

Theorem: The variance (\rightarrow I/1.13.1) of the sum of two random variables (\rightarrow I/1.2.2) equals the sum of the variances of those random variables, plus two times their covariance (\rightarrow I/1.15.1):

$$\text{Var}(X + Y) = \text{Var}(X) + \text{Var}(Y) + 2 \text{Cov}(X, Y) . \tag{1}$$

Proof: The variance (\rightarrow I/1.13.1) is defined in terms of the expected value (\rightarrow I/1.12.1) as

$$\text{Var}(X) = E[(X - E(X))^2] . \quad (2)$$

Using the linearity of the expected value (\rightarrow I/1.12.5) and the definition of the covariance (\rightarrow I/1.15.1), we can derive (1) as follows:

$$\begin{aligned} \text{Var}(X + Y) &\stackrel{(2)}{=} E[((X + Y) - E(X + Y))^2] \\ &= E[(X - E(X) + Y - E(Y))^2] \\ &= E[(X - E(X))^2 + (Y - E(Y))^2 + 2(X - E(X))(Y - E(Y))] \\ &= E[(X - E(X))^2] + E[(Y - E(Y))^2] + E[2(X - E(X))(Y - E(Y))] \\ &\stackrel{(2)}{=} \text{Var}(X) + \text{Var}(Y) + 2 \text{Cov}(X, Y) . \end{aligned} \quad (3)$$

■

Sources:

- Wikipedia (2020): “Variance”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-07-07; URL: https://en.wikipedia.org/wiki/Variance#Basic_properties.

1.13.10 Variance of linear combination

Theorem: The variance (\rightarrow I/1.13.1) of the linear combination of two random variables (\rightarrow I/1.2.2) is a function of the variances as well as the covariance (\rightarrow I/1.15.1) of those random variables:

$$\text{Var}(aX + bY) = a^2 \text{Var}(X) + b^2 \text{Var}(Y) + 2ab \text{Cov}(X, Y) . \quad (1)$$

Proof: The variance (\rightarrow I/1.13.1) is defined in terms of the expected value (\rightarrow I/1.12.1) as

$$\text{Var}(X) = E[(X - E(X))^2] . \quad (2)$$

Using this and the linearity of the expected value (\rightarrow I/1.12.5), we can derive (1) as follows:

$$\begin{aligned} \text{Var}(aX + bY) &\stackrel{(2)}{=} E[((aX + bY) - E(aX + bY))^2] \\ &= E[(a(X - E(X)) + b(Y - E(Y)))^2] \\ &= E[a^2(X - E(X))^2 + b^2(Y - E(Y))^2 + 2ab(X - E(X))(Y - E(Y))] \\ &= E[a^2(X - E(X))^2] + E[b^2(Y - E(Y))^2] + E[2ab(X - E(X))(Y - E(Y))] \\ &\stackrel{(2)}{=} a^2 \text{Var}(X) + b^2 \text{Var}(Y) + 2ab \text{Cov}(X, Y) . \end{aligned} \quad (3)$$

■

Sources:

- Wikipedia (2020): “Variance”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-07-07; URL: https://en.wikipedia.org/wiki/Variance#Basic_properties.

1.13.11 Additivity under independence

Theorem: The variance (\rightarrow I/1.13.1) is additive for independent (\rightarrow I/1.3.6) random variables (\rightarrow I/1.2.2):

$$p(X, Y) = p(X)p(Y) \quad \Rightarrow \quad \text{Var}(X + Y) = \text{Var}(X) + \text{Var}(Y) . \quad (1)$$

Proof: The variance of the sum of two random variables (\rightarrow I/1.13.9) is given by

$$\text{Var}(X + Y) = \text{Var}(X) + \text{Var}(Y) + 2 \text{Cov}(X, Y) . \quad (2)$$

The covariance of independent random variables (\rightarrow I/1.15.6) is zero:

$$p(X, Y) = p(X)p(Y) \quad \Rightarrow \quad \text{Cov}(X, Y) = 0 . \quad (3)$$

Combining (2) and (3), we have:

$$\text{Var}(X + Y) = \text{Var}(X) + \text{Var}(Y) . \quad (4)$$

■

Sources:

- Wikipedia (2020): “Variance”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-07-07; URL: https://en.wikipedia.org/wiki/Variance#Basic_properties.

1.13.12 Law of total variance

Theorem: (law of total variance, also called “conditional variance formula”) Let X and Y be random variables (\rightarrow I/1.2.2) defined on the same probability space (\rightarrow I/1.1.4) and assume that the variance (\rightarrow I/1.13.1) of Y is finite. Then, the sum of the expectation (\rightarrow I/1.12.1) of the conditional variance and the variance (\rightarrow I/1.13.1) of the conditional expectation of Y given X is equal to the variance (\rightarrow I/1.13.1) of Y :

$$\text{Var}(Y) = \text{E}[\text{Var}(Y|X)] + \text{Var}[\text{E}(Y|X)] . \quad (1)$$

Proof: The variance can be decomposed into expected values (\rightarrow I/1.13.4) as follows:

$$\text{Var}(Y) = \text{E}(Y^2) - \text{E}(Y)^2 . \quad (2)$$

This can be rearranged into:

$$\text{E}(Y^2) = \text{Var}(Y) + \text{E}(Y)^2 . \quad (3)$$

Applying the law of total expectation (\rightarrow I/1.12.8), we have:

$$\text{E}(Y^2) = \text{E} [\text{Var}(Y|X) + \text{E}(Y|X)^2] . \quad (4)$$

Now subtract the second term from (2):

$$\text{E}(Y^2) - \text{E}(Y)^2 = \text{E} [\text{Var}(Y|X) + \text{E}(Y|X)^2] - \text{E}(Y)^2 . \quad (5)$$

Again applying the law of total expectation (\rightarrow I/1.12.8), we have:

$$E(Y^2) - E(Y)^2 = E [\text{Var}(Y|X) + E(Y|X)^2] - E [E(Y|X)]^2 . \quad (6)$$

With the linearity of the expected value (\rightarrow I/1.12.5), the terms can be regrouped to give:

$$E(Y^2) - E(Y)^2 = E [\text{Var}(Y|X)] + (E [E(Y|X)^2] - E [E(Y|X)]^2) . \quad (7)$$

Using the decomposition of variance into expected values (\rightarrow I/1.13.4), we finally have:

$$\text{Var}(Y) = E[\text{Var}(Y|X)] + \text{Var}[E(Y|X)] . \quad (8)$$

■

Sources:

- Wikipedia (2021): “Law of total variance”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-11-26; URL: https://en.wikipedia.org/wiki/Law_of_total_variance#Proof.

1.13.13 Precision

Definition: The precision of a random variable (\rightarrow I/1.2.2) X is defined as the inverse of the variance (\rightarrow I/1.13.1), i.e. one divided by the expected value (\rightarrow I/1.12.1) of the squared deviation from its expected value (\rightarrow I/1.12.1):

$$\text{Prec}(X) = \text{Var}(X)^{-1} = \frac{1}{E [(X - E(X))^2]} . \quad (1)$$

Sources:

- Wikipedia (2020): “Precision (statistics)”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-04-21; URL: [https://en.wikipedia.org/wiki/Precision_\(statistics\)](https://en.wikipedia.org/wiki/Precision_(statistics)).

1.14 Skewness

1.14.1 Definition

Definition: Let X be a random variable (\rightarrow I/1.2.2) with expected value (\rightarrow I/1.12.1) μ and standard deviation (\rightarrow I/1.19.1) σ . Then, the skewness of X is defined as the third standardized moment (\rightarrow I/1.21.9) of X :

$$\text{Skew}(X) = \frac{E[(X - \mu)^3]}{\sigma^3} . \quad (1)$$

Sources:

- Wikipedia (2023): “Skewness”; in: *Wikipedia, the free encyclopedia*, retrieved on 2023-04-20; URL: <https://en.wikipedia.org/wiki/Skewness>.

1.14.2 Sample skewness

Definition: Let $x = \{x_1, \dots, x_n\}$ be a sample (\rightarrow I/1.1.6) from a random variable (\rightarrow I/1.2.2) X . Then, the sample skewness of x is given by

$$\hat{s} = \frac{\frac{1}{n} \sum_{i=1}^n (x_i - \bar{x})^3}{\left[\frac{1}{n} \sum_{i=1}^n (x_i - \bar{x})^2 \right]^{3/2}}, \quad (1)$$

where \bar{x} is the sample mean (\rightarrow I/1.12.2).

Sources:

- Joanes, D. N. and Gill, C. A. (1998): “Comparing measures of sample skewness and kurtosis”; in: *The Statistician*, vol. 47, part 1, pp. 183-189; URL: <https://www.jstor.org/stable/2988433>.

1.14.3 Partition into expected values

Theorem: Let X be a random variable (\rightarrow I/1.2.2) with expected value (\rightarrow I/1.12.1) μ and standard deviation (\rightarrow I/1.19.1) σ . Then, the skewness (\rightarrow I/1.14.1) of X can be computed as:

$$\text{Skew}(X) = \frac{E(X^3) - 3\mu\sigma^2 - \mu^3}{\sigma^3}. \quad (1)$$

Proof: The skewness (\rightarrow I/1.14.1) of X is defined as

$$\text{Skew}(X) = \frac{E[(X - \mu)^3]}{\sigma^3}. \quad (2)$$

Because the expected value is a linear operator (\rightarrow I/1.12.5), we can rewrite (2) as

$$\begin{aligned} \text{Skew}(X) &= \frac{E[(X - \mu)^3]}{\sigma^3} \\ &= \frac{E[X^3 - 3X^2\mu + 3X\mu^2 - \mu^3]}{\sigma^3} \\ &= \frac{E(X^3) - 3E(X^2)\mu + 3E(X)\mu^2 - \mu^3}{\sigma^3} \\ &= \frac{E(X^3) - 3\mu[E(X^2) - E(X)\mu] - \mu^3}{\sigma^3} \\ &= \frac{E(X^3) - 3\mu[E(X^2) - E(X)^2] - \mu^3}{\sigma^3}. \end{aligned} \quad (3)$$

Because the variance can be written in terms of expected values (\rightarrow I/1.13.4) as

$$\sigma^2 = E(X^2) - E(X)^2, \quad (4)$$

we can rewrite (3) as

$$\text{Skew}(X) = \frac{E(X^3) - 3\mu\sigma^2 - \mu^3}{\sigma^3}. \quad (5)$$

This finishes the proof of (1). ■

Sources:

- Wikipedia (2023): “Skewness”; in: *Wikipedia, the free encyclopedia*, retrieved on 2023-04-20; URL: <https://en.wikipedia.org/wiki/Skewness>.

1.15 Covariance**1.15.1 Definition**

Definition: The covariance of two random variables (\rightarrow I/1.2.2) X and Y is defined as the expected value (\rightarrow I/1.12.1) of the product of their deviations from their individual expected values (\rightarrow I/1.12.1):

$$\text{Cov}(X, Y) = E[(X - E[X])(Y - E[Y])] . \quad (1)$$

Sources:

- Wikipedia (2020): “Covariance”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-02-06; URL: <https://en.wikipedia.org/wiki/Covariance#Definition>.

1.15.2 Sample covariance

Definition: Let $x = \{x_1, \dots, x_n\}$ and $y = \{y_1, \dots, y_n\}$ be samples (\rightarrow I/1.1.6) from random variables (\rightarrow I/1.2.2) X and Y . Then, the sample covariance of x and y is given by

$$\hat{\sigma}_{xy} = \frac{1}{n} \sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y}) \quad (1)$$

and the unbiased sample covariance of x and y is given by

$$s_{xy} = \frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y}) \quad (2)$$

where \bar{x} and \bar{y} are the sample means (\rightarrow I/1.12.2).

Sources:

- Wikipedia (2021): “Covariance”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-05-20; URL: https://en.wikipedia.org/wiki/Covariance#Calculating_the_sample_covariance.

1.15.3 Partition into expected values

Theorem: Let X and Y be random variables (\rightarrow I/1.2.2). Then, the covariance (\rightarrow I/1.15.1) of X and Y is equal to the mean (\rightarrow I/1.12.1) of the product of X and Y minus the product of the means (\rightarrow I/1.12.1) of X and Y :

$$\text{Cov}(X, Y) = E(XY) - E(X)E(Y) . \quad (1)$$

Proof: The covariance (\rightarrow I/1.15.1) of X and Y is defined as

$$\text{Cov}(X, Y) = E[(X - E[X])(Y - E[Y])] . \quad (2)$$

which, due to the linearity of the expected value (\rightarrow I/1.12.5), can be rewritten as

$$\begin{aligned} \text{Cov}(X, Y) &= E[(X - E[X])(Y - E[Y])] \\ &= E[XY - X E(Y) - E(X) Y + E(X)E(Y)] \\ &= E(XY) - E(X)E(Y) - E(X)E(Y) + E(X)E(Y) \\ &= E(XY) - E(X)E(Y) . \end{aligned} \quad (3)$$

■

Sources:

- Wikipedia (2020): “Covariance”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-06-02; URL: <https://en.wikipedia.org/wiki/Covariance#Definition>.

1.15.4 Symmetry

Theorem: The covariance (\rightarrow I/1.15.1) of two random variables (\rightarrow I/1.2.2) is a symmetric function:

$$\text{Cov}(X, Y) = \text{Cov}(Y, X) . \quad (1)$$

Proof: The covariance (\rightarrow I/1.15.1) of random variables (\rightarrow I/1.2.2) X and Y is defined as:

$$\text{Cov}(X, Y) = E[(X - E[X])(Y - E[Y])] . \quad (2)$$

Switching X and Y in (2), we can easily see:

$$\begin{aligned} \text{Cov}(Y, X) &\stackrel{(2)}{=} E[(Y - E[Y])(X - E[X])] \\ &= E[(X - E[X])(Y - E[Y])] \\ &= \text{Cov}(X, Y) . \end{aligned} \quad (3)$$

■

Sources:

- Wikipedia (2022): “Covariance”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-09-26; URL: https://en.wikipedia.org/wiki/Covariance#Covariance_of_linear_combinations.

1.15.5 Self-covariance

Theorem: The covariance (\rightarrow I/1.15.1) of a random variable (\rightarrow I/1.2.2) with itself is equal to the variance (\rightarrow I/1.13.1):

$$\text{Cov}(X, X) = \text{Var}(X) . \quad (1)$$

Proof: The covariance (\rightarrow I/1.15.1) of random variables (\rightarrow I/1.2.2) X and Y is defined as:

$$\text{Cov}(X, Y) = E[(X - E[X])(Y - E[Y])] . \quad (2)$$

Inserting X for Y in (2), the result is the variance (\rightarrow I/1.13.1) of X :

$$\begin{aligned}\text{Cov}(X, X) &\stackrel{(2)}{=} \text{E}[(X - \text{E}[X])(X - \text{E}[X])] \\ &= \text{E}[(X - \text{E}[X])^2] \\ &= \text{Var}(X) .\end{aligned}\tag{3}$$

■

Sources:

- Wikipedia (2022): “Covariance”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-09-26; URL: https://en.wikipedia.org/wiki/Covariance#Covariance_with_itself.

1.15.6 Covariance under independence

Theorem: Let X and Y be independent (\rightarrow I/1.3.6) random variables (\rightarrow I/1.2.2). Then, the covariance (\rightarrow I/1.15.1) of X and Y is zero:

$$X, Y \text{ independent} \quad \Rightarrow \quad \text{Cov}(X, Y) = 0 .\tag{1}$$

Proof: The covariance can be expressed in terms of expected values (\rightarrow I/1.15.3) as

$$\text{Cov}(X, Y) = \text{E}(X Y) - \text{E}(X) \text{E}(Y) .\tag{2}$$

For independent random variables, the expected value of the product is equal to the product of the expected values (\rightarrow I/1.12.7):

$$\text{E}(X Y) = \text{E}(X) \text{E}(Y) .\tag{3}$$

Taking (2) and (3) together, we have

$$\begin{aligned}\text{Cov}(X, Y) &\stackrel{(2)}{=} \text{E}(X Y) - \text{E}(X) \text{E}(Y) \\ &\stackrel{(3)}{=} \text{E}(X) \text{E}(Y) - \text{E}(X) \text{E}(Y) \\ &= 0 .\end{aligned}\tag{4}$$

■

Sources:

- Wikipedia (2020): “Covariance”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-09-03; URL: https://en.wikipedia.org/wiki/Covariance#Uncorrelatedness_and_independence.

1.15.7 Law of total covariance

Theorem: (law of total covariance, also called “conditional covariance formula”) Let X , Y and Z be random variables (\rightarrow I/1.2.2) defined on the same probability space (\rightarrow I/1.1.4) and assume that the covariance (\rightarrow I/1.15.1) of X and Y is finite. Then, the sum of the expectation (\rightarrow I/1.12.1) of the conditional covariance and the covariance (\rightarrow I/1.15.1) of the conditional expectations of X and Y given Z is equal to the covariance (\rightarrow I/1.15.1) of X and Y :

$$\text{Cov}(X, Y) = E[\text{Cov}(X, Y|Z)] + \text{Cov}[E(X|Z), E(Y|Z)] . \quad (1)$$

Proof: The covariance can be decomposed into expected values (\rightarrow I/1.15.3) as follows:

$$\text{Cov}(X, Y) = E(XY) - E(X)E(Y) . \quad (2)$$

Then, conditioning on Z and applying the law of total expectation (\rightarrow I/1.12.8), we have:

$$\text{Cov}(X, Y) = E[E(XY|Z)] - E[E(X|Z)] E[E(Y|Z)] . \quad (3)$$

Applying the decomposition of covariance into expected values (\rightarrow I/1.15.3) to the first term gives:

$$\text{Cov}(X, Y) = E[\text{Cov}(X, Y|Z) + E(X|Z)E(Y|Z)] - E[E(X|Z)] E[E(Y|Z)] . \quad (4)$$

With the linearity of the expected value (\rightarrow I/1.12.5), the terms can be regrouped to give:

$$\text{Cov}(X, Y) = E[\text{Cov}(X, Y|Z)] + (E[E(X|Z)E(Y|Z)] - E[E(X|Z)] E[E(Y|Z)]) . \quad (5)$$

Once more using the decomposition of covariance into expected values (\rightarrow I/1.15.3), we finally have:

$$\text{Cov}(X, Y) = E[\text{Cov}(X, Y|Z)] + \text{Cov}[E(X|Z), E(Y|Z)] . \quad (6)$$

■

Sources:

- Wikipedia (2021): “Law of total covariance”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-11-26; URL: https://en.wikipedia.org/wiki/Law_of_total_covariance#Proof.

1.15.8 Relationship to correlation

Theorem: Let X and Y be random variables (\rightarrow I/1.2.2). Then, the covariance (\rightarrow I/1.15.1) of X and Y is equal to the product of their correlation (\rightarrow I/1.17.1) and the standard deviations (\rightarrow I/1.19.1) of X and Y :

$$\text{Cov}(X, Y) = \text{Corr}(X, Y) \sigma_X \sigma_Y . \quad (1)$$

Proof: The correlation (\rightarrow I/1.17.1) of X and Y is defined as

$$\text{Corr}(X, Y) = \frac{\text{Cov}(X, Y)}{\sigma_X \sigma_Y} . \quad (2)$$

which can be rearranged for the covariance (\rightarrow I/1.15.1) to give

$$\text{Cov}(X, Y) = \text{Corr}(X, Y) \sigma_X \sigma_Y . \quad (3)$$

■

1.16 Covariance matrix

1.16.1 Definition

Definition: Let $X = [X_1, \dots, X_n]^T$ be a random vector (\rightarrow I/1.2.3). Then, the covariance matrix of X is defined as the $n \times n$ matrix in which the entry (i, j) is the covariance (\rightarrow I/1.15.1) of X_i and X_j :

$$\Sigma_{XX} = \begin{bmatrix} \text{Cov}(X_1, X_1) & \dots & \text{Cov}(X_1, X_n) \\ \vdots & \ddots & \vdots \\ \text{Cov}(X_n, X_1) & \dots & \text{Cov}(X_n, X_n) \end{bmatrix} = \begin{bmatrix} E[(X_1 - E[X_1])(X_1 - E[X_1])] & \dots & E[(X_1 - E[X_1])(X_n - E[X_n])] \\ \vdots & \ddots & \vdots \\ E[(X_n - E[X_n])(X_1 - E[X_1])] & \dots & E[(X_n - E[X_n])(X_n - E[X_n])] \end{bmatrix} \quad (1)$$

Sources:

- Wikipedia (2020): “Covariance matrix”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-06-06; URL: https://en.wikipedia.org/wiki/Covariance_matrix#Definition.

1.16.2 Sample covariance matrix

Definition: Let $x = \{x_1, \dots, x_n\}$ be a sample (\rightarrow I/1.1.6) from a random vector (\rightarrow I/1.2.3) $X \in \mathbb{R}^{p \times 1}$. Then, the sample covariance matrix of x is given by

$$\hat{\Sigma} = \frac{1}{n} \sum_{i=1}^n (x_i - \bar{x})(x_i - \bar{x})^T \quad (1)$$

and the unbiased sample covariance matrix of x is given by

$$S = \frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x})(x_i - \bar{x})^T \quad (2)$$

where \bar{x} is the sample mean (\rightarrow I/1.12.2).

Sources:

- Wikipedia (2021): “Sample mean and covariance”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-05-20; URL: https://en.wikipedia.org/wiki/Sample_mean_and_covariance#Definition_of_sample_covariance.

1.16.3 Partition into expected values

Theorem: Let X be a random vector (\rightarrow I/1.2.3). Then, the covariance matrix (\rightarrow I/1.16.1) of X is equal to the mean (\rightarrow I/1.12.1) of the outer product of X with itself minus the outer product of the mean (\rightarrow I/1.12.1) of X with itself:

$$\Sigma_{XX} = E(XX^T) - E(X)E(X)^T. \quad (1)$$

Proof: The covariance matrix (\rightarrow I/1.16.1) of X is defined as

$$\Sigma_{XX} = \begin{bmatrix} E[(X_1 - E[X_1])(X_1 - E[X_1])] & \dots & E[(X_1 - E[X_1])(X_n - E[X_n])] \\ \vdots & \ddots & \vdots \\ E[(X_n - E[X_n])(X_1 - E[X_1])] & \dots & E[(X_n - E[X_n])(X_n - E[X_n])] \end{bmatrix} \quad (2)$$

which can also be expressed using matrix multiplication as

$$\Sigma_{XX} = E[(X - E[X])(X - E[X])^T] . \quad (3)$$

Due to the linearity of the expected value (\rightarrow I/1.12.5), this can be rewritten as

$$\begin{aligned} \Sigma_{XX} &= E[(X - E[X])(X - E[X])^T] \\ &= E[XX^T - XE(X)^T - E(X)X^T + E(X)E(X)^T] \\ &= E(XX^T) - E(X)E(X)^T - E(X)E(X)^T + E(X)E(X)^T \\ &= E(XX^T) - E(X)E(X)^T . \end{aligned} \quad (4)$$

■

Sources:

- Taboga, Marco (2010): “Covariance matrix”; in: *Lectures on probability and statistics*, retrieved on 2020-06-06; URL: <https://www.statlect.com/fundamentals-of-probability/covariance-matrix>.

1.16.4 Symmetry

Theorem: Each covariance matrix (\rightarrow I/1.16.1) is symmetric:

$$\Sigma_{XX}^T = \Sigma_{XX} . \quad (1)$$

Proof: The covariance matrix (\rightarrow I/1.16.1) of a random vector (\rightarrow I/1.2.3) X is defined as

$$\Sigma_{XX} = \begin{bmatrix} \text{Cov}(X_1, X_1) & \dots & \text{Cov}(X_1, X_n) \\ \vdots & \ddots & \vdots \\ \text{Cov}(X_n, X_1) & \dots & \text{Cov}(X_n, X_n) \end{bmatrix} . \quad (2)$$

A symmetric matrix is a matrix whose transpose is equal to itself. The transpose of Σ_{XX} is

$$\Sigma_{XX}^T = \begin{bmatrix} \text{Cov}(X_1, X_1) & \dots & \text{Cov}(X_n, X_1) \\ \vdots & \ddots & \vdots \\ \text{Cov}(X_1, X_n) & \dots & \text{Cov}(X_n, X_n) \end{bmatrix} . \quad (3)$$

Because the covariance is a symmetric function (\rightarrow I/1.15.4), i.e. $\text{Cov}(X, Y) = \text{Cov}(Y, X)$, this matrix is equal to

$$\Sigma_{XX}^T = \begin{bmatrix} \text{Cov}(X_1, X_1) & \dots & \text{Cov}(X_1, X_n) \\ \vdots & \ddots & \vdots \\ \text{Cov}(X_n, X_1) & \dots & \text{Cov}(X_n, X_n) \end{bmatrix} \quad (4)$$

which is equivalent to our original definition in (2). ■

Sources:

- Wikipedia (2022): “Covariance matrix”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-09-26; URL: https://en.wikipedia.org/wiki/Covariance_matrix#Basic_properties.

1.16.5 Positive semi-definiteness

Theorem: Each covariance matrix (\rightarrow I/1.16.1) is positive semi-definite:

$$a^T \Sigma_{XX} a \geq 0 \quad \text{for all } a \in \mathbb{R}^n. \quad (1)$$

Proof: The covariance matrix (\rightarrow I/1.16.1) of X can be expressed (\rightarrow I/1.16.3) in terms of expected values (\rightarrow I/1.12.1) as follows

$$\Sigma_{XX} = \Sigma(X) = E[(X - E[X])(X - E[X])^T] \quad (2)$$

A positive semi-definite matrix is a matrix whose eigenvalues are all non-negative or, equivalently,

$$M \text{ pos. semi-def.} \Leftrightarrow x^T M x \geq 0 \quad \text{for all } x \in \mathbb{R}^n. \quad (3)$$

Here, for an arbitrary real column vector $a \in \mathbb{R}^n$, we have:

$$a^T \Sigma_{XX} a \stackrel{(2)}{=} a^T E[(X - E[X])(X - E[X])^T] a. \quad (4)$$

Because the expected value is a linear operator (\rightarrow I/1.12.5), we can write:

$$a^T \Sigma_{XX} a = E[a^T (X - E[X])(X - E[X])^T a]. \quad (5)$$

Now define the scalar random variable (\rightarrow I/1.2.2)

$$Y = a^T (X - \mu_X). \quad (6)$$

where $\mu_X = E[X]$ and note that

$$a^T (X - \mu_X) = (X - \mu_X)^T a. \quad (7)$$

Thus, combining (5) with (6), we have:

$$a^T \Sigma_{XX} a = E[Y^2]. \quad (8)$$

Because Y^2 is a random variable that cannot become negative and the expected value of a strictly non-negative random variable is also non-negative (\rightarrow I/1.12.4), we finally have

$$a^T \Sigma_{XX} a \geq 0 \quad (9)$$

for any $a \in \mathbb{R}^n$. ■

Sources:

- hkBattousai (2013): “What is the proof that covariance matrices are always semi-definite?”; in: *StackExchange Mathematics*, retrieved on 2022-09-26; URL: <https://math.stackexchange.com/a/327872>.
- Wikipedia (2022): “Covariance matrix”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-09-26; URL: https://en.wikipedia.org/wiki/Covariance_matrix#Basic_properties.

1.16.6 Invariance under addition of vector

Theorem: The covariance matrix (\rightarrow I/1.16.1) Σ_{XX} of a random vector (\rightarrow I/1.2.3) X is invariant under addition of a constant vector (\rightarrow I/1.2.5) a :

$$\Sigma(X + a) = \Sigma(X) . \quad (1)$$

Proof: The covariance matrix (\rightarrow I/1.16.1) of X can be expressed (\rightarrow I/1.16.3) in terms of expected values (\rightarrow I/1.12.1) as follows:

$$\Sigma_{XX} = \Sigma(X) = E [(X - E[X])(X - E[X])^T] . \quad (2)$$

Using this and the linearity of the expected value (\rightarrow I/1.12.5), we can derive (1) as follows:

$$\begin{aligned} \Sigma(X + a) &\stackrel{(2)}{=} E [([X + a] - E[X + a])([X + a] - E[X + a])^T] \\ &= E [(X + a - E[X] - a)(X + a - E[X] - a)^T] \\ &= E [(X - E[X])(X - E[X])^T] \\ &\stackrel{(2)}{=} \Sigma(X) . \end{aligned} \quad (3)$$

■

Sources:

- Wikipedia (2022): “Covariance matrix”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-09-22; URL: https://en.wikipedia.org/wiki/Covariance_matrix#Basic_properties.

1.16.7 Scaling upon multiplication with matrix

Theorem: The covariance matrix (\rightarrow I/1.16.1) Σ_{XX} of a random vector (\rightarrow I/1.2.3) X scales upon multiplication with a constant matrix (\rightarrow I/1.2.5) A :

$$\Sigma(AX) = A \Sigma(X) A^T . \quad (1)$$

Proof: The covariance matrix (\rightarrow I/1.16.1) of X can be expressed (\rightarrow I/1.16.3) in terms of expected values (\rightarrow I/1.12.1) as follows:

$$\Sigma_{XX} = \Sigma(X) = E [(X - E[X])(X - E[X])^T] . \quad (2)$$

Using this and the linearity of the expected value (\rightarrow I/1.12.5), we can derive (1) as follows:

$$\begin{aligned}
\Sigma(AX) &\stackrel{(2)}{=} E [(AX) - E[AX]](AX) - E[AX]]^T] \\
&= E [(A[X - E[X]]) (A[X - E[X]])^T] \\
&= E [A(X - E[X])(X - E[X])^T A^T] \\
&= A E [(X - E[X])(X - E[X])^T] A^T \\
&\stackrel{(2)}{=} A \Sigma(X) A^T .
\end{aligned} \tag{3}$$

■

Sources:

- Wikipedia (2022): “Covariance matrix”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-09-22; URL: https://en.wikipedia.org/wiki/Covariance_matrix#Basic_properties.

1.16.8 Covariance matrix and correlation matrix

Theorem: Let X be a random vector (\rightarrow I/1.2.3). Then, the covariance matrix (\rightarrow I/1.16.1) Σ_{XX} of X can be expressed in terms of its correlation matrix (\rightarrow I/1.17.6) C_{XX} as follows

$$\Sigma_{XX} = D_X \cdot C_{XX} \cdot D_X , \tag{1}$$

where D_X is a diagonal matrix with the standard deviations (\rightarrow I/1.19.1) of X_1, \dots, X_n as entries on the diagonal:

$$D_X = \text{diag}(\sigma_{X_1}, \dots, \sigma_{X_n}) = \begin{bmatrix} \sigma_{X_1} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \sigma_{X_n} \end{bmatrix} . \tag{2}$$

Proof: Reiterating (1) and applying (2), we have:

$$\Sigma_{XX} = \begin{bmatrix} \sigma_{X_1} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \sigma_{X_n} \end{bmatrix} \cdot C_{XX} \cdot \begin{bmatrix} \sigma_{X_1} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \sigma_{X_n} \end{bmatrix} . \tag{3}$$

Together with the definition of the correlation matrix (\rightarrow I/1.17.6), this gives

$$\begin{aligned}
\Sigma_{XX} &= \begin{bmatrix} \sigma_{X_1} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \sigma_{X_n} \end{bmatrix} \cdot \begin{bmatrix} \frac{E[(X_1 - E[X_1])(X_1 - E[X_1])]}{\sigma_{X_1} \sigma_{X_1}} & \dots & \frac{E[(X_1 - E[X_1])(X_n - E[X_n])]}{\sigma_{X_1} \sigma_{X_n}} \\ \vdots & \ddots & \vdots \\ \frac{E[(X_n - E[X_n])(X_1 - E[X_1])]}{\sigma_{X_n} \sigma_{X_1}} & \dots & \frac{E[(X_n - E[X_n])(X_n - E[X_n])]}{\sigma_{X_n} \sigma_{X_n}} \end{bmatrix} \cdot \begin{bmatrix} \sigma_{X_1} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \sigma_{X_n} \end{bmatrix} \\
&= \begin{bmatrix} \frac{\sigma_{X_1} \cdot E[(X_1 - E[X_1])(X_1 - E[X_1])]}{\sigma_{X_1} \sigma_{X_1}} & \dots & \frac{\sigma_{X_1} \cdot E[(X_1 - E[X_1])(X_n - E[X_n])]}{\sigma_{X_1} \sigma_{X_n}} \\ \vdots & \ddots & \vdots \\ \frac{\sigma_{X_n} \cdot E[(X_n - E[X_n])(X_1 - E[X_1])]}{\sigma_{X_n} \sigma_{X_1}} & \dots & \frac{\sigma_{X_n} \cdot E[(X_n - E[X_n])(X_n - E[X_n])]}{\sigma_{X_n} \sigma_{X_n}} \end{bmatrix} \cdot \begin{bmatrix} \sigma_{X_1} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \sigma_{X_n} \end{bmatrix} \\
&= \begin{bmatrix} \frac{\sigma_{X_1} \cdot E[(X_1 - E[X_1])(X_1 - E[X_1]) \cdot \sigma_{X_1}]}{\sigma_{X_1} \sigma_{X_1}} & \dots & \frac{\sigma_{X_1} \cdot E[(X_1 - E[X_1])(X_n - E[X_n]) \cdot \sigma_{X_n}]}{\sigma_{X_1} \sigma_{X_n}} \\ \vdots & \ddots & \vdots \\ \frac{\sigma_{X_n} \cdot E[(X_n - E[X_n])(X_1 - E[X_1]) \cdot \sigma_{X_1}]}{\sigma_{X_n} \sigma_{X_1}} & \dots & \frac{\sigma_{X_n} \cdot E[(X_n - E[X_n])(X_n - E[X_n]) \cdot \sigma_{X_n}]}{\sigma_{X_n} \sigma_{X_n}} \end{bmatrix} \\
&= \begin{bmatrix} E[(X_1 - E[X_1])(X_1 - E[X_1])] & \dots & E[(X_1 - E[X_1])(X_n - E[X_n])] \\ \vdots & \ddots & \vdots \\ E[(X_n - E[X_n])(X_1 - E[X_1])] & \dots & E[(X_n - E[X_n])(X_n - E[X_n])] \end{bmatrix}
\end{aligned} \tag{4}$$

which is nothing else than the definition of the covariance matrix (\rightarrow I/1.16.1).

■

Sources:

- Penny, William (2006): “The correlation matrix”; in: *Mathematics for Brain Imaging*, ch. 1.4.5, p. 28, eq. 1.60; URL: https://ueapsylabs.co.uk/sites/wpenny/mbi/mbi_course.pdf.

1.16.9 Cross-covariance matrix

Definition: Let $X = [X_1, \dots, X_n]^T$ and $Y = [Y_1, \dots, Y_m]^T$ be two random vectors (\rightarrow I/1.2.3) that can or cannot be of equal size. Then, the cross-covariance matrix of X and Y is defined as the $n \times m$ matrix in which the entry (i, j) is the covariance (\rightarrow I/1.15.1) of X_i and Y_j :

$$\Sigma_{XY} = \begin{bmatrix} \text{Cov}(X_1, Y_1) & \dots & \text{Cov}(X_1, Y_m) \\ \vdots & \ddots & \vdots \\ \text{Cov}(X_n, Y_1) & \dots & \text{Cov}(X_n, Y_m) \end{bmatrix} = \begin{bmatrix} E[(X_1 - E[X_1])(Y_1 - E[Y_1])] & \dots & E[(X_1 - E[X_1])(Y_m - E[Y_m])] \\ \vdots & \ddots & \vdots \\ E[(X_n - E[X_n])(Y_1 - E[Y_1])] & \dots & E[(X_n - E[X_n])(Y_m - E[Y_m])] \end{bmatrix} \tag{1}$$

Sources:

- Wikipedia (2022): “Cross-covariance matrix”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-09-26; URL: https://en.wikipedia.org/wiki/Cross-covariance_matrix#Definition.

1.16.10 Cross-covariance and expected values

Theorem: Let X and Y be a random vectors (\rightarrow I/1.2.3). Then, the cross-covariance matrix (\rightarrow I/1.16.9) of X and Y is equal to the mean (\rightarrow I/1.12.1) of the outer product of X with Y minus the outer product of the means (\rightarrow I/1.12.1) of X and Y :

$$\Sigma_{XY} = E(XY^T) - E(X)E(Y)^T. \quad (1)$$

Proof: The cross-covariance matrix (\rightarrow I/1.16.9) of X and Y is defined as

$$\Sigma_{XY} = \begin{bmatrix} E[(X_1 - E[X_1])(Y_1 - E[Y_1])] & \dots & E[(X_1 - E[X_1])(Y_m - E[Y_m])] \\ \vdots & \ddots & \vdots \\ E[(X_n - E[X_n])(Y_1 - E[Y_1])] & \dots & E[(X_n - E[X_n])(Y_m - E[Y_m])] \end{bmatrix} \quad (2)$$

which can also be expressed using matrix multiplication as

$$\Sigma_{XY} = E[(X - E[X])(Y - E[Y])^T]. \quad (3)$$

Due to the linearity of the expected value (\rightarrow I/1.12.5), this can be rewritten as

$$\begin{aligned} \Sigma_{XY} &= E[(X - E[X])(Y - E[Y])^T] \\ &= E[XY^T - XE(Y)^T - E(X)Y^T + E(X)E(Y)^T] \\ &= E(XY^T) - E(X)E(Y)^T - E(X)E(Y)^T + E(X)E(Y)^T \\ &= E(XY^T) - E(X)E(Y)^T. \end{aligned} \quad (4)$$

■

1.16.11 Covariance matrix of a sum

Theorem: The covariance matrix (\rightarrow I/1.16.1) of the sum of two random vectors (\rightarrow I/1.2.3) of the same dimension equals the sum of the covariances of those random vectors, plus the sum of their cross-covariances (\rightarrow I/1.16.9):

$$\Sigma(X + Y) = \Sigma_{XX} + \Sigma_{YY} + \Sigma_{XY} + \Sigma_{YX}. \quad (1)$$

Proof: The covariance matrix (\rightarrow I/1.16.1) of X can be expressed (\rightarrow I/1.16.3) in terms of expected values (\rightarrow I/1.12.1) as follows

$$\Sigma_{XX} = \Sigma(X) = E[(X - E[X])(X - E[X])^T] \quad (2)$$

and the cross-covariance matrix (\rightarrow I/1.16.9) of X and Y can similarly be written as

$$\Sigma_{XY} = \Sigma(X, Y) = E[(X - E[X])(Y - E[Y])^T] \quad (3)$$

Using this and the linearity of the expected value (\rightarrow I/1.12.5) as well as the definitions of covariance matrix (\rightarrow I/1.16.1) and cross-covariance matrix (\rightarrow I/1.16.9), we can derive (1) as follows:

$$\begin{aligned}
\Sigma(X+Y) &\stackrel{(2)}{=} \mathbb{E} [([X+Y] - \mathbb{E}[X+Y])([X+Y] - \mathbb{E}[X+Y])^T] \\
&= \mathbb{E} [(X - \mathbb{E}[X]) + (Y - \mathbb{E}[Y])(X - \mathbb{E}[X]) + (Y - \mathbb{E}[Y])^T] \\
&= \mathbb{E} [(X - \mathbb{E}[X])(X - \mathbb{E}[X])^T + (X - \mathbb{E}[X])(Y - \mathbb{E}[Y])^T + (Y - \mathbb{E}[Y])(X - \mathbb{E}[X])^T + (Y - \mathbb{E}[Y])(Y - \mathbb{E}[Y])^T] \\
&= \mathbb{E} [(X - \mathbb{E}[X])(X - \mathbb{E}[X])^T] + \mathbb{E} [(X - \mathbb{E}[X])(Y - \mathbb{E}[Y])^T] + \mathbb{E} [(Y - \mathbb{E}[Y])(X - \mathbb{E}[X])^T] + \mathbb{E} [(Y - \mathbb{E}[Y])(Y - \mathbb{E}[Y])^T] \\
&\stackrel{(2)}{=} \Sigma_{XX} + \Sigma_{YY} + \mathbb{E} [(X - \mathbb{E}[X])(Y - \mathbb{E}[Y])^T] + \mathbb{E} [(Y - \mathbb{E}[Y])(X - \mathbb{E}[X])^T] \\
&\stackrel{(3)}{=} \Sigma_{XX} + \Sigma_{YY} + \Sigma_{XY} + \Sigma_{YX} .
\end{aligned} \tag{4}$$

Sources:

- Wikipedia (2022): “Covariance matrix”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-09-26; URL: https://en.wikipedia.org/wiki/Covariance_matrix#Basic_properties.

1.16.12 Precision matrix

Definition: Let $X = [X_1, \dots, X_n]^T$ be a random vector (\rightarrow I/1.2.3). Then, the precision matrix of X is defined as the inverse of the covariance matrix (\rightarrow I/1.16.1) of X :

$$\Lambda_{XX} = \Sigma_{XX}^{-1} = \begin{bmatrix} \text{Cov}(X_1, X_1) & \dots & \text{Cov}(X_1, X_n) \\ \vdots & \ddots & \vdots \\ \text{Cov}(X_n, X_1) & \dots & \text{Cov}(X_n, X_n) \end{bmatrix}^{-1} . \tag{1}$$

Sources:

- Wikipedia (2020): “Precision (statistics)”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-06-06; URL: [https://en.wikipedia.org/wiki/Precision_\(statistics\)](https://en.wikipedia.org/wiki/Precision_(statistics)).

1.16.13 Precision matrix and correlation matrix

Theorem: Let X be a random vector (\rightarrow I/1.2.3). Then, the precision matrix (\rightarrow I/1.16.12) Λ_{XX} of X can be expressed in terms of its correlation matrix (\rightarrow I/1.17.6) C_{XX} as follows

$$\Lambda_{XX} = D_X^{-1} \cdot C_{XX}^{-1} \cdot D_X^{-1} , \tag{1}$$

where D_X^{-1} is a diagonal matrix with the inverse standard deviations (\rightarrow I/1.19.1) of X_1, \dots, X_n as entries on the diagonal:

$$D_X^{-1} = \text{diag}(1/\sigma_{X_1}, \dots, 1/\sigma_{X_n}) = \begin{bmatrix} \frac{1}{\sigma_{X_1}} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \frac{1}{\sigma_{X_n}} \end{bmatrix} . \tag{2}$$

Proof: The precision matrix (\rightarrow I/1.16.12) is defined as the inverse of the covariance matrix (\rightarrow I/1.16.1)

$$\Lambda_{XX} = \Sigma_{XX}^{-1} \quad (3)$$

and the relation between covariance matrix and correlation matrix (\rightarrow I/1.16.8) is given by

$$\Sigma_{XX} = D_X \cdot C_{XX} \cdot D_X \quad (4)$$

where

$$D_X = \text{diag}(\sigma_{X_1}, \dots, \sigma_{X_n}) = \begin{bmatrix} \sigma_{X_1} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \sigma_{X_n} \end{bmatrix}. \quad (5)$$

Using the matrix product property

$$(A \cdot B \cdot C)^{-1} = C^{-1} \cdot B^{-1} \cdot A^{-1} \quad (6)$$

and the diagonal matrix property

$$\text{diag}(a_1, \dots, a_n)^{-1} = \begin{bmatrix} a_1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & a_n \end{bmatrix}^{-1} = \begin{bmatrix} \frac{1}{a_1} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \frac{1}{a_n} \end{bmatrix} = \text{diag}(1/a_1, \dots, 1/a_n), \quad (7)$$

we obtain

$$\begin{aligned} \Lambda_{XX} &\stackrel{(3)}{=} \Sigma_{XX}^{-1} \\ &\stackrel{(4)}{=} (D_X \cdot C_{XX} \cdot D_X)^{-1} \\ &\stackrel{(6)}{=} D_X^{-1} \cdot C_{XX}^{-1} \cdot D_X^{-1} \\ &\stackrel{(7)}{=} \begin{bmatrix} \frac{1}{\sigma_{X_1}} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \frac{1}{\sigma_{X_n}} \end{bmatrix} \cdot C_{XX}^{-1} \cdot \begin{bmatrix} \frac{1}{\sigma_{X_1}} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \frac{1}{\sigma_{X_n}} \end{bmatrix} \end{aligned} \quad (8)$$

which conforms to equation (1). ■

1.17 Correlation

1.17.1 Definition

Definition: The correlation of two random variables (\rightarrow I/1.2.2) X and Y , also called Pearson product-moment correlation coefficient (PPMCC), is defined as the ratio of the covariance (\rightarrow I/1.15.1) of X and Y relative to the product of their standard deviations (\rightarrow I/1.19.1):

$$\text{Corr}(X, Y) = \frac{\sigma_{XY}}{\sigma_X \sigma_Y} = \frac{\text{Cov}(X, Y)}{\sqrt{\text{Var}(X)} \sqrt{\text{Var}(Y)}} = \frac{\text{E}[(X - \text{E}[X])(Y - \text{E}[Y])]}{\sqrt{\text{E}[(X - \text{E}[X])^2]} \sqrt{\text{E}[(Y - \text{E}[Y])^2]}}. \quad (1)$$

Two random variables are called uncorrelated, if $\text{Corr}(X, Y) = 0$.

Sources:

- Wikipedia (2020): “Correlation and dependence”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-02-06; URL: https://en.wikipedia.org/wiki/Correlation_and_dependence#Pearson's_product-moment_coefficient.

1.17.2 Range

Theorem: Let X and Y be two random variables (\rightarrow I/1.2.2). Then, the correlation of X and Y is between and including -1 and $+1$:

$$-1 \leq \text{Corr}(X, Y) \leq +1 . \quad (1)$$

Proof: Consider the variance (\rightarrow I/1.13.1) of X plus or minus Y , each divided by their standard deviations (\rightarrow I/1.19.1):

$$\text{Var} \left(\frac{X}{\sigma_X} \pm \frac{Y}{\sigma_Y} \right) . \quad (2)$$

Because the variance is non-negative (\rightarrow I/1.13.5), this term is larger than or equal to zero:

$$0 \leq \text{Var} \left(\frac{X}{\sigma_X} \pm \frac{Y}{\sigma_Y} \right) . \quad (3)$$

Using the variance of a linear combination (\rightarrow I/1.13.10), it can also be written as:

$$\begin{aligned} \text{Var} \left(\frac{X}{\sigma_X} \pm \frac{Y}{\sigma_Y} \right) &= \text{Var} \left(\frac{X}{\sigma_X} \right) + \text{Var} \left(\frac{Y}{\sigma_Y} \right) \pm 2 \text{Cov} \left(\frac{X}{\sigma_X}, \frac{Y}{\sigma_Y} \right) \\ &= \frac{1}{\sigma_X^2} \text{Var}(X) + \frac{1}{\sigma_Y^2} \text{Var}(Y) \pm 2 \frac{1}{\sigma_X \sigma_Y} \text{Cov}(X, Y) \\ &= \frac{1}{\sigma_X^2} \sigma_X^2 + \frac{1}{\sigma_Y^2} \sigma_Y^2 \pm 2 \frac{1}{\sigma_X \sigma_Y} \sigma_{XY} . \end{aligned} \quad (4)$$

Using the relationship between covariance and correlation (\rightarrow I/1.15.8), we have:

$$\text{Var} \left(\frac{X}{\sigma_X} \pm \frac{Y}{\sigma_Y} \right) = 1 + 1 \pm 2 \text{Corr}(X, Y) . \quad (5)$$

Thus, the combination of (3) with (5) yields

$$0 \leq 2 \pm 2 \text{Corr}(X, Y) \quad (6)$$

which is equivalent to

$$-1 \leq \text{Corr}(X, Y) \leq +1 . \quad (7)$$

Sources:

- Dor Leventer (2021): “How can I simply prove that the pearson correlation coefficient is between -1 and 1?”; in: *StackExchange Mathematics*, retrieved on 2021-12-14; URL: <https://math.stackexchange.com/a/4260655/480910>.

1.17.3 Correlation under independence

Theorem: Independent (\rightarrow I/1.3.6) random variables (\rightarrow I/1.2.2) are uncorrelated.

Proof: The correlation (\rightarrow I/1.17.1) of two random variables is defined as:

$$\text{Corr}(X, Y) = \frac{\text{Cov}(X, Y)}{\sqrt{\text{Var}(X)}\sqrt{\text{Var}(Y)}}. \quad (1)$$

The covariance of independent random variables is zero (\rightarrow I/1.15.6):

$$X, Y \text{ independent} \Rightarrow \text{Cov}(X, Y) = 0. \quad (2)$$

Thus, the correlation of independent random variables is also zero:

$$X, Y \text{ independent} \Rightarrow \text{Corr}(X, Y) = 0. \quad (3)$$

■

Sources:

- StatProofBook (2022): “Uncorrelated random variables are not necessarily independent.”; in: *X*, Nov 22, 2022, 06:34 AM; URL: <https://x.com/StatProofBook/status/1594927275514134528>.

1.17.4 Sample correlation coefficient

Definition: Let $x = \{x_1, \dots, x_n\}$ and $y = \{y_1, \dots, y_n\}$ be samples (\rightarrow I/1.1.6) from random variables (\rightarrow I/1.2.2) X and Y . Then, the sample correlation coefficient of x and y is given by

$$r_{xy} = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^n (x_i - \bar{x})^2} \sqrt{\sum_{i=1}^n (y_i - \bar{y})^2}} \quad (1)$$

where \bar{x} and \bar{y} are the sample means (\rightarrow I/1.12.2).

Sources:

- Wikipedia (2021): “Pearson correlation coefficient”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-12-14; URL: https://en.wikipedia.org/wiki/Pearson_correlation_coefficient#For_a_sample.

1.17.5 Relationship to standard scores

Theorem: Let $x = \{x_1, \dots, x_n\}$ and $y = \{y_1, \dots, y_n\}$ be samples (\rightarrow I/1.1.6) from random variables (\rightarrow I/1.2.2) X and Y . Then, the sample correlation coefficient (\rightarrow I/1.17.4) r_{xy} can be expressed in terms of the standard scores of x and y :

$$r_{xy} = \frac{1}{n-1} \sum_{i=1}^n z_i^{(x)} \cdot z_i^{(y)} = \frac{1}{n-1} \sum_{i=1}^n \left(\frac{x_i - \bar{x}}{s_x} \right) \left(\frac{y_i - \bar{y}}{s_y} \right) \quad (1)$$

where \bar{x} and \bar{y} are the sample means (\rightarrow I/1.12.2) and s_x and s_y are the sample variances (\rightarrow I/1.13.2).

Proof: The sample correlation coefficient (\rightarrow I/1.17.4) is defined as

$$r_{xy} = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^n (x_i - \bar{x})^2} \sqrt{\sum_{i=1}^n (y_i - \bar{y})^2}} . \quad (2)$$

Using the sample variances (\rightarrow I/1.13.2) of x and y , we can write:

$$r_{xy} = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{(n-1)s_x^2} \sqrt{(n-1)s_y^2}} . \quad (3)$$

Rearranging the terms, we arrive at:

$$r_{xy} = \frac{1}{(n-1)s_x s_y} \sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y}) . \quad (4)$$

Further simplifying, the result is:

$$r_{xy} = \frac{1}{n-1} \sum_{i=1}^n \left(\frac{x_i - \bar{x}}{s_x} \right) \left(\frac{y_i - \bar{y}}{s_y} \right) . \quad (5)$$

■

Sources:

- Wikipedia (2021): “Pearson correlation coefficient”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-12-14; URL: https://en.wikipedia.org/wiki/Pearson_correlation_coefficient#For_a_sample.

1.17.6 Correlation matrix

Definition: Let $X = [X_1, \dots, X_n]^T$ be a random vector (\rightarrow I/1.2.3). Then, the correlation matrix of X is defined as the $n \times n$ matrix in which the entry (i, j) is the correlation (\rightarrow I/1.17.1) of X_i and X_j :

$$C_{XX} = \begin{bmatrix} \text{Corr}(X_1, X_1) & \dots & \text{Corr}(X_1, X_n) \\ \vdots & \ddots & \vdots \\ \text{Corr}(X_n, X_1) & \dots & \text{Corr}(X_n, X_n) \end{bmatrix} = \begin{bmatrix} \frac{\text{E}[(X_1 - \text{E}[X_1])(X_1 - \text{E}[X_1])]}{\sigma_{X_1} \sigma_{X_1}} & \dots & \frac{\text{E}[(X_1 - \text{E}[X_1])(X_n - \text{E}[X_n])]}{\sigma_{X_1} \sigma_{X_n}} \\ \vdots & \ddots & \vdots \\ \frac{\text{E}[(X_n - \text{E}[X_n])(X_1 - \text{E}[X_1])]}{\sigma_{X_n} \sigma_{X_1}} & \dots & \frac{\text{E}[(X_n - \text{E}[X_n])(X_n - \text{E}[X_n])]}{\sigma_{X_n} \sigma_{X_n}} \end{bmatrix} . \quad (1)$$

Sources:

- Wikipedia (2020): “Correlation and dependence”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-06-06; URL: https://en.wikipedia.org/wiki/Correlation_and_dependence#Correlation_matrices.

1.17.7 Sample correlation matrix

Definition: Let $x = \{x_1, \dots, x_n\}$ be a sample (\rightarrow I/1.1.6) from a random vector (\rightarrow I/1.2.3) $X \in \mathbb{R}^{p \times 1}$. Then, the sample correlation matrix of x is the matrix whose entries are the sample correlation coefficients (\rightarrow I/1.17.4) between pairs of entries of x_1, \dots, x_n :

$$R_{xx} = \begin{bmatrix} r_{x^{(1)},x^{(1)}} & \dots & r_{x^{(1)},x^{(n)}} \\ \vdots & \ddots & \vdots \\ r_{x^{(n)},x^{(1)}} & \dots & r_{x^{(n)},x^{(n)}} \end{bmatrix} \quad (1)$$

where the $r_{x^{(j)},x^{(k)}}$ is the sample correlation (\rightarrow I/1.17.4) between the j -th and the k -th entry of X given by

$$r_{x^{(j)},x^{(k)}} = \frac{\sum_{i=1}^n (x_{ij} - \bar{x}^{(j)})(x_{ik} - \bar{x}^{(k)})}{\sqrt{\sum_{i=1}^n (x_{ij} - \bar{x}^{(j)})^2} \sqrt{\sum_{i=1}^n (x_{ik} - \bar{x}^{(k)})^2}} \quad (2)$$

in which $\bar{x}^{(j)}$ and $\bar{x}^{(k)}$ are the sample means (\rightarrow I/1.12.2)

$$\begin{aligned} \bar{x}^{(j)} &= \frac{1}{n} \sum_{i=1}^n x_{ij} \\ \bar{x}^{(k)} &= \frac{1}{n} \sum_{i=1}^n x_{ik} . \end{aligned} \quad (3)$$

1.18 Measures of central tendency

1.18.1 Median

Definition: The median of a sample or random variable is the value separating the higher half from the lower half of its values.

1) Let $x = \{x_1, \dots, x_n\}$ be a sample (\rightarrow I/1.1.6) from a random variable (\rightarrow I/1.2.2) X . Then, the median of x is

$$\text{median}(x) = \begin{cases} x_{(n+1)/2} , & \text{if } n \text{ is odd} \\ \frac{1}{2}(x_{n/2} + x_{n/2+1}) , & \text{if } n \text{ is even} , \end{cases} \quad (1)$$

i.e. the median is the “middle” number when all numbers are sorted from smallest to largest.

2) Let X be a continuous random variable (\rightarrow I/1.2.2) with cumulative distribution function (\rightarrow I/1.8.1) $F_X(x)$. Then, the median of X is

$$\text{median}(X) = x, \quad \text{s.t.} \quad F_X(x) = \frac{1}{2} , \quad (2)$$

i.e. the median is the value at which the CDF is $1/2$.

Sources:

- Wikipedia (2020): “Median”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-10-15; URL: <https://en.wikipedia.org/wiki/Median>.

1.18.2 Median minimizes mean absolute error

Theorem: Let X_1, \dots, X_n be a collection of continuous (\rightarrow I/1.2.6) random variables (\rightarrow I/1.2.2) drawn from a probability distribution (\rightarrow I/1.5.1) with the probability density function (\rightarrow I/1.7.1) $f(x)$ supported on $(-\infty, \infty)$ with common median (\rightarrow I/1.18.1) m . Then, m minimizes the mean absolute error:

$$m = \arg \min_{a \in \mathbb{R}} E[|X_i - a|] . \quad (1)$$

Proof: We can find the optimum by performing a derivative test. First, since an absolute value function is not differentiable at 0, we simplify the objective function by splitting it into two separate integrals:

$$E(|X_i - a|) = \int_{-\infty}^a (a - x)f(x) dx + \int_a^{\infty} (x - a)f(x) dx . \quad (2)$$

Now note that $|\frac{\partial}{\partial a}(a - x)f(x)| = |\frac{\partial}{\partial a}(x - a)f(x)| = f(x)$. Consequently, $\int_{-\infty}^a f(x) dx = \Pr(X_i < a)$ and $\int_a^{\infty} f(x) dx = \Pr(X_i > a)$, both of which must be finite by the axioms of probability (\rightarrow I/1.4.1). Therefore, these integrals meet the conditions for application of Leibniz's rule.

Applying Leibniz's integral rule, we can differentiate the objective function as follows:

$$\begin{aligned} & \frac{\partial}{\partial a} \left(\int_{-\infty}^a (a - x)f(x) dx + \int_a^{\infty} (x - a)f(x) dx \right) \\ &= (a - x)f(x) \Big|_{x=a} + \int_{-\infty}^a f(x) dx - (x - a)f(x) \Big|_{x=a} - \int_a^{\infty} f(x) dx . \end{aligned} \quad (3)$$

Canceling non-integral terms and setting this derivative to 0, it must be true that

$$\int_{-\infty}^a f(x) dx - \int_a^{\infty} f(x) dx = 0 \quad \Rightarrow \quad \Pr(X_i < a) = \Pr(X_i > a) . \quad (4)$$

Together with the probability of the complement (\rightarrow I/1.4.6), this yields the implication

$$\Pr(X_i < a) = \Pr(X_i > a) \quad \Rightarrow \quad \Pr(X_i < a) = 1 - \Pr(X_i < a) \quad \Rightarrow \quad \Pr(X_i < a) = 0.5 \quad (5)$$

As a result, a satisfies the definition of a median (\rightarrow I/1.18.1) at the critical point of the objective function.

Finally, the absolute value is a convex function. Thus, by Jensen's inequality, its expected value is also convex. This implies, since the median is the sole critical point, that it must be a global minimum. Therefore, the median must minimize the mean absolute error, completing the proof. ■

Sources:

- Wikipedia (2024): "Derivative test"; in: *Wikipedia, the free encyclopedia*, retrieved on 2024-09-23; URL: https://en.wikipedia.org/wiki/Derivative_test.
- Wikipedia (2024): "Leibniz integral rule"; in: *Wikipedia, the free encyclopedia*, retrieved on 2024-09-23; URL: https://en.wikipedia.org/wiki/Leibniz_integral_rule.
- Wikipedia (2024): "Jensen's inequality"; in: *Wikipedia, the free encyclopedia*, retrieved on 2024-09-23; URL: https://en.wikipedia.org/wiki/Jensen%27s_inequality.
- Wikipedia (2024): "Convex function"; in: *Wikipedia, the free encyclopedia*, retrieved on 2024-09-23; URL: https://en.wikipedia.org/wiki/Convex_function.

1.18.3 Mode

Definition: The mode of a sample or random variable is the value which occurs most often or with largest probability among all its values.

1) Let $x = \{x_1, \dots, x_n\}$ be a sample (\rightarrow I/1.1.6) from a random variable (\rightarrow I/1.2.2) X . Then, the mode of x is the value which occurs most often in the list x_1, \dots, x_n .

2) Let X be a random variable (\rightarrow I/1.2.2) with probability mass function (\rightarrow I/1.6.1) or probability density function (\rightarrow I/1.7.1) $f_X(x)$. Then, the mode of X is the value which maximizes the PMF or PDF:

$$\text{mode}(X) = \arg \max_x f_X(x) . \quad (1)$$

Sources:

- Wikipedia (2020): “Mode (statistics)”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-10-15; URL: [https://en.wikipedia.org/wiki/Mode_\(statistics\)](https://en.wikipedia.org/wiki/Mode_(statistics)).

1.19 Measures of statistical dispersion

1.19.1 Standard deviation

Definition: The standard deviation σ of a random variable (\rightarrow I/1.2.2) X with expected value (\rightarrow I/1.12.1) μ is defined as the square root of the variance (\rightarrow I/1.13.1), i.e.

$$\sigma(X) = \sqrt{\text{E}[(X - \mu)^2]} . \quad (1)$$

Sources:

- Wikipedia (2020): “Standard deviation”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-09-03; URL: https://en.wikipedia.org/wiki/Standard_deviation#Definition_of_population_values.

1.19.2 Sample standard deviation

Definition: Let $x = \{x_1, \dots, x_n\}$ be a sample (\rightarrow I/1.1.6) from a random variable (\rightarrow I/1.2.2) X . Then, the sample standard deviation of x is given by

$$\hat{\sigma} = \sqrt{\frac{1}{n} \sum_{i=1}^n (x_i - \bar{x})^2} \quad (1)$$

and the unbiased sample standard deviation of x is given by

$$s = \sqrt{\frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x})^2} \quad (2)$$

where \bar{x} is the sample mean (\rightarrow I/1.12.2).

Sources:

- Ostwald, Dirk (2023): “Erwartungswerte”; in: *Wahrscheinlichkeitstheorie und Frequentistische Inferenz*, Einheit (5), Folie 32; URL: https://www.ipsy.ovgu.de/ipsy_media/Methodenlehre+I/Wintersemester+2324/Wahrscheinlichkeitstheorie+und+Frequentistische+Inferenz/5_Erwartungswerte.pdf.
- Wikipedia (2025): “Standard deviation”; in: *Wikipedia, the free encyclopedia*, retrieved on 2025-01-10; URL: https://en.wikipedia.org/wiki/Standard_deviation#Estimation.

1.19.3 Pooled sample standard deviation

Definition: Let $x_i = \{x_{i1}, \dots, x_{in_i}\}$ for $i = 1, \dots, k$ be samples (\rightarrow I/1.1.6) from a random variable (\rightarrow I/1.2.2) X whose expected value (\rightarrow I/1.12.1), but not variance (\rightarrow I/1.13.1) potentially depends on sample index i . Then, the pooled sample standard deviation (\rightarrow I/1.19.2) is defined as the square root of the pooled sample variance (\rightarrow I/1.13.3), i.e.

$$s_{1\dots k} = \sqrt{s_{1\dots k}^2} = \sqrt{\frac{1}{n-k} \sum_{i=1}^k \sum_{j=1}^{n_i} (x_{ij} - \bar{x}_i)^2} \quad (1)$$

where \bar{x}_i is the sample mean (\rightarrow I/1.12.2) of the i -th sample

$$\bar{x}_i = \frac{1}{n_i} \sum_{j=1}^{n_i} x_{ij} \quad (2)$$

and n is the total sample size (\rightarrow I/1.1.7):

$$n = \sum_{i=1}^k n_i . \quad (3)$$

Sources:

- Ostwald, Dirk (2023): “T-Tests”; in: *Allgemeines Lineares Modell*, Einheit (9), Folien 66/73; URL: https://www.ipsy.ovgu.de/ipsy_media/Methodenlehre+I/Sommersemester+2023/Allgemeines+Lineares+Modell/9_T_Tests.pdf.
- Wikipedia (2025): “Pooled variance”; in: *Wikipedia, the free encyclopedia*, retrieved on 2025-01-10; URL: https://en.wikipedia.org/wiki/Pooled_variance#Definition_and_computation.

1.19.4 Full width at half maximum

Definition: Let X be a continuous random variable (\rightarrow I/1.2.2) with a unimodal probability density function (\rightarrow I/1.7.1) $f_X(x)$ and mode (\rightarrow I/1.18.3) x_M . Then, the full width at half maximum of X is defined as

$$\text{FWHM}(X) = \Delta x = x_2 - x_1 \quad (1)$$

where x_1 and x_2 are specified, such that

$$f_X(x_1) = f_X(x_2) = \frac{1}{2} f_X(x_M) \quad \text{and} \quad x_1 < x_M < x_2 . \quad (2)$$

Sources:

- Wikipedia (2020): “Full width at half maximum”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-08-19; URL: https://en.wikipedia.org/wiki/Full_width_at_half_maximum.

1.20 Further summary statistics

1.20.1 Minimum

Definition: The minimum of a sample or random variable is its lowest observed or possible value.

1) Let $x = \{x_1, \dots, x_n\}$ be a sample (\rightarrow I/1.1.6) from a random variable (\rightarrow I/1.2.2) X . Then, the minimum of x is

$$\min(x) = x_j, \quad \text{such that } x_j \leq x_i \quad \text{for all } i = 1, \dots, n, i \neq j, \quad (1)$$

i.e. the minimum is the value which is smaller than or equal to all other observed values.

2) Let X be a random variable (\rightarrow I/1.2.2) with possible values \mathcal{X} . Then, the minimum of X is

$$\min(X) = \tilde{x}, \quad \text{such that } \tilde{x} < x \quad \text{for all } x \in \mathcal{X} \setminus \{\tilde{x}\}, \quad (2)$$

i.e. the minimum is the value which is smaller than all other possible values.

Sources:

- Wikipedia (2020): “Sample maximum and minimum”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-11-12; URL: https://en.wikipedia.org/wiki/Sample_maximum_and_minimum.

1.20.2 Maximum

Definition: The maximum of a sample or random variable is its highest observed or possible value.

1) Let $x = \{x_1, \dots, x_n\}$ be a sample (\rightarrow I/1.1.6) from a random variable (\rightarrow I/1.2.2) X . Then, the maximum of x is

$$\max(x) = x_j, \quad \text{such that } x_j \geq x_i \quad \text{for all } i = 1, \dots, n, i \neq j, \quad (1)$$

i.e. the maximum is the value which is larger than or equal to all other observed values.

2) Let X be a random variable (\rightarrow I/1.2.2) with possible values \mathcal{X} . Then, the maximum of X is

$$\max(X) = \tilde{x}, \quad \text{such that } \tilde{x} > x \quad \text{for all } x \in \mathcal{X} \setminus \{\tilde{x}\}, \quad (2)$$

i.e. the maximum is the value which is larger than all other possible values.

Sources:

- Wikipedia (2020): “Sample maximum and minimum”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-11-12; URL: https://en.wikipedia.org/wiki/Sample_maximum_and_minimum.

1.21 Further moments

1.21.1 Moment

Definition: Let X be a random variable (\rightarrow I/1.2.2), let c be a constant (\rightarrow I/1.2.5) and let n be a positive integer. Then, the n -th moment of X about c is defined as the expected value (\rightarrow I/1.12.1) of the n -th power of X minus c :

$$\mu_n(c) = E[(X - c)^n] . \quad (1)$$

The “ n -th moment of X ” may also refer to:

- the n -th raw moment (\rightarrow I/1.21.3) $\mu'_n = \mu_n(0)$;
- the n -th central moment (\rightarrow I/1.21.6) $\mu_n = \mu_n(\mu)$;
- the n -th standardized moment (\rightarrow I/1.21.9) $\mu_n^* = \mu_n/\sigma^n$.

Sources:

- Wikipedia (2020): “Moment (mathematics)”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-08-19; URL: [https://en.wikipedia.org/wiki/Moment_\(mathematics\)#Significance_of_the_moments](https://en.wikipedia.org/wiki/Moment_(mathematics)#Significance_of_the_moments).

1.21.2 Moment in terms of moment-generating function

Theorem: Let X be a scalar random variable (\rightarrow I/1.2.2) with the moment-generating function (\rightarrow I/1.9.1) $M_X(t)$. Then, the n -th raw moment (\rightarrow I/1.21.3) of X can be calculated from the moment-generating function via

$$E(X^n) = M_X^{(n)}(0) \quad (1)$$

where n is a positive integer and $M_X^{(n)}(t)$ is the n -th derivative of $M_X(t)$.

Proof: Using the definition of the moment-generating function (\rightarrow I/1.9.1), we can write:

$$M_X^{(n)}(t) = \frac{d^n}{dt^n} E(e^{tX}) . \quad (2)$$

Using the power series expansion of the exponential function

$$e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!} , \quad (3)$$

equation (2) becomes

$$M_X^{(n)}(t) = \frac{d^n}{dt^n} E \left(\sum_{m=0}^{\infty} \frac{t^m X^m}{m!} \right) . \quad (4)$$

Because the expected value is a linear operator (\rightarrow I/1.12.5), we have:

$$\begin{aligned} M_X^{(n)}(t) &= \frac{d^n}{dt^n} \sum_{m=0}^{\infty} E \left(\frac{t^m X^m}{m!} \right) \\ &= \sum_{m=0}^{\infty} \frac{d^n}{dt^n} \frac{t^m}{m!} E(X^m) . \end{aligned} \quad (5)$$

Using the n -th derivative of the m -th power

$$\frac{d^n}{dx^n} x^m = \begin{cases} m^n x^{m-n}, & \text{if } n \leq m \\ 0, & \text{if } n > m. \end{cases} \quad (6)$$

with the falling factorial

$$m^n = \prod_{i=0}^{n-1} (m-i) = \frac{m!}{(m-n)!}, \quad (7)$$

equation (5) becomes

$$\begin{aligned} M_X^{(n)}(t) &= \sum_{m=n}^{\infty} \frac{m^n t^{m-n}}{m!} E(X^m) \\ &\stackrel{(7)}{=} \sum_{m=n}^{\infty} \frac{m! t^{m-n}}{(m-n)! m!} E(X^m) \\ &= \sum_{m=n}^{\infty} \frac{t^{m-n}}{(m-n)!} E(X^m) \\ &= \frac{t^{n-n}}{(n-n)!} E(X^n) + \sum_{m=n+1}^{\infty} \frac{t^{m-n}}{(m-n)!} E(X^m) \\ &= \frac{t^0}{0!} E(X^n) + \sum_{m=n+1}^{\infty} \frac{t^{m-n}}{(m-n)!} E(X^m) \\ &= E(X^n) + \sum_{m=n+1}^{\infty} \frac{t^{m-n}}{(m-n)!} E(X^m). \end{aligned} \quad (8)$$

Setting $t = 0$ in (8) yields

$$\begin{aligned} M_X^{(n)}(0) &= E(X^n) + \sum_{m=n+1}^{\infty} \frac{0^{m-n}}{(m-n)!} E(X^m) \\ &= E(X^n) \end{aligned} \quad (9)$$

which conforms to equation (1). ■

Sources:

- ProofWiki (2020): “Moment in terms of Moment Generating Function”; in: *ProofWiki*, retrieved on 2020-08-19; URL: https://proofwiki.org/wiki/Moment_in_terms_of_Moment_Generating_Function.

1.21.3 Raw moment

Definition: Let X be a random variable (\rightarrow I/1.2.2) and let n be a positive integer. Then, the n -th raw moment of X , also called (n -th) “crude moment”, is defined as the n -th moment (\rightarrow I/1.21.1) of X about the value 0:

$$\mu'_n = \mu_n(0) = E[(X - 0)^n] = E[X^n] . \quad (1)$$

Sources:

- Wikipedia (2020): “Moment (mathematics)” ; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-10-08; URL: [https://en.wikipedia.org/wiki/Moment_\(mathematics\)#Significance_of_the_moments](https://en.wikipedia.org/wiki/Moment_(mathematics)#Significance_of_the_moments).

1.21.4 First raw moment is mean

Theorem: The first raw moment (\rightarrow I/1.21.3) equals the mean (\rightarrow I/1.12.1), i.e.

$$\mu'_1 = \mu . \quad (1)$$

Proof: The first raw moment (\rightarrow I/1.21.3) of a random variable (\rightarrow I/1.2.2) X is defined as

$$\mu'_1 = E[(X - 0)^1] \quad (2)$$

which is equal to the expected value (\rightarrow I/1.12.1) of X :

$$\mu'_1 = E[X] = \mu . \quad (3)$$

■

1.21.5 Second raw moment and variance

Theorem: The second raw moment (\rightarrow I/1.21.3) can be expressed as

$$\mu'_2 = \text{Var}(X) + E(X)^2 \quad (1)$$

where $\text{Var}(X)$ is the variance (\rightarrow I/1.13.1) of X and $E(X)$ is the expected value (\rightarrow I/1.12.1) of X .

Proof: The second raw moment (\rightarrow I/1.21.3) of a random variable (\rightarrow I/1.2.2) X is defined as

$$\mu'_2 = E[(X - 0)^2] . \quad (2)$$

Using the partition of variance into expected values (\rightarrow I/1.13.4)

$$\text{Var}(X) = E(X^2) - E(X)^2 , \quad (3)$$

the second raw moment can be rearranged into:

$$\mu'_2 \stackrel{(2)}{=} E(X^2) \stackrel{(3)}{=} \text{Var}(X) + E(X)^2 . \quad (4)$$

■

1.21.6 Central moment

Definition: Let X be a random variable (\rightarrow I/1.2.2) with expected value (\rightarrow I/1.12.1) μ and let n be a positive integer. Then, the n -th central moment of X is defined as the n -th moment (\rightarrow I/1.21.1) of X about the value μ :

$$\mu_n = E[(X - \mu)^n] . \quad (1)$$

Sources:

- Wikipedia (2020): “Moment (mathematics)” ; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-10-08; URL: [https://en.wikipedia.org/wiki/Moment_\(mathematics\)#Significance_of_the_moments](https://en.wikipedia.org/wiki/Moment_(mathematics)#Significance_of_the_moments).

1.21.7 First central moment is zero

Theorem: The first central moment (\rightarrow I/1.21.6) is zero, i.e.

$$\mu_1 = 0 . \quad (1)$$

Proof: The first central moment (\rightarrow I/1.21.6) of a random variable (\rightarrow I/1.2.2) X with mean (\rightarrow I/1.12.1) μ is defined as

$$\mu_1 = E[(X - \mu)^1] . \quad (2)$$

Due to the linearity of the expected value (\rightarrow I/1.12.5) and by plugging in $\mu = E(X)$, we have

$$\begin{aligned} \mu_1 &= E[X - \mu] \\ &= E(X) - \mu \\ &= E(X) - E(X) \\ &= 0 . \end{aligned} \quad (3)$$

■

Sources:

- ProofWiki (2020): “First Central Moment is Zero”; in: *ProofWiki*, retrieved on 2020-09-09; URL: https://proofwiki.org/wiki/First_Central_Moment_is_Zero.

1.21.8 Second central moment is variance

Theorem: The second central moment (\rightarrow I/1.21.6) equals the variance (\rightarrow I/1.13.1), i.e.

$$\mu_2 = \text{Var}(X) . \quad (1)$$

Proof: The second central moment (\rightarrow I/1.21.6) of a random variable (\rightarrow I/1.2.2) X with mean (\rightarrow I/1.12.1) μ is defined as

$$\mu_2 = E[(X - \mu)^2] \quad (2)$$

which is equivalent to the definition of the variance (\rightarrow I/1.13.1):

$$\mu_2 = E[(X - E(X))^2] = \text{Var}(X) . \quad (3)$$

■

Sources:

- Wikipedia (2020): “Moment (mathematics)”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-10-08; URL: [https://en.wikipedia.org/wiki/Moment_\(mathematics\)#Significance_of_the_moments](https://en.wikipedia.org/wiki/Moment_(mathematics)#Significance_of_the_moments).

1.21.9 Standardized moment

Definition: Let X be a random variable (\rightarrow I/1.2.2) with expected value (\rightarrow I/1.12.1) μ and standard deviation (\rightarrow I/1.19.1) σ and let n be a positive integer. Then, the n -th standardized moment of X is defined as the n -th moment (\rightarrow I/1.21.1) of X about the value μ , divided by the n -th power of σ :

$$\mu_n^* = \frac{\mu_n}{\sigma^n} = \frac{E[(X - \mu)^n]}{\sigma^n} . \quad (1)$$

Sources:

- Wikipedia (2020): “Moment (mathematics)”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-10-08; URL: [https://en.wikipedia.org/wiki/Moment_\(mathematics\)#Standardized_moments](https://en.wikipedia.org/wiki/Moment_(mathematics)#Standardized_moments).

2 Information theory

2.1 Shannon entropy

2.1.1 Definition

Definition: Let X be a discrete random variable (\rightarrow I/1.2.2) with possible outcomes \mathcal{X} and the (observed or assumed) probability mass function (\rightarrow I/1.6.1) $p(x) = f_X(x)$. Then, the entropy (also referred to as “Shannon entropy”) of X is defined as

$$H(X) = - \sum_{x \in \mathcal{X}} p(x) \cdot \log_b p(x) \quad (1)$$

where b is the base of the logarithm specifying in which unit the entropy is determined. By convention, $0 \cdot \log 0$ is taken to be zero when calculating the entropy of X .

Sources:

- Shannon CE (1948): “A Mathematical Theory of Communication”; in: *Bell System Technical Journal*, vol. 27, iss. 3, pp. 379-423; URL: <https://ieeexplore.ieee.org/document/6773024>; DOI: 10.1002/j.1538-7305.1948.tb01338.x.

2.1.2 Non-negativity

Theorem: The entropy of a discrete random variable (\rightarrow I/1.2.2) is a non-negative number:

$$H(X) \geq 0 . \quad (1)$$

Proof: The entropy of a discrete random variable (\rightarrow I/2.1.1) is defined as

$$H(X) = - \sum_{x \in \mathcal{X}} p(x) \cdot \log_b p(x) \quad (2)$$

The minus sign can be moved into the sum:

$$H(X) = \sum_{x \in \mathcal{X}} [p(x) \cdot (-\log_b p(x))] \quad (3)$$

Because the co-domain of probability mass functions (\rightarrow I/1.6.1) is $[0, 1]$, we can deduce:

$$\begin{aligned} 0 &\leq p(x) \leq 1 \\ -\infty &\leq \log_b p(x) \leq 0 \\ 0 &\leq -\log_b p(x) \leq +\infty \\ 0 &\leq p(x) \cdot (-\log_b p(x)) \leq +\infty . \end{aligned} \quad (4)$$

By convention, $0 \cdot \log_b(0)$ is taken to be 0 when calculating entropy, consistent with

$$\lim_{p \rightarrow 0} [p \log_b(p)] = 0 . \quad (5)$$

Taking this together, each addend in (3) is positive or zero and thus, the entire sum must also be non-negative.

Sources:

- Cover TM, Thomas JA (1991): “Elements of Information Theory”, p. 15; URL: <https://www.wiley.com/en-us/Elements+of+Information+Theory%2C+2nd+Edition-p-9780471241959>.

2.1.3 Concavity

Theorem: The entropy (\rightarrow I/2.1.1) is concave in the probability mass function (\rightarrow I/1.6.1) p , i.e.

$$H[\lambda p_1 + (1 - \lambda)p_2] \geq \lambda H[p_1] + (1 - \lambda)H[p_2] \quad (1)$$

where p_1 and p_2 are probability mass functions and $0 \leq \lambda \leq 1$.

Proof: Let X be a discrete random variable (\rightarrow I/1.2.2) with possible outcomes \mathcal{X} and let $u(x)$ be the probability mass function (\rightarrow I/1.6.1) of a discrete uniform distribution (\rightarrow II/1.1.1) on $X \in \mathcal{X}$. Then, the entropy (\rightarrow I/2.1.1) of an arbitrary probability mass function (\rightarrow I/1.6.1) $p(x)$ can be rewritten as

$$\begin{aligned} H[p] &= - \sum_{x \in \mathcal{X}} p(x) \cdot \log p(x) \\ &= - \sum_{x \in \mathcal{X}} p(x) \cdot \log \frac{p(x)}{u(x)} u(x) \\ &= - \sum_{x \in \mathcal{X}} p(x) \cdot \log \frac{p(x)}{u(x)} - \sum_{x \in \mathcal{X}} p(x) \cdot \log u(x) \\ &= -\text{KL}[p||u] - \log \frac{1}{|\mathcal{X}|} \sum_{x \in \mathcal{X}} p(x) \\ &= \log |\mathcal{X}| - \text{KL}[p||u] \end{aligned} \quad (2)$$

$$\log |\mathcal{X}| - H[p] = \text{KL}[p||u]$$

where we have applied the definition of the Kullback-Leibler divergence (\rightarrow I/2.5.1), the probability mass function of the discrete uniform distribution (\rightarrow II/1.1.2) and the total sum over the probability mass function (\rightarrow I/1.6.1).

Note that the KL divergence is convex (\rightarrow I/2.5.6) in the pair of probability distributions (\rightarrow I/1.5.1) (p, q) :

$$\text{KL}[\lambda p_1 + (1 - \lambda)p_2 || \lambda q_1 + (1 - \lambda)q_2] \leq \lambda \text{KL}[p_1 || q_1] + (1 - \lambda) \text{KL}[p_2 || q_2] \quad (3)$$

A special case of this is given by

$$\begin{aligned} \text{KL}[\lambda p_1 + (1 - \lambda)p_2 || \lambda u + (1 - \lambda)u] &\leq \lambda \text{KL}[p_1 || u] + (1 - \lambda) \text{KL}[p_2 || u] \\ \text{KL}[\lambda p_1 + (1 - \lambda)p_2 || u] &\leq \lambda \text{KL}[p_1 || u] + (1 - \lambda) \text{KL}[p_2 || u] \end{aligned} \quad (4)$$

and applying equation (2), we have

$$\begin{aligned} \log |\mathcal{X}| - H[\lambda p_1 + (1 - \lambda)p_2] &\leq \lambda (\log |\mathcal{X}| - H[p_1]) + (1 - \lambda) (\log |\mathcal{X}| - H[p_2]) \\ \log |\mathcal{X}| - H[\lambda p_1 + (1 - \lambda)p_2] &\leq \log |\mathcal{X}| - \lambda H[p_1] - (1 - \lambda)H[p_2] \\ -H[\lambda p_1 + (1 - \lambda)p_2] &\leq -\lambda H[p_1] - (1 - \lambda)H[p_2] \\ H[\lambda p_1 + (1 - \lambda)p_2] &\geq \lambda H[p_1] + (1 - \lambda)H[p_2] \end{aligned} \quad (5)$$

which is equivalent to (1). ■

Sources:

- Wikipedia (2020): “Entropy (information theory)”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-08-11; URL: [https://en.wikipedia.org/wiki/Entropy_\(information_theory\)#Further_properties](https://en.wikipedia.org/wiki/Entropy_(information_theory)#Further_properties).
- Cover TM, Thomas JA (1991): “Elements of Information Theory”, p. 30; URL: <https://www.wiley.com/en-us/Elements+of+Information+Theory%2C+2nd+Edition-p-9780471241959>.
- Xie, Yao (2012): “Chain Rules and Inequalities”; in: *ECE587: Information Theory*, Lecture 3, Slide 25; URL: <https://www2.isye.gatech.edu/~yxie77/ece587/Lecture3.pdf>.
- Goh, Siong Thye (2016): “Understanding the proof of the concavity of entropy”; in: *StackExchange Mathematics*, retrieved on 2020-11-08; URL: <https://math.stackexchange.com/questions/2000194/understanding-the-proof-of-the-concavity-of-entropy>.

2.1.4 Conditional entropy

Definition: Let X and Y be discrete random variables (\rightarrow I/1.2.2) with possible outcomes \mathcal{X} and \mathcal{Y} and probability mass functions (\rightarrow I/1.6.1) $p(x)$ and $p(y)$. Then, the conditional entropy of Y given X or, entropy of Y conditioned on X , is defined as

$$H(Y|X) = \sum_{x \in \mathcal{X}} p(x) \cdot H(Y|X = x) \quad (1)$$

where $H(Y|X = x)$ is the (marginal) entropy (\rightarrow I/2.1.1) of Y , evaluated at x .

Sources:

- Cover TM, Thomas JA (1991): “Joint Entropy and Conditional Entropy”; in: *Elements of Information Theory*, ch. 2.2, p. 15; URL: <https://www.wiley.com/en-us/Elements+of+Information+Theory%2C+2nd+Edition-p-9780471241959>.

2.1.5 Joint entropy

Definition: Let X and Y be discrete random variables (\rightarrow I/1.2.2) with possible outcomes \mathcal{X} and \mathcal{Y} and joint probability (\rightarrow I/1.3.2) mass function (\rightarrow I/1.6.1) $p(x, y)$. Then, the joint entropy of X and Y is defined as

$$H(X, Y) = - \sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} p(x, y) \cdot \log_b p(x, y) \quad (1)$$

where b is the base of the logarithm specifying in which unit the entropy is determined.

Sources:

- Cover TM, Thomas JA (1991): “Joint Entropy and Conditional Entropy”; in: *Elements of Information Theory*, ch. 2.2, p. 16; URL: <https://www.wiley.com/en-us/Elements+of+Information+Theory%2C+2nd+Edition-p-9780471241959>.

2.1.6 Cross-entropy

Definition: Let X be a discrete random variable (\rightarrow I/1.2.2) with possible outcomes \mathcal{X} and let P and Q be two probability distributions (\rightarrow I/1.5.1) on X with the probability mass functions (\rightarrow I/1.6.1) $p(x)$ and $q(x)$. Then, the cross-entropy of Q relative to P is defined as

$$H(P, Q) = - \sum_{x \in \mathcal{X}} p(x) \cdot \log_b q(x) \quad (1)$$

where b is the base of the logarithm specifying in which unit the cross-entropy is determined.

Sources:

- Wikipedia (2020): “Cross entropy”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-07-28; URL: https://en.wikipedia.org/wiki/Cross_entropy#Definition.

2.1.7 Convexity of cross-entropy

Theorem: The cross-entropy (\rightarrow I/2.1.6) is convex in the second probability distribution (\rightarrow I/1.5.1), i.e.

$$H[p, \lambda q_1 + (1 - \lambda)q_2] \leq \lambda H[p, q_1] + (1 - \lambda)H[p, q_2] \quad (1)$$

where p is a fixed and q_1 and q_2 are any two probability mass functions (\rightarrow I/1.6.1) and $0 \leq \lambda \leq 1$.

Proof: The relationship between Kullback-Leibler divergence, entropy and cross-entropy (\rightarrow I/2.5.9) is:

$$\text{KL}[P||Q] = H(P, Q) - H(P) . \quad (2)$$

Note that the KL divergence is convex (\rightarrow I/2.5.6) in the pair of probability distributions (\rightarrow I/1.5.1) (p, q) :

$$\text{KL}[\lambda p_1 + (1 - \lambda)p_2 || \lambda q_1 + (1 - \lambda)q_2] \leq \lambda \text{KL}[p_1 || q_1] + (1 - \lambda)\text{KL}[p_2 || q_2] . \quad (3)$$

A special case of this is given by

$$\begin{aligned} \text{KL}[\lambda p + (1 - \lambda)p || \lambda q_1 + (1 - \lambda)q_2] &\leq \lambda \text{KL}[p || q_1] + (1 - \lambda)\text{KL}[p || q_2] \\ \text{KL}[p || \lambda q_1 + (1 - \lambda)q_2] &\leq \lambda \text{KL}[p || q_1] + (1 - \lambda)\text{KL}[p || q_2] \end{aligned} \quad (4)$$

and applying equation (2), we have

$$\begin{aligned} H[p, \lambda q_1 + (1 - \lambda)q_2] - H[p] &\leq \lambda (H[p, q_1] - H[p]) + (1 - \lambda) (H[p, q_2] - H[p]) \\ H[p, \lambda q_1 + (1 - \lambda)q_2] - H[p] &\leq \lambda H[p, q_1] + (1 - \lambda)H[p, q_2] - H[p] \\ H[p, \lambda q_1 + (1 - \lambda)q_2] &\leq \lambda H[p, q_1] + (1 - \lambda)H[p, q_2] \end{aligned} \quad (5)$$

which is equivalent to (1). ■

Sources:

- Wikipedia (2020): “Cross entropy”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-08-11; URL: https://en.wikipedia.org/wiki/Cross_entropy#Definition.
- gunes (2019): “Convexity of cross entropy”; in: *StackExchange CrossValidated*, retrieved on 2020-11-08; URL: <https://stats.stackexchange.com/questions/394463/convexity-of-cross-entropy>.

2.1.8 Gibbs’ inequality

Theorem: Let X be a discrete random variable (\rightarrow I/1.2.2) and consider two probability distributions (\rightarrow I/1.5.1) with probability mass functions (\rightarrow I/1.6.1) $p(x)$ and $q(x)$. Then, Gibbs’ inequality states that the entropy (\rightarrow I/2.1.1) of X according to P is smaller than or equal to the cross-entropy (\rightarrow I/2.1.6) of P and Q :

$$-\sum_{x \in \mathcal{X}} p(x) \log_b p(x) \leq -\sum_{x \in \mathcal{X}} p(x) \log_b q(x) . \quad (1)$$

Proof: Without loss of generality, we will use the natural logarithm, because a change in the base of the logarithm only implies multiplication by a constant:

$$\log_b a = \frac{\ln a}{\ln b} . \quad (2)$$

Let I be the set of all x for which $p(x)$ is non-zero. Then, proving (1) requires to show that

$$\sum_{x \in I} p(x) \ln \frac{p(x)}{q(x)} \geq 0 . \quad (3)$$

For all $x > 0$, it holds that $\ln x \leq x - 1$, with equality only if $x = 1$. Multiplying this with -1 , we have $\ln \frac{1}{x} \geq 1 - x$. Applying this to (3), we can say about the left-hand side that

$$\begin{aligned} \sum_{x \in I} p(x) \ln \frac{p(x)}{q(x)} &\geq \sum_{x \in I} p(x) \left(1 - \frac{q(x)}{p(x)} \right) \\ &= \sum_{x \in I} p(x) - \sum_{x \in I} q(x) . \end{aligned} \quad (4)$$

Finally, since $p(x)$ and $q(x)$ are probability mass functions (\rightarrow I/1.6.1), we have

$$\begin{aligned} 0 \leq p(x) \leq 1, \quad \sum_{x \in I} p(x) &= 1 \quad \text{and} \\ 0 \leq q(x) \leq 1, \quad \sum_{x \in I} q(x) &\leq 1 , \end{aligned} \quad (5)$$

such that it follows from (4) that

$$\begin{aligned} \sum_{x \in I} p(x) \ln \frac{p(x)}{q(x)} &\geq \sum_{x \in I} p(x) - \sum_{x \in I} q(x) \\ &= 1 - \sum_{x \in I} q(x) \geq 0 . \end{aligned} \quad (6)$$

**Sources:**

- Wikipedia (2020): “Gibbs’ inequality”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-09-09; URL: https://en.wikipedia.org/wiki/Gibbs%27_inequality#Proof.

2.1.9 Log sum inequality

Theorem: Let a_1, \dots, a_n and b_1, \dots, b_n be non-negative real numbers and define $a = \sum_{i=1}^n a_i$ and $b = \sum_{i=1}^n b_i$. Then, the log sum inequality states that

$$\sum_{i=1}^n a_i \log_c \frac{a_i}{b_i} \geq a \log_c \frac{a}{b} . \quad (1)$$

Proof: Without loss of generality, we will use the natural logarithm, because a change in the base of the logarithm only implies multiplication by a constant:

$$\log_c a = \frac{\ln a}{\ln c} . \quad (2)$$

Let $f(x) = x \ln x$. Then, the left-hand side of (1) can be rewritten as

$$\begin{aligned} \sum_{i=1}^n a_i \ln \frac{a_i}{b_i} &= \sum_{i=1}^n b_i f\left(\frac{a_i}{b_i}\right) \\ &= b \sum_{i=1}^n \frac{b_i}{b} f\left(\frac{a_i}{b_i}\right) . \end{aligned} \quad (3)$$

Because $f(x)$ is a convex function and

$$\begin{aligned} \frac{b_i}{b} &\geq 0 \\ \sum_{i=1}^n \frac{b_i}{b} &= 1 , \end{aligned} \quad (4)$$

applying Jensen’s inequality (\rightarrow I/1.12.11) yields

$$\begin{aligned} b \sum_{i=1}^n \frac{b_i}{b} f\left(\frac{a_i}{b_i}\right) &\geq b f\left(\sum_{i=1}^n \frac{b_i}{b} \frac{a_i}{b_i}\right) \\ &= b f\left(\frac{1}{b} \sum_{i=1}^n a_i\right) \\ &= b f\left(\frac{a}{b}\right) \\ &= a \ln \frac{a}{b} . \end{aligned} \quad (5)$$

Finally, combining (3) and (5), this demonstrates (1).

Sources:

- Wikipedia (2020): “Log sum inequality”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-09-09; URL: https://en.wikipedia.org/wiki/Log_sum_inequality#Proof.

2.2 Differential entropy**2.2.1 Definition**

Definition: Let X be a continuous random variable (\rightarrow I/1.2.2) with possible outcomes \mathcal{X} and the (estimated or assumed) probability density function (\rightarrow I/1.7.1) $p(x) = f_X(x)$. Then, the differential entropy (also referred to as “continuous entropy”) of X is defined as

$$h(X) = - \int_{\mathcal{X}} p(x) \log_b p(x) dx \quad (1)$$

where b is the base of the logarithm specifying in which unit the entropy is determined.

Sources:

- Cover TM, Thomas JA (1991): “Differential Entropy”; in: *Elements of Information Theory*, ch. 8.1, p. 243; URL: <https://www.wiley.com/en-us/Elements+of+Information+Theory%2C+2nd+Edition-p-9780471241959>.

2.2.2 Negativity

Theorem: Unlike its discrete analogue (\rightarrow I/2.1.2), the differential entropy (\rightarrow I/2.2.1) can become negative.

Proof: Let X be a random variable (\rightarrow I/1.2.2) following a continuous uniform distribution (\rightarrow II/3.1.1) with minimum 0 and maximum $1/2$:

$$X \sim \mathcal{U}(0, 1/2) . \quad (1)$$

Then, its probability density function (\rightarrow II/3.1.3) is:

$$f_X(x) = 2 \quad \text{for} \quad 0 \leq x \leq \frac{1}{2} . \quad (2)$$

Thus, the differential entropy (\rightarrow I/2.2.1) follows as

$$\begin{aligned} h(X) &= - \int_{\mathcal{X}} f_X(x) \log_b f_X(x) dx \\ &= - \int_0^{\frac{1}{2}} 2 \log_b(2) dx \\ &= - \log_b(2) \int_0^{\frac{1}{2}} 2 dx \\ &= - \log_b(2) [2x]_0^{\frac{1}{2}} \\ &= - \log_b(2) \end{aligned} \quad (3)$$

which is negative for any base $b > 1$.

**Sources:**

- Wikipedia (2020): “Differential entropy”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-03-02; URL: https://en.wikipedia.org/wiki/Differential_entropy#Definition.

2.2.3 Invariance under addition

Theorem: Let X be a continuous (\rightarrow I/1.2.6) random variable (\rightarrow I/1.2.2). Then, the differential entropy (\rightarrow I/2.2.1) of X remains constant under addition of a constant:

$$h(X + c) = h(X) . \quad (1)$$

Proof: By definition, the differential entropy (\rightarrow I/2.2.1) of X is

$$h(X) = - \int_{\mathcal{X}} p(x) \log p(x) dx \quad (2)$$

where $p(x) = f_X(x)$ is the probability density function (\rightarrow I/1.7.1) of X . Define the mappings between X and $Y = X + c$ as

$$Y = g(X) = X + c \quad \Leftrightarrow \quad X = g^{-1}(Y) = Y - c . \quad (3)$$

Note that $g(X)$ is a strictly increasing function, such that the probability density function (\rightarrow I/1.7.3) of Y is

$$f_Y(y) = f_X(g^{-1}(y)) \frac{dg^{-1}(y)}{dy} \stackrel{(3)}{=} f_X(y - c) . \quad (4)$$

Writing down the differential entropy for Y , we have:

$$\begin{aligned} h(Y) &= - \int_{\mathcal{Y}} f_Y(y) \log f_Y(y) dy \\ &\stackrel{(4)}{=} - \int_{\mathcal{Y}} f_X(y - c) \log f_X(y - c) dy \end{aligned} \quad (5)$$

Substituting $x = y - c$, such that $y = x + c$, this yields:

$$\begin{aligned} h(Y) &= - \int_{\{y-c \mid y \in \mathcal{Y}\}} f_X(x + c - c) \log f_X(x + c - c) d(x + c) \\ &= - \int_{\mathcal{X}} f_X(x) \log f_X(x) dx \\ &\stackrel{(2)}{=} h(X) . \end{aligned} \quad (6)$$

**Sources:**

- Wikipedia (2020): “Differential entropy”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-02-12; URL: https://en.wikipedia.org/wiki/Differential_entropy#Properties_of_differential_entropy.

2.2.4 Addition upon multiplication

Theorem: Let X be a continuous (\rightarrow I/1.2.6) random variable (\rightarrow I/1.2.2). Then, the differential entropy (\rightarrow I/2.2.1) of X increases additively upon multiplication with a constant:

$$h(aX) = h(X) + \log |a| . \quad (1)$$

Proof: By definition, the differential entropy (\rightarrow I/2.2.1) of X is

$$h(X) = - \int_{\mathcal{X}} p(x) \log p(x) dx \quad (2)$$

where $p(x) = f_X(x)$ is the probability density function (\rightarrow I/1.7.1) of X .

Define the mappings between X and $Y = aX$ as

$$Y = g(X) = aX \quad \Leftrightarrow \quad X = g^{-1}(Y) = \frac{Y}{a} . \quad (3)$$

If $a > 0$, then $g(X)$ is a strictly increasing function, such that the probability density function (\rightarrow I/1.7.3) of Y is

$$f_Y(y) = f_X(g^{-1}(y)) \frac{dg^{-1}(y)}{dy} \stackrel{(3)}{=} \frac{1}{a} f_X\left(\frac{y}{a}\right) ; \quad (4)$$

if $a < 0$, then $g(X)$ is a strictly decreasing function, such that the probability density function (\rightarrow I/1.7.4) of Y is

$$f_Y(y) = -f_X(g^{-1}(y)) \frac{dg^{-1}(y)}{dy} \stackrel{(3)}{=} -\frac{1}{a} f_X\left(\frac{y}{a}\right) ; \quad (5)$$

thus, we can write

$$f_Y(y) = \frac{1}{|a|} f_X\left(\frac{y}{a}\right) . \quad (6)$$

Writing down the differential entropy for Y , we have:

$$\begin{aligned} h(Y) &= - \int_{\mathcal{Y}} f_Y(y) \log f_Y(y) dy \\ &\stackrel{(6)}{=} - \int_{\mathcal{Y}} \frac{1}{|a|} f_X\left(\frac{y}{a}\right) \log \left[\frac{1}{|a|} f_X\left(\frac{y}{a}\right) \right] dy \end{aligned} \quad (7)$$

Substituting $x = y/a$, such that $y = ax$, this yields:

$$\begin{aligned} h(Y) &= - \int_{\{y/a \mid y \in \mathcal{Y}\}} \frac{1}{|a|} f_X\left(\frac{ax}{a}\right) \log \left[\frac{1}{|a|} f_X\left(\frac{ax}{a}\right) \right] d(ax) \\ &= - \int_{\mathcal{X}} f_X(x) \log \left[\frac{1}{|a|} f_X(x) \right] dx \\ &= - \int_{\mathcal{X}} f_X(x) [\log f_X(x) - \log |a|] dx \\ &= - \int_{\mathcal{X}} f_X(x) \log f_X(x) dx + \log |a| \int_{\mathcal{X}} f_X(x) dx \\ &\stackrel{(2)}{=} h(X) + \log |a| . \end{aligned} \quad (8)$$

**Sources:**

- Wikipedia (2020): “Differential entropy”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-02-12; URL: https://en.wikipedia.org/wiki/Differential_entropy#Properties_of_differential_entropy.

2.2.5 Addition upon matrix multiplication

Theorem: Let X be a continuous (\rightarrow I/1.2.6) random vector (\rightarrow I/1.2.3). Then, the differential entropy (\rightarrow I/2.2.1) of X increases additively when multiplied with an invertible matrix A :

$$h(AX) = h(X) + \log |A| . \quad (1)$$

Proof: By definition, the differential entropy (\rightarrow I/2.2.1) of X is

$$h(X) = - \int_{\mathcal{X}} f_X(x) \log f_X(x) dx \quad (2)$$

where $f_X(x)$ is the probability density function (\rightarrow I/1.7.1) of X and \mathcal{X} is the set of possible values of X .

The probability density function of a linear function of a continuous random vector (\rightarrow I/1.7.6) $Y = g(X) = \Sigma X + \mu$ is

$$f_Y(y) = \begin{cases} \frac{1}{|\Sigma|} f_X(\Sigma^{-1}(y - \mu)) , & \text{if } y \in \mathcal{Y} \\ 0 , & \text{if } y \notin \mathcal{Y} \end{cases} \quad (3)$$

where $\mathcal{Y} = \{y = \Sigma x + \mu : x \in \mathcal{X}\}$ is the set of possible outcomes of Y .

Therefore, with $Y = g(X) = AX$, i.e. $\Sigma = A$ and $\mu = 0_n$, the probability density function (\rightarrow I/1.7.1) of Y is given by

$$f_Y(y) = \begin{cases} \frac{1}{|A|} f_X(A^{-1}y) , & \text{if } y \in \mathcal{Y} \\ 0 , & \text{if } y \notin \mathcal{Y} \end{cases} \quad (4)$$

where $\mathcal{Y} = \{y = Ax : x \in \mathcal{X}\}$.

Thus, the differential entropy (\rightarrow I/2.2.1) of Y is

$$\begin{aligned} h(Y) &\stackrel{(2)}{=} - \int_{\mathcal{Y}} f_Y(y) \log f_Y(y) dy \\ &\stackrel{(4)}{=} - \int_{\mathcal{Y}} \left[\frac{1}{|A|} f_X(A^{-1}y) \right] \log \left[\frac{1}{|A|} f_X(A^{-1}y) \right] dy . \end{aligned} \quad (5)$$

Substituting $y = Ax$ into the integral, we obtain

$$\begin{aligned} h(Y) &= - \int_{\mathcal{X}} \left[\frac{1}{|A|} f_X(A^{-1}Ax) \right] \log \left[\frac{1}{|A|} f_X(A^{-1}Ax) \right] d(Ax) \\ &= - \frac{1}{|A|} \int_{\mathcal{X}} f_X(x) \log \left[\frac{1}{|A|} f_X(x) \right] d(Ax) . \end{aligned} \quad (6)$$

Using the differential $d(Ax) = |A|dx$, this becomes

$$\begin{aligned} h(Y) &= -\frac{|A|}{|A|} \int_{\mathcal{X}} f_X(x) \log \left[\frac{1}{|A|} f_X(x) \right] dx \\ &= - \int_{\mathcal{X}} f_X(x) \log f_X(x) dx - \int_{\mathcal{X}} f_X(x) \log \frac{1}{|A|} dx . \end{aligned} \quad (7)$$

Finally, employing the fact (\rightarrow I/1.7.1) that $\int_{\mathcal{X}} f_X(x) dx = 1$, we can derive the differential entropy (\rightarrow I/2.2.1) of Y as

$$\begin{aligned} h(Y) &= - \int_{\mathcal{X}} f_X(x) \log f_X(x) dx + \log |A| \int_{\mathcal{X}} f_X(x) dx \\ &\stackrel{(2)}{=} h(X) + \log |A| . \end{aligned} \quad (8)$$

■

Sources:

- Cover, Thomas M. & Thomas, Joy A. (1991): “Properties of Differential Entropy, Relative Entropy, and Mutual Information”; in: *Elements of Information Theory*, sect. 8.6, p. 253; URL: https://www.google.de/books/edition/Elements_of_Information_Theory/j0DBDwAAQBAJ.
- Wikipedia (2021): “Differential entropy”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-10-07; URL: https://en.wikipedia.org/wiki/Differential_entropy#Properties_of_differential_entropy.

2.2.6 Non-invariance and transformation

Theorem: The differential entropy (\rightarrow I/2.2.1) is not invariant under change of variables, i.e. there exist random variables X and $Y = g(X)$, such that

$$h(Y) \neq h(X) . \quad (1)$$

In particular, for an invertible transformation $g : \mathcal{X} \rightarrow \mathcal{Y}$ from a random vector X to another random vector of the same dimension Y , it holds that

$$h(Y) = h(X) + \int_{\mathcal{X}} f_X(x) \log |J_g(x)| dx . \quad (2)$$

where $J_g(x)$ is the Jacobian matrix of the vector-valued function g and \mathcal{X} and \mathcal{Y} are the sets of possible values of X of Y , respectively.

Proof: By definition, the differential entropy (\rightarrow I/2.2.1) of X is

$$h(X) = - \int_{\mathcal{X}} f_X(x) \log f_X(x) dx \quad (3)$$

where $f_X(x)$ is the probability density function (\rightarrow I/1.7.1) of X .

The probability density function of an invertible function of a continuous random vector (\rightarrow I/1.7.5) $Y = g(X)$ is

$$f_Y(y) = \begin{cases} f_X(g^{-1}(y)) |J_{g^{-1}}(y)| , & \text{if } y \in \mathcal{Y} \\ 0 , & \text{if } y \notin \mathcal{Y} \end{cases} \quad (4)$$

where $\mathcal{Y} = \{y = g(x) : x \in \mathcal{X}\}$ is the set of possible outcomes of Y and $J_{g^{-1}}(y)$ is the Jacobian matrix of $g^{-1}(y)$

$$J_{g^{-1}}(y) = \begin{bmatrix} \frac{dx_1}{dy_1} & \cdots & \frac{dx_1}{dy_n} \\ \vdots & \ddots & \vdots \\ \frac{dx_n}{dy_1} & \cdots & \frac{dx_n}{dy_n} \end{bmatrix}. \quad (5)$$

Thus, the differential entropy (\rightarrow I/2.2.1) of Y is

$$\begin{aligned} h(Y) &\stackrel{(3)}{=} - \int_{\mathcal{Y}} f_Y(y) \log f_Y(y) dy \\ &\stackrel{(4)}{=} - \int_{\mathcal{Y}} [f_X(g^{-1}(y)) |J_{g^{-1}}(y)|] \log [f_X(g^{-1}(y)) |J_{g^{-1}}(y)|] dy. \end{aligned} \quad (6)$$

Substituting $y = g(x)$ into the integral and applying $J_{f^{-1}}(y) = J_f^{-1}(x)$, we obtain

$$\begin{aligned} h(Y) &= - \int_{\mathcal{X}} [f_X(g^{-1}(g(x))) |J_{g^{-1}}(y)|] \log [f_X(g^{-1}(g(x))) |J_{g^{-1}}(y)|] d[g(x)] \\ &= - \int_{\mathcal{X}} [f_X(x) |J_g^{-1}(x)|] \log [f_X(x) |J_g^{-1}(x)|] d[g(x)]. \end{aligned} \quad (7)$$

Using the relations $y = f(x) \Rightarrow dy = |J_f(x)| dx$ and $|A||B| = |AB|$, this becomes

$$\begin{aligned} h(Y) &= - \int_{\mathcal{X}} [f_X(x) |J_g^{-1}(x)| |J_g(x)|] \log [f_X(x) |J_g^{-1}(x)|] dx \\ &= - \int_{\mathcal{X}} f_X(x) \log f_X(x) dx - \int_{\mathcal{X}} f_X(x) \log |J_g^{-1}(x)| dx. \end{aligned} \quad (8)$$

Finally, employing the fact (\rightarrow I/1.7.8) that $\int_{\mathcal{X}} f_X(x) dx = 1$ and the determinant property $|A^{-1}| = 1/|A|$, we can derive the differential entropy (\rightarrow I/2.2.1) of Y as

$$\begin{aligned} h(Y) &= - \int_{\mathcal{X}} f_X(x) \log f_X(x) dx - \int_{\mathcal{X}} f_X(x) \log \frac{1}{|J_g(x)|} dx \\ &\stackrel{(3)}{=} h(X) + \int_{\mathcal{X}} f_X(x) \log |J_g(x)| dx. \end{aligned} \quad (9)$$

Because there exist X and Y , such that the integral term in (9) is non-zero, this also demonstrates that there exist X and Y , such that (1) is fulfilled. ■

Sources:

- Wikipedia (2021): “Differential entropy”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-10-07; URL: https://en.wikipedia.org/wiki/Differential_entropy#Properties_of_differential_entropy.
- Bernhard (2016): “proof of upper bound on differential entropy of $f(X)$ ”; in: *StackExchange Mathematics*, retrieved on 2021-10-07; URL: <https://math.stackexchange.com/a/1759531>.

- peek-a-boo (2019): “How to come up with the Jacobian in the change of variables formula”; in: *StackExchange Mathematics*, retrieved on 2021-08-30; URL: <https://math.stackexchange.com/a/3239222>.
- Wikipedia (2021): “Jacobian matrix and determinant”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-10-07; URL: https://en.wikipedia.org/wiki/Jacobian_matrix_and_determinant#Inverse.
- Wikipedia (2021): “Inverse function theorem”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-10-07; URL: https://en.wikipedia.org/wiki/Inverse_function_theorem#Statement.
- Wikipedia (2021): “Determinant”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-10-07; URL: https://en.wikipedia.org/wiki/Determinant#Properties_of_the_determinant.

2.2.7 Conditional differential entropy

Definition: Let X and Y be continuous random variables (\rightarrow I/1.2.2) with possible outcomes \mathcal{X} and \mathcal{Y} and probability density functions (\rightarrow I/1.7.1) $p(x)$ and $p(y)$. Then, the conditional differential entropy of Y given X or, differential entropy of Y conditioned on X , is defined as

$$h(Y|X) = \int_{x \in \mathcal{X}} p(x) \cdot h(Y|X = x) dx \quad (1)$$

where $h(Y|X = x)$ is the (marginal) differential entropy (\rightarrow I/2.2.1) of Y , evaluated at x .

2.2.8 Joint differential entropy

Definition: Let X and Y be continuous random variables (\rightarrow I/1.2.2) with possible outcomes \mathcal{X} and \mathcal{Y} and joint probability (\rightarrow I/1.3.2) density function (\rightarrow I/1.7.1) $p(x, y)$. Then, the joint differential entropy of X and Y is defined as

$$h(X, Y) = - \int_{x \in \mathcal{X}} \int_{y \in \mathcal{Y}} p(x, y) \cdot \log_b p(x, y) dy dx \quad (1)$$

where b is the base of the logarithm specifying in which unit the differential entropy is determined.

2.2.9 Differential cross-entropy

Definition: Let X be a continuous random variable (\rightarrow I/1.2.2) with possible outcomes \mathcal{X} and let P and Q be two probability distributions (\rightarrow I/1.5.1) on X with the probability density functions (\rightarrow I/1.7.1) $p(x)$ and $q(x)$. Then, the differential cross-entropy of Q relative to P is defined as

$$h(P, Q) = - \int_{\mathcal{X}} p(x) \log_b q(x) dx \quad (1)$$

where b is the base of the logarithm specifying in which unit the differential cross-entropy is determined.

Sources:

- Wikipedia (2020): “Cross entropy”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-07-28; URL: https://en.wikipedia.org/wiki/Cross_entropy#Definition.

2.3 Discrete mutual information

2.3.1 Definition

Definition:

1) The mutual information of two discrete random variables (\rightarrow I/1.2.2) X and Y is defined as

$$I(X, Y) = - \sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} p(x, y) \cdot \log \frac{p(x, y)}{p(x) \cdot p(y)} \quad (1)$$

where $p(x)$ and $p(y)$ are the probability mass functions (\rightarrow I/1.6.1) of X and Y and $p(x, y)$ is the joint probability (\rightarrow I/1.3.2) mass function of X and Y .

2) The mutual information of two continuous random variables (\rightarrow I/1.2.2) X and Y is defined as

$$I(X, Y) = - \int_{\mathcal{X}} \int_{\mathcal{Y}} p(x, y) \cdot \log \frac{p(x, y)}{p(x) \cdot p(y)} dy dx \quad (2)$$

where $p(x)$ and $p(y)$ are the probability density functions (\rightarrow I/1.6.1) of X and Y and $p(x, y)$ is the joint probability (\rightarrow I/1.3.2) density function of X and Y .

Sources:

- Cover TM, Thomas JA (1991): “Relative Entropy and Mutual Information”; in: *Elements of Information Theory*, ch. 2.3/8.5, p. 20/251; URL: <https://www.wiley.com/en-us/Elements+of+Information+Theory%2C+2nd+Edition-p-9780471241959>.

2.3.2 Relation to marginal and conditional entropy

Theorem: Let X and Y be discrete random variables (\rightarrow I/1.2.2) with the joint probability (\rightarrow I/1.3.2) $p(x, y)$ for $x \in \mathcal{X}$ and $y \in \mathcal{Y}$. Then, the mutual information (\rightarrow I/2.4.1) of X and Y can be expressed as

$$\begin{aligned} I(X, Y) &= H(X) - H(X|Y) \\ &= H(Y) - H(Y|X) \end{aligned} \quad (1)$$

where $H(X)$ and $H(Y)$ are the marginal entropies (\rightarrow I/2.1.1) of X and Y and $H(X|Y)$ and $H(Y|X)$ are the conditional entropies (\rightarrow I/2.1.4).

Proof: The mutual information (\rightarrow I/2.4.1) of X and Y is defined as

$$I(X, Y) = \sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} p(x, y) \log \frac{p(x, y)}{p(x) p(y)} . \quad (2)$$

Separating the logarithm, we have:

$$I(X, Y) = \sum_x \sum_y p(x, y) \log \frac{p(x, y)}{p(y)} - \sum_x \sum_y p(x, y) \log p(x) . \quad (3)$$

Applying the law of conditional probability (\rightarrow I/1.3.4), i.e. $p(x, y) = p(x|y) p(y)$, we get:

$$I(X, Y) = \sum_x \sum_y p(x|y) p(y) \log p(x|y) - \sum_x \sum_y p(x, y) \log p(x) . \quad (4)$$

Regrouping the variables, we have:

$$I(X, Y) = \sum_y p(y) \sum_x p(x|y) \log p(x|y) - \sum_x \left(\sum_y p(x, y) \right) \log p(x) . \quad (5)$$

Applying the law of marginal probability (\rightarrow I/1.3.3), i.e. $p(x) = \sum_y p(x, y)$, we get:

$$I(X, Y) = \sum_y p(y) \sum_x p(x|y) \log p(x|y) - \sum_x p(x) \log p(x) . \quad (6)$$

Now considering the definitions of marginal (\rightarrow I/2.1.1) and conditional (\rightarrow I/2.1.4) entropy

$$\begin{aligned} H(X) &= - \sum_{x \in \mathcal{X}} p(x) \log p(x) \\ H(X|Y) &= \sum_{y \in \mathcal{Y}} p(y) H(X|Y = y) , \end{aligned} \quad (7)$$

we can finally show:

$$\begin{aligned} I(X, Y) &= -H(X|Y) + H(X) \\ &= H(X) - H(X|Y) . \end{aligned} \quad (8)$$

The conditioning of X on Y in this proof is without loss of generality. Thus, the proof for the expression using the reverse conditional entropy of Y given X is obtained by simply switching x and y in the derivation. ■

Sources:

- Wikipedia (2020): “Mutual information”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-01-13; URL: https://en.wikipedia.org/wiki/Mutual_information#Relation_to_conditional_and_joint_entropy.

2.3.3 Relation to marginal and joint entropy

Theorem: Let X and Y be discrete random variables (\rightarrow I/1.2.2) with the joint probability (\rightarrow I/1.3.2) $p(x, y)$ for $x \in \mathcal{X}$ and $y \in \mathcal{Y}$. Then, the mutual information (\rightarrow I/2.4.1) of X and Y can be expressed as

$$I(X, Y) = H(X) + H(Y) - H(X, Y) \quad (1)$$

where $H(X)$ and $H(Y)$ are the marginal entropies (\rightarrow I/2.1.1) of X and Y and $H(X, Y)$ is the joint entropy (\rightarrow I/2.1.5).

Proof: The mutual information (\rightarrow I/2.4.1) of X and Y is defined as

$$I(X, Y) = \sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} p(x, y) \log \frac{p(x, y)}{p(x)p(y)} . \quad (2)$$

Separating the logarithm, we have:

$$I(X, Y) = \sum_x \sum_y p(x, y) \log p(x, y) - \sum_x \sum_y p(x, y) \log p(x) - \sum_x \sum_y p(x, y) \log p(y) . \quad (3)$$

Regrouping the variables, this reads:

$$I(X, Y) = \sum_x \sum_y p(x, y) \log p(x, y) - \sum_x \left(\sum_y p(x, y) \right) \log p(x) - \sum_y \left(\sum_x p(x, y) \right) \log p(y) . \quad (4)$$

Applying the law of marginal probability (\rightarrow I/1.3.3), i.e. $p(x) = \sum_y p(x, y)$, we get:

$$I(X, Y) = \sum_x \sum_y p(x, y) \log p(x, y) - \sum_x p(x) \log p(x) - \sum_y p(y) \log p(y) . \quad (5)$$

Now considering the definitions of marginal (\rightarrow I/2.1.1) and joint (\rightarrow I/2.1.5) entropy

$$\begin{aligned} H(X) &= - \sum_{x \in \mathcal{X}} p(x) \log p(x) \\ H(X, Y) &= - \sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} p(x, y) \log p(x, y) , \end{aligned} \quad (6)$$

we can finally show:

$$\begin{aligned} I(X, Y) &= -H(X, Y) + H(X) + H(Y) \\ &= H(X) + H(Y) - H(X, Y) . \end{aligned} \quad (7)$$

■

Sources:

- Wikipedia (2020): “Mutual information”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-01-13; URL: https://en.wikipedia.org/wiki/Mutual_information#Relation_to_conditional_and_joint_entropy.

2.3.4 Relation to joint and conditional entropy

Theorem: Let X and Y be discrete random variables (\rightarrow I/1.2.2) with the joint probability (\rightarrow I/1.3.2) $p(x, y)$ for $x \in \mathcal{X}$ and $y \in \mathcal{Y}$. Then, the mutual information (\rightarrow I/2.4.1) of X and Y can be expressed as

$$I(X, Y) = H(X, Y) - H(X|Y) - H(Y|X) \quad (1)$$

where $H(X, Y)$ is the joint entropy (\rightarrow I/2.1.5) of X and Y and $H(X|Y)$ and $H(Y|X)$ are the conditional entropies (\rightarrow I/2.1.4).

Proof: The existence of the joint probability mass function (\rightarrow I/1.6.1) ensures that the mutual information (\rightarrow I/2.4.1) is defined:

$$I(X, Y) = \sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} p(x, y) \log \frac{p(x, y)}{p(x) p(y)} . \quad (2)$$

The relation of mutual information to conditional entropy (\rightarrow I/2.3.2) is:

$$I(X, Y) = H(X) - H(X|Y) \quad (3)$$

$$I(X, Y) = H(Y) - H(Y|X) \quad (4)$$

The relation of mutual information to joint entropy (\rightarrow I/2.3.3) is:

$$I(X, Y) = H(X) + H(Y) - H(X, Y) . \quad (5)$$

It is true that

$$I(X, Y) = I(X, Y) + I(X, Y) - I(X, Y) . \quad (6)$$

Plugging in (3), (4) and (5) on the right-hand side, we have

$$\begin{aligned} I(X, Y) &= H(X) - H(X|Y) + H(Y) - H(Y|X) - H(X) - H(Y) + H(X, Y) \\ &= H(X, Y) - H(X|Y) - H(Y|X) \end{aligned} \quad (7)$$

which proves the identity given above. ■

Sources:

- Wikipedia (2020): “Mutual information”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-01-13; URL: https://en.wikipedia.org/wiki/Mutual_information#Relation_to_conditional_and_joint_entropy.

2.4 Continuous mutual information

2.4.1 Definition

Definition:

1) The mutual information of two discrete random variables (\rightarrow I/1.2.2) X and Y is defined as

$$I(X, Y) = - \sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} p(x, y) \cdot \log \frac{p(x, y)}{p(x) \cdot p(y)} \quad (1)$$

where $p(x)$ and $p(y)$ are the probability mass functions (\rightarrow I/1.6.1) of X and Y and $p(x, y)$ is the joint probability (\rightarrow I/1.3.2) mass function of X and Y .

2) The mutual information of two continuous random variables (\rightarrow I/1.2.2) X and Y is defined as

$$I(X, Y) = - \int_{\mathcal{X}} \int_{\mathcal{Y}} p(x, y) \cdot \log \frac{p(x, y)}{p(x) \cdot p(y)} dy dx \quad (2)$$

where $p(x)$ and $p(y)$ are the probability density functions (\rightarrow I/1.6.1) of X and Y and $p(x, y)$ is the joint probability (\rightarrow I/1.3.2) density function of X and Y .

Sources:

- Cover TM, Thomas JA (1991): “Relative Entropy and Mutual Information”; in: *Elements of Information Theory*, ch. 2.3/8.5, p. 20/251; URL: <https://www.wiley.com/en-us/Elements+of+Information+Theory%2C+2nd+Edition-p-9780471241959>.

2.4.2 Relation to marginal and conditional differential entropy

Theorem: Let X and Y be continuous (\rightarrow I/1.2.6) random variables (\rightarrow I/1.2.2) with the joint probability (\rightarrow I/1.3.2) $p(x, y)$ for $x \in \mathcal{X}$ and $y \in \mathcal{Y}$. Then, the mutual information (\rightarrow I/2.4.1) of X and Y can be expressed as

$$\begin{aligned} I(X, Y) &= h(X) - h(X|Y) \\ &= h(Y) - h(Y|X) \end{aligned} \quad (1)$$

where $h(X)$ and $h(Y)$ are the marginal differential entropies (\rightarrow I/2.2.1) of X and Y and $h(X|Y)$ and $h(Y|X)$ are the conditional differential entropies (\rightarrow I/2.2.7).

Proof: The mutual information (\rightarrow I/2.4.1) of X and Y is defined as

$$I(X, Y) = \int_{\mathcal{X}} \int_{\mathcal{Y}} p(x, y) \log \frac{p(x, y)}{p(x)p(y)} dy dx . \quad (2)$$

Separating the logarithm, we have:

$$I(X, Y) = \int_{\mathcal{X}} \int_{\mathcal{Y}} p(x, y) \log \frac{p(x, y)}{p(y)} dy dx - \int_{\mathcal{X}} \int_{\mathcal{Y}} p(x, y) \log p(x) dx dy . \quad (3)$$

Applying the law of conditional probability (\rightarrow I/1.3.4), i.e. $p(x, y) = p(x|y)p(y)$, we get:

$$I(X, Y) = \int_{\mathcal{X}} \int_{\mathcal{Y}} p(x|y)p(y) \log p(x|y) dy dx - \int_{\mathcal{X}} \int_{\mathcal{Y}} p(x, y) \log p(x) dy dx . \quad (4)$$

Regrouping the variables, we have:

$$I(X, Y) = \int_{\mathcal{Y}} p(y) \int_{\mathcal{X}} p(x|y) \log p(x|y) dx dy - \int_{\mathcal{X}} \left(\int_{\mathcal{Y}} p(x, y) dy \right) \log p(x) dx . \quad (5)$$

Applying the law of marginal probability (\rightarrow I/1.3.3), i.e. $p(x) = \int_{\mathcal{Y}} p(x, y) dy$, we get:

$$I(X, Y) = \int_{\mathcal{Y}} p(y) \int_{\mathcal{X}} p(x|y) \log p(x|y) dx dy - \int_{\mathcal{X}} p(x) \log p(x) dx . \quad (6)$$

Now considering the definitions of marginal (\rightarrow I/2.2.1) and conditional (\rightarrow I/2.2.7) differential entropy

$$\begin{aligned} h(X) &= - \int_{\mathcal{X}} p(x) \log p(x) dx \\ h(X|Y) &= \int_{\mathcal{Y}} p(y) h(X|Y = y) dy , \end{aligned} \quad (7)$$

we can finally show:

$$I(X, Y) = -h(X|Y) + h(X) = h(X) - h(X|Y) . \quad (8)$$

The conditioning of X on Y in this proof is without loss of generality. Thus, the proof for the expression using the reverse conditional differential entropy of Y given X is obtained by simply switching x and y in the derivation.



Sources:

- Wikipedia (2020): “Mutual information”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-02-21; URL: https://en.wikipedia.org/wiki/Mutual_information#Relation_to_conditional_and_joint_entropy.

2.4.3 Relation to marginal and joint differential entropy

Theorem: Let X and Y be continuous (\rightarrow I/1.2.6) random variables (\rightarrow I/1.2.2) with the joint probability (\rightarrow I/1.3.2) $p(x, y)$ for $x \in \mathcal{X}$ and $y \in \mathcal{Y}$. Then, the mutual information (\rightarrow I/2.4.1) of X and Y can be expressed as

$$I(X, Y) = h(X) + h(Y) - h(X, Y) \quad (1)$$

where $h(X)$ and $h(Y)$ are the marginal differential entropies (\rightarrow I/2.2.1) of X and Y and $h(X, Y)$ is the joint differential entropy (\rightarrow I/2.2.8).

Proof: The mutual information (\rightarrow I/2.4.1) of X and Y is defined as

$$I(X, Y) = \int_{\mathcal{X}} \int_{\mathcal{Y}} p(x, y) \log \frac{p(x, y)}{p(x)p(y)} dy dx . \quad (2)$$

Separating the logarithm, we have:

$$I(X, Y) = \int_{\mathcal{X}} \int_{\mathcal{Y}} p(x, y) \log p(x, y) dy dx - \int_{\mathcal{X}} \int_{\mathcal{Y}} p(x, y) \log p(x) dy dx - \int_{\mathcal{X}} \int_{\mathcal{Y}} p(x, y) \log p(y) dy dx . \quad (3)$$

Regrouping the variables, this reads:

$$I(X, Y) = \int_{\mathcal{X}} \int_{\mathcal{Y}} p(x, y) \log p(x, y) dy dx - \int_{\mathcal{X}} \left(\int_{\mathcal{Y}} p(x, y) dy \right) \log p(x) dx - \int_{\mathcal{Y}} \left(\int_{\mathcal{X}} p(x, y) dx \right) \log p(y) dy . \quad (4)$$

Applying the law of marginal probability (\rightarrow I/1.3.3), i.e. $p(x) = \int_{\mathcal{Y}} p(x, y) dy$, we get:

$$I(X, Y) = \int_{\mathcal{X}} \int_{\mathcal{Y}} p(x, y) \log p(x, y) dy dx - \int_{\mathcal{X}} p(x) \log p(x) dx - \int_{\mathcal{Y}} p(y) \log p(y) dy . \quad (5)$$

Now considering the definitions of marginal (\rightarrow I/2.2.1) and joint (\rightarrow I/2.2.8) differential entropy

$$\begin{aligned} h(X) &= - \int_{\mathcal{X}} p(x) \log p(x) dx \\ h(X, Y) &= - \int_{\mathcal{X}} \int_{\mathcal{Y}} p(x, y) \log p(x, y) dy dx , \end{aligned} \quad (6)$$

we can finally show:

$$\begin{aligned} I(X, Y) &= -h(X, Y) + h(X) + h(Y) \\ &= h(X) + h(Y) - h(X, Y) . \end{aligned} \quad (7)$$

■

Sources:

- Wikipedia (2020): “Mutual information”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-02-21; URL: https://en.wikipedia.org/wiki/Mutual_information#Relation_to_conditional_and_joint_entropy.

2.4.4 Relation to joint and conditional differential entropy

Theorem: Let X and Y be continuous (\rightarrow I/1.2.6) random variables (\rightarrow I/1.2.2) with the joint probability (\rightarrow I/1.3.2) $p(x, y)$ for $x \in \mathcal{X}$ and $y \in \mathcal{Y}$. Then, the mutual information (\rightarrow I/2.4.1) of X and Y can be expressed as

$$I(X, Y) = h(X, Y) - h(X|Y) - h(Y|X) \quad (1)$$

where $h(X, Y)$ is the joint differential entropy (\rightarrow I/2.2.8) of X and Y and $h(X|Y)$ and $h(Y|X)$ are the conditional differential entropies (\rightarrow I/2.2.7).

Proof: The existence of the joint probability density function (\rightarrow I/1.7.1) ensures that the mutual information (\rightarrow I/2.4.1) is defined:

$$I(X, Y) = \int_{\mathcal{X}} \int_{\mathcal{Y}} p(x, y) \log \frac{p(x, y)}{p(x)p(y)} dy dx . \quad (2)$$

The relation of mutual information to conditional differential entropy (\rightarrow I/2.4.2) is:

$$I(X, Y) = h(X) - h(X|Y) \quad (3)$$

$$I(X, Y) = h(Y) - h(Y|X) \quad (4)$$

The relation of mutual information to joint differential entropy (\rightarrow I/2.4.3) is:

$$I(X, Y) = h(X) + h(Y) - h(X, Y) . \quad (5)$$

It is true that

$$I(X, Y) = I(X, Y) + I(X, Y) - I(X, Y) . \quad (6)$$

Plugging in (3), (4) and (5) on the right-hand side, we have

$$\begin{aligned} I(X, Y) &= h(X) - h(X|Y) + h(Y) - h(Y|X) - h(X) - h(Y) + h(X, Y) \\ &= h(X, Y) - h(X|Y) - h(Y|X) \end{aligned} \quad (7)$$

which proves the identity given above.

■

Sources:

- Wikipedia (2020): “Mutual information”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-02-21; URL: https://en.wikipedia.org/wiki/Mutual_information#Relation_to_conditional_and_joint_entropy.

2.5 Kullback-Leibler divergence

2.5.1 Definition

Definition: Let X be a random variable (\rightarrow I/1.2.2) with possible outcomes \mathcal{X} and let P and Q be two probability distributions (\rightarrow I/1.5.1) on X .

1) The Kullback-Leibler divergence of P from Q for a discrete random variable X is defined as

$$\text{KL}[P||Q] = \sum_{x \in \mathcal{X}} p(x) \cdot \log \frac{p(x)}{q(x)} \quad (1)$$

where $p(x)$ and $q(x)$ are the probability mass functions (\rightarrow I/1.6.1) of P and Q .

2) The Kullback-Leibler divergence of P from Q for a continuous random variable X is defined as

$$\text{KL}[P||Q] = \int_{\mathcal{X}} p(x) \cdot \log \frac{p(x)}{q(x)} dx \quad (2)$$

where $p(x)$ and $q(x)$ are the probability density functions (\rightarrow I/1.7.1) of P and Q .

By convention (\rightarrow I/2.1.1), $0 \cdot \log 0$ is taken to be zero when calculating the divergence between P and Q .

Sources:

- MacKay, David J.C. (2003): “Probability, Entropy, and Inference”; in: *Information Theory, Inference, and Learning Algorithms*, ch. 2.6, eq. 2.45, p. 34; URL: <https://www.inference.org.uk/itprnn/book.pdf>.

2.5.2 Non-negativity

Theorem: The Kullback-Leibler divergence (\rightarrow I/2.5.1) is always non-negative

$$\text{KL}[P||Q] \geq 0 \quad (1)$$

with $\text{KL}[P||Q] = 0$, if and only if $P = Q$.

Proof: The discrete Kullback-Leibler divergence (\rightarrow I/2.5.1) is defined as

$$\text{KL}[P||Q] = \sum_{x \in \mathcal{X}} p(x) \cdot \log \frac{p(x)}{q(x)} \quad (2)$$

which can be reformulated into

$$\text{KL}[P||Q] = \sum_{x \in \mathcal{X}} p(x) \cdot \log p(x) - \sum_{x \in \mathcal{X}} p(x) \cdot \log q(x) . \quad (3)$$

Gibbs’ inequality (\rightarrow I/2.1.8) states that the entropy (\rightarrow I/2.1.1) of a probability distribution is always less than or equal to the cross-entropy (\rightarrow I/2.1.6) with another probability distribution – with equality only if the distributions are identical –,

$$-\sum_{i=1}^n p(x_i) \log p(x_i) \leq -\sum_{i=1}^n p(x_i) \log q(x_i) \quad (4)$$

which can be reformulated into

$$\sum_{i=1}^n p(x_i) \log p(x_i) - \sum_{i=1}^n p(x_i) \log q(x_i) \geq 0 . \quad (5)$$

Applying (5) to (3), this proves equation (1). ■

Sources:

- Wikipedia (2020): “Kullback-Leibler divergence”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-05-31; URL: https://en.wikipedia.org/wiki/Kullback%E2%80%93Leibler_divergence#Properties.

2.5.3 Non-negativity

Theorem: The Kullback-Leibler divergence (\rightarrow I/2.5.1) is always non-negative

$$\text{KL}[P||Q] \geq 0 \quad (1)$$

with $\text{KL}[P||Q] = 0$, if and only if $P = Q$.

Proof: The discrete Kullback-Leibler divergence (\rightarrow I/2.5.1) is defined as

$$\text{KL}[P||Q] = \sum_{x \in \mathcal{X}} p(x) \cdot \log \frac{p(x)}{q(x)} . \quad (2)$$

The log sum inequality (\rightarrow I/2.1.9) states that

$$\sum_{i=1}^n a_i \log_c \frac{a_i}{b_i} \geq a \log_c \frac{a}{b} . \quad (3)$$

where a_1, \dots, a_n and b_1, \dots, b_n are non-negative real numbers as well as $a = \sum_{i=1}^n a_i$ and $b = \sum_{i=1}^n b_i$. Because $p(x)$ and $q(x)$ are probability mass functions (\rightarrow I/1.6.1), such that

$$\begin{aligned} p(x) &\geq 0, & \sum_{x \in \mathcal{X}} p(x) &= 1 & \text{ and} \\ q(x) &\geq 0, & \sum_{x \in \mathcal{X}} q(x) &= 1 , \end{aligned} \quad (4)$$

theorem (1) is simply a special case of (3), i.e.

$$\text{KL}[P||Q] \stackrel{(2)}{=} \sum_{x \in \mathcal{X}} p(x) \cdot \log \frac{p(x)}{q(x)} \stackrel{(3)}{\geq} 1 \log \frac{1}{1} = 0 . \quad (5)$$

Sources:

- Wikipedia (2020): “Log sum inequality”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-09-09; URL: https://en.wikipedia.org/wiki/Log_sum_inequality#Applications. ■

2.5.4 Non-negativity

Theorem: The Kullback-Leibler divergence (\rightarrow I/2.5.1) is always non-negative

$$\text{KL}[P||Q] \geq 0 \quad (1)$$

with $\text{KL}[P||Q] = 0$, if and only if $P = Q$.

Proof: The continuous Kullback-Leibler divergence (\rightarrow I/2.5.1) is defined as

$$\text{KL}[P||Q] = \int_{\mathcal{X}} p(x) \cdot \log \frac{p(x)}{q(x)} dx . \quad (2)$$

For a continuous random variable (\rightarrow I/1.2.6) X with possible values $x \in \mathcal{X}$, Jensen's inequality (\rightarrow I/1.12.11) implies that

$$\int_{\mathcal{X}} q(x)g(x) dx \geq g\left(\int_{\mathcal{X}} q(x)x dx\right) \quad (3)$$

where $g(x)$ is a convex function and $q(x)$ is the probability density function (\rightarrow I/1.7.1) of X . The negative KL divergence is equal to

$$\begin{aligned} -\text{KL}[P||Q] &= -\int_{\mathcal{X}} p(x) \cdot \log \frac{p(x)}{q(x)} dx \\ &= \int_{\mathcal{X}} p(x) \cdot \log \frac{q(x)}{p(x)} dx . \end{aligned} \quad (4)$$

Applying (3) to (4), we have

$$\begin{aligned} -\text{KL}[P||Q] &\leq \log \int_{\mathcal{X}} p(x) \cdot \frac{q(x)}{p(x)} dx \\ &= \log \int_{\mathcal{X}} q(x) dx \\ &= \log 1 = 0 \end{aligned} \quad (5)$$

where the inequality sign has been reversed, because $\log(x)$ is a concave function, and we have used the fact that a PDF integrates to one (\rightarrow I/1.7.1). From (5), we get

$$\begin{aligned} -\text{KL}[P||Q] &\leq 0 \\ \text{KL}[P||Q] &\geq 0 . \end{aligned} \quad (6)$$

■

Sources:

- Ostwald et al. (2014): “A tutorial on variational Bayes for latent linear stochastic time-series models”; in: *Journal of Mathematical Psychology*, vol. 60, pp. 1-19, App. A; URL: <https://www.sciencedirect.com/science/article/pii/S0022249614000352>; DOI: 10.1016/j.jmp.2014.04.0.

2.5.5 Non-symmetry

Theorem: The Kullback-Leibler divergence (\rightarrow I/2.5.1) is non-symmetric, i.e.

$$\text{KL}[P||Q] \neq \text{KL}[Q||P] \quad (1)$$

for some probability distributions (\rightarrow I/1.5.1) P and Q .

Proof: Let $X \in \mathcal{X} = \{0, 1, 2\}$ be a discrete random variable (\rightarrow I/1.2.2) and consider the two probability distributions (\rightarrow I/1.5.1)

$$\begin{aligned} P : X &\sim \text{Bin}(2, 0.5) \\ Q : X &\sim \mathcal{U}(0, 2) \end{aligned} \quad (2)$$

where $\text{Bin}(n, p)$ indicates a binomial distribution (\rightarrow II/1.3.1) and $\mathcal{U}(a, b)$ indicates a discrete uniform distribution (\rightarrow II/1.1.1).

Then, the probability mass function of the binomial distribution (\rightarrow II/1.3.3) entails that

$$p(x) = \begin{cases} 1/4, & \text{if } x = 0 \\ 1/2, & \text{if } x = 1 \\ 1/4, & \text{if } x = 2 \end{cases} \quad (3)$$

and the probability mass function of the discrete uniform distribution (\rightarrow II/1.1.2) entails that

$$q(x) = \frac{1}{3}, \quad (4)$$

such that the Kullback-Leibler divergence (\rightarrow I/2.5.1) of P from Q is

$$\begin{aligned} \text{KL}[P||Q] &= \sum_{x \in \mathcal{X}} p(x) \cdot \log \frac{p(x)}{q(x)} \\ &= \frac{1}{4} \log \frac{3}{4} + \frac{1}{2} \log \frac{3}{2} + \frac{1}{4} \log \frac{3}{4} \\ &= \frac{1}{2} \log \frac{3}{4} + \frac{1}{2} \log \frac{3}{2} \\ &= \frac{1}{2} \left(\log \frac{3}{4} + \log \frac{3}{2} \right) \\ &= \frac{1}{2} \log \left(\frac{3}{4} \cdot \frac{3}{2} \right) \\ &= \frac{1}{2} \log \frac{9}{8} = 0.0589 \end{aligned} \quad (5)$$

and the Kullback-Leibler divergence (\rightarrow I/2.5.1) of Q from P is

$$\begin{aligned}
\text{KL}[Q||P] &= \sum_{x \in \mathcal{X}} q(x) \cdot \log \frac{q(x)}{p(x)} \\
&= \frac{1}{3} \log \frac{4}{3} + \frac{1}{3} \log \frac{2}{3} + \frac{1}{3} \log \frac{4}{3} \\
&= \frac{1}{3} \left(\log \frac{4}{3} + \log \frac{2}{3} + \log \frac{4}{3} \right) \\
&= \frac{1}{3} \log \left(\frac{4}{3} \cdot \frac{2}{3} \cdot \frac{4}{3} \right) \\
&= \frac{1}{3} \log \frac{32}{27} = 0.0566
\end{aligned} \tag{6}$$

which provides an example for

$$\text{KL}[P||Q] \neq \text{KL}[Q||P] \tag{7}$$

and thus proves the theorem. ■

Sources:

- Kullback, Solomon (1959): “Divergence”; in: *Information Theory and Statistics*, ch. 1.3, pp. 6ff.; URL: <http://index-of.co.uk/Information-Theory/Information%20theory%20and%20statistics%20-%20Solomon%20Kullback.pdf>.
- Wikipedia (2020): “Kullback-Leibler divergence”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-08-11; URL: https://en.wikipedia.org/wiki/Kullback%E2%80%93Leibler_divergence#Basic_example.

2.5.6 Convexity

Theorem: The Kullback-Leibler divergence (\rightarrow I/2.5.1) is convex in pairs of probability distributions (\rightarrow I/1.5.1), i.e.

$$\text{KL}[\lambda p_1 + (1 - \lambda)p_2 || \lambda q_1 + (1 - \lambda)q_2] \leq \lambda \text{KL}[p_1 || q_1] + (1 - \lambda) \text{KL}[p_2 || q_2] \tag{1}$$

where (p_1, q_1) and (p_2, q_2) are two pairs of probability density functions (\rightarrow I/1.7.1) and $0 \leq \lambda \leq 1$.

Proof: The Kullback-Leibler divergence (\rightarrow I/2.5.1) of P from Q is defined as

$$\text{KL}[P||Q] = \sum_{x \in \mathcal{X}} p(x) \cdot \log \frac{p(x)}{q(x)} \tag{2}$$

and the log sum inequality (\rightarrow I/2.1.9) states that

$$\sum_{i=1}^n a_i \log \frac{a_i}{b_i} \geq \left(\sum_{i=1}^n a_i \right) \log \frac{\sum_{i=1}^n a_i}{\sum_{i=1}^n b_i} \tag{3}$$

where a_1, \dots, a_n and b_1, \dots, b_n are non-negative real numbers.

Thus, we can rewrite the KL divergence of the mixture distribution as

$$\begin{aligned}
& \text{KL}[\lambda p_1 + (1 - \lambda)p_2 || \lambda q_1 + (1 - \lambda)q_2] \\
& \stackrel{(2)}{=} \sum_{x \in \mathcal{X}} \left[[\lambda p_1(x) + (1 - \lambda)p_2(x)] \cdot \log \frac{\lambda p_1(x) + (1 - \lambda)p_2(x)}{\lambda q_1(x) + (1 - \lambda)q_2(x)} \right] \\
& \stackrel{(3)}{\leq} \sum_{x \in \mathcal{X}} \left[\lambda p_1(x) \cdot \log \frac{\lambda p_1(x)}{\lambda q_1(x)} + (1 - \lambda)p_2(x) \cdot \log \frac{(1 - \lambda)p_2(x)}{(1 - \lambda)q_2(x)} \right] \\
& = \lambda \sum_{x \in \mathcal{X}} p_1(x) \cdot \log \frac{p_1(x)}{q_1(x)} + (1 - \lambda) \sum_{x \in \mathcal{X}} p_2(x) \cdot \log \frac{p_2(x)}{q_2(x)} \\
& \stackrel{(2)}{=} \lambda \text{KL}[p_1 || q_1] + (1 - \lambda) \text{KL}[p_2 || q_2]
\end{aligned} \tag{4}$$

which is equivalent to (1). ■

Sources:

- Wikipedia (2020): “Kullback-Leibler divergence”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-08-11; URL: https://en.wikipedia.org/wiki/Kullback%E2%80%93Leibler_divergence#Properties.
- Xie, Yao (2012): “Chain Rules and Inequalities”; in: *ECE587: Information Theory*, Lecture 3, Slides 22/24; URL: <https://www2.isye.gatech.edu/~yxie77/ece587/Lecture3.pdf>.

2.5.7 Additivity for independent distributions

Theorem: The Kullback-Leibler divergence (\rightarrow I/2.5.1) is additive for independent distributions, i.e.

$$\text{KL}[P || Q] = \text{KL}[P_1 || Q_1] + \text{KL}[P_2 || Q_2] \tag{1}$$

where P_1 and P_2 are independent (\rightarrow I/1.3.6) distributions (\rightarrow I/1.5.1) with the joint distribution (\rightarrow I/1.5.2) P , such that $p(x, y) = p_1(x) p_2(y)$, and equivalently for Q_1 , Q_2 and Q .

Proof: The continuous Kullback-Leibler divergence (\rightarrow I/2.5.1) is defined as

$$\text{KL}[P || Q] = \int_{\mathcal{X}} p(x) \cdot \log \frac{p(x)}{q(x)} dx \tag{2}$$

which, applied to the joint distributions P and Q , yields

$$\text{KL}[P || Q] = \int_{\mathcal{X}} \int_{\mathcal{Y}} p(x, y) \cdot \log \frac{p(x, y)}{q(x, y)} dy dx . \tag{3}$$

Applying $p(x, y) = p_1(x) p_2(y)$ and $q(x, y) = q_1(x) q_2(y)$, we have

$$\text{KL}[P || Q] = \int_{\mathcal{X}} \int_{\mathcal{Y}} p_1(x) p_2(y) \cdot \log \frac{p_1(x) p_2(y)}{q_1(x) q_2(y)} dy dx . \tag{4}$$

Now we can separate the logarithm and evaluate the integrals:

$$\begin{aligned}
\text{KL}[P||Q] &= \int_{\mathcal{X}} \int_{\mathcal{Y}} p_1(x) p_2(y) \cdot \left(\log \frac{p_1(x)}{q_1(x)} + \log \frac{p_2(y)}{q_2(y)} \right) dy dx \\
&= \int_{\mathcal{X}} \int_{\mathcal{Y}} p_1(x) p_2(y) \cdot \log \frac{p_1(x)}{q_1(x)} dy dx + \int_{\mathcal{X}} \int_{\mathcal{Y}} p_1(x) p_2(y) \cdot \log \frac{p_2(y)}{q_2(y)} dy dx \\
&= \int_{\mathcal{X}} p_1(x) \cdot \log \frac{p_1(x)}{q_1(x)} \int_{\mathcal{Y}} p_2(y) dy dx + \int_{\mathcal{Y}} p_2(y) \cdot \log \frac{p_2(y)}{q_2(y)} \int_{\mathcal{X}} p_1(x) dx dy \\
&= \int_{\mathcal{X}} p_1(x) \cdot \log \frac{p_1(x)}{q_1(x)} dx + \int_{\mathcal{Y}} p_2(y) \cdot \log \frac{p_2(y)}{q_2(y)} dy \\
&\stackrel{(2)}{=} \text{KL}[P_1||Q_1] + \text{KL}[P_2||Q_2] .
\end{aligned} \tag{5}$$

■

Sources:

- Wikipedia (2020): “Kullback-Leibler divergence”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-05-31; URL: https://en.wikipedia.org/wiki/Kullback%E2%80%93Leibler_divergence#Properties.

2.5.8 Invariance under parameter transformation

Theorem: The Kullback-Leibler divergence (\rightarrow I/2.5.1) is invariant under parameter transformation, i.e.

$$\text{KL}[p(x)||q(x)] = \text{KL}[p(y)||q(y)] \tag{1}$$

where $y(x) = mx + n$ is an affine transformation of x and $p(x)$ and $q(x)$ are the probability density functions (\rightarrow I/1.7.1) of the probability distributions (\rightarrow I/1.5.1) P and Q on the continuous random variable (\rightarrow I/1.2.2) X .

Proof: The continuous Kullback-Leibler divergence (\rightarrow I/2.5.1) (KL divergence) is defined as

$$\text{KL}[p(x)||q(x)] = \int_a^b p(x) \cdot \log \frac{p(x)}{q(x)} dx \tag{2}$$

where $a = \min(\mathcal{X})$ and $b = \max(\mathcal{X})$ are the lower and upper bound of the possible outcomes \mathcal{X} of X . Since $y(x) = mx + n$ is a strictly increasing (\rightarrow I/1.7.3) or strictly decreasing (\rightarrow I/1.7.4) function, we have the identity of the differentials

$$\begin{aligned}
p(x) dx &= p(y) dy \\
q(x) dx &= q(y) dy
\end{aligned} \tag{3}$$

which can be rearranged into

$$\begin{aligned}
p(x) &= p(y) \frac{dy}{dx} \\
q(x) &= q(y) \frac{dy}{dx} ,
\end{aligned} \tag{4}$$

the KL divergence can be evaluated as follows:

$$\begin{aligned}
\text{KL}[p(x)||q(x)] &= \int_a^b p(x) \cdot \log \frac{p(x)}{q(x)} dx \\
&= \int_{y(a)}^{y(b)} p(y) \frac{dy}{dx} \cdot \log \left(\frac{p(y) \frac{dy}{dx}}{q(y) \frac{dy}{dx}} \right) dx \\
&= \int_{y(a)}^{y(b)} p(y) \cdot \log \frac{p(y)}{q(y)} dy \\
&= \text{KL}[p(y)||q(y)] .
\end{aligned} \tag{5}$$

■

Sources:

- Wikipedia (2020): “Kullback-Leibler divergence”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-05-27; URL: https://en.wikipedia.org/wiki/Kullback%E2%80%93Leibler_divergence#Properties.
- shimao (2018): “KL divergence invariant to affine transformation?”; in: *StackExchange CrossValidated*, retrieved on 2020-05-28; URL: <https://stats.stackexchange.com/questions/341922/kl-divergence-invariant-to-affine-transformation>.

2.5.9 Relation to discrete entropy

Theorem: Let X be a discrete random variable (\rightarrow I/1.2.2) with possible outcomes \mathcal{X} and let P and Q be two probability distributions (\rightarrow I/1.5.1) on X . Then, the Kullback-Leibler divergence (\rightarrow I/2.5.1) of P from Q can be expressed as

$$\text{KL}[P||Q] = H(P, Q) - H(P) \tag{1}$$

where $H(P, Q)$ is the cross-entropy (\rightarrow I/2.1.6) of P and Q and $H(P)$ is the marginal entropy (\rightarrow I/2.1.1) of P .

Proof: The discrete Kullback-Leibler divergence (\rightarrow I/2.5.1) is defined as

$$\text{KL}[P||Q] = \sum_{x \in \mathcal{X}} p(x) \cdot \log \frac{p(x)}{q(x)} \tag{2}$$

where $p(x)$ and $q(x)$ are the probability mass functions (\rightarrow I/1.6.1) of P and Q . Separating the logarithm, we have:

$$\text{KL}[P||Q] = - \sum_{x \in \mathcal{X}} p(x) \log q(x) + \sum_{x \in \mathcal{X}} p(x) \log p(x) . \tag{3}$$

Now considering the definitions of marginal entropy (\rightarrow I/2.1.1) and cross-entropy (\rightarrow I/2.1.6)

$$\begin{aligned}
H(P) &= - \sum_{x \in \mathcal{X}} p(x) \log p(x) \\
H(P, Q) &= - \sum_{x \in \mathcal{X}} p(x) \log q(x) ,
\end{aligned} \tag{4}$$

we can finally show:

$$\text{KL}[P||Q] = H(P, Q) - H(P) . \tag{5}$$

**Sources:**

- Wikipedia (2020): “Kullback-Leibler divergence”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-05-27; URL: https://en.wikipedia.org/wiki/Kullback%E2%80%93Leibler_divergence#Motivation.

2.5.10 Relation to differential entropy

Theorem: Let X be a continuous random variable (\rightarrow I/1.2.2) with possible outcomes \mathcal{X} and let P and Q be two probability distributions (\rightarrow I/1.5.1) on X . Then, the Kullback-Leibler divergence (\rightarrow I/2.5.1) of P from Q can be expressed as

$$\text{KL}[P||Q] = h(P, Q) - h(P) \quad (1)$$

where $h(P, Q)$ is the differential cross-entropy (\rightarrow I/2.2.9) of P and Q and $h(P)$ is the marginal differential entropy (\rightarrow I/2.2.1) of P .

Proof: The continuous Kullback-Leibler divergence (\rightarrow I/2.5.1) is defined as

$$\text{KL}[P||Q] = \int_{\mathcal{X}} p(x) \cdot \log \frac{p(x)}{q(x)} dx \quad (2)$$

where $p(x)$ and $q(x)$ are the probability density functions (\rightarrow I/1.7.1) of P and Q . Separating the logarithm, we have:

$$\text{KL}[P||Q] = - \int_{\mathcal{X}} p(x) \log q(x) dx + \int_{\mathcal{X}} p(x) \log p(x) dx . \quad (3)$$

Now considering the definitions of marginal differential entropy (\rightarrow I/2.2.1) and differential cross-entropy (\rightarrow I/2.2.9)

$$\begin{aligned} h(P) &= - \int_{\mathcal{X}} p(x) \log p(x) dx \\ h(P, Q) &= - \int_{\mathcal{X}} p(x) \log q(x) dx , \end{aligned} \quad (4)$$

we can finally show:

$$\text{KL}[P||Q] = h(P, Q) - h(P) . \quad (5)$$

**Sources:**

- Wikipedia (2020): “Kullback-Leibler divergence”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-05-27; URL: https://en.wikipedia.org/wiki/Kullback%E2%80%93Leibler_divergence#Motivation.

3 Estimation theory

3.1 Basic concepts of estimation

3.1.1 Estimator

Definition: Let $y \in \mathcal{Y}$ be measured data (\rightarrow I/1.1.5), governed by a probability distribution (\rightarrow I/1.5.1) described by some statistical parameter (\rightarrow I/1.5.7) $\theta \in \Theta$. Then, a function $\hat{\theta} : \mathcal{Y} \rightarrow \Theta$ exemplifying a rule for calculating an estimate of θ from y is called an “estimator”. Estimation theory distinguishes:

- the quantify of interest θ is called the “estimand”;
- the rule $\hat{\theta}$ for estimating it is called “estimator”;
- the result of estimation $\hat{\theta}(y)$ is called “estimate”.

Sources:

- Ostwald, Dirk (2023): “Punktschätzung”; in: *Wahrscheinlichkeitstheorie und Frequentistische Inferenz*, Einheit (9), Folie 7; URL: https://www.ipsy.ovgu.de/ipsy__media/Methodenlehre+I/Wintersemester2324/Wahrscheinlichkeitstheorie+und+Frequentistische+Inferenz/9_Punktsch%C3%A4tzung.pdf.
- Wikipedia (2024): “Estimator”; in: *Wikipedia, the free encyclopedia*, retrieved on 2024-11-01; URL: <https://en.wikipedia.org/wiki/Estimator#Definition>.

3.1.2 Biased vs. unbiased

Definition: Let $\hat{\theta} : \mathcal{Y} \rightarrow \Theta$ be an estimator (\rightarrow I/3.1.1) of a parameter (\rightarrow I/1.5.7) $\theta \in \Theta$ from data (\rightarrow I/1.1.5) $y \in \mathcal{Y}$. Then,

- $\hat{\theta}$ is called an unbiased estimator when its expected value (\rightarrow I/1.12.1) is equal to the parameter that it is estimating: $E_{\hat{\theta}}(\hat{\theta}) = \theta$, where the expectation is calculated over all possible samples y leading to values of $\hat{\theta}$.
- $\hat{\theta}$ is called a biased estimator otherwise, i.e. when $E_{\hat{\theta}}(\hat{\theta}) \neq \theta$.

Sources:

- Wikipedia (2024): “Estimator”; in: *Wikipedia, the free encyclopedia*, retrieved on 2024-11-08; URL: <https://en.wikipedia.org/wiki/Estimator#Bias>.

3.2 Point estimates

3.2.1 Mean squared error

Definition: Let $\hat{\theta}$ be an estimator (\rightarrow I/3.1.1) of an unknown parameter (\rightarrow I/1.5.7) θ based on measured data (\rightarrow I/1.1.5) y . Then, the mean squared error is defined as the expected value (\rightarrow I/1.12.1) of the squared difference between the estimated value and the true value of the parameter:

$$\text{MSE} = E_{\hat{\theta}} \left[\left(\hat{\theta} - \theta \right)^2 \right] . \quad (1)$$

where $E_{\hat{\theta}} [\cdot]$ is expectation calculated over all possible samples (\rightarrow I/1.1.6) y leading to values of $\hat{\theta}$.

Sources:

- Wikipedia (2022): “Estimator”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-03-27; URL: https://en.wikipedia.org/wiki/Estimator#Mean_squared_error.

3.2.2 Partition of the mean squared error into bias and variance

Theorem: The mean squared error (\rightarrow I/3.2.1) can be partitioned into variance and squared bias

$$\text{MSE}(\hat{\theta}) = \text{Var}(\hat{\theta}) + \text{Bias}(\hat{\theta}, \theta)^2 \quad (1)$$

where the variance (\rightarrow I/1.13.1) is given by

$$\text{Var}(\hat{\theta}) = E_{\hat{\theta}} \left[\left(\hat{\theta} - E_{\hat{\theta}}(\hat{\theta}) \right)^2 \right] \quad (2)$$

and the bias is given by

$$\text{Bias}(\hat{\theta}, \theta) = \left(E_{\hat{\theta}}(\hat{\theta}) - \theta \right). \quad (3)$$

Proof: The mean squared error (\rightarrow I/3.2.1) (MSE) is defined as the expected value (\rightarrow I/1.12.1) of the squared deviation of the estimated value $\hat{\theta}$ from the true value θ of a parameter, over all values $\hat{\theta}$:

$$\text{MSE}(\hat{\theta}) = E_{\hat{\theta}} \left[\left(\hat{\theta} - \theta \right)^2 \right]. \quad (4)$$

This formula can be evaluated in the following way:

$$\begin{aligned} \text{MSE}(\hat{\theta}) &= E_{\hat{\theta}} \left[\left(\hat{\theta} - \theta \right)^2 \right] \\ &= E_{\hat{\theta}} \left[\left(\hat{\theta} - E_{\hat{\theta}}(\hat{\theta}) + E_{\hat{\theta}}(\hat{\theta}) - \theta \right)^2 \right] \\ &= E_{\hat{\theta}} \left[\left(\hat{\theta} - E_{\hat{\theta}}(\hat{\theta}) \right)^2 + 2 \left(\hat{\theta} - E_{\hat{\theta}}(\hat{\theta}) \right) \left(E_{\hat{\theta}}(\hat{\theta}) - \theta \right) + \left(E_{\hat{\theta}}(\hat{\theta}) - \theta \right)^2 \right] \\ &= E_{\hat{\theta}} \left[\left(\hat{\theta} - E_{\hat{\theta}}(\hat{\theta}) \right)^2 \right] + E_{\hat{\theta}} \left[2 \left(\hat{\theta} - E_{\hat{\theta}}(\hat{\theta}) \right) \left(E_{\hat{\theta}}(\hat{\theta}) - \theta \right) \right] + E_{\hat{\theta}} \left[\left(E_{\hat{\theta}}(\hat{\theta}) - \theta \right)^2 \right]. \end{aligned} \quad (5)$$

Because $E_{\hat{\theta}}(\hat{\theta}) - \theta$ is constant as a function of $\hat{\theta}$, we have:

$$\begin{aligned} \text{MSE}(\hat{\theta}) &= E_{\hat{\theta}} \left[\left(\hat{\theta} - E_{\hat{\theta}}(\hat{\theta}) \right)^2 \right] + 2 \left(E_{\hat{\theta}}(\hat{\theta}) - \theta \right) E_{\hat{\theta}} \left[\hat{\theta} - E_{\hat{\theta}}(\hat{\theta}) \right] + \left(E_{\hat{\theta}}(\hat{\theta}) - \theta \right)^2 \\ &= E_{\hat{\theta}} \left[\left(\hat{\theta} - E_{\hat{\theta}}(\hat{\theta}) \right)^2 \right] + 2 \left(E_{\hat{\theta}}(\hat{\theta}) - \theta \right) \left(E_{\hat{\theta}}(\hat{\theta}) - E_{\hat{\theta}}(\hat{\theta}) \right) + \left(E_{\hat{\theta}}(\hat{\theta}) - \theta \right)^2 \\ &= E_{\hat{\theta}} \left[\left(\hat{\theta} - E_{\hat{\theta}}(\hat{\theta}) \right)^2 \right] + \left(E_{\hat{\theta}}(\hat{\theta}) - \theta \right)^2. \end{aligned} \quad (6)$$

This proves the partition given by (1). ■

Sources:

- Wikipedia (2019): “Mean squared error”; in: *Wikipedia, the free encyclopedia*, retrieved on 2019-11-27; URL: https://en.wikipedia.org/wiki/Mean_squared_error#Proof_of_variance_and_bias_relationship.

3.3 Interval estimates**3.3.1 Confidence interval**

Definition: Let y be a random sample (\rightarrow I/1.1.6) from a probability distributions (\rightarrow I/1.5.1) governed by a parameter (\rightarrow I/1.5.7) of interest θ and quantities not of interest φ . A confidence interval for θ is defined as an interval $[u(y), v(y)]$ determined by the random variables (\rightarrow I/1.2.2) $u(y)$ and $v(y)$ with the property

$$\Pr(u(y) < \theta < v(y) \mid \theta, \varphi) = \gamma \quad \text{for all } (\theta, \varphi). \quad (1)$$

where $\gamma = 1 - \alpha$ is called the confidence level.

Sources:

- Wikipedia (2022): “Confidence interval”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-03-27; URL: https://en.wikipedia.org/wiki/Confidence_interval#Definition.

3.3.2 Construction of confidence intervals using Wilks’ theorem

Theorem: Let m be a generative model (\rightarrow I/5.1.1) for measured data y with model parameters $\theta \in \Theta$, consisting of a parameter of interest $\phi \in \Phi$ and nuisance parameters $\lambda \in \Lambda$:

$$m : p(y \mid \theta) = \mathcal{D}(y; \theta), \quad \theta = \{\phi, \lambda\}. \quad (1)$$

Further, let $\hat{\theta}$ be an estimate of θ , obtained using maximum-likelihood-estimation (\rightarrow I/4.1.3):

$$\hat{\theta} = \arg \max_{\theta} \log p(y \mid \theta), \quad \hat{\theta} = \{\hat{\phi}, \hat{\lambda}\}. \quad (2)$$

Then, an asymptotic confidence interval (\rightarrow I/3.3.1) for θ is given by

$$\text{CI}_{1-\alpha}(\hat{\phi}) = \left\{ \phi \mid \log p(y \mid \phi, \hat{\lambda}) \geq \log p(y \mid \hat{\phi}, \hat{\lambda}) - \frac{1}{2} \chi_{1,1-\alpha}^2 \right\} \quad (3)$$

where $1 - \alpha$ is the confidence level and $\chi_{1,1-\alpha}^2$ is the $(1 - \alpha)$ -quantile of the chi-squared distribution (\rightarrow II/3.7.1) with 1 degree of freedom (\rightarrow I/1.5.12).

Proof: The confidence interval (\rightarrow I/3.3.1) is defined as the interval that, under infinitely repeated random experiments (\rightarrow I/1.1.1), contains the true parameter value with a certain probability.

Let us define the likelihood ratio (\rightarrow I/4.1.6)

$$\Lambda(\phi) = \frac{p(y \mid \phi, \hat{\lambda})}{p(y \mid \hat{\phi}, \hat{\lambda})} \quad \text{for all } \phi \in \Phi \quad (4)$$

and compute the log-likelihood ratio (\rightarrow I/4.1.7)

$$\log \Lambda(\phi) = \log p(y|\phi, \hat{\lambda}) - \log p(y|\hat{\phi}, \hat{\lambda}) . \quad (5)$$

Wilks' theorem states that, when comparing two statistical models with parameter spaces Θ_1 and $\Theta_0 \subset \Theta_1$, as the sample size (\rightarrow I/1.1.7) approaches infinity, the quantity calculated as -2 times the log-ratio of maximum likelihoods follows a chi-squared distribution (\rightarrow II/3.7.1), if the null hypothesis is true:

$$H_0 : \theta \in \Theta_0 \quad \Rightarrow \quad -2 \log \frac{\max_{\theta \in \Theta_0} p(y|\theta)}{\max_{\theta \in \Theta_1} p(y|\theta)} \sim \chi_{\Delta k}^2 \quad \text{as } n \rightarrow \infty \quad (6)$$

where Δk is the difference in dimensionality between Θ_0 and Θ_1 . Applied to our example in (5), we note that $\Theta_1 = \{\phi, \hat{\phi}\}$ and $\Theta_0 = \{\phi\}$, such that $\Delta k = 1$ and Wilks' theorem implies:

$$-2 \log \Lambda(\phi) \sim \chi_1^2 . \quad (7)$$

Using the quantile function (\rightarrow I/1.11.1) $\chi_{k,p}^2$ of the chi-squared distribution (\rightarrow II/3.7.1), an $(1 - \alpha)$ -confidence interval is therefore given by all values ϕ that satisfy

$$-2 \log \Lambda(\phi) \leq \chi_{1,1-\alpha}^2 . \quad (8)$$

Applying (5) and rearranging, we can evaluate

$$\begin{aligned} -2 \left[\log p(y|\phi, \hat{\lambda}) - \log p(y|\hat{\phi}, \hat{\lambda}) \right] &\leq \chi_{1,1-\alpha}^2 \\ \log p(y|\phi, \hat{\lambda}) - \log p(y|\hat{\phi}, \hat{\lambda}) &\geq -\frac{1}{2} \chi_{1,1-\alpha}^2 \\ \log p(y|\phi, \hat{\lambda}) &\geq \log p(y|\hat{\phi}, \hat{\lambda}) - \frac{1}{2} \chi_{1,1-\alpha}^2 \end{aligned} \quad (9)$$

which is equivalent to the confidence interval given by (3). ■

Sources:

- Wikipedia (2020): “Confidence interval”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-02-19; URL: https://en.wikipedia.org/wiki/Confidence_interval#Methods_of_derivation.
- Wikipedia (2020): “Likelihood-ratio test”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-02-19; URL: https://en.wikipedia.org/wiki/Likelihood-ratio_test#Definition.
- Wikipedia (2020): “Wilks' theorem”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-02-19; URL: https://en.wikipedia.org/wiki/Wilks%27_theorem.

4 Frequentist statistics

4.1 Likelihood theory

4.1.1 Likelihood function

Definition: Let there be a generative model (\rightarrow I/5.1.1) m describing measured data y using model parameters θ . Then, the probability density function (\rightarrow I/1.7.1) of the distribution of y given θ is called the likelihood function of m :

$$\mathcal{L}_m(\theta) = p(y|\theta, m) = \mathcal{D}(y; \theta) . \quad (1)$$

4.1.2 Log-likelihood function

Definition: Let there be a generative model (\rightarrow I/5.1.1) m describing measured data y using model parameters θ . Then, the logarithm of the probability density function (\rightarrow I/1.7.1) of the distribution of y given θ is called the log-likelihood function (\rightarrow I/5.1.2) of m :

$$\text{LL}_m(\theta) = \log p(y|\theta, m) = \log \mathcal{D}(y; \theta) . \quad (1)$$

4.1.3 Maximum likelihood estimation

Definition: Let there be a generative model (\rightarrow I/5.1.1) m describing measured data y using model parameters θ . Then, the parameter values maximizing the likelihood function (\rightarrow I/5.1.2) or log-likelihood function (\rightarrow I/4.1.2) are called “maximum likelihood estimates” of θ :

$$\hat{\theta} = \arg \max_{\theta} \mathcal{L}_m(\theta) = \arg \max_{\theta} \text{LL}_m(\theta) . \quad (1)$$

The process of calculating $\hat{\theta}$ is called “maximum likelihood estimation” and the functional form leading from y to $\hat{\theta}$ given m is called “maximum likelihood estimator”. Maximum likelihood estimation, estimator and estimates may all be abbreviated as “MLE”.

4.1.4 Maximum log-likelihood

Definition: Let there be a generative model (\rightarrow I/5.1.1) m describing measured data y using model parameters θ . Then, the maximum log-likelihood (MLL) of m is the maximal value of the log-likelihood function (\rightarrow I/4.1.2) of this model:

$$\text{MLL}(m) = \max_{\theta} \text{LL}_m(\theta) . \quad (1)$$

The maximum log-likelihood can be obtained by plugging the maximum likelihood estimates (\rightarrow I/4.1.3) into the log-likelihood function (\rightarrow I/4.1.2).

4.1.5 MLE can be biased

Theorem: Maximum likelihood estimation (\rightarrow I/4.1.3) can result in biased estimates (\rightarrow I/3.1.2) of model parameters (\rightarrow I/1.5.7), i.e. estimates (\rightarrow I/3.1.1) whose long-term expected value (\rightarrow I/1.12.1) is unequal to the quantities they estimate:

$$\text{E} \left[\hat{\theta}_{\text{MLE}} \right] = \text{E} \left[\arg \max_{\theta} \text{LL}_m(\theta) \right] \neq \theta . \quad (1)$$

Proof: Consider a set of independent and identical normally distributed observations (\rightarrow III/1.1.1) $x = \{x_1, \dots, x_n\}$ with unknown mean (\rightarrow I/1.12.1) μ and variance (\rightarrow I/1.13.1) σ^2 :

$$x_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(\mu, \sigma^2), \quad i = 1, \dots, n. \quad (2)$$

Then, we know that the maximum likelihood estimator for the variance (\rightarrow III/1.1.2) σ^2 is underestimating the true variance of the data distribution (\rightarrow IV/1.1.2):

$$\mathbb{E} [\hat{\sigma}_{\text{MLE}}^2] = \frac{n-1}{n} \sigma^2 \neq \sigma^2. \quad (3)$$

This proves the existence of cases such as those stated by the theorem. ■

4.1.6 Likelihood ratio

Definition: Let m_0 and m_1 be two generative models (\rightarrow I/5.1.1) describing the same measured data y using different model parameters $\theta_0 \in \Theta_0$ and $\theta_1 \in \Theta_1$. Then, the quotient of the maximized likelihood functions (\rightarrow I/4.1.3) of these two models is denoted as Λ_{01} and is called the likelihood (\rightarrow I/5.1.2) ratio of m_0 relative to m_1 :

$$\Lambda_{01} = \frac{\max_{\theta_0 \in \Theta_0} \mathcal{L}_{m_0}(\theta_0)}{\max_{\theta_1 \in \Theta_1} \mathcal{L}_{m_1}(\theta_1)} = \frac{p(y|\hat{\theta}_0, m_0)}{p(y|\hat{\theta}_1, m_1)}. \quad (1)$$

Sources:

- Wikipedia (2024): “Neyman-Pearson lemma”; in: *Wikipedia, the free encyclopedia*, retrieved on 2024-06-14; URL: https://en.wikipedia.org/wiki/Neyman%E2%80%93Pearson_lemma#Example.

4.1.7 Log-likelihood ratio

Definition: Let m_0 and m_1 be two generative models (\rightarrow I/5.1.1) describing the same measured data y using different model parameters $\theta_0 \in \Theta_0$ and $\theta_1 \in \Theta_1$. Then, the logarithmized quotient of the maximized likelihood functions (\rightarrow I/4.1.3) of these two models is denoted as $\log \Lambda_{01}$ and is called the log-likelihood (\rightarrow I/4.1.2) ratio of m_0 relative to m_1 :

$$\log \Lambda_{01} = \log \frac{\max_{\theta_0 \in \Theta_0} \mathcal{L}_{m_0}(\theta_0)}{\max_{\theta_1 \in \Theta_1} \mathcal{L}_{m_1}(\theta_1)} = \log p(y|\hat{\theta}_0, m_0) - \log p(y|\hat{\theta}_1, m_1). \quad (1)$$

Sources:

- Wikipedia (2024): “Likelihood-ratio test”; in: *Wikipedia, the free encyclopedia*, retrieved on 2024-06-14; URL: https://en.wikipedia.org/wiki/Likelihood-ratio_test#Definition.

4.1.8 Method of moments

Definition: Let measured data y follow a probability distribution (\rightarrow I/1.5.1) with probability mass (\rightarrow I/1.6.1) or probability density (\rightarrow I/1.7.1) $p(y|\theta)$ governed by unknown parameters $\theta_1, \dots, \theta_k$. Then, method-of-moments estimation, also referred to as “method of moments” or “matching the moments”, consists in

1) expressing the first k moments (\rightarrow I/1.21.1) of y in terms of θ

$$\begin{aligned}\mu_1 &= f_1(\theta_1, \dots, \theta_k) \\ &\vdots \\ \mu_k &= f_k(\theta_1, \dots, \theta_k) ,\end{aligned}\tag{1}$$

2) calculating the first k sample moments (\rightarrow I/1.21.1) from y

$$\hat{\mu}_1(y), \dots, \hat{\mu}_k(y)\tag{2}$$

3) and solving the system of k equations

$$\begin{aligned}\hat{\mu}_1(y) &= f_1(\hat{\theta}_1, \dots, \hat{\theta}_k) \\ &\vdots \\ \hat{\mu}_k(y) &= f_k(\hat{\theta}_1, \dots, \hat{\theta}_k)\end{aligned}\tag{3}$$

for $\hat{\theta}_1, \dots, \hat{\theta}_k$, which are subsequently referred to as “method-of-moments estimates”.

Sources:

- Wikipedia (2021): “Method of moments (statistics)”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-04-29; URL: [https://en.wikipedia.org/wiki/Method_of_moments_\(statistics\)#Method](https://en.wikipedia.org/wiki/Method_of_moments_(statistics)#Method).

4.2 Statistical hypotheses

4.2.1 Statistical hypothesis

Definition: A statistical hypothesis is a statement about the parameters of a distribution describing a population from which observations can be sampled as measured data (\rightarrow I/1.1.5).

More precisely, let m be a generative model (\rightarrow I/5.1.1) describing measured data y in terms of a distribution $\mathcal{D}(\theta)$ with model parameters $\theta \in \Theta$. Then, a statistical hypothesis is formally specified as

$$H : \theta \in \Theta^* \quad \text{where} \quad \Theta^* \subset \Theta .\tag{1}$$

Sources:

- Wikipedia (2021): “Statistical hypothesis testing”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-03-19; URL: https://en.wikipedia.org/wiki/Statistical_hypothesis_testing#Definition_of_terms.

4.2.2 Simple vs. composite

Definition: Let H be a statistical hypothesis (\rightarrow I/4.2.1). Then,

- H is called a simple hypothesis, if it completely specifies the population distribution; in this case, the sampling distribution (\rightarrow I/1.5.6) of the test statistic (\rightarrow I/4.3.5) is a function of sample size (\rightarrow I/1.1.7) alone.
- H is called a composite hypothesis, if it does not completely specify the population distribution; for example, the hypothesis may only specify one parameter of the distribution and leave others unspecified.

Sources:

- Wikipedia (2021): “Exclusion of the null hypothesis”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-03-19; URL: https://en.wikipedia.org/wiki/Exclusion_of_the_null_hypothesis#Terminology.

4.2.3 Point/exact vs. set/inexact

Definition: Let H be a statistical hypothesis (\rightarrow I/4.2.1). Then,

- H is called a point hypothesis or exact hypothesis, if it specifies an exact parameter value:

$$H : \theta = \theta^* ; \quad (1)$$

- H is called a set hypothesis or inexact hypothesis, if it specifies a set of possible values with more than one element for the parameter value (e.g. a range or an interval):

$$H : \theta \in \Theta^* . \quad (2)$$

Sources:

- Wikipedia (2021): “Exclusion of the null hypothesis”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-03-19; URL: https://en.wikipedia.org/wiki/Exclusion_of_the_null_hypothesis#Terminology.

4.2.4 One-tailed vs. two-tailed

Definition: Let H_0 be a point (\rightarrow I/4.2.3) null hypothesis (\rightarrow I/4.3.2)

$$H_0 : \theta = \theta_0 \quad (1)$$

and consider a set (\rightarrow I/4.2.3) alternative hypothesis (\rightarrow I/4.3.3) H_1 . Then,

- H_1 is called a left-sided one-tailed hypothesis, if θ is assumed to be smaller than θ_0 :

$$H_1 : \theta < \theta_0 ; \quad (2)$$

- H_1 is called a right-sided one-tailed hypothesis, if θ is assumed to be larger than θ_0 :

$$H_1 : \theta > \theta_0 ; \quad (3)$$

- H_1 is called a two-tailed hypothesis, if θ is assumed to be unequal to θ_0 :

$$H_1 : \theta \neq \theta_0 . \quad (4)$$

Sources:

- Wikipedia (2021): “One- and two-tailed tests”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-03-31; URL: https://en.wikipedia.org/wiki/One_and_two-tailed_tests.

4.3 Hypothesis testing

4.3.1 Statistical test

Definition: Let y be a set of measured data (\rightarrow I/1.1.5). Then, a statistical hypothesis test consists of the following:

- an assumption about the distribution (\rightarrow I/1.5.1) of the data, often expressed in terms of a statistical model (\rightarrow I/5.1.1) m ;
- a null hypothesis (\rightarrow I/4.3.2) H_0 and an alternative hypothesis (\rightarrow I/4.3.3) H_1 which make specific statements about the distribution of the data;
- a test statistic (\rightarrow I/4.3.5) $T(Y)$ which is a function of the data and whose distribution under the null hypothesis (\rightarrow I/4.3.2) is known;
- a significance level (\rightarrow I/4.3.8) α which imposes an upper bound on the probability (\rightarrow I/1.3.1) of rejecting H_0 , given that H_0 is true.

Procedurally, the statistical hypothesis test works as follows:

- Given the null hypothesis H_0 and the significance level α , a critical value (\rightarrow I/4.3.9) t_{crit} is determined which partitions the set of possible values of $T(Y)$ into “acceptance region” and “rejection region”.
- Then, the observed test statistic (\rightarrow I/4.3.5) $t_{\text{obs}} = T(y)$ is calculated from the actually measured data y . If it is in the rejection region, H_0 is rejected in favor of H_1 . Otherwise, the test fails to reject H_0 .

Sources:

- Wikipedia (2021): “Statistical hypothesis testing”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-03-19; URL: https://en.wikipedia.org/wiki/Statistical_hypothesis_testing#The_testing_process.

4.3.2 Null hypothesis

Definition: The statement which is tested in a statistical hypothesis test (\rightarrow I/4.3.1) is called the “null hypothesis”, denoted as H_0 . The test is designed to assess the strength of evidence against H_0 and possibly reject it. The opposite of H_0 is called the “alternative hypothesis (\rightarrow I/4.3.3)”. Usually, H_0 is a statement that a particular parameter is zero, that there is no effect of a particular treatment or that there is no difference between particular conditions.

More precisely, let m be a generative model (\rightarrow I/5.1.1) describing measured data y using model parameters $\theta \in \Theta$. Then, a null hypothesis is formally specified as

$$H_0 : \theta \in \Theta_0 \quad \text{where} \quad \Theta_0 \subset \Theta . \quad (1)$$

Sources:

- Wikipedia (2021): “Exclusion of the null hypothesis”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-03-12; URL: https://en.wikipedia.org/wiki/Exclusion_of_the_null_hypothesis#Basic_definitions.

4.3.3 Alternative hypothesis

Definition: Let H_0 be a null hypothesis (\rightarrow I/4.3.2) of a statistical hypothesis test (\rightarrow I/4.3.1). Then, the corresponding alternative hypothesis, denoted as H_1 , is either the negation of H_0 or an interesting sub-case in the negation of H_0 , depending on context. The test is designed to assess the strength of evidence against H_0 and possibly reject it in favor of H_1 . Usually, H_1 is a statement that a particular parameter is non-zero, that there is an effect of a particular treatment or that there is a difference between particular conditions.

More precisely, let m be a generative model (\rightarrow I/5.1.1) describing measured data y using model parameters $\theta \in \Theta$. Then, null and alternative hypothesis are formally specified as

$$\begin{aligned} H_0 : \theta \in \Theta_0 \quad \text{where} \quad \Theta_0 \subset \Theta \\ H_1 : \theta \in \Theta_1 \quad \text{where} \quad \Theta_1 = \Theta \setminus \Theta_0 . \end{aligned} \tag{1}$$

Sources:

- Wikipedia (2021): “Exclusion of the null hypothesis”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-03-12; URL: https://en.wikipedia.org/wiki/Exclusion_of_the_null_hypothesis#Basic_definitions.

4.3.4 One-tailed vs. two-tailed

Definition: Let there be a statistical test (\rightarrow I/4.3.1) of an alternative hypothesis (\rightarrow I/4.3.3) H_1 against a null hypothesis (\rightarrow I/4.3.2) H_0 . Then,

- the test is called a one-tailed test, if H_1 is a one-tailed hypothesis (\rightarrow I/4.2.4);
- the test is called a two-tailed test, if H_1 is a two-tailed hypothesis (\rightarrow I/4.2.4).

The fact whether a test (\rightarrow I/4.3.1) is one-tailed or two-tailed has consequences for the computation of critical value (\rightarrow I/4.3.9) and p-value (\rightarrow I/4.3.10).

Sources:

- Wikipedia (2021): “One- and two-tailed tests”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-03-31; URL: https://en.wikipedia.org/wiki/One-_and_two-tailed_tests.

4.3.5 Test statistic

Definition: In a statistical hypothesis test (\rightarrow I/4.3.1), the test statistic $T(Y)$ is a scalar function of the measured data (\rightarrow I/1.1.5) y whose distribution under the null hypothesis (\rightarrow I/4.3.2) H_0 can be established. Together with a significance level (\rightarrow I/4.3.8) α , this distribution implies a critical value (\rightarrow I/4.3.9) t_{crit} of the test statistic which determines whether the test rejects or fails to reject H_0 .

Sources:

- Wikipedia (2021): “Statistical hypothesis testing”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-03-19; URL: https://en.wikipedia.org/wiki/Statistical_hypothesis_testing#The_testing_process.

4.3.6 Size of a test

Definition: Let there be a statistical hypothesis test (\rightarrow I/4.3.1) with null hypothesis (\rightarrow I/4.3.2) H_0 . Then, the size of the test is the probability of a false-positive result or making a type I error, i.e. the probability (\rightarrow I/1.3.1) of rejecting the null hypothesis (\rightarrow I/4.3.2) H_0 , given that H_0 is actually true.

For a simple null hypothesis (\rightarrow I/4.2.2), the size is determined by the following conditional probability (\rightarrow I/1.3.4):

$$\Pr(\text{test rejects } H_0 | H_0) . \quad (1)$$

For a composite null hypothesis (\rightarrow I/4.2.2), the size is the supremum over all possible realizations of the null hypothesis (\rightarrow I/4.3.2):

$$\sup_{h \in H_0} \Pr(\text{test rejects } H_0 | h) . \quad (2)$$

Sources:

- Wikipedia (2021): “Size (statistics)”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-03-19; URL: [https://en.wikipedia.org/wiki/Size_\(statistics\)](https://en.wikipedia.org/wiki/Size_(statistics)).

4.3.7 Power of a test

Definition: Let there be a statistical hypothesis test (\rightarrow I/4.3.1) with null hypothesis (\rightarrow I/4.3.2) H_0 and alternative hypothesis (\rightarrow I/4.3.3) H_1 . Then, the power of the test is the probability of a true-positive result or not making a type II error, i.e. the probability (\rightarrow I/1.3.1) of rejecting H_0 , given that H_1 is actually true.

For given null (\rightarrow I/4.3.2) and alternative (\rightarrow I/4.3.3) hypothesis (\rightarrow I/4.2.1), the size is determined by the following conditional probability (\rightarrow I/1.3.4):

$$\Pr(\text{test rejects } H_0 | H_1) . \quad (1)$$

Sources:

- Wikipedia (2021): “Power of a test”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-03-31; URL: https://en.wikipedia.org/wiki/Power_of_a_test#Description.

4.3.8 Significance level

Definition: Let the size (\rightarrow I/4.3.6) of a statistical hypothesis test (\rightarrow I/4.3.1) be the probability of a false-positive result or making a type I error, i.e. the probability (\rightarrow I/1.3.1) of rejecting the null hypothesis (\rightarrow I/4.3.2) H_0 , given that H_0 is actually true:

$$\Pr(\text{test rejects } H_0 | H_0) . \quad (1)$$

Then, the test is said to have significance level α , if the size is less than or equal to α :

$$\Pr(\text{test rejects } H_0 | H_0) \leq \alpha . \quad (2)$$

Sources:

- Wikipedia (2021): “Statistical hypothesis testing”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-03-19; URL: https://en.wikipedia.org/wiki/Statistical_hypothesis_testing#Definition_of_terms.

4.3.9 Critical value

Definition: In a statistical hypothesis test (\rightarrow I/4.3.1), the critical value (\rightarrow I/4.3.9) t_{crit} is that value of the test statistic (\rightarrow I/4.3.5) $T(Y)$ which partitions the set of possible test statistics into “acceptance region” and “rejection region” based on a significance level (\rightarrow I/4.3.8) α . Put differently, if the observed test statistic $t_{\text{obs}} = T(y)$ computed from actually measured data (\rightarrow I/1.1.5) y is as extreme or more extreme than the critical value, the test rejects the null hypothesis (\rightarrow I/4.3.2) H_0 in favor of the alternative hypothesis (\rightarrow I/4.3.3).

Sources:

- Wikipedia (2021): “Statistical hypothesis testing”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-03-19; URL: https://en.wikipedia.org/wiki/Statistical_hypothesis_testing#Definition_of_terms.

4.3.10 p-value

Definition: Let there be a statistical test (\rightarrow I/4.3.1) of the null hypothesis (\rightarrow I/4.3.2) H_0 and the alternative hypothesis (\rightarrow I/4.3.3) H_1 using the test statistic (\rightarrow I/4.3.5) $T(Y)$. Let y be the measured data (\rightarrow I/1.1.5) and let $t_{\text{obs}} = T(y)$ be the observed test statistic computed from y . Moreover, assume that $F_T(t)$ is the cumulative distribution function (\rightarrow I/1.8.1) (CDF) of the distribution of $T(Y)$ under H_0 .

Then, the p-value is the probability of obtaining a test statistic more extreme than or as extreme as t_{obs} , given that the null hypothesis H_0 is true:

- $p = F_T(t_{\text{obs}})$, if H_1 is a left-sided one-tailed hypothesis (\rightarrow I/4.2.4);
- $p = 1 - F_T(t_{\text{obs}})$, if H_1 is a right-sided one-tailed hypothesis (\rightarrow I/4.2.4);
- $p = 2 \cdot \min([F_T(t_{\text{obs}}), 1 - F_T(t_{\text{obs}})])$, if H_1 is a two-tailed hypothesis (\rightarrow I/4.2.4).

Sources:

- Wikipedia (2021): “Statistical hypothesis testing”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-03-19; URL: https://en.wikipedia.org/wiki/Statistical_hypothesis_testing#Definition_of_terms.

4.3.11 Distribution of p-value under null hypothesis

Theorem: Under the null hypothesis (\rightarrow I/4.3.2), the p-value (\rightarrow I/4.3.10) in a statistical test (\rightarrow I/4.3.1) follows a continuous uniform distribution (\rightarrow II/3.1.1):

$$p \sim \mathcal{U}(0, 1) . \quad (1)$$

Proof: Without loss of generality, consider a left-sided one-tailed hypothesis test (\rightarrow I/4.2.4). Then, the p-value is a function of the test statistic (\rightarrow I/4.3.10)

$$\begin{aligned} P &= F_T(T) \\ p &= F_T(t_{\text{obs}}) \end{aligned} \tag{2}$$

where t_{obs} is the observed test statistic (\rightarrow I/4.3.5) and $F_T(t)$ is the cumulative distribution function (\rightarrow I/1.8.1) of the test statistic (\rightarrow I/4.3.5) under the null hypothesis (\rightarrow I/4.3.2).

Then, we can obtain the cumulative distribution function (\rightarrow I/1.8.1) of the p-value (\rightarrow I/4.3.10) as

$$\begin{aligned} F_P(p) &= \Pr(P < p) \\ &= \Pr(F_T(T) < p) \\ &= \Pr(T < F_T^{-1}(p)) \\ &= F_T(F_T^{-1}(p)) \\ &= p \end{aligned} \tag{3}$$

which is the cumulative distribution function of a continuous uniform distribution (\rightarrow II/3.1.4) over the interval $[0, 1]$:

$$F_X(x) = \int_{-\infty}^x \mathcal{U}(z; 0, 1) dz = x \quad \text{where} \quad 0 \leq x \leq 1. \tag{4}$$

■

Sources:

- jll (2018): “Why are p-values uniformly distributed under the null hypothesis?”; in: *StackExchange Cross Validated*, retrieved on 2022-03-18; URL: <https://stats.stackexchange.com/a/345763/270304>.

4.3.12 Minimum detectable effect

Definition: Consider a hypothesis test (\rightarrow I/4.3.1) concerning parameter θ . We have $H_0 : \theta \in \Theta_0$ versus $H_1 : \theta \in \Theta_1$, where $\{\Theta_0, \Theta_1\}$ is a partition of Θ . Let the probability of rejecting the null hypothesis for the test with n observations be $\kappa_n(\theta)$. The number of samples n is fixed.

The effect size for a parameter $\theta \in \Theta_1$ is the distance of θ from the null parameter space Θ_0 , $d(\theta, \Theta_0)$. It can be defined as

$$d(\theta, \Theta_0) = \inf_{\theta_0 \in \Theta_0} \|\theta - \theta_0\|. \tag{1}$$

Let the test have a given significance level (\rightarrow I/4.3.8) α and desired power (\rightarrow I/4.3.7) $1 - \beta$. The minimum detectable effect, δ , is the smallest δ so that the hypothesis test simultaneously has size (\rightarrow I/4.3.6) less than or equal to α and power at least $1 - \beta$:

$$\left(\sup_{\theta \in \Theta_0} \kappa_n(\theta) \leq \alpha \right) \wedge \left(\inf_{\theta: d(\theta, \Theta_0) \leq \delta} \kappa_n(\theta) \geq 1 - \beta \right). \tag{2}$$

Sources:

- Sylvain Chabé-Ferret (2025): “Power Analysis”; in: *Statistical Tools for Causal Inference*, retrieved on 2025-07-05; URL: <https://chabefer.github.io/STCI/Power.html>.

4.3.13 Minimum required sample size

Definition: Consider a hypothesis test (\rightarrow I/4.3.1) concerning parameter θ . We have $H_0 : \theta \in \Theta_0$ versus $H_1 : \theta \in \Theta_1$, where $\{\Theta_0, \Theta_1\}$ is a partition of Θ . Let the probability of rejecting the null hypothesis for the test with n observations be $\kappa_n(\theta)$.

Given a pre-specified significance level (\rightarrow I/4.3.8) $\alpha \in [0, 1]$ and a desired power (\rightarrow I/4.3.7) $1 - \beta \in [0, 1]$, the test must satisfy two conditions:

1. significance constraint: The probability of a type I error must not exceed α :

$$\sup_{\theta \in \Theta_0} \kappa_n(\theta) \leq \alpha . \quad (1)$$

2. power constraint: The power of the test must be at least $1 - \beta$ for all parameters corresponding to a minimum detectable effect (\rightarrow I/4.3.12), δ . This is represented by a specified subset of the alternative hypothesis space, $\Theta_{1,\delta} \subset \Theta_1$:

$$\inf_{\theta \in \Theta_{1,\delta}} \kappa_n(\theta) \geq 1 - \beta . \quad (2)$$

The minimum required sample size, n_m , is the smallest integer n so that the hypothesis test simultaneously satisfies both the significance and power constraint.

Sources:

- Sylvain Chabé-Ferret (2025): “Power Analysis”; in: *Statistical Tools for Causal Inference*, retrieved on 2025-07-05; URL: <https://chabefer.github.io/STCI/Power.html>.

5 Bayesian statistics

5.1 Probabilistic modeling

5.1.1 Generative model

Definition: Consider measured data (\rightarrow I/1.1.5) y and some unknown latent parameters (\rightarrow I/1.5.7) θ . A statement about the distribution (\rightarrow I/1.5.1) of y given θ is called a generative model m

$$m : y \sim \mathcal{D}(\theta) , \quad (1)$$

where \mathcal{D} denotes an arbitrary probability distribution (\rightarrow I/1.5.1) and θ are the parameters of this distribution.

Sources:

- Friston et al. (2008): “Bayesian decoding of brain images”; in: *NeuroImage*, vol. 39, pp. 181-205;
URL: <https://www.sciencedirect.com/science/article/abs/pii/S1053811907007203>; DOI: 10.1016/j.neuroim

5.1.2 Likelihood function

Definition: Let there be a generative model (\rightarrow I/5.1.1) m describing measured data y using model parameters θ . Then, the probability density function (\rightarrow I/1.7.1) of the distribution of y given θ is called the likelihood function of m :

$$\mathcal{L}_m(\theta) = p(y|\theta, m) = \mathcal{D}(y; \theta) . \quad (1)$$

5.1.3 Prior distribution

Definition: Consider measured data y and some unknown latent parameters θ . A distribution (\rightarrow I/1.5.1) of θ unconditional on y is called a prior distribution:

$$\theta \sim \mathcal{D}(\lambda) . \quad (1)$$

The parameters λ of this distribution are called the prior hyperparameters and the probability density function (\rightarrow I/1.7.1) is called the prior density:

$$p(\theta|m) = \mathcal{D}(\theta; \lambda) . \quad (2)$$

5.1.4 Prior predictive distribution

Definition: Consider a full probability model (\rightarrow I/5.1.6) with likelihood function (\rightarrow I/5.1.2) $p(y|\theta)$ and prior distribution (\rightarrow I/5.1.3) $p(\theta)$. Then, the marginal distribution (\rightarrow I/1.5.3) of any data point (\rightarrow I/1.1.5) y_{new} , accounting for the prior distribution, is called the prior predictive distribution:

$$p(y_{\text{new}}) = \int p(y_{\text{new}}|\theta) p(\theta) d\theta . \quad (1)$$

5.1.5 Prior predictive distribution is marginal of joint likelihood

Theorem: The prior predictive distribution (\rightarrow I/5.1.4) is the marginal distribution (\rightarrow I/1.5.3) of the joint likelihood (\rightarrow I/5.1.15) of the new data (\rightarrow I/1.1.5) y_{new} , unconditional on the measured data y :

$$p(y_{\text{new}}) = \int p(y_{\text{new}}, \theta) d\theta \quad (1)$$

Proof: The prior predictive distribution (\rightarrow I/5.1.4) is defined as the marginal distribution (\rightarrow I/1.5.3) of new data y_{new} , predicted based on the prior distribution (\rightarrow I/5.1.3) before seeing the measured data y :

$$p(y_{\text{new}}) = \int p(y_{\text{new}}|\theta) p(\theta) d\theta . \quad (2)$$

By using the law of conditional probability (\rightarrow I/1.3.4), we can write the integrand as

$$p(y_{\text{new}}|\theta) p(\theta) = p(y_{\text{new}}, \theta) \quad (3)$$

which is the joint likelihood (\rightarrow I/5.1.7). Thus, expression (2) can be written as:

$$p(y_{\text{new}}) = \int p(y_{\text{new}}, \theta) d\theta . \quad (4)$$

■

5.1.6 Full probability model

Definition: Consider measured data y and some unknown latent parameters θ . The combination of a generative model (\rightarrow I/5.1.1) for y in terms of the parameters θ and a prior distribution (\rightarrow I/5.1.3) on θ in terms of hyperparameters λ is called a full probability model m :

$$m : y \sim \mathcal{D}_1(\theta), \theta \sim \mathcal{D}_2(\lambda) . \quad (1)$$

Sources:

- Gelman A, Carlin JB, Stern HS, Dunson DB, Vehtari A, Rubin DB (2014): “Probability and inference”; in: *Bayesian Data Analysis*, ch. 1, p. 3; URL: <http://www.stat.columbia.edu/~gelman/book/>.

5.1.7 Joint likelihood

Definition: Let there be a generative model (\rightarrow I/5.1.1) m describing measured data y using model parameters θ and a prior distribution (\rightarrow I/5.1.3) on θ . Then, the joint probability (\rightarrow I/1.3.2) distribution (\rightarrow I/1.5.1) of y and θ is called the joint likelihood:

$$p(y, \theta|m) = p(y|\theta, m) p(\theta|m) . \quad (1)$$

5.1.8 Joint likelihood is product of likelihood and prior

Theorem: Let there be a generative model (\rightarrow I/5.1.1) m describing measured data y using model parameters θ and a prior distribution (\rightarrow I/5.1.3) on θ . Then, the joint likelihood (\rightarrow I/5.1.7) is equal to the product of likelihood function (\rightarrow I/5.1.2) and prior density (\rightarrow I/5.1.3):

$$p(y, \theta|m) = p(y|\theta, m) p(\theta|m) . \quad (1)$$

Proof: The joint likelihood (\rightarrow I/5.1.7) is defined as the joint probability (\rightarrow I/1.3.2) distribution (\rightarrow I/1.5.1) of data y and parameters θ :

$$p(y, \theta|m) . \quad (2)$$

Applying the law of conditional probability (\rightarrow I/1.3.4), we have:

$$\begin{aligned} p(y|\theta, m) &= \frac{p(y, \theta|m)}{p(\theta|m)} \\ &\Leftrightarrow \\ p(y, \theta|m) &= p(y|\theta, m) p(\theta|m) . \end{aligned} \quad (3)$$

■

5.1.9 Posterior distribution

Definition: Consider measured data y and some unknown latent parameters θ . The distribution (\rightarrow I/1.5.1) of θ conditional (\rightarrow I/1.5.4) on y is called the posterior distribution:

$$\theta|y \sim \mathcal{D}(\phi) . \quad (1)$$

The parameters ϕ of this distribution are called the posterior hyperparameters and the probability density function (\rightarrow I/1.7.1) is called the posterior density:

$$p(\theta|y, m) = \mathcal{D}(\theta; \phi) . \quad (2)$$

5.1.10 Posterior density is proportional to joint likelihood

Theorem: In a full probability model (\rightarrow I/5.1.6) m describing measured data y using model parameters θ , the posterior density (\rightarrow I/5.1.9) over the model parameters is proportional to the joint likelihood (\rightarrow I/5.1.7):

$$p(\theta|y, m) \propto p(y, \theta|m) . \quad (1)$$

Proof: In a full probability model (\rightarrow I/5.1.6), the posterior distribution (\rightarrow I/5.1.9) can be expressed using Bayes' theorem (\rightarrow I/5.3.2):

$$p(\theta|y, m) = \frac{p(y|\theta, m) p(\theta|m)}{p(y|m)} . \quad (2)$$

Applying the law of conditional probability (\rightarrow I/1.3.4) to the numerator, we have:

$$p(\theta|y, m) = \frac{p(y, \theta|m)}{p(y|m)} . \quad (3)$$

Because the denominator does not depend on θ , it is constant in θ and thus acts a proportionality factor between the posterior distribution and the joint likelihood:

$$p(\theta|y, m) \propto p(y, \theta|m) . \quad (4)$$

■

5.1.11 Combined posterior distribution from independent data

Theorem: Let $p(\theta|y_1)$ and $p(\theta|y_2)$ be posterior distributions (\rightarrow I/5.1.9), obtained using the same prior distribution (\rightarrow I/5.1.3) from conditionally independent (\rightarrow I/1.3.7) data sets y_1 and y_2 :

$$p(y_1, y_2|\theta) = p(y_1|\theta) \cdot p(y_2|\theta) . \quad (1)$$

Then, the combined posterior distribution (\rightarrow I/1.5.1) is proportional to the product of the individual posterior densities (\rightarrow I/1.7.1), divided by the prior density:

$$p(\theta|y_1, y_2) \propto \frac{p(\theta|y_1) \cdot p(\theta|y_2)}{p(\theta)} . \quad (2)$$

Proof: Since $p(\theta|y_1)$ and $p(\theta|y_2)$ are posterior distributions (\rightarrow I/5.1.9), Bayes' theorem (\rightarrow I/5.3.2) holds for them:

$$\begin{aligned} p(\theta|y_1) &= \frac{p(y_1|\theta) \cdot p(\theta)}{p(y_1)} \\ p(\theta|y_2) &= \frac{p(y_2|\theta) \cdot p(\theta)}{p(y_2)} . \end{aligned} \quad (3)$$

Moreover, Bayes' theorem must also hold for the combined posterior distribution (\rightarrow I/5.1.10):

$$p(\theta|y_1, y_2) = \frac{p(y_1, y_2|\theta) \cdot p(\theta)}{p(y_1, y_2)} . \quad (4)$$

With that, we can express the combined posterior distribution as follows:

$$\begin{aligned} p(\theta|y_1, y_2) &\stackrel{(4)}{=} \frac{p(y_1, y_2|\theta) \cdot p(\theta)}{p(y_1, y_2)} \\ &\stackrel{(1)}{=} p(y_1|\theta) \cdot p(y_2|\theta) \cdot \frac{p(\theta)}{p(y_1, y_2)} \\ &\stackrel{(3)}{=} \frac{p(\theta|y_1) \cdot p(y_1)}{p(\theta)} \cdot \frac{p(\theta|y_2) \cdot p(y_2)}{p(\theta)} \cdot \frac{p(\theta)}{p(y_1, y_2)} \\ &= \frac{p(\theta|y_1) \cdot p(\theta|y_2)}{p(\theta)} \cdot \frac{p(y_1) \cdot p(y_2)}{p(y_1, y_2)} . \end{aligned} \quad (5)$$

Note that the second fraction does not depend on θ and thus, the posterior distribution over θ is proportional to the first fraction:

$$p(\theta|y_1, y_2) \propto \frac{p(\theta|y_1) \cdot p(\theta|y_2)}{p(\theta)} . \quad (6)$$

■

5.1.12 Posterior predictive distribution

Definition: Consider a full probability model (\rightarrow I/5.1.6) with likelihood function (\rightarrow I/5.1.2) $p(y|\theta)$ and posterior distribution (\rightarrow I/5.1.9) $p(\theta|y)$ based on measured data (\rightarrow I/1.1.5) y . Then, the marginal distribution (\rightarrow I/1.5.3) of new data y_{new} , predicted based on the posterior distribution, is called the posterior predictive distribution:

$$p(y_{\text{new}}|y) = \int p(y_{\text{new}}|\theta) p(\theta|y) d\theta . \quad (1)$$

5.1.13 Posterior predictive distribution is marginal of joint likelihood

Theorem: The posterior predictive distribution (\rightarrow I/5.1.12) is the marginal distribution (\rightarrow I/1.5.3) of the joint likelihood (\rightarrow I/5.1.15) of the new data (\rightarrow I/1.1.5) y_{new} , conditional on the measured data y :

$$p(y_{\text{new}}|y) = \int p(y_{\text{new}}, \theta|y) d\theta \quad (1)$$

Proof: The posterior predictive distribution (\rightarrow I/5.1.12) is defined as the marginal distribution (\rightarrow I/1.5.3) of new data y_{new} , predicted based on the posterior distribution (\rightarrow I/5.1.9) obtained from the measured data y :

$$p(y_{\text{new}}|y) = \int p(y_{\text{new}}|\theta) p(\theta|y) d\theta . \quad (2)$$

We notice that y_{new} is independent (\rightarrow I/1.3.9) of y , so we can write:

$$p(y_{\text{new}}|y) = \int p(y_{\text{new}}|\theta, y) p(\theta|y) d\theta . \quad (3)$$

By using the law of conditional probability (\rightarrow I/1.3.4), we can write the integrand as:

$$p(y_{\text{new}}|\theta, y) p(\theta|y) = p(y_{\text{new}}, \theta|y) . \quad (4)$$

This is the posterior (\rightarrow I/5.1.9) joint likelihood (\rightarrow I/5.1.7). Thus, expression (2) can be written as:

$$p(y_{\text{new}}|y) = \int p(y_{\text{new}}, \theta|y) d\theta . \quad (5)$$

■

5.1.14 Maximum-a-posteriori estimation

Definition: Consider a posterior distribution (\rightarrow I/5.1.9) of an unknown parameter θ , given measured data y , parametrized by posterior hyperparameters ϕ :

$$\theta|y \sim \mathcal{D}(\phi) . \quad (1)$$

Then, the value of θ at which the posterior density (\rightarrow I/5.1.9) attains its maximum is called the “maximum-a-posteriori estimate”, “MAP estimate” or “posterior mode” of θ :

$$\hat{\theta}_{\text{MAP}} = \arg \max_{\theta} \mathcal{D}(\theta; \phi) . \quad (2)$$

Sources:

- Wikipedia (2023): “Maximum a posteriori estimation”; in: *Wikipedia, the free encyclopedia*, retrieved on 2023-12-01; URL: https://en.wikipedia.org/wiki/Maximum_a_posteriori_estimation#Description.

5.1.15 Marginal likelihood

Definition: Let there be a generative model (\rightarrow I/5.1.1) m describing measured data y using model parameters θ and a prior distribution (\rightarrow I/5.1.3) on θ . Then, the marginal probability (\rightarrow I/1.3.3) distribution (\rightarrow I/1.5.1) of y across the parameter space Θ is called the marginal likelihood:

$$p(y|m) = \int_{\Theta} p(y, \theta|m) d\theta . \quad (1)$$

5.1.16 Marginal likelihood is integral of joint likelihood

Theorem: In a full probability model (\rightarrow I/5.1.6) m describing measured data y using model parameters θ , the marginal likelihood (\rightarrow I/5.1.15) is the integral of the joint likelihood (\rightarrow I/5.1.7) across the parameter space Θ

$$p(y|m) = \int_{\Theta} p(y, \theta|m) d\theta \quad (1)$$

and related to likelihood function (\rightarrow I/5.1.2) and prior distribution (\rightarrow I/5.1.3) as follows:

$$p(y|m) = \int_{\Theta} p(y|\theta, m) p(\theta|m) d\theta . \quad (2)$$

Proof: In a full probability model (\rightarrow I/5.1.6), the marginal likelihood (\rightarrow I/5.1.15) is defined as the marginal probability of the data y , given only the model m :

$$p(y|m) . \quad (3)$$

Using the law of marginal probability (\rightarrow I/1.3.3), this can be obtained by integrating the joint likelihood (\rightarrow I/5.1.7) function over the entire parameter space:

$$p(y|m) = \int_{\Theta} p(y, \theta|m) d\theta . \quad (4)$$

Applying the law of conditional probability (\rightarrow I/1.3.4), the integrand can also be written as the product of likelihood function (\rightarrow I/5.1.2) and prior density (\rightarrow I/5.1.3):

$$p(y|m) = \int_{\Theta} p(y|\theta, m) p(\theta|m) d\theta . \quad (5)$$

■

5.2 Prior distributions

5.2.1 Flat vs. hard vs. soft

Definition: Let $p(\theta|m)$ be a prior distribution (\rightarrow I/5.1.3) for the parameter θ of a generative model (\rightarrow I/5.1.1) m . Then,

- the distribution is called a “flat prior”, if its precision (\rightarrow I/1.13.13) is zero or variance (\rightarrow I/1.13.1) is infinite;
- the distribution is called a “hard prior”, if its precision (\rightarrow I/1.13.13) is infinite or variance (\rightarrow I/1.13.1) is zero;
- the distribution is called a “soft prior”, if its precision (\rightarrow I/1.13.13) and variance (\rightarrow I/1.13.1) are non-zero and finite.

Sources:

- Friston et al. (2002): “Classical and Bayesian Inference in Neuroimaging: Theory”; in: *NeuroImage*, vol. 16, iss. 2, pp. 465-483, fn. 1; URL: <https://www.sciencedirect.com/science/article/pii/S1053811902910906>; DOI: 10.1006/nimg.2002.1090.
- Friston et al. (2002): “Classical and Bayesian Inference in Neuroimaging: Applications”; in: *NeuroImage*, vol. 16, iss. 2, pp. 484-512, fn. 10; URL: <https://www.sciencedirect.com/science/article/pii/S1053811902910918>; DOI: 10.1006/nimg.2002.1091.

5.2.2 Uniform vs. non-uniform

Definition: Let $p(\theta|m)$ be a prior distribution (\rightarrow I/5.1.3) for the parameter θ of a generative model (\rightarrow I/5.1.1) m where θ belongs to the parameter space Θ . Then,

- the distribution is called a “uniform prior”, if its density (\rightarrow I/1.7.1) or mass (\rightarrow I/1.6.1) is constant over Θ ;
- the distribution is called a “non-uniform prior”, if its density (\rightarrow I/1.7.1) or mass (\rightarrow I/1.6.1) is not constant over Θ .

Sources:

- Wikipedia (2020): “Lindley’s paradox”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-11-25; URL: https://en.wikipedia.org/wiki/Lindley%27s_paradox#Bayesian_approach.

5.2.3 Informative vs. non-informative

Definition: Let $p(\theta|m)$ be a prior distribution (\rightarrow I/5.1.3) for the parameter θ of a generative model (\rightarrow I/5.1.1) m . Then,

- the distribution is called an “informative prior”, if it biases the parameter towards particular values;

- the distribution is called a “weakly informative prior”, if it mildly influences the posterior distribution (\rightarrow I/5.1.10);
- the distribution is called a “non-informative prior”, if it does not influence (\rightarrow I/5.1.10) the posterior hyperparameters (\rightarrow I/5.1.9).

Sources:

- Soch J, Allefeld C, Haynes JD (2016): “How to avoid mismodelling in GLM-based fMRI data analysis: cross-validated Bayesian model selection”; in: *NeuroImage*, vol. 141, pp. 469-489, eq. 15, p. 473; URL: <https://www.sciencedirect.com/science/article/pii/S1053811916303615>; DOI: 10.1016/j.neuroimage.2016.07.047.

5.2.4 Empirical vs. non-empirical

Definition: Let $p(\theta|m)$ be a prior distribution (\rightarrow I/5.1.3) for the parameter θ of a generative model (\rightarrow I/5.1.1) m . Then,

- the distribution is called an “empirical prior”, if it has been derived from empirical data (\rightarrow I/5.1.10);
- the distribution is called a “theoretical prior”, if it was specified without regard to empirical data.

Sources:

- Soch J, Allefeld C, Haynes JD (2016): “How to avoid mismodelling in GLM-based fMRI data analysis: cross-validated Bayesian model selection”; in: *NeuroImage*, vol. 141, pp. 469-489, eq. 13, p. 473; URL: <https://www.sciencedirect.com/science/article/pii/S1053811916303615>; DOI: 10.1016/j.neuroimage.2016.07.047.

5.2.5 Conjugate vs. non-conjugate

Definition: Let m be a generative model (\rightarrow I/5.1.1) with likelihood function (\rightarrow I/5.1.2) $p(y|\theta, m)$ and prior distribution (\rightarrow I/5.1.3) $p(\theta|m)$. Then,

- the prior distribution (\rightarrow I/5.1.3) is called “conjugate”, if it, when combined with the likelihood function (\rightarrow I/5.1.2), leads to a posterior distribution (\rightarrow I/5.1.9) that belongs to the same family of probability distributions (\rightarrow I/1.5.1);
- the prior distribution is called “non-conjugate”, if this is not the case.

Sources:

- Wikipedia (2020): “Conjugate prior”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-12-02; URL: https://en.wikipedia.org/wiki/Conjugate_prior.

5.2.6 Maximum entropy priors

Definition: Let m be a generative model (\rightarrow I/5.1.1) with likelihood function (\rightarrow I/5.1.2) $p(y|\theta, m)$ and prior distribution (\rightarrow I/5.1.3) $p(\theta|\lambda, m)$ using prior hyperparameters (\rightarrow I/5.1.3) λ . Then, the prior distribution is called a “maximum entropy prior”, if

1) when θ is a discrete random variable (\rightarrow I/1.2.6), it maximizes the entropy (\rightarrow I/2.1.1) of the prior probability mass function (\rightarrow I/1.6.1):

$$\lambda_{\text{maxent}} = \arg \max_{\lambda} H[p(\theta|\lambda, m)] ; \quad (1)$$

2) when θ is a continuous random variable (\rightarrow I/1.2.6), it maximizes the differential entropy (\rightarrow I/2.2.1) of the prior probability density function (\rightarrow I/1.7.1):

$$\lambda_{\text{maxent}} = \arg \max_{\lambda} h[p(\theta|\lambda, m)] . \quad (2)$$

Sources:

- Wikipedia (2020): “Prior probability”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-12-02; URL: https://en.wikipedia.org/wiki/Prior_probability#Uninformative_priors.

5.2.7 Empirical Bayes priors

Definition: Let m be a generative model (\rightarrow I/5.1.1) with likelihood function (\rightarrow I/5.1.2) $p(y|\theta, m)$ and prior distribution (\rightarrow I/5.1.3) $p(\theta|\lambda, m)$ using prior hyperparameters (\rightarrow I/5.1.3) λ . Let $p(y|\lambda, m)$ be the marginal likelihood (\rightarrow I/5.1.15) when integrating the parameters out of the joint likelihood (\rightarrow I/5.1.16). Then, the prior distribution is called an “Empirical Bayes (\rightarrow I/5.3.4) prior”, if it maximizes the logarithmized marginal likelihood:

$$\lambda_{\text{EB}} = \arg \max_{\lambda} \log p(y|\lambda, m) . \quad (1)$$

Sources:

- Wikipedia (2020): “Empirical Bayes method”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-12-02; URL: https://en.wikipedia.org/wiki/Empirical_Bayes_method#Introduction.

5.2.8 Reference priors

Definition: Let m be a generative model (\rightarrow I/5.1.1) with likelihood function (\rightarrow I/5.1.2) $p(y|\theta, m)$ and prior distribution (\rightarrow I/5.1.3) $p(\theta|\lambda, m)$ using prior hyperparameters (\rightarrow I/5.1.3) λ . Let $p(\theta|y, \lambda, m)$ be the posterior distribution (\rightarrow I/5.1.9) that is proportional to the the joint likelihood (\rightarrow I/5.1.10). Then, the prior distribution is called a “reference prior”, if it maximizes the expected (\rightarrow I/1.12.1) Kullback-Leibler divergence (\rightarrow I/2.5.1) of the posterior distribution relative to the prior distribution:

$$\lambda_{\text{ref}} = \arg \max_{\lambda} \langle \text{KL} [p(\theta|y, \lambda, m) || p(\theta|\lambda, m)] \rangle . \quad (1)$$

Sources:

- Wikipedia (2020): “Prior probability”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-12-02; URL: https://en.wikipedia.org/wiki/Prior_probability#Uninformative_priors.

5.3 Bayesian inference

5.3.1 Odds ratios

Definition: Let A_1 , A_2 and B be arbitrary statements about random variables (\rightarrow I/1.2.2) where A_1 and A_2 are mutually exclusive (\rightarrow I/1.3.10), but not necessarily collectively exhaustive (\rightarrow I/1.4.12). Then, the “odds” or “prior (\rightarrow I/5.1.3) odds ratio” in favor of A_1 against A_2 is defined as the ratio of the probabilities of A_1 and A_2 , unconditional on B

$$\frac{p(A_1)}{p(A_2)} \quad (1)$$

and the “posterior (\rightarrow I/5.1.9) odds ratio” in favor of A_1 against A_2 is defined as the ratio of the probabilities of A_1 and A_2 , conditional on B

$$\frac{p(A_1|B)}{p(A_2|B)} \quad (2)$$

where $p(\cdot)$ is a probability mass function (\rightarrow I/1.6.1) or probability density function (\rightarrow I/1.7.1). Prior and posterior odds ratio are related to each other via the Bayes factor (\rightarrow IV/3.3.1) through Bayes’ rule (\rightarrow I/5.3.3).

Sources:

- Wikipedia (2025): “Odds ratio”; in: *Wikipedia, the free encyclopedia*, retrieved on 2025-02-06; URL: https://en.wikipedia.org/wiki/Odds_ratio.

5.3.2 Bayes’ theorem

Theorem: Let A and B be two arbitrary statements about random variables (\rightarrow I/1.2.2), such as statements about the presence or absence of an event or about the value of a scalar, vector or matrix. Then, the conditional probability that A is true, given that B is true, is equal to

$$p(A|B) = \frac{p(B|A)p(A)}{p(B)} . \quad (1)$$

Proof: The conditional probability (\rightarrow I/1.3.4) is defined as the ratio of joint probability (\rightarrow I/1.3.2), i.e. the probability of both statements being true, and marginal probability (\rightarrow I/1.3.3), i.e. the probability of only the second one being true:

$$p(A|B) = \frac{p(A, B)}{p(B)} . \quad (2)$$

It can also be written down for the reverse situation, i.e. to calculate the probability that B is true, given that A is true:

$$p(B|A) = \frac{p(A, B)}{p(A)} . \quad (3)$$

Both equations can be rearranged for the joint probability

$$p(A|B)p(B) \stackrel{(2)}{=} p(A, B) \stackrel{(3)}{=} p(B|A)p(A) \quad (4)$$

from which Bayes’ theorem can be directly derived:

$$p(A|B) \stackrel{(4)}{=} \frac{p(B|A)p(A)}{p(B)} . \quad (5)$$

■

Sources:

- Koch, Karl-Rudolf (2007): “Rules of Probability”; in: *Introduction to Bayesian Statistics*, Springer, Berlin/Heidelberg, 2007, pp. 6/13, eqs. 2.12/2.38; URL: <https://www.springer.com/de/book/9783540727231>; DOI: 10.1007/978-3-540-72726-2.

5.3.3 Bayes’ rule

Theorem: Let A_1 , A_2 and B be arbitrary statements about random variables (\rightarrow I/1.2.2) where A_1 and A_2 are mutually exclusive. Then, Bayes’ rule states that the posterior odds (\rightarrow I/5.3.1) are equal to the Bayes factor (\rightarrow IV/3.3.1) times the prior odds (\rightarrow I/5.3.1), i.e.

$$\frac{p(A_1|B)}{p(A_2|B)} = \frac{p(B|A_1)}{p(B|A_2)} \cdot \frac{p(A_1)}{p(A_2)} . \quad (1)$$

Proof: Using Bayes’ theorem (\rightarrow I/5.3.2), the conditional probabilities (\rightarrow I/1.3.4) on the left are given by

$$p(A_1|B) = \frac{p(B|A_1) \cdot p(A_1)}{p(B)} \quad (2)$$

$$p(A_2|B) = \frac{p(B|A_2) \cdot p(A_2)}{p(B)} . \quad (3)$$

Dividing the two conditional probabilities by each other

$$\begin{aligned} \frac{p(A_1|B)}{p(A_2|B)} &= \frac{p(B|A_1) \cdot p(A_1)/p(B)}{p(B|A_2) \cdot p(A_2)/p(B)} \\ &= \frac{p(B|A_1)}{p(B|A_2)} \cdot \frac{p(A_1)}{p(A_2)} , \end{aligned} \quad (4)$$

one obtains the posterior odds ratio as given by the theorem. ■

Sources:

- Wikipedia (2019): “Bayes’ theorem”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-01-06; URL: https://en.wikipedia.org/wiki/Bayes%27_theorem#Bayes%E2%80%99_rule.

5.3.4 Empirical Bayes

Definition: Let m be a generative model (\rightarrow I/5.1.1) with model parameters θ and hyper-parameters λ implying the likelihood function (\rightarrow I/5.1.2) $p(y|\theta, \lambda, m)$ and prior distribution (\rightarrow I/5.1.3) $p(\theta|\lambda, m)$. Then, an Empirical Bayes treatment of m , also referred to as “type II maximum likelihood (\rightarrow I/4.1.3)” or “evidence (\rightarrow IV/3.1.3) approximation”, consists in

1) evaluating the marginal likelihood (\rightarrow I/5.1.15) of the model m

$$p(y|\lambda, m) = \int p(y|\theta, \lambda, m) (\theta|\lambda, m) d\theta , \quad (1)$$

2) maximizing the log model evidence (\rightarrow IV/3.1.3) with respect to λ

$$\hat{\lambda} = \arg \max_{\lambda} \log p(y|\lambda, m) \quad (2)$$

3) and using the prior distribution (\rightarrow I/5.1.3) at this maximum

$$p(\theta|m) = p(\theta|\hat{\lambda}, m) \quad (3)$$

for Bayesian inference (\rightarrow I/5.3.2), i.e. obtaining the posterior distribution (\rightarrow I/5.1.10) and computing the marginal likelihood (\rightarrow I/5.1.16).

Sources:

- Wikipedia (2021): “Empirical Bayes method”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-04-29; URL: https://en.wikipedia.org/wiki/Empirical_Bayes_method#Introduction.
- Bishop CM (2006): “The Evidence Approximation”; in: *Pattern Recognition for Machine Learning*, ch. 3.5, pp. 165-172; URL: <https://www.springer.com/gp/book/9780387310732>.

5.3.5 Variational Bayes

Definition: Let m be a generative model (\rightarrow I/5.1.1) with model parameters (\rightarrow I/1.5.7) $\theta \in \Theta$ implying the likelihood function (\rightarrow I/5.1.2) $p(y|\theta, m)$ and prior distribution (\rightarrow I/5.1.3) $p(\theta|m)$. Then, a Variational Bayes treatment of m , also referred to as “approximate inference” or “variational inference”, consists in

1) constructing an approximate posterior distribution (\rightarrow I/5.1.9)

$$q(\theta) \approx p(\theta|y, m), \quad (1)$$

2) evaluating the variational free energy (\rightarrow IV/3.1.11)

$$F_m[q(\theta)] = \int_{\Theta} q(\theta) \log \frac{p(\theta|y, m)}{q(\theta)} d\theta \quad (2)$$

3) and maximizing this function with respect to $q(\theta)$

$$\hat{q}(\theta) = \arg \max_q F_m[q(\theta)] \quad (3)$$

for Bayesian inference (\rightarrow I/5.3.2), i.e. obtaining the posterior distribution (\rightarrow I/5.1.9) (from eq. (3)) and approximating the marginal likelihood (\rightarrow I/5.1.15) (by plugging eq. (3) into eq. (2)).

Sources:

- Wikipedia (2021): “Variational Bayesian methods”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-04-29; URL: https://en.wikipedia.org/wiki/Variational_Bayesian_methods#Evidence_lower_bound.
- Bishop CM (2006): “Variational Inference”; in: *Pattern Recognition for Machine Learning*, ch. 10.1, pp. 462-474; URL: <https://www.springer.com/gp/book/9780387310732>.
- Penny W, Flandin G, Trujillo-Barreto N (2007): “Bayesian Comparison of Spatially Regularised General Linear Models”; in: *Human Brain Mapping*, vol. 28, pp. 275–293, eqs. 2-9; URL: <https://onlinelibrary.wiley.com/doi/full/10.1002/hbm.20327>; DOI: 10.1002/hbm.20327.

- Ostwald D, Kirilina E, Starke L, Blankenburg F (2014): “A tutorial on variational Bayes for latent linear stochastic time-series models”; in: *Journal of Mathematical Psychology*, vol. 60, pp. 1-14, eqs. 10-17; URL: <https://www.sciencedirect.com/science/article/abs/pii/S0022249614000352>; DOI: 10.1016/j.jmp.2014.04.003.

5.3.6 Decomposition of the free energy

Theorem: Let m be a generative model (\rightarrow I/5.1.1) with likelihood function (\rightarrow I/5.1.2) $p(y|\theta, m) = p(y|\theta)$, prior distribution (\rightarrow I/5.1.3) $p(\theta|m) = p(\theta)$, joint likelihood (\rightarrow I/5.1.7) $p(y, \theta|m) = p(y, \theta)$, true posterior distribution (\rightarrow I/5.1.9) $p(\theta|y, m) = p(\theta|y)$ and approximate posterior (\rightarrow I/5.3.5) distribution $q(\theta|m) = q(\theta) \approx p(\theta|y)$. Then, the variational free energy (\rightarrow IV/3.1.11) can be decomposed as

1) the difference between log model evidence and KL divergence of approximate from true posterior

$$F[q(\theta)] = \log p(y) - \text{KL}[q(\theta)||p(\theta|y)] , \quad (1)$$

2) the difference of expected log-likelihood and KL divergence of approximate posterior from prior

$$F[q(\theta)] = \langle \log p(y|\theta) \rangle_{q(\theta)} - \text{KL}[q(\theta)||p(\theta)] \quad (2)$$

3) the sum of expected joint log-likelihood and approximate posterior differential entropy

$$F[q(\theta)] = \langle \log p(y, \theta) \rangle_{q(\theta)} - h[q(\theta)] \quad (3)$$

where $p(y|m) = p(y)$ is the marginal likelihood (\rightarrow I/5.1.15), $\langle \cdot \rangle_{p(x)}$ denotes an expectation (\rightarrow I/1.12.1) with respect to the density (\rightarrow I/1.7.1) $p(x)$, $\text{KL}[\cdot||\cdot]$ denotes the Kullback-Leibler divergence (\rightarrow I/2.5.1) and $h[\cdot]$ denotes the differential entropy (\rightarrow I/2.2.1).

Proof: The log model evidence (\rightarrow IV/3.1.3) is defined as

$$\log p(y) = \log \int_{\Theta} p(y, \theta) d\theta \quad (4)$$

and using the approximate posterior density $q(\theta)$, this can be rewritten as

$$\begin{aligned} \log p(y) &= \log \int_{\Theta} \frac{q(\theta)}{q(\theta)} p(y, \theta) d\theta \\ &= \log \left\langle \frac{p(y, \theta)}{q(\theta)} \right\rangle_{q(\theta)} . \end{aligned} \quad (5)$$

By Jensen's inequality (\rightarrow I/1.12.11) and because the logarithm is a concave function (\rightarrow I/2.5.4), we have:

$$\log \left\langle \frac{p(y, \theta)}{q(\theta)} \right\rangle_{q(\theta)} \geq \left\langle \log \frac{p(y, \theta)}{q(\theta)} \right\rangle_{q(\theta)} . \quad (6)$$

The right-hand side of this equation is referred to as the free energy (\rightarrow IV/3.1.11):

$$F[q(\theta)] = \left\langle \log \frac{p(y, \theta)}{q(\theta)} \right\rangle_{q(\theta)} . \quad (7)$$

With that, we can show the above identities:

1) the difference between log model evidence and KL divergence of approximate from true posterior

$$\begin{aligned}
 F[q(\theta)] &= \left\langle \log \frac{p(y, \theta)}{q(\theta)} \right\rangle_{q(\theta)} \\
 &= \left\langle \log \frac{p(\theta|y)p(y)}{q(\theta)} \right\rangle_{q(\theta)} \\
 &= \left\langle \log p(y) - \log \frac{q(\theta)}{p(\theta|y)} \right\rangle_{q(\theta)} \\
 &= \langle \log p(y) \rangle_{q(\theta)} - \int_{\Theta} q(\theta) \log \frac{q(\theta)}{p(\theta|y)} d\theta \\
 &= \log p(y) - \text{KL}[q(\theta)||p(\theta|y)]
 \end{aligned} \tag{8}$$

where the first term is the log model evidence (\rightarrow IV/3.1.3) (= log marginal likelihood) and the second term can be seen as an approximation error (= divergence of approximate from true posterior distribution);

2) the difference of expected log-likelihood and KL divergence of approximate posterior from prior

$$\begin{aligned}
 F[q(\theta)] &= \left\langle \log \frac{p(y, \theta)}{q(\theta)} \right\rangle_{q(\theta)} \\
 &= \left\langle \log \frac{p(y|\theta)p(\theta)}{q(\theta)} \right\rangle_{q(\theta)} \\
 &= \left\langle \log p(y|\theta) - \log \frac{q(\theta)}{p(\theta)} \right\rangle_{q(\theta)} \\
 &= \int_{\Theta} q(\theta) \log p(y|\theta) d\theta - \int_{\Theta} q(\theta) \log \frac{q(\theta)}{p(\theta)} d\theta \\
 &= \langle \log p(y|\theta) \rangle_{q(\theta)} - \text{KL}[q(\theta)||p(\theta)]
 \end{aligned} \tag{9}$$

where the first term can be seen as an accuracy term (\rightarrow IV/3.1.6) (= posterior expected log-likelihood) and the second term can be seen as a complexity penalty (\rightarrow IV/3.1.6) (= divergence of posterior from prior distribution);

3) the sum of expected joint log-likelihood and approximate posterior entropy

$$\begin{aligned}
 F[q(\theta)] &= \left\langle \log \frac{p(y, \theta)}{q(\theta)} \right\rangle_{q(\theta)} \\
 &= \langle \log p(y, \theta) - \log q(\theta) \rangle_{q(\theta)} \\
 &= \int_{\Theta} q(\theta) \log p(y, \theta) d\theta - \int_{\Theta} q(\theta) \log q(\theta) d\theta \\
 &= \langle \log p(y, \theta) \rangle_{q(\theta)} + h[q(\theta)]
 \end{aligned} \tag{10}$$

where the first term represents the negative energy (= posterior expected joint log-likelihood) and the second term presents the posterior entropy (\rightarrow I/2.2.1) (= differential entropy of the approximate posterior distribution).

**Sources:**

- Zeidman et al. (2023): “A primer on Variational Laplace (VL)” ; in: *NeuroImage*, vol. 279, art. 120310, p. 5, eqs. 12-14; URL: <https://www.sciencedirect.com/science/article/pii/S1053811923004615>; DOI: 10.1016/j.neuroimage.2023.120310.

5.3.7 Free energy is lower bound on log model evidence

Theorem: Let m be a generative model (\rightarrow I/5.1.1) with likelihood function (\rightarrow I/5.1.2) $p(y|\theta, m) = p(y|\theta)$ and prior distribution (\rightarrow I/5.1.3) $p(\theta|m) = p(\theta)$. Then, under a variational Bayesian (\rightarrow I/5.3.5) treatment using the approximate posterior (\rightarrow I/5.3.5) distribution $q(\theta|m) = q(\theta) \approx p(\theta|y)$, the variational free energy (\rightarrow IV/3.1.11) is a lower bound on the log model evidence (\rightarrow IV/3.1.3):

$$F[q(\theta)] \leq \log p(y) = \log \int_{\Theta} p(y, \theta|m) d\theta . \quad (1)$$

Proof: Using a decomposition of the variational free energy (\rightarrow I/5.3.6), it can be shown that the free energy is equal to the difference between the log model evidence (\rightarrow IV/3.1.3) and the Kullback-Leibler divergence (\rightarrow I/2.5.1) of approximate from true posterior distribution:

$$F[q(\theta)] = \log p(y) - \text{KL}[q(\theta)||p(\theta|y)] \quad (2)$$

Since the KL divergence is zero or positive for any two distributions (\rightarrow I/2.5.4)

$$\text{KL}[P||Q] \geq 0 , \quad (3)$$

the free energy must be smaller than or equal to the log model evidence:

$$F[q(\theta)] \leq \log p(y) . \quad (4)$$

**Sources:**

- Zeidman et al. (2023): “A primer on Variational Laplace (VL)” ; in: *NeuroImage*, vol. 279, art. 120310, pp. 4-5, eqs. 9-11; URL: <https://www.sciencedirect.com/science/article/pii/S1053811923004615>; DOI: 10.1016/j.neuroimage.2023.120310.

6 Machine learning

6.1 Scoring rules

6.1.1 Scoring rule

Definition: A scoring rule is any extended real-valued function $\mathbf{S} : \mathcal{Q} \times \Omega \rightarrow \mathbb{R}$ where \mathcal{Q} is a family of probability distributions over the space Ω , such that $\mathbf{S}(Q, \cdot)$ is \mathcal{Q} -quasi-integrable for all $Q \in \mathcal{Q}$. Output of the function $\mathbf{S}(Q, y)$ represents the loss or penalty when the forecast $Q \in \mathcal{Q}$ is issued and the observation $y \in \Omega$ is realized.

Sources:

- Bálint Mucsányi, Michael Kirchhof, Elisa Nguyen, Alexander Rubinstein, Seong Joon Oh (2023): “Proper/Strictly Proper Scoring Rule”; in: *Trustworthy Machine Learning*; URL: <https://trustworthyml.io/>; DOI: 10.48550/arXiv.2310.08215.
- Wikipedia (2024): “Scoring rule”; in: *Wikipedia, the free encyclopedia*, retrieved on 2024-02-28; URL: https://en.wikipedia.org/wiki/Scoring_rule.

6.1.2 Proper scoring rule

Definition: A scoring rule (\rightarrow I/6.1.1) \mathbf{S} is called a proper scoring rule, if and only if

$$\max_{Q \in \mathcal{Q}} \mathbb{E}_{Y \sim P}[\mathbf{S}(Q, Y)] = \mathbb{E}_{Y \sim P}[\mathbf{S}(P, Y)] . \quad (1)$$

In other words, score function \mathbf{S} is a proper scoring rule, if it is maximized when the forecaster gives exactly the ground truth distribution $P(Y)$ as its probabilistic forecast $Q \in \mathcal{Q}$.

Sources:

- Bálint Mucsányi, Michael Kirchhof, Elisa Nguyen, Alexander Rubinstein, Seong Joon Oh (2023): “Proper/Strictly Proper Scoring Rule”; in: *Trustworthy Machine Learning*; URL: <https://trustworthyml.io/>; DOI: 10.48550/arXiv.2310.08215.

6.1.3 Strictly proper scoring rule

Definition: A scoring rule (\rightarrow I/6.1.1) \mathbf{S} is called a strictly proper scoring rule, if and only if

- \mathbf{S} is a proper scoring rule (\rightarrow I/6.1.2), and
- $\arg \max_{Q \in \mathcal{Q}} \mathbb{E}_{Y \sim P}[\mathbf{S}(Q, Y)] = P$ is the unique maximizer of \mathbf{S} in \mathcal{Q} .

In other words, a strictly proper scoring rule is maximized only when the the forecaster gives exactly the ground truth distribution $P(Y)$ as its probabilistic forecast $Q \in \mathcal{Q}$.

Sources:

- Bálint Mucsányi, Michael Kirchhof, Elisa Nguyen, Alexander Rubinstein, Seong Joon Oh (2023): “Proper/Strictly Proper Scoring Rule”; in: *Trustworthy Machine Learning*; URL: <https://trustworthyml.io/>; DOI: 10.48550/arXiv.2310.08215.

6.1.4 Log probability scoring rule

Definition: A log (probability) scoring rule (\rightarrow I/6.1.1) $S(q, y)$ is as a scoring rule that measures the quality of a probabilistic forecast in decision theory. Formally, it can be defined in discrete or continuous form as follows:

1) Log scoring rule for binary classification:

$$S(q, y) = \begin{cases} \log q, & \text{if } y = 1 \\ \log(1 - q), & \text{if } y = 0 \end{cases} \quad (1)$$

which can be expressed as

$$S(q, y) = y \log q + (1 - y) \log(1 - q) \quad (2)$$

Note that the expressions given above have slightly different domains. For the first equation, the domain is $D_1 = ([0, 1) \times \{0\}) \cup ((0, 1] \times \{1\})$, while for the second equation, the domain is $D_2 = (0, 1) \times \{0, 1\}$.

2) Log scoring rule for multiclass classification:

$$S(q, y) = \sum_k y_k \log q_k(x) = \log q_{y^*}(x) \quad (3)$$

where y^* is the true class and q is the predicted probability distribution over the classes. We have $y_k = 1$, if the true class is k and $y_k = 0$ otherwise.

3) Log scoring rule for regression (continuous case):

$$S(q, y) = \log q(y) \quad (4)$$

where q is the predicted probability distribution over the continuous space and y is the true value.

Sources:

- Bálint Mucsányi, Michael Kirchhof, Elisa Nguyen, Alexander Rubinstein, Seong Joon Oh (2023): “Proper/Strictly Proper Scoring Rule”; in: *Trustworthy Machine Learning*; URL: <https://trustworthyml.io/>; DOI: 10.48550/arXiv.2310.08215.

6.1.5 Log probability is strictly proper scoring rule

Theorem: The log (probability) scoring rule (\rightarrow I/6.1.4) is a strictly proper scoring rule (\rightarrow I/6.1.3).

Proof: We will show that all versions of the log probability scoring rule (binary/multiclass/regression) are strictly proper scoring rules.

1) Binary log probability scoring rule:

$$\mathbb{E}_{Y \sim P}[\mathbf{S}(Q, Y)] = P(Y = 1) \log q + P(Y = 0) \log(1 - q) \quad (1)$$

Let p be the true probability of the event $Y = 1$. Then, the expected score is:

$$\mathbb{E}_{Y \sim P}[\mathbf{S}(Q, Y)] = p \log q + (1 - p) \log(1 - q) \quad (2)$$

To find the maxima, take the derivative with respect to q and set it to zero:

$$\begin{aligned}
\frac{\partial}{\partial q} \mathbb{E}_{Y \sim P}[\mathbf{S}(Q, Y)] &= \frac{p}{q} - \frac{1-p}{1-q} \\
0 &= \frac{p - pq - q + pq}{q(1-q)} \\
0 &= \frac{p-q}{q(1-q)} \\
\Rightarrow p - q &= 0 \\
\Rightarrow p &= q
\end{aligned} \tag{3}$$

Now, we need to check the second derivative to see, if it is a maximum for the properness condition and if it is the only maximizer for the strictness condition:

$$\begin{aligned}
\frac{\partial^2}{\partial q^2} \mathbb{E}_{Y \sim P}[\mathbf{S}(Q, Y)] &= -\frac{p}{q^2} - \frac{1-p}{(1-q)^2} \\
&= -\left(\underbrace{\frac{p}{q^2}}_{>0} + \underbrace{\frac{1-p}{(1-q)^2}}_{>0} \right) < 0
\end{aligned} \tag{4}$$

Except for the cases $q = 0$ and $q = 1$, the second derivative is always negative, which means that the function is concave and the maximum is unique. For $q = 1$, maximum is achieved only if $p = 1$, and similarly for $q = 0$, maximum is achieved only if $p = 0$. Therefore, $p = q$ is the only maximizer and the log probability scoring rule for binary classification is strictly proper.

2a) Multiclass log probability scoring rule (Proof 1):

$$S(q, y) = \sum_k^K y_k \log q_k(x) \tag{5}$$

Let p_k be the true probability of the event $Y = k$. Since q_k is the predicted probability for class k , we know that $\sum_i q_i = 1$. Then, the expected score is:

$$\begin{aligned}
\mathbb{E}_{Y \sim P}[\mathbf{S}(Q, Y)] &= \sum_k P(Y = k|x) \log(q_k(x)) \\
&= p_1 \log(q_1(x)) + p_2 \log(q_2(x)) + \dots + p_K \log(q_K(x)) \\
&= p_1 \log(q_1(x)) + p_2 \log(q_2(x)) + \dots + p_K \log\left(1 - \sum_{i \neq K} q_i(x)\right)
\end{aligned} \tag{6}$$

Taking the derivative with respect to q_j and setting it to zero:

$$\begin{aligned}
\frac{\partial}{\partial q_j} \mathbb{E}_{Y \sim P}[\mathbf{S}(Q, Y)] &= \frac{p_j}{q_j} - \frac{p_K}{1 - \sum_{i \neq K} q_i(x)} \\
0 &= \frac{p_j}{q_j} - \frac{p_K}{q_K} \\
\Rightarrow \frac{p_j}{q_j} &= \frac{p_K}{q_K}
\end{aligned} \tag{7}$$

This equality holds for any j :

$$\frac{p_1}{q_1} = \frac{p_2}{q_2} = \dots = \frac{p_K}{q_K} = \lambda \quad (8)$$

Each q_i can be represented as a constant multiple of p_i as follows: $q_i = \lambda p_i$

$$\begin{aligned} \sum_i q_i &= 1 \\ \sum_i \lambda p_i &= 1 \\ \lambda \sum_i p_i &= 1 \\ \lambda &= 1 \end{aligned} \quad (9)$$

Since $\lambda = 1$, we have $p_i = q_i$ for all i . Now, we need to check the second derivative to see, if it is a maximum for the properness condition and if it is the only maximizer for the strictness condition:

$$\begin{aligned} \frac{\partial^2}{\partial q_j^2} \mathbb{E}_{Y \sim P}[\mathbf{S}(Q, Y)] &= -\frac{p_j}{q_j^2} - \frac{p_K}{(1 - \sum_{i \neq K} q_i(x))^2} \\ &= -\left(\underbrace{\frac{p_j}{q_j^2}}_{> 0} + \underbrace{\frac{p_K}{(1 - \sum_{i \neq K} q_i(x))^2}}_{> 0} \right) < 0 \end{aligned} \quad (10)$$

Except for the cases $q_j = 0$ and $q_j = 1$, the second derivative is always negative, which means that the function is concave and the maximum is unique. For $q_j = 1$, maximum is achieved only if $p_j = 1$, and similarly for $q_j = 0$ maximum is achieved only if $p_j = 0$. Therefore, $p_j = q_j$ is the only maximizer and the log probability scoring rule for multiclass classification is strictly proper.

2b) Multiclass log probability scoring rule (Proof 2):

Alternatively, we can solve the optimization problem with Lagrange multipliers. The Lagrangian is:

$$\mathcal{L}(q, \lambda) = \sum_k P(Y = k|x) \log(q_k(x)) + \lambda \left(1 - \sum_k q_k(x) \right) \quad (11)$$

Taking the derivative with respect to q_j and setting it to zero:

$$\begin{aligned} \frac{\partial}{\partial q_j} \mathcal{L}(q, \lambda) &= \frac{p_j}{q_j} - \lambda \\ 0 &= \frac{p_j}{q_j} - \lambda \\ \Rightarrow \frac{p_j}{q_j} &= \lambda \end{aligned} \quad (12)$$

The rest of the proof follows as in the first proof.

3) Continuous log probability scoring rule:

$$S(q, y) = \log q(y) \quad (13)$$

Let $p(y)$ be the true probability density function (\rightarrow I/1.7.1) of the event $Y = y$. Then, the expected (\rightarrow I/1.12.1) score (\rightarrow I/6.1.1) is:

$$\mathbb{E}_{Y \sim P}[\mathbf{S}(Q, Y)] = \int p(y) \log q(y) dy \quad (14)$$

Let $X = \frac{q(y)}{p(y)}$ and $\phi = \log(\cdot)$ (a concave function). By Jensen's inequality, we know that $f(\mathbb{E}[X]) \leq \mathbb{E}[f(X)]$, if f is concave. Therefore, we have:

$$\begin{aligned} \int p(y) \log \frac{q(y)}{p(y)} dy &\leq \log \int p(y) \frac{q(y)}{p(y)} dy \\ \int p(y) \log \frac{q(y)}{p(y)} dy &\leq \log \int q(y) dy \\ \int p(y) \log \frac{q(y)}{p(y)} dy &\leq \log(1) \\ \int p(y) \log \frac{q(y)}{p(y)} dy &\leq 0 \end{aligned} \quad (15)$$

The same result can be obtained by using the Kullback-Leibler divergence (\rightarrow I/2.5.1). The Kullback-Leibler divergence is always non-negative (\rightarrow I/2.5.3), therefore $E - CE = KL \geq 0$. The resulting expression is $-KL$, which is always non-positive. It is maximized only when $q(y) = p(y)$ which means that the log probability scoring rule for continuous classification is strictly proper.

An alternative argument for uniqueness of the maximum point can be proposed as follows: $\int p(y) \log \frac{q(y)}{p(y)} dy$ can be equal to 0 in two cases: Either $\frac{q(y)}{p(y)}$ is equal to 1 for each value or the expression $\log(\frac{q(y)}{p(y)})$ takes positive and negative values summing up to 0 at the end. The second case cannot occur, because it means that there exists a y_0 such that $q(y_0) > p(y_0)$, implying that Jensen's inequality is violated. Therefore, the maximum is achieved, if and only if $q = p$. ■

Sources:

- Bálint Mucsányi, Michael Kirchhof, Elisa Nguyen, Alexander Rubinstein, Seong Joon Oh (2023): "Proper/Strictly Proper Scoring Rule"; in: *Trustworthy Machine Learning*; URL: <https://trustworthyml.io/>; DOI: 10.48550/arXiv.2310.08215.

6.1.6 Brier scoring rule

Definition: A Brier scoring rule (\rightarrow I/6.1.1) $S(q, y)$ is as a scoring rule that measures the quality of a probabilistic forecast in decision theory. Formally, it can be defined for binary or multiclass classification as follows:

1) Brier scoring rule for binary classification:

$$S(q, y) = -(q - y)^2 \quad (1)$$

q represents the predicted probability of the positive class ($Y = 1$) and y is the true class label. Since we want the output of the scoring rule to be maximized when the predicted probability is close to the true class label, we use the negative of the squared difference between the predicted probability and the true class label.

2) Brier scoring rule for multiclass classification:

$$S(q, y) = - \sum_k (q_k - y_k)^2 = -(q_{y^*} - 1)^2 - \sum_{k \neq y^*} q_k^2 \quad (2)$$

where q_k is the predicted probability of class k and y^* is the true class label. Similar to the log probability scoring rule, we have $y_k = 1$, if the true class is k and $y_k = 0$ otherwise.

3) Regression (continuous case):

Although there is no direct version of Brier score for regression, we can use the squared error loss as a scoring rule for regression problems as well.

Sources:

- Bálint Mucsányi, Michael Kirchhof, Elisa Nguyen, Alexander Rubinstein, Seong Joon Oh (2023): “Proper/Strictly Proper Scoring Rule”; in: *Trustworthy Machine Learning*; URL: <https://trustworthyml.io/>; DOI: 10.48550/arXiv.2310.08215.

6.1.7 Brier scoring rule is strictly proper scoring rule

Theorem: The brier scoring rule (\rightarrow I/6.1.6) is a strictly proper scoring rule (\rightarrow I/6.1.3).

Proof: We will show that both versions of the brier scoring rule (binary/multiclass) are strictly proper scoring rules.

1) Brier scoring rule for binary classification:

$$\mathbb{E}_{Y \sim P}[\mathbf{S}(Q, Y)] = -P(Y = 1)(q - 1)^2 + P(Y = 0) - q^2 \quad (1)$$

Let p be the true probability of the event $Y = 1$. Then, the expected score is:

$$\mathbb{E}_{Y \sim P}[\mathbf{S}(Q, Y)] = -p(q - 1)^2 - (1 - p)q^2 \quad (2)$$

To find the maxima, take the derivative with respect to q and set it to zero:

$$\begin{aligned} \frac{\partial}{\partial q} \mathbb{E}_{Y \sim P}[\mathbf{S}(Q, Y)] &= -2p(q - 1) - 2(1 - p)q \\ &= -2pq + 2p - 2q + 2pq \\ &= 2p - 2q \\ 0 &= 2p - 2q \\ \Rightarrow p &= q \end{aligned} \quad (3)$$

We need to check the second derivative to see if it is a maximum (for the properness condition) and if it is the only maximizer (for the strictness condition):

$$\frac{\partial^2}{\partial q^2} \mathbb{E}_{Y \sim P}[\mathbf{S}(Q, Y)] = -2 < 0 \quad (4)$$

The second derivative is always negative which means that the function is concave and the maximum is unique. Therefore, $p = q$ is the only maximizer and the Brier scoring rule for binary classification is strictly proper.

2) Brier scoring rule for multiclass classification:

$$\begin{aligned}
\mathbb{E}_{Y \sim P}[\mathbf{S}(Q, Y)] &= \sum_k P(Y = k) \left[- \sum_i (q_i - y_i)^2 \right] \\
&= \sum_k P(Y = k) \left[- (q_k - 1)^2 - \sum_{i \neq k} q_i^2 \right] \\
&= \sum_k P(Y = k) \left[- (q_k - 1)^2 + q_k^2 - \sum_i q_i^2 \right] \\
&= \sum_k P(Y = k) \left[- q_k^2 - 1 + 2q_k + q_k^2 - \sum_i q_i^2 \right] \\
&= \sum_k P(Y = k) \left[2q_k - 1 - \sum_i q_i^2 \right] \\
&= \sum_k P(Y = k) (2q_k - 1) - \sum_k P(Y = k) \left(\sum_i q_i^2 \right) \\
&= \sum_k P(Y = k) (2q_k - 1) - \sum_i q_i^2 \underbrace{\left(\sum_k P(Y = k) \right)}_1 \\
&= \sum_k P(Y = k) (2q_k - 1) - \sum_i q_i^2 \\
&= \sum_k P(Y = k) (2q_k - 1) - q_k^2
\end{aligned} \tag{5}$$

Similar to what we did for log probability (\rightarrow I/6.1.5), this expression can be rewritten as follows (replacing q_K with $1 - \sum_{i \neq K} q_i$):

$$\begin{aligned}
\mathbb{E}_{Y \sim P}[\mathbf{S}(Q, Y)] &= p_1(2q_1 - 1) - q_1^2 + p_2(2q_2 - 1) - q_2^2 + \dots + p_K(2q_K - 1) - q_K^2 \\
&= p_1(2q_1 - 1) - q_1^2 + p_2(2q_2 - 1) - q_2^2 + \dots + p_K \left(1 - 2 \sum_{i \neq K} q_i \right) - \left(1 - \sum_{i \neq K} q_i \right)^2
\end{aligned} \tag{6}$$

Taking the derivative with respect to q_j and setting it to zero, we obtain:

$$\begin{aligned}
\frac{\partial}{\partial q_j} \mathbb{E}_{Y \sim P}[\mathbf{S}(Q, Y)] &= 2p_j - 2q_j - 2p_K + 2 \left(1 - \sum_{i \neq K} q_i \right) \\
&= 2p_j - 2q_j - 2p_K + 2q_K \\
&= (p_j - q_j) + (q_K - p_K) \\
(p_j - q_j) &= (p_K - q_K)
\end{aligned} \tag{7}$$

We know that $\sum_i p_i = 1$ and $\sum_i q_i = 1$, therefore:

$$\begin{aligned}
p_1 - q_1 &= p_2 - q_2 = \dots = p_K - q_K = \lambda \\
\sum_i p_i - q_i &= K \cdot \lambda = 0 \\
&\Rightarrow \lambda = 0 \quad \text{since } K \neq 0 \\
&\Rightarrow p_i = q_i \quad \text{for all } i = 1, \dots, K
\end{aligned} \tag{8}$$

Now, we need to check the second derivative to see, if it is a maximum for the properness condition and if it is the only maximizer for the strictness condition:

$$\frac{\partial^2}{\partial q_j^2} \mathbb{E}_{Y \sim P}[\mathbf{S}(Q, Y)] = -2 - 2 = -4 < 0 \tag{9}$$

The second derivative is always negative which means that the function is concave and the maximum is unique. Therefore, $p = q$ is the only maximizer and the Brier scoring rule for multiclass classification is strictly proper.

■

Sources:

- Bálint Mucsányi, Michael Kirchhof, Elisa Nguyen, Alexander Rubinstein, Seong Joon Oh (2023): “Proper/Strictly Proper Scoring Rule”; in: *Trustworthy Machine Learning*; URL: <https://trustworthyml.io/>; DOI: 10.48550/arXiv.2310.08215.

Chapter II

Probability Distributions

1 Univariate discrete distributions

1.1 Discrete uniform distribution

1.1.1 Definition

Definition: Let X be a discrete random variable (\rightarrow I/1.2.2). Then, X is said to be uniformly distributed with minimum a and maximum b

$$X \sim \mathcal{U}(a, b) , \quad (1)$$

if and only if each integer between and including a and b occurs with the same probability.

Sources:

- Wikipedia (2020): “Discrete uniform distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-07-28; URL: https://en.wikipedia.org/wiki/Discrete_uniform_distribution.

1.1.2 Probability mass function

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a discrete uniform distribution (\rightarrow II/1.1.1):

$$X \sim \mathcal{U}(a, b) . \quad (1)$$

Then, the probability mass function (\rightarrow I/1.6.1) of X is

$$f_X(x) = \frac{1}{b - a + 1} \quad \text{where} \quad x \in \{a, a + 1, \dots, b - 1, b\} . \quad (2)$$

Proof: A discrete uniform variable is defined as (\rightarrow II/1.1.1) having the same probability for each integer between and including a and b . The number of integers between and including a and b is

$$n = b - a + 1 \quad (3)$$

and because the sum across all probabilities (\rightarrow I/1.6.1) is

$$\sum_{x=a}^b f_X(x) = 1 , \quad (4)$$

we have

$$f_X(x) = \frac{1}{n} = \frac{1}{b - a + 1} . \quad (5)$$

■

1.1.3 Cumulative distribution function

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a discrete uniform distribution (\rightarrow II/1.1.1):

$$X \sim \mathcal{U}(a, b) . \quad (1)$$

Then, the cumulative distribution function (\rightarrow I/1.8.1) of X is

$$F_X(x) = \begin{cases} 0, & \text{if } x < a \\ \frac{\lfloor x \rfloor - a + 1}{b - a + 1}, & \text{if } a \leq x \leq b \\ 1, & \text{if } x > b. \end{cases} \quad (2)$$

Proof: The probability mass function of the discrete uniform distribution (\rightarrow II/1.1.2) is

$$\mathcal{U}(x; a, b) = \frac{1}{b - a + 1} \quad \text{where } x \in \{a, a + 1, \dots, b - 1, b\}. \quad (3)$$

Thus, the cumulative distribution function (\rightarrow I/1.8.1) is:

$$F_X(x) = \int_{-\infty}^x \mathcal{U}(z; a, b) dz \quad (4)$$

From (3), it follows that the cumulative probability increases step-wise by $1/n$ at each integer between and including a and b where

$$n = b - a + 1 \quad (5)$$

is the number of integers between and including a and b . This can be expressed by noting that

$$F_X(x) \stackrel{(3)}{=} \frac{\lfloor x \rfloor - a + 1}{n}, \quad \text{if } a \leq x \leq b. \quad (6)$$

Also, because $\Pr(X < a) = 0$, we have

$$F_X(x) \stackrel{(4)}{=} \int_{-\infty}^x 0 dz = 0, \quad \text{if } x < a \quad (7)$$

and because $\Pr(X > b) = 0$, we have

$$\begin{aligned} F_X(x) &\stackrel{(4)}{=} \int_{-\infty}^x \mathcal{U}(z; a, b) dz \\ &= \int_{-\infty}^b \mathcal{U}(z; a, b) dz + \int_b^x \mathcal{U}(z; a, b) dz \\ &= F_X(b) + \int_b^x 0 dz \stackrel{(6)}{=} 1 + 0 \\ &= 1, \quad \text{if } x > b. \end{aligned} \quad (8)$$

This completes the proof. ■

1.1.4 Quantile function

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a discrete uniform distribution (\rightarrow II/1.1.1):

$$X \sim \mathcal{U}(a, b) . \quad (1)$$

Then, the quantile function (\rightarrow I/1.11.1) of X is

$$Q_X(p) = \begin{cases} -\infty , & \text{if } p = 0 \\ a(1-p) + (b+1)p - 1 , & \text{when } p \in \left\{ \frac{1}{n}, \frac{2}{n}, \dots, \frac{b-a}{n}, 1 \right\} . \end{cases} \quad (2)$$

with $n = b - a + 1$.

Proof: The cumulative distribution function of the discrete uniform distribution (\rightarrow II/1.1.3) is:

$$F_X(x) = \begin{cases} 0 , & \text{if } x < a \\ \frac{\lfloor x \rfloor - a + 1}{b - a + 1} , & \text{if } a \leq x \leq b \\ 1 , & \text{if } x > b . \end{cases} \quad (3)$$

The quantile function (\rightarrow I/1.11.1) $Q_X(p)$ is defined as the smallest x , such that $F_X(x) = p$:

$$Q_X(p) = \min \{x \in \mathbb{R} \mid F_X(x) = p\} . \quad (4)$$

Because the CDF only returns (\rightarrow II/1.1.3) multiples of $1/n$ with $n = b - a + 1$, the quantile function (\rightarrow I/1.11.1) is only defined for such values. First, we have $Q_X(p) = -\infty$, if $p = 0$. Second, since the cumulative probability increases step-wise (\rightarrow II/1.1.3) by $1/n$ at each integer between and including a and b , the minimum x at which

$$F_X(x) = \frac{c}{n} \quad \text{where } c \in \{1, \dots, n\} \quad (5)$$

is given by

$$Q_X\left(\frac{c}{n}\right) = a + \frac{c}{n} \cdot n - 1 . \quad (6)$$

Substituting $p = c/n$ and $n = b - a + 1$, we can finally show:

$$\begin{aligned} Q_X(p) &= a + p \cdot (b - a + 1) - 1 \\ &= a + pb - pa + p - 1 \\ &= a(1-p) + (b+1)p - 1 . \end{aligned} \quad (7)$$

■

1.1.5 Shannon entropy

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a discrete uniform distribution (\rightarrow II/1.1.1):

$$X \sim \mathcal{U}(a, b) . \quad (1)$$

Then, the (Shannon) entropy (\rightarrow I/2.1.1) of X in nats is

$$H(X) = \ln(b - a + 1) . \quad (2)$$

Proof: The entropy (\rightarrow I/2.1.1) is defined as the probability-weighted average of the logarithmized probabilities for all possible values:

$$H(X) = - \sum_{x \in \mathcal{X}} p(x) \cdot \log_b p(x) . \quad (3)$$

Entropy is measured in nats by setting $b = e$. Then, with the probability mass function of the discrete uniform distribution (\rightarrow II/1.1.2), we have:

$$\begin{aligned} H(X) &= - \sum_{x \in \mathcal{X}} p(x) \cdot \log_e p(x) \\ &= - \sum_{x=a}^b p(x) \cdot \ln p(x) \\ &= - \sum_{x=a}^b \frac{1}{b-a+1} \cdot \ln \frac{1}{b-a+1} \\ &= -(b-a+1) \cdot \frac{1}{b-a+1} \cdot \ln \frac{1}{b-a+1} \\ &= - \ln \frac{1}{b-a+1} \\ &= \ln(b-a+1) . \end{aligned} \quad (4)$$

■

1.1.6 Kullback-Leibler divergence

Theorem: Let X be a random variable (\rightarrow I/1.2.2). Assume two discrete uniform distributions (\rightarrow II/1.1.1) P and Q specifying the probability distribution of X as

$$\begin{aligned} P : X &\sim \mathcal{U}(a_1, b_1) \\ Q : X &\sim \mathcal{U}(a_2, b_2) . \end{aligned} \quad (1)$$

Then, the Kullback-Leibler divergence (\rightarrow I/2.5.1) of P from Q is given by

$$\text{KL}[P \parallel Q] = \ln \frac{b_2 - a_2 + 1}{b_1 - a_1 + 1} . \quad (2)$$

Proof: The KL divergence for a discrete random variable (\rightarrow I/2.5.1) with possible values \mathcal{X} is given by

$$\text{KL}[P \parallel Q] = \sum_{x \in \mathcal{X}} p(x) \ln \frac{p(x)}{q(x)} . \quad (3)$$

This means that the KL divergence of P from Q is only defined, if for all $x \in \mathcal{X}$, $q(x) = 0$ implies $p(x) = 0$. Thus, $\text{KL}[P \parallel Q]$ only exists, if $a_2 \leq a_1$ and $b_1 \leq b_2$, i.e. if P only places non-zero probability

where Q also places non-zero probability, such that $q(x)$ is not zero for any $x \in \mathcal{X}$ where $p(x)$ is positive.

If this requirement is fulfilled, we can write

$$\text{KL}[P \parallel Q] = \sum_{x=-\infty}^{a_1} p(x) \ln \frac{p(x)}{q(x)} + \sum_{x=a_1}^{b_1} p(x) \ln \frac{p(x)}{q(x)} + \sum_{x=b_1}^{+\infty} p(x) \ln \frac{p(x)}{q(x)} \quad (4)$$

and because $p(x) = 0$ for any $x < a_1$ and any $x > b_1$, we have

$$\text{KL}[P \parallel Q] = \sum_{x=-\infty}^{a_1} 0 \cdot \ln \frac{0}{q(x)} + \sum_{x=a_1}^{b_1} p(x) \ln \frac{p(x)}{q(x)} + \sum_{x=b_1}^{+\infty} 0 \cdot \ln \frac{0}{q(x)}. \quad (5)$$

Now, $(0 \cdot \ln 0)$ is taken to be 0 by convention (\rightarrow I/2.1.1), such that

$$\text{KL}[P \parallel Q] = \sum_{x=a_1}^{b_1} p(x) \ln \frac{p(x)}{q(x)} \quad (6)$$

and we can use the probability mass function of the discrete uniform distribution (\rightarrow II/1.1.2) to evaluate:

$$\begin{aligned} \text{KL}[P \parallel Q] &= \sum_{x=a_1}^{b_1} \frac{1}{b_1 - a_1 + 1} \cdot \ln \frac{\frac{1}{b_1 - a_1 + 1}}{\frac{1}{b_2 - a_2 + 1}} \\ &= \frac{1}{b_1 - a_1 + 1} \cdot \ln \frac{b_2 - a_2 + 1}{b_1 - a_1 + 1} \sum_{x=a_1}^{b_1} 1 \\ &= \frac{1}{b_1 - a_1 + 1} \cdot \ln \frac{b_2 - a_2 + 1}{b_1 - a_1 + 1} \cdot (b_1 - a_1 + 1) \\ &= \ln \frac{b_2 - a_2 + 1}{b_1 - a_1 + 1}. \end{aligned} \quad (7)$$

■

1.1.7 Maximum entropy distribution

Theorem: The discrete uniform distribution (\rightarrow II/1.1.1) maximizes (Shannon) entropy (\rightarrow I/2.1.1) for a random variable (\rightarrow I/1.2.2) with finite support.

Proof: A random variable with finite support is a discrete random variable (\rightarrow I/1.2.6). Let X be such a random variable. Without loss of generality, we can assume that the possible values of the X can be enumerated from 1 to n .

Let $g(x)$ be the discrete uniform distribution with minimum $a = 1$ and maximum $b = n$ which assigns to equal probability to all n possible values and let $f(x)$ be an arbitrary discrete (\rightarrow I/1.2.6) probability distribution (\rightarrow I/1.5.1) on the set $\{1, 2, \dots, n-1, n\}$.

For a discrete random variable (\rightarrow I/1.2.6) X with set of possible values \mathcal{X} and probability mass function (\rightarrow I/1.6.1) $p(x)$, the Shannon entropy (\rightarrow I/2.1.1) is defined as:

$$H(X) = - \sum_{x \in \mathcal{X}} p(x) \log p(x) \quad (1)$$

Consider the Kullback-Leibler divergence (\rightarrow I/2.5.1) of distribution $f(x)$ from distribution $g(x)$ which is non-negative (\rightarrow I/2.5.2):

$$\begin{aligned} 0 \leq \text{KL}[f||g] &= \sum_{x \in \mathcal{X}} f(x) \log \frac{f(x)}{g(x)} \\ &= \sum_{x \in \mathcal{X}} f(x) \log f(x) - \sum_{x \in \mathcal{X}} f(x) \log g(x) \\ &\stackrel{(1)}{=} -H[f(x)] - \sum_{x \in \mathcal{X}} f(x) \log g(x) . \end{aligned} \quad (2)$$

By plugging the probability mass function of the discrete uniform distribution (\rightarrow II/1.1.2) into the second term, we obtain:

$$\begin{aligned} \sum_{x \in \mathcal{X}} f(x) \log g(x) &= \sum_{x=1}^n f(x) \log \frac{1}{n-1+1} \\ &= \log \frac{1}{n} \sum_{x=1}^n f(x) \\ &= -\log(n) . \end{aligned} \quad (3)$$

This is actually the negative of the entropy of the discrete uniform distribution (\rightarrow II/1.1.5), such that:

$$\sum_{x \in \mathcal{X}} f(x) \log g(x) = -H[\mathcal{U}(1, n)] = -H[g(x)] . \quad (4)$$

Combining (2) with (4), we can show that

$$\begin{aligned} 0 &\leq \text{KL}[f||g] \\ 0 &\leq -H[f(x)] - (-H[g(x)]) \\ H[g(x)] &\geq H[f(x)] \end{aligned} \quad (5)$$

which means that the entropy (\rightarrow I/2.1.1) of the discrete uniform distribution (\rightarrow II/1.1.1) $\mathcal{U}(a, b)$ will be larger than or equal to any other distribution (\rightarrow I/1.5.1) defined on the same set of values $\{a, \dots, b\}$. ■

Sources:

- Probability Fact (2023): “The entropy of a distribution with finite domain”; in: *Twitter*, retrieved on 2023-08-18; URL: <https://twitter.com/ProbFact/status/1673787091610750980>.

1.2 Bernoulli distribution

1.2.1 Definition

Definition: Let X be a random variable (\rightarrow I/1.2.2). Then, X is said to follow a Bernoulli distribution with success probability p

$$X \sim \text{Bern}(p) , \quad (1)$$

if $X = 1$ with probability (\rightarrow I/1.3.1) p and $X = 0$ with probability (\rightarrow I/1.3.1) $q = 1 - p$.

Sources:

- Wikipedia (2020): “Bernoulli distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-03-22; URL: https://en.wikipedia.org/wiki/Bernoulli_distribution.

1.2.2 Special case of categorical distribution

Theorem: The Bernoulli distribution (\rightarrow II/1.2.1) with success probability p is a special case of the categorical distribution (\rightarrow II/2.1.1) with category probabilities $p_1 = p$ and $p_2 = 1 - p$:

$$X \sim \text{Cat}([p, 1 - p]) \quad \Rightarrow \quad X \sim \text{Bern}(p) . \quad (1)$$

Proof: The probability mass function of the categorical distribution (\rightarrow II/2.1.2), where x is a $1 \times k$ vector and e_1, \dots, e_k are the $1 \times k$ elementary row vectors, is as follows:

$$\text{Cat}(x; [p_1, \dots, p_k]) = \begin{cases} p_1 , & \text{if } x = e_1 \\ \vdots & \vdots \\ p_k , & \text{if } x = e_k . \end{cases} \quad (2)$$

If we let $k = 2$, $p_1 = p$ and $p_2 = 1 - p$, we obtain

$$\text{Cat}(x; [p, 1 - p]) = \begin{cases} p , & \text{if } x = [1, 0] \\ 1 - p , & \text{if } x = [0, 1] . \end{cases} \quad (3)$$

Writing this in terms of the first entry $x_1 \in \{0, 1\}$, we get

$$\text{Cat}(x; [p, 1 - p]) = \begin{cases} p , & \text{if } x_1 = 1 \\ 1 - p , & \text{if } x_1 = 0 \end{cases} \quad (4)$$

which is equivalent to the probability mass function of the Bernoulli distribution (\rightarrow II/1.2.3). ■

1.2.3 Probability mass function

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a Bernoulli distribution (\rightarrow II/1.2.1):

$$X \sim \text{Bern}(p) . \quad (1)$$

Then, the probability mass function (\rightarrow I/1.6.1) of X is

$$f_X(x) = \begin{cases} p , & \text{if } x = 1 \\ 1 - p , & \text{if } x = 0 . \end{cases} \quad (2)$$

Proof: This follows directly from the definition of the Bernoulli distribution (\rightarrow II/1.2.1). ■

1.2.4 Mean

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a Bernoulli distribution (\rightarrow II/1.2.1):

$$X \sim \text{Bern}(p) . \quad (1)$$

Then, the mean or expected value (\rightarrow I/1.12.1) of X is

$$E(X) = p . \quad (2)$$

Proof: The expected value (\rightarrow I/1.12.1) is the probability-weighted average of all possible values:

$$E(X) = \sum_{x \in \mathcal{X}} x \cdot \Pr(X = x) . \quad (3)$$

Since there are only two possible outcomes for a Bernoulli random variable (\rightarrow II/1.2.3), we have:

$$\begin{aligned} E(X) &= 0 \cdot \Pr(X = 0) + 1 \cdot \Pr(X = 1) \\ &= 0 \cdot (1 - p) + 1 \cdot p \\ &= p . \end{aligned} \quad (4)$$

Sources:

- Wikipedia (2020): “Bernoulli distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-01-16; URL: https://en.wikipedia.org/wiki/Bernoulli_distribution#Mean.

1.2.5 Variance

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a Bernoulli distribution (\rightarrow II/1.2.1):

$$X \sim \text{Bern}(p) . \quad (1)$$

Then, the variance (\rightarrow I/1.12.1) of X is

$$\text{Var}(X) = p(1 - p) . \quad (2)$$

Proof: The variance (\rightarrow I/1.13.1) is the probability-weighted average of the squared deviation from the expected value (\rightarrow I/1.12.1) across all possible values

$$\text{Var}(X) = \sum_{x \in \mathcal{X}} (x - E(X))^2 \cdot \Pr(X = x) \quad (3)$$

and can also be written in terms of the expected values (\rightarrow I/1.13.4):

$$\text{Var}(X) = E(X^2) - E(X)^2 . \quad (4)$$

The mean of a Bernoulli random variable (\rightarrow II/1.2.4) is

$$X \sim \text{Bern}(p) \quad \Rightarrow \quad E(X) = p \quad (5)$$

and the mean of a squared Bernoulli random variable is

$$E(X^2) = 0^2 \cdot \Pr(X = 0) + 1^2 \cdot \Pr(X = 1) = 0 \cdot (1 - p) + 1 \cdot p = p. \quad (6)$$

Combining (4), (5) and (6), we have:

$$\text{Var}(X) = p - p^2 = p(1 - p). \quad (7)$$

■

Sources:

- Wikipedia (2022): “Bernoulli distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-01-20; URL: https://en.wikipedia.org/wiki/Bernoulli_distribution#Variance.

1.2.6 Range of variance

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a Bernoulli distribution (\rightarrow II/1.2.1):

$$X \sim \text{Bern}(p). \quad (1)$$

Then, the variance (\rightarrow I/1.13.1) of X is necessarily between 0 and 1/4:

$$0 \leq \text{Var}(X) \leq \frac{1}{4}. \quad (2)$$

Proof: The variance of a Bernoulli random variable (\rightarrow II/1.2.5) is

$$X \sim \text{Bern}(p) \quad \Rightarrow \quad \text{Var}(X) = p(1 - p) \quad (3)$$

which can also be understood as a function of the success probability (\rightarrow II/1.2.1) p :

$$\text{Var}(X) = \text{Var}(p) = -p^2 + p. \quad (4)$$

The first derivative of this function is

$$\frac{d\text{Var}(p)}{dp} = -2p + 1 \quad (5)$$

and setting this derivative to zero

$$\begin{aligned} \frac{d\text{Var}(p_M)}{dp} &= 0 \\ 0 &= -2p_M + 1 \\ p_M &= \frac{1}{2}, \end{aligned} \quad (6)$$

we obtain the maximum possible variance

$$\max [\text{Var}(X)] = \text{Var}(p_M) = -\left(\frac{1}{2}\right)^2 + \frac{1}{2} = \frac{1}{4} . \quad (7)$$

The function $\text{Var}(p)$ is monotonically increasing for $0 < p < p_M$ as $d\text{Var}(p)/dp > 0$ in this interval and it is monotonically decreasing for $p_M < p < 1$ as $d\text{Var}(p)/dp < 0$ in this interval. Moreover, as variance is always non-negative (\rightarrow I/1.13.5), the minimum variance is

$$\min [\text{Var}(X)] = \text{Var}(0) = \text{Var}(1) = 0 . \quad (8)$$

Thus, we have:

$$\text{Var}(p) \in \left[0, \frac{1}{4}\right] . \quad (9)$$

■

Sources:

- Wikipedia (2022): “Bernoulli distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-01-27; URL: https://en.wikipedia.org/wiki/Bernoulli_distribution#Variance.

1.2.7 Shannon entropy

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a Bernoulli distribution (\rightarrow II/1.2.1):

$$X \sim \text{Bern}(p) . \quad (1)$$

Then, the (Shannon) entropy (\rightarrow I/2.1.1) of X in bits is

$$H(X) = -p \log_2 p - (1 - p) \log_2 (1 - p) . \quad (2)$$

Proof: The entropy (\rightarrow I/2.1.1) is defined as the probability-weighted average of the logarithmized probabilities for all possible values:

$$H(X) = - \sum_{x \in \mathcal{X}} p(x) \cdot \log_b p(x) . \quad (3)$$

Entropy is measured in bits by setting $b = 2$. Since there are only two possible outcomes for a Bernoulli random variable (\rightarrow II/1.2.3), we have:

$$\begin{aligned} H(X) &= -\Pr(X = 0) \cdot \log_2 \Pr(X = 0) - \Pr(X = 1) \cdot \log_2 \Pr(X = 1) \\ &= -p \log_2 p - (1 - p) \log_2 (1 - p) . \end{aligned} \quad (4)$$

■

Sources:

- Wikipedia (2022): “Bernoulli distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-09-02; URL: https://en.wikipedia.org/wiki/Bernoulli_distribution.
- Wikipedia (2022): “Binary entropy function”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-09-02; URL: https://en.wikipedia.org/wiki/Binary_entropy_function.

1.2.8 Kullback-Leibler divergence

Theorem: Let X be a random variable (\rightarrow I/1.2.2). Assume two Bernoulli distributions (\rightarrow II/1.2.1) P and Q specifying the probability distribution of X as

$$\begin{aligned} P : X &\sim \text{Bern}(p_1) \\ Q : X &\sim \text{Bern}(p_2) . \end{aligned} \tag{1}$$

Then, the Kullback-Leibler divergence (\rightarrow I/2.5.1) of P from Q is given by

$$\text{KL}[P \parallel Q] = \ln \frac{1-p_1}{1-p_2} + p_1 \cdot \ln \frac{p_1(1-p_2)}{p_2(1-p_1)} . \tag{2}$$

Proof: The KL divergence for a discrete random variable (\rightarrow I/2.5.1) is given by

$$\text{KL}[P \parallel Q] = \sum_{x \in \mathcal{X}} p(x) \ln \frac{p(x)}{q(x)} \tag{3}$$

which, applied to the Bernoulli distributions (\rightarrow II/1.2.1) in (1), yields

$$\begin{aligned} \text{KL}[P \parallel Q] &= \sum_{x \in \{0,1\}} p(x) \ln \frac{p(x)}{q(x)} \\ &= p(X=0) \cdot \ln \frac{p(X=0)}{q(X=0)} + p(X=1) \cdot \ln \frac{p(X=1)}{q(X=1)} . \end{aligned} \tag{4}$$

Using the probability mass function of the Bernoulli distribution (\rightarrow II/1.2.3), this becomes:

$$\begin{aligned} \text{KL}[P \parallel Q] &= (1-p_1) \cdot \ln \frac{1-p_1}{1-p_2} + p_1 \cdot \ln \frac{p_1}{p_2} \\ &= \ln \frac{1-p_1}{1-p_2} + p_1 \cdot \ln \frac{p_1}{p_2} - p_1 \cdot \ln \frac{1-p_1}{1-p_2} \\ &= \ln \frac{1-p_1}{1-p_2} + p_1 \cdot \left(\ln \frac{p_1}{p_2} + \ln \frac{1-p_2}{1-p_1} \right) \\ &= \ln \frac{1-p_1}{1-p_2} + p_1 \cdot \ln \frac{p_1(1-p_2)}{p_2(1-p_1)} \end{aligned} \tag{5}$$

■

1.3 Binomial distribution

1.3.1 Definition

Definition: Let X be a random variable (\rightarrow I/1.2.2). Then, X is said to follow a binomial distribution with number of trials n and success probability p

$$X \sim \text{Bin}(n, p) , \tag{1}$$

if X is the number of successes observed in n independent (\rightarrow I/1.3.6) trials, where each trial has two possible outcomes (\rightarrow II/1.2.1) (success/failure) and the probability of success and failure are identical across trials ($p/q = 1 - p$).

Sources:

- Wikipedia (2020): “Binomial distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-03-22; URL: https://en.wikipedia.org/wiki/Binomial_distribution.

1.3.2 Special case of multinomial distribution

Theorem: The binomial distribution (\rightarrow II/1.3.1) with sample size n and success probability p is a special case of the multinomial distribution (\rightarrow II/2.2.1) with sample size n category probabilities $p_1 = p$ and $p_2 = 1 - p$:

$$X \sim \text{Mult}(n, [p, 1 - p]) \quad \Rightarrow \quad X \sim \text{Bin}(p) . \quad (1)$$

Proof: The probability mass function of the multinomial distribution (\rightarrow II/2.2.2), where x is a $1 \times k$ vector with $x_i \in \{0, 1, \dots, n\}$, is as follows:

$$\text{Mult}(x; n, [p_1, \dots, p_k]) = \binom{n}{x_1, \dots, x_k} \prod_{i=1}^k p_i^{x_i} . \quad (2)$$

If we let $k = 2$, $p_1 = p$ and $p_2 = 1 - p$, we obtain

$$\text{Mult}(x; n, [p, 1 - p]) = \binom{n}{x_1, x_2} p^{x_1} (1 - p)^{n - x_1} . \quad (3)$$

Recognizing that $\sum_{i=1}^k x_i = n$, such that $x_2 = n - x_1$, we get

$$\begin{aligned} \text{Mult}(x; n, [p, 1 - p]) &= \binom{n}{x_1, n - x_1} p^{x_1} (1 - p)^{n - x_1} \\ &= \binom{n}{x_1} p^{x_1} (1 - p)^{n - x_1} \end{aligned} \quad (4)$$

which is equivalent to the probability mass function of the binomial distribution (\rightarrow II/1.3.3). ■

1.3.3 Probability mass function

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a binomial distribution (\rightarrow II/1.3.1):

$$X \sim \text{Bin}(n, p) . \quad (1)$$

Then, the probability mass function (\rightarrow I/1.6.1) of X is

$$f_X(x) = \binom{n}{x} p^x (1 - p)^{n - x} . \quad (2)$$

Proof: A binomial variable (\rightarrow II/1.3.1) is defined as the number of successes observed in n independent (\rightarrow I/1.3.6) trials, where each trial has two possible outcomes (\rightarrow II/1.2.1) (success/failure) and the probability (\rightarrow I/1.3.1) of success and failure are identical across trials ($p, q = 1 - p$).

If one has obtained x successes in n trials, one has also obtained $(n - x)$ failures. The probability of a particular series of x successes and $(n - x)$ failures, when order does matter, is

$$p^x (1 - p)^{n-x} . \quad (3)$$

When order does not matter, there is a number of series consisting of x successes and $(n - x)$ failures. This number is equal to the number of possibilities in which x objects can be chosen from n objects which is given by the binomial coefficient:

$$\binom{n}{x} . \quad (4)$$

In order to obtain the probability of x successes and $(n - x)$ failures, when order does not matter, the probability in (3) has to be multiplied with the number of possibilities in (4) which gives

$$p(X = x|n, p) = \binom{n}{x} p^x (1 - p)^{n-x} \quad (5)$$

which is equivalent to the expression above. ■

1.3.4 Cumulative distribution function

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a binomial distribution (\rightarrow II/1.3.1):

$$X \sim \text{Bin}(n, p) . \quad (1)$$

Then, the cumulative distribution function (\rightarrow I/1.8.1) of X is

$$F_X(x) = \sum_{k=0}^x \binom{n}{k} p^k (1 - p)^{n-k} . \quad (2)$$

Proof: The cumulative distribution function (\rightarrow I/1.8.1) is defined as

$$F_X(x) = \Pr(X \leq x) \quad (3)$$

which, in terms of the probability mass function, is given by (\rightarrow I/1.8.5)

$$F_X(x) = \sum_{\substack{t \in \mathcal{X} \\ t \leq x}} f_X(t) . \quad (4)$$

The probability mass function of the binomial distribution (\rightarrow II/1.3.3) is

$$f_X(x) = \binom{n}{x} p^x (1 - p)^{n-x} , \quad (5)$$

so that the cumulative distribution function of the binomial distribution becomes

$$\begin{aligned}
F_X(x) &\stackrel{(4)}{=} \sum_{k=0}^x f_X(k) \\
&\stackrel{(5)}{=} \sum_{k=0}^x \binom{n}{k} p^k (1-p)^{n-k} .
\end{aligned} \tag{6}$$

■

Sources:

- Wikipedia (2025): “Binomial distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2025-02-06; URL: https://en.wikipedia.org/wiki/Binomial_distribution#Cumulative_distribution_function.

1.3.5 Probability-generating function

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a binomial distribution (\rightarrow II/1.3.1):

$$X \sim \text{Bin}(n, p) . \tag{1}$$

Then, the probability-generating function (\rightarrow I/1.10.1) of X is

$$G_X(z) = (q + pz)^n \tag{2}$$

where $q = 1 - p$.

Proof: The probability-generating function (\rightarrow I/1.10.1) of X is defined as

$$G_X(z) = \sum_{x=0}^{\infty} f_X(x) z^x \tag{3}$$

With the probability mass function of the binomial distribution (\rightarrow II/1.3.3)

$$f_X(x) = \binom{n}{x} p^x (1-p)^{n-x} , \tag{4}$$

we obtain:

$$\begin{aligned}
G_X(z) &= \sum_{x=0}^n \binom{n}{x} p^x (1-p)^{n-x} z^x \\
&= \sum_{x=0}^n \binom{n}{x} (pz)^x (1-p)^{n-x} .
\end{aligned} \tag{5}$$

According to the binomial theorem

$$(x + y)^n = \sum_{k=0}^n \binom{n}{k} x^{n-k} y^k , \tag{6}$$

the sum in equation (5) equals

$$G_X(z) = ((1-p) + (pz))^n \tag{7}$$

which is equivalent to the result in (2).

**Sources:**

- ProofWiki (2022): “Probability Generating Function of Binomial Distribution”; in: *ProofWiki*, retrieved on 2022-10-11; URL: https://proofwiki.org/wiki/Probability_Generating_Function_of_Binomial_Distribution.

1.3.6 Mean

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a binomial distribution (\rightarrow II/1.3.1):

$$X \sim \text{Bin}(n, p) . \quad (1)$$

Then, the mean or expected value (\rightarrow I/1.12.1) of X is

$$E(X) = np . \quad (2)$$

Proof: By definition, a binomial random variable (\rightarrow II/1.3.1) is the sum of n independent and identical (\rightarrow I/1.2.8) Bernoulli trials (\rightarrow II/1.2.1) with success probability p . Therefore, the expected value is

$$E(X) = E(X_1 + \dots + X_n) \quad (3)$$

and because the expected value is a linear operator (\rightarrow I/1.12.5), this is equal to

$$E(X) = E(X_1) + \dots + E(X_n) = \sum_{i=1}^n E(X_i) . \quad (4)$$

With the expected value of the Bernoulli distribution (\rightarrow II/1.2.4), we have:

$$E(X) = \sum_{i=1}^n p = np . \quad (5)$$

**Sources:**

- Wikipedia (2020): “Binomial distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-01-16; URL: https://en.wikipedia.org/wiki/Binomial_distribution#Expected_value_and_variance.

1.3.7 Variance

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a binomial distribution (\rightarrow II/1.3.1):

$$X \sim \text{Bin}(n, p) . \quad (1)$$

Then, the variance (\rightarrow I/1.13.1) of X is

$$\text{Var}(X) = np(1 - p) . \quad (2)$$

Proof: By definition, a binomial random variable (\rightarrow II/1.3.1) is the sum of n independent and identical (\rightarrow I/1.2.8) Bernoulli trials (\rightarrow II/1.2.1) with success probability p . Therefore, the variance is

$$\text{Var}(X) = \text{Var}(X_1 + \dots + X_n) \quad (3)$$

and because variances add up under independence (\rightarrow I/1.13.11), this is equal to

$$\text{Var}(X) = \text{Var}(X_1) + \dots + \text{Var}(X_n) = \sum_{i=1}^n \text{Var}(X_i) . \quad (4)$$

With the variance of the Bernoulli distribution (\rightarrow II/1.2.5), we have:

$$\text{Var}(X) = \sum_{i=1}^n p(1-p) = np(1-p) . \quad (5)$$

■

Sources:

- Wikipedia (2022): “Binomial distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-01-20; URL: https://en.wikipedia.org/wiki/Binomial_distribution#Expected_value_and_variance.

1.3.8 Range of variance

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a binomial distribution (\rightarrow II/1.3.1):

$$X \sim \text{Bin}(n, p) . \quad (1)$$

Then, the variance (\rightarrow I/1.13.1) of X is necessarily between 0 and $n/4$:

$$0 \leq \text{Var}(X) \leq \frac{n}{4} . \quad (2)$$

Proof: By definition, a binomial random variable (\rightarrow II/1.3.1) is the sum of n independent and identical (\rightarrow I/1.2.8) Bernoulli trials (\rightarrow II/1.2.1) with success probability p . Therefore, the variance is

$$\text{Var}(X) = \text{Var}(X_1 + \dots + X_n) \quad (3)$$

and because variances add up under independence (\rightarrow I/1.13.11), this is equal to

$$\text{Var}(X) = \text{Var}(X_1) + \dots + \text{Var}(X_n) = \sum_{i=1}^n \text{Var}(X_i) . \quad (4)$$

As the variance of a Bernoulli random variable is always between 0 and $1/4$ (\rightarrow II/1.2.6)

$$0 \leq \text{Var}(X_i) \leq \frac{1}{4} \quad \text{for all } i = 1, \dots, n , \quad (5)$$

the minimum variance of X is

$$\min [\text{Var}(X)] = n \cdot 0 = 0 \quad (6)$$

and the maximum variance of X is

$$\max [\text{Var}(X)] = n \cdot \frac{1}{4} = \frac{n}{4} . \quad (7)$$

Thus, we have:

$$\text{Var}(X) \in \left[0, \frac{n}{4}\right] . \quad (8)$$

■

1.3.9 Shannon entropy

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a binomial distribution (\rightarrow II/1.3.1):

$$X \sim \text{Bin}(n, p) . \quad (1)$$

Then, the (Shannon) entropy (\rightarrow I/2.1.1) of X in bits is

$$H(X) = n \cdot H_{\text{bern}}(p) - E_{\text{lbc}}(n, p) \quad (2)$$

where $H_{\text{bern}}(p)$ is the binary entropy function, i.e. the (Shannon) entropy of the Bernoulli distribution (\rightarrow II/1.2.7) with success probability p

$$H_{\text{bern}}(p) = -p \cdot \log_2 p - (1-p) \log_2 (1-p) \quad (3)$$

and $E_{\text{lbc}}(n, p)$ is the expected value (\rightarrow I/1.12.1) of the logarithmized binomial coefficient (\rightarrow II/1.3.3) with superset size n

$$E_{\text{lbc}}(n, p) = E \left[\log_2 \binom{n}{X} \right] \quad \text{where } X \sim \text{Bin}(n, p) . \quad (4)$$

Proof: The entropy (\rightarrow I/2.1.1) is defined as the probability-weighted average of the logarithmized probabilities for all possible values:

$$H(X) = - \sum_{x \in \mathcal{X}} p(x) \cdot \log_b p(x) . \quad (5)$$

Entropy is measured in bits by setting $b = 2$. Then, with the probability mass function of the binomial distribution (\rightarrow II/1.3.3), we have:

$$\begin{aligned} H(X) &= - \sum_{x \in \mathcal{X}} f_X(x) \cdot \log_2 f_X(x) \\ &= - \sum_{x=0}^n \binom{n}{x} p^x (1-p)^{n-x} \cdot \log_2 \left[\binom{n}{x} p^x (1-p)^{n-x} \right] \\ &= - \sum_{x=0}^n \binom{n}{x} p^x (1-p)^{n-x} \cdot \left[\log_2 \binom{n}{x} + x \cdot \log_2 p + (n-x) \cdot \log_2 (1-p) \right] \\ &= - \sum_{x=0}^n \binom{n}{x} p^x (1-p)^{n-x} \cdot \left[\log_2 \binom{n}{x} + x \cdot \log_2 p + n \cdot \log_2 (1-p) - x \cdot \log_2 (1-p) \right] . \end{aligned} \quad (6)$$

Since the first factor in the sum corresponds to the probability mass (\rightarrow I/1.6.1) of $X = x$, we can rewrite this as the sum of the expected values (\rightarrow I/1.12.1) of the functions (\rightarrow I/1.12.9) of the discrete random variable (\rightarrow I/1.2.6) x in the square bracket:

$$\begin{aligned} H(X) &= - \left\langle \log_2 \binom{n}{x} \right\rangle_{p(x)} - \langle x \cdot \log_2 p \rangle_{p(x)} - \langle n \cdot \log_2(1-p) \rangle_{p(x)} + \langle x \cdot \log_2(1-p) \rangle_{p(x)} \\ &= - \left\langle \log_2 \binom{n}{x} \right\rangle_{p(x)} - \log_2 p \cdot \langle x \rangle_{p(x)} - n \cdot \log_2(1-p) + \log_2(1-p) \cdot \langle x \rangle_{p(x)} . \end{aligned} \quad (7)$$

Using the expected value of the binomial distribution (\rightarrow II/1.3.6), i.e. $X \sim \text{Bin}(n, p) \Rightarrow \langle x \rangle = np$, this gives:

$$\begin{aligned} H(X) &= - \left\langle \log_2 \binom{n}{x} \right\rangle_{p(x)} - np \cdot \log_2 p - n \cdot \log_2(1-p) + np \cdot \log_2(1-p) \\ &= - \left\langle \log_2 \binom{n}{x} \right\rangle_{p(x)} + n [-p \cdot \log_2 p - (1-p) \log_2(1-p)] . \end{aligned} \quad (8)$$

Finally, we note that the first term is the negative expected value (\rightarrow I/1.12.1) of the logarithm of a binomial coefficient (\rightarrow II/1.3.3) and that the term in square brackets is the entropy of the Bernoulli distribution (\rightarrow II/1.3.9), such that we finally get:

$$H(X) = n \cdot H_{\text{bern}}(p) - E_{\text{lbc}}(n, p) . \quad (9)$$

Note that, because $0 \leq H_{\text{bern}}(p) \leq 1$, we have $0 \leq n \cdot H_{\text{bern}}(p) \leq n$, and because the entropy is non-negative (\rightarrow I/2.1.2), it must hold that $n \geq E_{\text{lbc}}(n, p) \geq 0$.

■

1.3.10 Kullback-Leibler divergence

Theorem: Let X be a random variable (\rightarrow I/1.2.2). Assume two binomial distributions (\rightarrow II/1.3.1) P and Q specifying the probability distribution of X as

$$\begin{aligned} P : X &\sim \text{Bin}(n, p_1) \\ Q : X &\sim \text{Bin}(n, p_2) . \end{aligned} \quad (1)$$

Then, the Kullback-Leibler divergence (\rightarrow I/2.5.1) of P from Q is given by

$$\text{KL}[P \parallel Q] = np_1 \cdot \ln \frac{p_1}{p_2} + n(1-p_1) \cdot \ln \frac{1-p_1}{1-p_2} . \quad (2)$$

Proof: The KL divergence for a discrete random variable (\rightarrow I/2.5.1) is given by

$$\text{KL}[P \parallel Q] = \sum_{x \in \mathcal{X}} p(x) \ln \frac{p(x)}{q(x)} \quad (3)$$

which, applied to the binomial distributions (\rightarrow II/1.3.1) in (1), yields

$$\begin{aligned}
\text{KL}[P \parallel Q] &= \sum_{x=0}^n p(x) \ln \frac{p(x)}{q(x)} \\
&= p(X=0) \cdot \ln \frac{p(X=0)}{q(X=0)} + \dots + p(X=n) \cdot \ln \frac{p(X=n)}{q(X=n)}.
\end{aligned} \tag{4}$$

Using the probability mass function of the binomial distribution (\rightarrow II/1.3.3), this becomes:

$$\begin{aligned}
\text{KL}[P \parallel Q] &= \sum_{x=0}^n \binom{n}{x} p_1^x (1-p_1)^{n-x} \cdot \ln \frac{\binom{n}{x} p_1^x (1-p_1)^{n-x}}{\binom{n}{x} p_2^x (1-p_2)^{n-x}} \\
&= \sum_{x=0}^n \binom{n}{x} p_1^x (1-p_1)^{n-x} \cdot \left[x \cdot \ln \frac{p_1}{p_2} + (n-x) \cdot \ln \frac{1-p_1}{1-p_2} \right] \\
&= \ln \frac{p_1}{p_2} \cdot \sum_{x=0}^n \binom{n}{x} p_1^x (1-p_1)^{n-x} x + \ln \frac{1-p_1}{1-p_2} \cdot \sum_{x=0}^n \binom{n}{x} p_1^x (1-p_1)^{n-x} (n-x).
\end{aligned} \tag{5}$$

We can now see that some terms in this sum are expected values (\rightarrow I/1.12.1) with respect to binomial distributions (\rightarrow II/1.3.1):

$$\begin{aligned}
\sum_{x=0}^n \binom{n}{x} p_1^x (1-p_1)^{n-x} x &= \text{E}[x]_{\text{Bin}(n, p_1)} \\
\sum_{x=0}^n \binom{n}{x} p_1^x (1-p_1)^{n-x} (n-x) &= \text{E}[n-x]_{\text{Bin}(n, p_1)}.
\end{aligned} \tag{6}$$

Using the expected value of the binomial distribution (\rightarrow II/1.3.6), these can be simplified to

$$\begin{aligned}
\text{E}[x]_{\text{Bin}(n, p_1)} &= np_1 \\
\text{E}[n-x]_{\text{Bin}(n, p_1)} &= n - np_1,
\end{aligned} \tag{7}$$

such that the Kullback-Leibler divergence finally becomes:

$$\text{KL}[P \parallel Q] = np_1 \cdot \ln \frac{p_1}{p_2} + n(1-p_1) \cdot \ln \frac{1-p_1}{1-p_2}. \tag{8}$$

■

Sources:

- PSPACEhard (2017): “Kullback-Leibler divergence for binomial distributions P and Q”; in: *Stack-Exchange Mathematics*, retrieved on 2023-10-20; URL: <https://math.stackexchange.com/a/2215384/480910>.

1.3.11 Conditional binomial

Theorem: Let X and Y be two random variables (\rightarrow I/1.2.2) where Y is binomially distributed (\rightarrow II/1.3.1) conditional on (\rightarrow I/1.5.4) X

$$Y|X \sim \text{Bin}(X, q) \quad (1)$$

and X also follows a binomial distribution (\rightarrow II/1.3.1), but with different success frequency (\rightarrow II/1.3.1):

$$X \sim \text{Bin}(n, p) . \quad (2)$$

Then, the maginal distribution (\rightarrow I/1.5.3) of Y unconditional on X is again a binomial distribution (\rightarrow II/1.3.1):

$$Y \sim \text{Bin}(n, pq) . \quad (3)$$

Proof: We are interested in the probability that Y equals a number m . According to the law of marginal probability (\rightarrow I/1.3.3) or the law of total probability (\rightarrow I/1.4.11), this probability can be expressed as:

$$\Pr(Y = m) = \sum_{k=0}^{\infty} \Pr(Y = m|X = k) \cdot \Pr(X = k) . \quad (4)$$

Since, by definitions (2) and (1), $\Pr(X = k) = 0$ when $k > n$ and $\Pr(Y = m|X = k) = 0$ when $k < m$, we have:

$$\Pr(Y = m) = \sum_{k=m}^n \Pr(Y = m|X = k) \cdot \Pr(X = k) . \quad (5)$$

Now we can take the probability mass function of the binomial distribution (\rightarrow II/1.3.3) and plug it in for the terms in the sum of (5) to get:

$$\Pr(Y = m) = \sum_{k=m}^n \binom{k}{m} q^m (1-q)^{k-m} \cdot \binom{n}{k} p^k (1-p)^{n-k} . \quad (6)$$

Applying the binomial coefficient identity $\binom{n}{k} \binom{k}{m} = \binom{n}{m} \binom{n-m}{k-m}$ and rearranging the terms, we have:

$$\Pr(Y = m) = \sum_{k=m}^n \binom{n}{m} \binom{n-m}{k-m} p^k q^m (1-p)^{n-k} (1-q)^{k-m} . \quad (7)$$

Now we partition $p^k = p^m \cdot p^{k-m}$ and pull all terms dependent on k out of the sum:

$$\begin{aligned} \Pr(Y = m) &= \binom{n}{m} p^m q^m \sum_{k=m}^n \binom{n-m}{k-m} p^{k-m} (1-p)^{n-k} (1-q)^{k-m} \\ &= \binom{n}{m} (pq)^m \sum_{k=m}^n \binom{n-m}{k-m} (p(1-q))^{k-m} (1-p)^{n-k} . \end{aligned} \quad (8)$$

Then we substitute $i = k - m$, such that $k = i + m$:

$$\Pr(Y = m) = \binom{n}{m} (pq)^m \sum_{i=0}^{n-m} \binom{n-m}{i} (p-pq)^i (1-p)^{n-m-i} . \quad (9)$$

According to the binomial theorem

$$(x + y)^n = \sum_{k=0}^n \binom{n}{k} x^{n-k} y^k, \quad (10)$$

the sum in equation (9) is equal to

$$\sum_{i=0}^{n-m} \binom{n-m}{i} (p-pq)^i (1-p)^{n-m-i} = ((p-pq) + (1-p))^{n-m}. \quad (11)$$

Thus, (9) develops into

$$\begin{aligned} \Pr(Y = m) &= \binom{n}{m} (pq)^m (p-pq + 1-p)^{n-m} \\ &= \binom{n}{m} (pq)^m (1-pq)^{n-m} \end{aligned} \quad (12)$$

which is the probability mass function of the binomial distribution (\rightarrow II/1.3.3) with parameters n and pq , such that

$$Y \sim \text{Bin}(n, pq). \quad (13)$$

■

Sources:

- Wikipedia (2022): “Binomial distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-10-07; URL: https://en.wikipedia.org/wiki/Binomial_distribution#Conditional_binomials.

1.4 Beta-binomial distribution

1.4.1 Definition

Definition: Let p be a random variable (\rightarrow I/1.2.2) following a beta distribution (\rightarrow II/3.9.1)

$$p \sim \text{Bet}(\alpha, \beta) \quad (1)$$

and let X be a random variable (\rightarrow I/1.2.2) following a binomial distribution (\rightarrow II/1.3.1) conditional on p

$$X \mid p \sim \text{Bin}(n, p). \quad (2)$$

Then, the marginal distribution (\rightarrow I/1.5.3) of X is called a beta-binomial distribution

$$X \sim \text{BetBin}(n, \alpha, \beta) \quad (3)$$

with number of trials (\rightarrow II/1.3.1) n and shape parameters (\rightarrow II/3.9.1) α and β .

Sources:

- Wikipedia (2022): “Beta-binomial distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-10-20; URL: https://en.wikipedia.org/wiki/Beta-binomial_distribution#Motivation_and_derivation.

1.4.2 Probability mass function

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a beta-binomial distribution (\rightarrow II/1.4.1):

$$X \sim \text{BetBin}(n, \alpha, \beta) . \quad (1)$$

Then, the probability mass function (\rightarrow I/1.6.1) of X is

$$f_X(x) = \binom{n}{x} \cdot \frac{B(\alpha + x, \beta + n - x)}{B(\alpha, \beta)} \quad (2)$$

where $B(x, y)$ is the beta function.

Proof: A beta-binomial random variable (\rightarrow II/1.4.1) is defined as a binomial variate (\rightarrow II/1.3.1) for which the success probability is following a beta distribution (\rightarrow II/3.9.1):

$$\begin{aligned} X | p &\sim \text{Bin}(n, p) \\ p &\sim \text{Bet}(\alpha, \beta) . \end{aligned} \quad (3)$$

Thus, we can combine the law of marginal probability (\rightarrow I/1.3.3) and the law of conditional probability (\rightarrow I/1.3.4) to derive the probability (\rightarrow I/1.3.1) of X as

$$\begin{aligned} p(x) &= \int_{\mathcal{P}} p(x, p) \, dp \\ &= \int_{\mathcal{P}} p(x|p) p(p) \, dp \end{aligned} \quad (4)$$

where $\mathcal{P} = [0, 1]$ is the set of possible values of p . Now, we can plug in the probability mass function of the binomial distribution (\rightarrow II/1.3.3) and the probability density function of the beta distribution (\rightarrow II/3.9.5) to get

$$\begin{aligned} p(x) &= \int_0^1 \binom{n}{x} p^x (1-p)^{n-x} \cdot \frac{1}{B(\alpha, \beta)} p^{\alpha-1} (1-p)^{\beta-1} \, dp \\ &= \binom{n}{x} \cdot \frac{1}{B(\alpha, \beta)} \int_0^1 p^{\alpha+x-1} (1-p)^{\beta+n-x-1} \, dp \\ &= \binom{n}{x} \cdot \frac{B(\alpha+x, \beta+n-x)}{B(\alpha, \beta)} \int_0^1 \frac{1}{B(\alpha+x, \beta+n-x)} p^{\alpha+x-1} (1-p)^{\beta+n-x-1} \, dp . \end{aligned} \quad (5)$$

Finally, we recognize that the integrand is equal to the probability density function of a beta distribution (\rightarrow II/3.9.5) and because probability density integrates to one (\rightarrow I/1.7.1), we have

$$p(x) = \binom{n}{x} \cdot \frac{B(\alpha+x, \beta+n-x)}{B(\alpha, \beta)} = f_X(x) . \quad (6)$$

This completes the proof. ■

Sources:

- Wikipedia (2022): “Beta-binomial distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-10-20; URL: https://en.wikipedia.org/wiki/Beta-binomial_distribution#As_a_compound_distribution.

1.4.3 Probability mass function in terms of gamma function

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a beta-binomial distribution (\rightarrow II/1.4.1):

$$X \sim \text{BetBin}(n, \alpha, \beta) . \quad (1)$$

Then, the probability mass function (\rightarrow I/1.6.1) of X can be expressed as

$$f_X(x) = \frac{\Gamma(n+1)}{\Gamma(x+1)\Gamma(n-x+1)} \cdot \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} \cdot \frac{\Gamma(\alpha+x)\Gamma(\beta+n-x)}{\Gamma(\alpha+\beta+n)} \quad (2)$$

where $\Gamma(x)$ is the gamma function.

Proof: The probability mass function of the beta-binomial distribution (\rightarrow II/1.4.2) is given by

$$f_X(x) = \binom{n}{x} \cdot \frac{B(\alpha+x, \beta+n-x)}{B(\alpha, \beta)} . \quad (3)$$

Note that the binomial coefficient can be expressed in terms of factorials

$$\binom{n}{x} = \frac{n!}{x!(n-x)!} , \quad (4)$$

that factorials are related to the gamma function via $n! = \Gamma(n+1)$

$$\frac{n!}{x!(n-x)!} = \frac{\Gamma(n+1)}{\Gamma(x+1)\Gamma(n-x+1)} \quad (5)$$

and that the beta function is related to the gamma function via

$$B(\alpha, \beta) = \frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha+\beta)} . \quad (6)$$

Applying (4), (5) and (6) to (3), we get

$$f_X(x) = \frac{\Gamma(n+1)}{\Gamma(x+1)\Gamma(n-x+1)} \cdot \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} \cdot \frac{\Gamma(\alpha+x)\Gamma(\beta+n-x)}{\Gamma(\alpha+\beta+n)} . \quad (7)$$

This completes the proof. ■

Sources:

- Wikipedia (2022): “Beta-binomial distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-10-20; URL: https://en.wikipedia.org/wiki/Beta-binomial_distribution#As_a_compound_distribution.

1.4.4 Cumulative distribution function

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a beta-binomial distribution (\rightarrow II/1.4.1):

$$X \sim \text{BetBin}(n, \alpha, \beta) . \quad (1)$$

Then, the cumulative distribution function (\rightarrow I/1.8.1) of X is

$$F_X(x) = \frac{1}{B(\alpha, \beta)} \cdot \frac{\Gamma(n+1)}{\Gamma(\alpha + \beta + n)} \cdot \sum_{i=0}^x \frac{\Gamma(\alpha + i) \cdot \Gamma(\beta + n - i)}{\Gamma(i+1) \cdot \Gamma(n - i + 1)} \quad (2)$$

where $B(x, y)$ is the beta function and $\Gamma(x)$ is the gamma function.

Proof: The cumulative distribution function (\rightarrow I/1.8.1) is defined as

$$F_X(x) = \Pr(X \leq x) \quad (3)$$

which, for a discrete random variable (\rightarrow I/1.2.6), evaluates to

$$F_X(x) = \sum_{i=-\infty}^x f_X(i) . \quad (4)$$

With the probability mass function of the beta-binomial distribution (\rightarrow II/1.4.2), this becomes

$$F_X(x) = \sum_{i=0}^x \binom{n}{i} \cdot \frac{B(\alpha + i, \beta + n - i)}{B(\alpha, \beta)} . \quad (5)$$

Using the expression of binomial coefficients in terms of factorials

$$\binom{n}{k} = \frac{n!}{k! (n - k)!} , \quad (6)$$

the relationship between factorials and the gamma function

$$n! = \Gamma(n + 1) \quad (7)$$

and the link between gamma function and beta function

$$B(\alpha, \beta) = \frac{\Gamma(\alpha) \Gamma(\beta)}{\Gamma(\alpha + \beta)} , \quad (8)$$

equation (5) can be further developped as follows:

$$\begin{aligned} F_X(x) &\stackrel{(6)}{=} \frac{1}{B(\alpha, \beta)} \cdot \sum_{i=0}^x \frac{n!}{i! (n - i)!} \cdot B(\alpha + i, \beta + n - i) \\ &\stackrel{(8)}{=} \frac{1}{B(\alpha, \beta)} \cdot \sum_{i=0}^x \frac{n!}{i! (n - i)!} \cdot \frac{\Gamma(\alpha + i) \cdot \Gamma(\beta + n - i)}{\Gamma(\alpha + \beta + n)} \\ &= \frac{1}{B(\alpha, \beta)} \cdot \frac{n!}{\Gamma(\alpha + \beta + n)} \cdot \sum_{i=0}^x \frac{\Gamma(\alpha + i) \cdot \Gamma(\beta + n - i)}{i! (n - i)!} \\ &\stackrel{(7)}{=} \frac{1}{B(\alpha, \beta)} \cdot \frac{\Gamma(n + 1)}{\Gamma(\alpha + \beta + n)} \cdot \sum_{i=0}^x \frac{\Gamma(\alpha + i) \cdot \Gamma(\beta + n - i)}{\Gamma(i + 1) \cdot \Gamma(n - i + 1)} . \end{aligned} \quad (9)$$

This completes the proof. ■

1.5 Poisson distribution

1.5.1 Definition

Definition: Let X be a random variable (\rightarrow I/1.2.2). Then, X is said to follow a Poisson distribution with rate λ

$$X \sim \text{Poiss}(\lambda) , \quad (1)$$

if and only if its probability mass function (\rightarrow I/1.6.1) is given by

$$\text{Poiss}(x; \lambda) = \frac{\lambda^x e^{-\lambda}}{x!} \quad (2)$$

where $x \in \mathbb{N}_0$ and $\lambda > 0$.

Sources:

- Wikipedia (2020): “Poisson distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-05-25; URL: https://en.wikipedia.org/wiki/Poisson_distribution#Definitions.

1.5.2 Probability mass function

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a Poisson distribution (\rightarrow II/1.5.1):

$$X \sim \text{Poiss}(\lambda) . \quad (1)$$

Then, the probability mass function (\rightarrow I/1.6.1) of X is

$$f_X(x) = \frac{\lambda^x e^{-\lambda}}{x!}, \quad x \in \mathbb{N}_0 . \quad (2)$$

Proof: This follows directly from the definition of the Poisson distribution (\rightarrow II/1.5.1). ■

1.5.3 Mean

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a Poisson distribution (\rightarrow II/1.5.1):

$$X \sim \text{Poiss}(\lambda) . \quad (1)$$

Then, the mean or expected value (\rightarrow I/1.12.1) of X is

$$\mathbb{E}(X) = \lambda . \quad (2)$$

Proof: The expected value of a discrete random variable (\rightarrow I/1.12.1) is defined as

$$\mathbb{E}(X) = \sum_{x \in \mathcal{X}} x \cdot f_X(x) , \quad (3)$$

such that, with the probability mass function of the Poisson distribution (\rightarrow II/1.5.2), we have:

$$\begin{aligned}
E(X) &= \sum_{x=0}^{\infty} x \cdot \frac{\lambda^x e^{-\lambda}}{x!} \\
&= \sum_{x=1}^{\infty} x \cdot \frac{\lambda^x e^{-\lambda}}{x!} \\
&= e^{-\lambda} \cdot \sum_{x=1}^{\infty} \frac{x}{x!} \lambda^x \\
&= \lambda e^{-\lambda} \cdot \sum_{x=1}^{\infty} \frac{\lambda^{x-1}}{(x-1)!} .
\end{aligned} \tag{4}$$

Substituting $z = x - 1$, such that $x = z + 1$, we get:

$$E(X) = \lambda e^{-\lambda} \cdot \sum_{z=0}^{\infty} \frac{\lambda^z}{z!} . \tag{5}$$

Using the power series expansion of the exponential function

$$e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!} , \tag{6}$$

the expected value of X finally becomes

$$\begin{aligned}
E(X) &= \lambda e^{-\lambda} \cdot e^{\lambda} \\
&= \lambda .
\end{aligned} \tag{7}$$

■

Sources:

- ProofWiki (2020): “Expectation of Poisson Distribution”; in: *ProofWiki*, retrieved on 2020-08-19; URL: https://proofwiki.org/wiki/Expectation_of_Poisson_Distribution.

1.5.4 Variance

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a Poisson distribution (\rightarrow II/1.5.1):

$$X \sim \text{Poiss}(\lambda) . \tag{1}$$

Then, the variance (\rightarrow I/1.13.1) of X is

$$\text{Var}(X) = \lambda . \tag{2}$$

Proof: The variance (\rightarrow I/1.13.1) can be expressed in terms of expected values (\rightarrow I/1.13.4) as

$$\text{Var}(X) = E(X^2) - E(X)^2 . \tag{3}$$

The expected value of a Poisson random variable (\rightarrow II/1.5.3) is

$$E(X) = \lambda . \tag{4}$$

Let us now consider the expectation (\rightarrow I/1.12.1) of $X(X-1)$ which is defined as

$$E[X(X-1)] = \sum_{x \in \mathcal{X}} x(x-1) \cdot f_X(x) , \quad (5)$$

such that, with the probability mass function of the Poisson distribution (\rightarrow II/1.5.2), we have:

$$\begin{aligned} E[X(X-1)] &= \sum_{x=0}^{\infty} x(x-1) \cdot \frac{\lambda^x e^{-\lambda}}{x!} \\ &= \sum_{x=2}^{\infty} x(x-1) \cdot \frac{\lambda^x e^{-\lambda}}{x!} \\ &= e^{-\lambda} \cdot \sum_{x=2}^{\infty} x(x-1) \cdot \frac{\lambda^x}{x \cdot (x-1) \cdot (x-2)!} \\ &= \lambda^2 \cdot e^{-\lambda} \cdot \sum_{x=2}^{\infty} \frac{\lambda^{x-2}}{(x-2)!} . \end{aligned} \quad (6)$$

Substituting $z = x - 2$, such that $x = z + 2$, we get:

$$E[X(X-1)] = \lambda^2 \cdot e^{-\lambda} \cdot \sum_{z=0}^{\infty} \frac{\lambda^z}{z!} . \quad (7)$$

Using the power series expansion of the exponential function

$$e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!} , \quad (8)$$

the expected value of $X(X-1)$ finally becomes

$$E[X(X-1)] = \lambda^2 \cdot e^{-\lambda} \cdot e^{\lambda} = \lambda^2 . \quad (9)$$

Note that this expectation can be written as

$$E[X(X-1)] = E(X^2 - X) = E(X^2) - E(X) , \quad (10)$$

such that, with (9) and (4), we have:

$$E(X^2) - E(X) = \lambda^2 \quad \Rightarrow \quad E(X^2) = \lambda^2 + \lambda . \quad (11)$$

Plugging (11) and (4) into (3), the variance of a Poisson random variable finally becomes

$$\text{Var}(X) = \lambda^2 + \lambda - \lambda^2 = \lambda . \quad (12)$$

■

Sources:

- jbststatistics (2013): “The Poisson Distribution: Mathematically Deriving the Mean and Variance”; in: *YouTube*, retrieved on 2021-04-29; URL: https://www.youtube.com/watch?v=65n_v92JZeE.

1.5.5 Shannon entropy

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a Poisson distribution (\rightarrow II/1.5.1):

$$X \sim \text{Poiss}(\lambda) . \quad (1)$$

Then, the (Shannon) entropy (\rightarrow I/2.1.1) of X in nats is

$$H(X) = \lambda(1 - \ln \lambda) + e^{-\lambda} \sum_{x=0}^{\infty} \frac{\lambda^x \ln x!}{x!} . \quad (2)$$

Proof: The entropy (\rightarrow I/2.1.1) is defined as the probability-weighted average of the logarithmized probabilities for all possible values:

$$H(X) = - \sum_{x \in \mathcal{X}} p(x) \cdot \log_b p(x) . \quad (3)$$

Entropy is measured in nats by setting $b = e$. Then, with the probability mass function of the Poisson distribution (\rightarrow II/1.5.2), we have:

$$\begin{aligned} H(X) &= - \sum_{x \in \mathcal{X}} p(x) \cdot \log_e p(x) \\ &= - \sum_{x=0}^{\infty} \frac{\lambda^x e^{-\lambda}}{x!} \cdot \ln \frac{\lambda^x e^{-\lambda}}{x!} \\ &= -e^{-\lambda} \sum_{x=0}^{\infty} \frac{\lambda^x}{x!} [\ln \lambda^x + \ln e^{-\lambda} - \ln x!] \\ &= -e^{-\lambda} \sum_{x=0}^{\infty} \frac{\lambda^x \ln \lambda^x}{x!} - e^{-\lambda} \sum_{x=0}^{\infty} \frac{\lambda^x \ln e^{-\lambda}}{x!} + e^{-\lambda} \sum_{x=0}^{\infty} \frac{\lambda^x \ln x!}{x!} \\ &= -e^{-\lambda} \sum_{x=0}^{\infty} \frac{\lambda^x x \cdot \ln \lambda}{x!} - e^{-\lambda} \sum_{x=0}^{\infty} \frac{\lambda^x (-\lambda) \cdot \ln e}{x!} + e^{-\lambda} \sum_{x=0}^{\infty} \frac{\lambda^x \ln x!}{x!} \\ &= -e^{-\lambda} \ln \lambda \sum_{x=0}^{\infty} \frac{\lambda^x \cdot x}{x!} + e^{-\lambda} \lambda \sum_{x=0}^{\infty} \frac{\lambda^x}{x!} + e^{-\lambda} \sum_{x=0}^{\infty} \frac{\lambda^x \ln x!}{x!} . \end{aligned} \quad (4)$$

Using the relation $x!/x = (x-1)!$, the first term can be developed as follows

$$\begin{aligned}
e^{-\lambda} \ln \lambda \sum_{x=0}^{\infty} \frac{\lambda^x \cdot x}{x!} &= e^{-\lambda} \cdot \ln \lambda \cdot \sum_{x=0}^{\infty} \lambda \cdot \frac{\lambda^x}{\lambda} \cdot \frac{x}{x!} \\
&= e^{-\lambda} \cdot \lambda \cdot \ln \lambda \cdot \sum_{x=0}^{\infty} \frac{\lambda^{x-1}}{(x-1)!} \\
&= e^{-\lambda} \cdot \lambda \cdot \ln \lambda \cdot \left(\frac{\lambda^{-1}}{(-1)!} + \sum_{x=0}^{\infty} \frac{\lambda^x}{x!} \right) \\
&= e^{-\lambda} \cdot \lambda \cdot \ln \lambda \cdot \left(\frac{1}{\lambda} \cdot \frac{0}{0!} + \sum_{x=0}^{\infty} \frac{\lambda^x}{x!} \right) \\
&= e^{-\lambda} \cdot \lambda \cdot \ln \lambda \cdot \sum_{x=0}^{\infty} \frac{\lambda^x}{x!} ,
\end{aligned} \tag{5}$$

such that equation (4) becomes

$$H(X) = -e^{-\lambda} \lambda \ln \lambda \sum_{x=0}^{\infty} \frac{\lambda^x}{x!} + e^{-\lambda} \lambda \sum_{x=0}^{\infty} \frac{\lambda^x}{x!} + e^{-\lambda} \sum_{x=0}^{\infty} \frac{\lambda^x \ln x!}{x!} . \tag{6}$$

Using the power series form of the exponential function

$$e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!} , \tag{7}$$

equation (6) finally becomes

$$\begin{aligned}
H(X) &= -e^{-\lambda} \lambda \ln \lambda e^{\lambda} + e^{-\lambda} \lambda e^{\lambda} + e^{-\lambda} \sum_{x=0}^{\infty} \frac{\lambda^x \ln x!}{x!} \\
&= -\lambda \ln \lambda + \lambda + e^{-\lambda} \sum_{x=0}^{\infty} \frac{\lambda^x \ln x!}{x!} \\
&= \lambda (1 - \ln \lambda) + e^{-\lambda} \sum_{x=0}^{\infty} \frac{\lambda^x \ln x!}{x!} .
\end{aligned} \tag{8}$$

■

2 Multivariate discrete distributions

2.1 Categorical distribution

2.1.1 Definition

Definition: Let X be a random vector (\rightarrow I/1.2.3). Then, X is said to follow a categorical distribution with category probabilities p_1, \dots, p_k

$$X \sim \text{Cat}([p_1, \dots, p_k]) , \quad (1)$$

if $X = e_i$ with probability (\rightarrow I/1.3.1) p_i for all $i = 1, \dots, k$, where e_i is the i -th elementary row vector, i.e. a $1 \times k$ vector of zeros with a one in i -th position.

Sources:

- Wikipedia (2020): “Categorical distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-03-22; URL: https://en.wikipedia.org/wiki/Categorical_distribution.

2.1.2 Probability mass function

Theorem: Let X be a random vector (\rightarrow I/1.2.3) following a categorical distribution (\rightarrow II/2.1.1):

$$X \sim \text{Cat}([p_1, \dots, p_k]) . \quad (1)$$

Then, the probability mass function (\rightarrow I/1.6.1) of X is

$$f_X(x) = \begin{cases} p_1 , & \text{if } x = e_1 \\ \vdots & \vdots \\ p_k , & \text{if } x = e_k . \end{cases} \quad (2)$$

where e_1, \dots, e_k are the $1 \times k$ elementary row vectors.

Proof: This follows directly from the definition of the categorical distribution (\rightarrow II/2.1.1). ■

2.1.3 Mean

Theorem: Let X be a random vector (\rightarrow I/1.2.3) following a categorical distribution (\rightarrow II/2.1.1):

$$X \sim \text{Cat}([p_1, \dots, p_k]) . \quad (1)$$

Then, the mean or expected value (\rightarrow I/1.12.1) of X is

$$E(X) = [p_1, \dots, p_k] . \quad (2)$$

Proof: If we conceive the outcome of a categorical distribution (\rightarrow II/2.1.1) to be a $1 \times k$ vector, then the elementary row vectors $e_1 = [1, 0, \dots, 0]$, ..., $e_k = [0, \dots, 0, 1]$ are all the possible outcomes and they occur with probabilities $\Pr(X = e_1) = p_1$, ..., $\Pr(X = e_k) = p_k$. Consequently, the expected value (\rightarrow I/1.12.1) is

$$\begin{aligned}
E(X) &= \sum_{x \in \mathcal{X}} x \cdot \Pr(X = x) \\
&= \sum_{i=1}^k e_i \cdot \Pr(X = e_i) \\
&= \sum_{i=1}^k e_i \cdot p_i \\
&= [p_1, \dots, p_k] .
\end{aligned} \tag{3}$$

■

2.1.4 Covariance

Theorem: Let X be a random vector (\rightarrow I/1.2.3) following a categorical distribution (\rightarrow II/2.1.1):

$$X \sim \text{Cat}(n, p) . \tag{1}$$

Then, the covariance matrix (\rightarrow I/1.16.1) of X is

$$\text{Cov}(X) = \text{diag}(p) - pp^T . \tag{2}$$

Proof: The categorical distribution (\rightarrow II/2.1.1) is a special case of the multinomial distribution (\rightarrow II/2.2.1) in which $n = 1$:

$$X \sim \text{Mult}(n, p) \quad \text{and} \quad n = 1 \quad \Rightarrow \quad X \sim \text{Cat}(p) . \tag{3}$$

The covariance matrix of the multinomial distribution (\rightarrow II/2.2.5) is

$$\text{Cov}(X) = n (\text{diag}(p) - pp^T) , \tag{4}$$

thus the covariance matrix of the categorical distribution is

$$\text{Cov}(X) = \text{diag}(p) - pp^T . \tag{5}$$

■

2.1.5 Shannon entropy

Theorem: Let X be a random vector (\rightarrow I/1.2.3) following a categorical distribution (\rightarrow II/2.1.1):

$$X \sim \text{Cat}(p) . \tag{1}$$

Then, the (Shannon) entropy (\rightarrow I/2.1.1) of X is

$$H(X) = - \sum_{i=1}^k p_i \cdot \log p_i . \tag{2}$$

Proof: The entropy (\rightarrow I/2.1.1) is defined as the probability-weighted average of the logarithmized probabilities for all possible values:

$$H(X) = - \sum_{x \in \mathcal{X}} p(x) \cdot \log_b p(x) . \quad (3)$$

Since there are k possible values for a categorical random vector (\rightarrow II/2.1.1) with probabilities given by the entries (\rightarrow II/2.1.2) of the $1 \times k$ vector p , we have:

$$\begin{aligned} H(X) &= -\Pr(X = e_1) \cdot \log \Pr(X = e_1) - \dots - \Pr(X = e_k) \cdot \log \Pr(X = e_k) \\ H(X) &= - \sum_{i=1}^k \Pr(X = e_i) \cdot \log \Pr(X = e_i) \\ H(X) &= - \sum_{i=1}^k p_i \cdot \log p_i . \end{aligned} \quad (4)$$

■

2.2 Multinomial distribution

2.2.1 Definition

Definition: Let X be a random vector (\rightarrow I/1.2.3). Then, X is said to follow a multinomial distribution with number of trials n and category probabilities p_1, \dots, p_k

$$X \sim \text{Mult}(n, [p_1, \dots, p_k]) , \quad (1)$$

if X are the numbers of observations belonging to k distinct categories in n independent (\rightarrow I/1.3.6) trials, where each trial has k possible outcomes (\rightarrow II/2.1.1) and the category probabilities are identical across trials.

Sources:

- Wikipedia (2020): “Binomial distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-03-22; URL: https://en.wikipedia.org/wiki/Multinomial_distribution.

2.2.2 Probability mass function

Theorem: Let X be a random vector (\rightarrow I/1.2.3) following a multinomial distribution (\rightarrow II/2.2.1):

$$X \sim \text{Mult}(n, [p_1, \dots, p_k]) . \quad (1)$$

Then, the probability mass function (\rightarrow I/1.6.1) of X is

$$f_X(x) = \binom{n}{x_1, \dots, x_k} \prod_{i=1}^k p_i^{x_i} . \quad (2)$$

Proof: A multinomial variable (\rightarrow II/2.2.1) is defined as a vector of the numbers of observations belonging to k distinct categories in n independent (\rightarrow I/1.3.6) trials, where each trial has k possible outcomes (\rightarrow II/2.1.1) and the category probabilities (\rightarrow I/1.3.1) are identical across trials.

Since the individual trials are independent (\rightarrow II/2.2.1) and joint probability factorizes under independence (\rightarrow I/1.3.9), the probability of a particular series of x_1 observations for category 1, x_2 observations for category 2, ... etc., when order does matter, is

$$\prod_{i=1}^k p_i^{x_i} . \quad (3)$$

When order does not matter, there is a number of series consisting of x_1 observations for category 1, x_2 observations for category 2, ... etc. This number is equal to the number of possibilities in which x_1 category 1 objects, x_2 category 2 objects, ... etc. can be distributed in a sequence of n objects which is given by the multinomial coefficient that can be expressed in terms of factorials:

$$\binom{n}{x_1, \dots, x_k} = \frac{n!}{x_1! \cdot \dots \cdot x_k!} . \quad (4)$$

In order to obtain the probability of x_1 observations for category 1, x_2 observations for category 2, ... etc., when order does not matter, the probability in (3) has to be multiplied with the number of possibilities in (4) which gives

$$p(X = x|n, [p_1, \dots, p_k]) = \binom{n}{x_1, \dots, x_k} \prod_{i=1}^k p_i^{x_i} \quad (5)$$

which is equivalent to the expression above. ■

2.2.3 Cumulative distribution function

Theorem: Let X be a random vector (\rightarrow I/1.2.3) following a multinomial distribution (\rightarrow II/2.2.1):

$$X \sim \text{Mult}(n, [p_1, \dots, p_k]) . \quad (1)$$

Then, 1) the joint cumulative distribution function (\rightarrow I/1.8.11) of X is

$$F_X(x) = \binom{n}{x_1, \dots, x_k} \prod_{i=1}^k p_i^{x_i} \quad (2)$$

and 2) the marginal (\rightarrow I/1.5.3) cumulative distribution function (\rightarrow I/1.8.1) of each X_i is

$$F_{X_i}(x_i) = \sum_{k=0}^{x_i} \binom{n}{k} p_i^k (1 - p_i)^{n-k} . \quad (3)$$

Proof: The probability mass function of the multinomial distribution (\rightarrow II/2.2.2) is

$$f_X(x) = \binom{n}{x_1, \dots, x_k} \prod_{i=1}^k p_i^{x_i} , \quad (4)$$

1) The joint cumulative distribution function (CDF) of a random vector (\rightarrow I/1.8.11) is defined as

$$F_X(x) = \Pr(X_1 \leq x_1, \dots, X_n \leq x_n) \quad (5)$$

which, in terms of the probability mass function, is given by (\rightarrow I/1.8.5)

$$F_X(x) = \sum_{t_1 \leq x_1} \dots \sum_{t_n \leq x_n} f_X(t_1, \dots, t_n) . \quad (6)$$

For a given set of counts x_1, \dots, x_k satisfying $\sum_{i=1}^k x_i = n$, we define the set of eligible values t_1, \dots, t_k for the CDF:

$$\mathcal{T}(x) = \left\{ (t_1, \dots, t_k) \mid t_i \in \mathbb{N}_0, 0 \leq t_i \leq x_i, \sum_{i=1}^k t_i = n \right\} . \quad (7)$$

Since any eligible set of counts t_1, \dots, t_k must add up to n , this set is equivalent to

$$\mathcal{T}(x) = \{(x_1, \dots, x_k)\} . \quad (8)$$

Therefore, the CDF is equal to the probability mass function at $t = x$:

$$F_X(x) \stackrel{(6)}{=} \sum_{t \in \mathcal{T}(x)} f_X(t_1, \dots, t_k) = f_X(x_1, \dots, x_k) . \quad (9)$$

so that the joint cumulative distribution function of the multinomial distribution becomes

$$F_X(x) \stackrel{(4)}{=} \binom{n}{x_1, \dots, x_k} \prod_{i=1}^k p_i^{x_i} . \quad (10)$$

2) The marginal distributions for the multinomial distribution (\rightarrow II/2.2.7) are

$$X_i \sim \text{Bin}(n, p_i) \quad \text{for all } i = 1, \dots, k . \quad (11)$$

Thus, the marginal cumulative distribution function of any entry X_i is equal to the cumulative distribution function of the binomial distribution (\rightarrow II/1.3.4):

$$F_{X_i}(x_i) = \sum_{k=0}^{x_i} \binom{n}{k} p_i^k (1 - p_i)^{n-k} . \quad (12)$$

■

2.2.4 Mean

Theorem: Let X be a random vector (\rightarrow I/1.2.3) following a multinomial distribution (\rightarrow II/2.2.1):

$$X \sim \text{Mult}(n, [p_1, \dots, p_k]) . \quad (1)$$

Then, the mean or expected value (\rightarrow I/1.12.1) of X is

$$\mathbb{E}(X) = [np_1, \dots, np_k] . \quad (2)$$

Proof: By definition, a multinomial random variable (\rightarrow II/2.2.1) is the sum of n independent and identical categorical trials (\rightarrow II/2.1.1) with category probabilities p_1, \dots, p_k . Therefore, the expected value is

$$\mathbb{E}(X) = \mathbb{E}(X_1 + \dots + X_n) \quad (3)$$

and because the expected value is a linear operator (\rightarrow I/1.12.5), this is equal to

$$\begin{aligned} E(X) &= E(X_1) + \dots + E(X_n) \\ &= \sum_{i=1}^n E(X_i) . \end{aligned} \quad (4)$$

With the expected value of the categorical distribution (\rightarrow II/2.1.3), we have:

$$E(X) = \sum_{i=1}^n [p_1, \dots, p_k] = n \cdot [p_1, \dots, p_k] = [np_1, \dots, np_k] . \quad (5)$$

■

2.2.5 Covariance

Theorem: Let X be a random vector (\rightarrow I/1.2.3) following a multinomial distribution (\rightarrow II/2.2.1):

$$[X_1, \dots, X_k] = X \sim \text{Mult}(n, p), \quad n \in \mathbb{N}, \quad p = [p_1, \dots, p_k]^T . \quad (1)$$

Then, the covariance matrix (\rightarrow I/1.16.1) of X is

$$\text{Cov}(X) = n (\text{diag}(p) - pp^T) . \quad (2)$$

Proof: We first observe that the sample space (\rightarrow I/1.1.2) of each coordinate X_i is $\{0, 1, \dots, n\}$ and X_i is the sum of independent draws of category i , which is drawn with probability p_i . Thus each coordinate follows a binomial distribution (\rightarrow II/1.3.1):

$$X_i \stackrel{\text{i.i.d.}}{\sim} \text{Bin}(n, p_i), \quad i = 1, \dots, k , \quad (3)$$

which has the variance (\rightarrow II/1.3.7) $\text{Var}(X_i) = np_i(1 - p_i) = n(p_i - p_i^2)$, constituting the elements of the main diagonal in $\text{Cov}(X)$ in (2). To prove $\text{Cov}(X_i, X_j) = -np_i p_j$ for $i \neq j$ (which constitutes the off-diagonal elements of the covariance matrix), we first recognize that

$$X_i = \sum_{k=1}^n \mathbb{I}_i(k), \quad \text{with} \quad \mathbb{I}_i(k) = \begin{cases} 1 & \text{if } k\text{-th draw was of category } i, \\ 0 & \text{otherwise} , \end{cases} \quad (4)$$

where the indicator function \mathbb{I}_i is a Bernoulli-distributed (\rightarrow II/1.2.1) random variable with the expected value (\rightarrow II/1.2.4) p_i . Then, we have

$$\begin{aligned}
\text{Cov}(X_i, X_j) &= \text{Cov} \left(\sum_{k=1}^n \mathbb{I}_i(k), \sum_{l=1}^n \mathbb{I}_j(l) \right) \\
&= \sum_{k=1}^n \sum_{l=1}^n \text{Cov}(\mathbb{I}_i(k), \mathbb{I}_j(l)) \\
&= \sum_{k=1}^n \left[\text{Cov}(\mathbb{I}_i(k), \mathbb{I}_j(k)) + \underbrace{\sum_{\substack{l=1 \\ l \neq k}}^n \text{Cov}(\mathbb{I}_i(k), \mathbb{I}_j(l))}_{=0} \right] \\
&\stackrel{i \neq j}{=} \sum_{k=1}^n \left(\text{E} \left(\underbrace{\mathbb{I}_i(k) \mathbb{I}_j(k)}_{=0} \right) - \text{E}(\mathbb{I}_i(k)) \text{E}(\mathbb{I}_j(k)) \right) \\
&= - \sum_{k=1}^n \text{E}(\mathbb{I}_i(k)) \text{E}(\mathbb{I}_j(k)) \\
&= -np_i p_j,
\end{aligned} \tag{5}$$

as desired. ■

Sources:

- Tutz G (2012): “Multinomial Response Models”; in: *Regression for Categorical Data*, pp. 209ff.;
URL: <https://www.cambridge.org/core/books/regression-for-categorical-data/B71F71F2A484E2DF88256>
DOI: 10.1017/CBO9780511842061.

2.2.6 Shannon entropy

Theorem: Let X be a random vector (\rightarrow I/1.2.3) following a multinomial distribution (\rightarrow II/2.2.1):

$$X \sim \text{Mult}(n, p). \tag{1}$$

Then, the (Shannon) entropy (\rightarrow I/2.1.1) of X is

$$H(X) = n \cdot H_{\text{cat}}(p) - E_{\text{lmc}}(n, p) \tag{2}$$

where $H_{\text{cat}}(p)$ is the categorical entropy function, i.e. the (Shannon) entropy of the categorical distribution (\rightarrow II/2.1.5) with category probabilities p

$$H_{\text{cat}}(p) = - \sum_{i=1}^k p_i \cdot \log p_i \tag{3}$$

and $E_{\text{lmc}}(n, p)$ is the expected value (\rightarrow I/1.12.1) of the logarithmized multinomial coefficient (\rightarrow II/2.2.2) with superset size n

$$E_{\text{lmc}}(n, p) = \text{E} \left[\log \binom{n}{X_1, \dots, X_k} \right] \quad \text{where } X \sim \text{Mult}(n, p). \tag{4}$$

Proof: The entropy (\rightarrow I/2.1.1) is defined as the probability-weighted average of the logarithmized probabilities for all possible values:

$$H(X) = - \sum_{x \in \mathcal{X}} p(x) \cdot \log_b p(x) . \quad (5)$$

The probability mass function of the multinomial distribution (\rightarrow II/2.2.2) is

$$f_X(x) = \binom{n}{x_1, \dots, x_k} \prod_{i=1}^k p_i^{x_i} \quad (6)$$

Let $\mathcal{X}_{n,k}$ be the set of all vectors $x \in \mathbb{N}^{1 \times k}$ satisfying $\sum_{i=1}^k x_i = n$. Then, we have:

$$\begin{aligned} H(X) &= - \sum_{x \in \mathcal{X}_{n,k}} f_X(x) \cdot \log f_X(x) \\ &= - \sum_{x \in \mathcal{X}_{n,k}} f_X(x) \cdot \log \left[\binom{n}{x_1, \dots, x_k} \prod_{i=1}^k p_i^{x_i} \right] \\ &= - \sum_{x \in \mathcal{X}_{n,k}} f_X(x) \cdot \left[\log \binom{n}{x_1, \dots, x_k} + \sum_{i=1}^k x_i \cdot \log p_i \right] . \end{aligned} \quad (7)$$

Since the first factor in the sum corresponds to the probability mass (\rightarrow I/1.6.1) of $X = x$, we can rewrite this as the sum of the expected values (\rightarrow I/1.12.1) of the functions (\rightarrow I/1.12.9) of the discrete random variable (\rightarrow I/1.2.6) x in the square bracket:

$$\begin{aligned} H(X) &= - \left\langle \log \binom{n}{x_1, \dots, x_k} \right\rangle_{p(x)} - \left\langle \sum_{i=1}^k x_i \cdot \log p_i \right\rangle_{p(x)} \\ &= - \left\langle \log \binom{n}{x_1, \dots, x_k} \right\rangle_{p(x)} - \sum_{i=1}^k \langle x_i \cdot \log p_i \rangle_{p(x)} . \end{aligned} \quad (8)$$

Using the expected value of the multinomial distribution (\rightarrow II/2.2.4), i.e. $X \sim \text{Mult}(n, p) \Rightarrow \langle x_i \rangle = np_i$, this gives:

$$\begin{aligned} H(X) &= - \left\langle \log \binom{n}{x_1, \dots, x_k} \right\rangle_{p(x)} - \sum_{i=1}^k np_i \cdot \log p_i \\ &= - \left\langle \log \binom{n}{x_1, \dots, x_k} \right\rangle_{p(x)} - n \sum_{i=1}^k p_i \cdot \log p_i . \end{aligned} \quad (9)$$

Finally, we note that the first term is the negative expected value (\rightarrow I/1.12.1) of the logarithm of a multinomial coefficient (\rightarrow II/2.2.2) and that the second term is the entropy of the categorical distribution (\rightarrow II/2.1.5), such that we finally get:

$$H(X) = n \cdot H_{\text{cat}}(p) - E_{\text{lmc}}(n, p) . \quad (10)$$

■

2.2.7 Marginal distributions

Theorem: Let X be a random vector (\rightarrow I/1.2.3) following a multinomial distribution (\rightarrow II/2.2.1):

$$X \sim \text{Mult}(n, [p_1, \dots, p_k]) . \quad (1)$$

Then, the marginal distribution (\rightarrow I/1.5.3) of any entry X_i is a binomial distribution (\rightarrow II/1.3.1):

$$X_i \sim \text{Bin}(n, p_i) \quad \text{for all } i = 1, \dots, k . \quad (2)$$

Proof: The entries of a multinomial (\rightarrow II/2.2.1) random vector X are the numbers of observations belonging to k distinct categories in n independent (\rightarrow I/1.3.6) trials where p_1, \dots, p_k are the category probabilities (\rightarrow II/2.2.1) identical across trials.

Let us define for each category $i = 1, \dots, k$ and each trial $j = 1, \dots, n$:

$$Y_{ij} = \begin{cases} 0 , & \text{if } X_i = 0 \text{ in trial } j \\ 1 , & \text{if } X_i = 1 \text{ in trial } j . \end{cases} \quad (3)$$

Since $\Pr(Y_{ij} = 1) = p_i$ and $\Pr(Y_{ij} = 0) = 1 - p_i$, Y_{ij} is a Bernoulli (\rightarrow II/1.2.1) random variable with success probability (\rightarrow II/1.2.1) p_i :

$$Y_{ij} \sim \text{Bern}(p_i) . \quad (4)$$

Moreover, each X_i is the sum of the corresponding Y_{ij} over all trials

$$X_i = \sum_{j=1}^n Y_{ij} , \quad (5)$$

i.e. X_i is a sum of independent Bernoulli random variables which, by definition, follows a binomial distribution (\rightarrow II/1.3.1):

$$X_i \sim \text{Bin}(n, p_i) . \quad (6)$$

■

3 Univariate continuous distributions

3.1 Continuous uniform distribution

3.1.1 Definition

Definition: Let X be a continuous random variable (\rightarrow I/1.2.2). Then, X is said to be uniformly distributed with minimum a and maximum b

$$X \sim \mathcal{U}(a, b) , \quad (1)$$

if and only if each value between and including a and b occurs with the same probability.

Sources:

- Wikipedia (2020): “Uniform distribution (continuous)”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-01-27; URL: [https://en.wikipedia.org/wiki/Uniform_distribution_\(continuous\)](https://en.wikipedia.org/wiki/Uniform_distribution_(continuous)).

3.1.2 Standard uniform distribution

Definition: Let X be a random variable (\rightarrow I/1.2.2). Then, X is said to be standard uniformly distributed, if X follows a continuous uniform distribution (\rightarrow II/3.1.1) with minimum $a = 0$ and maximum $b = 1$:

$$X \sim \mathcal{U}(0, 1) . \quad (1)$$

Sources:

- Wikipedia (2021): “Continuous uniform distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-07-23; URL: https://en.wikipedia.org/wiki/Continuous_uniform_distribution#Standard_uniform.

3.1.3 Probability density function

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a continuous uniform distribution (\rightarrow II/3.1.1):

$$X \sim \mathcal{U}(a, b) . \quad (1)$$

Then, the probability density function (\rightarrow I/1.7.1) of X is

$$f_X(x) = \begin{cases} \frac{1}{b-a} , & \text{if } a \leq x \leq b \\ 0 , & \text{otherwise .} \end{cases} \quad (2)$$

Proof: A continuous uniform variable is defined as (\rightarrow II/3.1.1) having a constant probability density between minimum a and maximum b . Therefore,

$$\begin{aligned} f_X(x) &\propto 1 \quad \text{for all } x \in [a, b] \quad \text{and} \\ f_X(x) &= 0, \quad \text{if } x < a \quad \text{or } x > b . \end{aligned} \quad (3)$$

To ensure that $f_X(x)$ is a proper probability density function (\rightarrow I/1.7.1), the integral over all non-zero probabilities has to sum to 1. Therefore,

$$f_X(x) = \frac{1}{c(a, b)} \quad \text{for all } x \in [a, b] \quad (4)$$

where the normalization factor $c(a, b)$ is specified, such that

$$\frac{1}{c(a, b)} \int_a^b 1 \, dx = 1 . \quad (5)$$

Solving this for $c(a, b)$, we obtain:

$$\begin{aligned} \int_a^b 1 \, dx &= c(a, b) \\ [x]_a^b &= c(a, b) \\ c(a, b) &= b - a . \end{aligned} \quad (6)$$

■

3.1.4 Cumulative distribution function

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a continuous uniform distribution (\rightarrow II/3.1.1):

$$X \sim \mathcal{U}(a, b) . \quad (1)$$

Then, the cumulative distribution function (\rightarrow I/1.8.1) of X is

$$F_X(x) = \begin{cases} 0 , & \text{if } x < a \\ \frac{x-a}{b-a} , & \text{if } a \leq x \leq b \\ 1 , & \text{if } x > b . \end{cases} \quad (2)$$

Proof: The probability density function of the continuous uniform distribution (\rightarrow II/3.1.3) is:

$$\mathcal{U}(x; a, b) = \begin{cases} \frac{1}{b-a} , & \text{if } a \leq x \leq b \\ 0 , & \text{otherwise} . \end{cases} \quad (3)$$

Thus, the cumulative distribution function (\rightarrow I/1.8.1) is:

$$F_X(x) = \int_{-\infty}^x \mathcal{U}(z; a, b) \, dz \quad (4)$$

First of all, if $x < a$, we have

$$F_X(x) = \int_{-\infty}^x 0 \, dz = 0 . \quad (5)$$

Moreover, if $a \leq x \leq b$, we have using (3)

$$\begin{aligned}
F_X(x) &= \int_{-\infty}^a \mathcal{U}(z; a, b) \, dz + \int_a^x \mathcal{U}(z; a, b) \, dz \\
&= \int_{-\infty}^a 0 \, dz + \int_a^x \frac{1}{b-a} \, dz \\
&= 0 + \frac{1}{b-a} [z]_a^x \\
&= \frac{x-a}{b-a} .
\end{aligned} \tag{6}$$

Finally, if $x > b$, we have

$$\begin{aligned}
F_X(x) &= \int_{-\infty}^b \mathcal{U}(z; a, b) \, dz + \int_b^x \mathcal{U}(z; a, b) \, dz \\
&= F_X(b) + \int_b^x 0 \, dz \\
&= \frac{b-a}{b-a} + 0 \\
&= 1 .
\end{aligned} \tag{7}$$

This completes the proof. ■

3.1.5 Quantile function

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a continuous uniform distribution (\rightarrow II/3.1.1):

$$X \sim \mathcal{U}(a, b) . \tag{1}$$

Then, the quantile function (\rightarrow I/1.11.1) of X is

$$Q_X(p) = \begin{cases} -\infty , & \text{if } p = 0 \\ bp + a(1-p) , & \text{if } p > 0 . \end{cases} \tag{2}$$

Proof: The cumulative distribution function of the continuous uniform distribution (\rightarrow II/3.1.4) is:

$$F_X(x) = \begin{cases} 0 , & \text{if } x < a \\ \frac{x-a}{b-a} , & \text{if } a \leq x \leq b \\ 1 , & \text{if } x > b . \end{cases} \tag{3}$$

The quantile function (\rightarrow I/1.11.1) $Q_X(p)$ is defined as the smallest x , such that $F_X(x) = p$:

$$Q_X(p) = \min \{x \in \mathbb{R} \mid F_X(x) = p\} . \tag{4}$$

Thus, we have $Q_X(p) = -\infty$, if $p = 0$. When $p > 0$, it holds that (\rightarrow I/1.11.2)

$$Q_X(p) = F_X^{-1}(x) . \quad (5)$$

This can be derived by rearranging equation (3):

$$\begin{aligned} p &= \frac{x - a}{b - a} \\ x &= p(b - a) + a \\ x &= bp + a(1 - p) . \end{aligned} \quad (6)$$

■

3.1.6 Mean

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a continuous uniform distribution (\rightarrow II/3.1.1):

$$X \sim \mathcal{U}(a, b) . \quad (1)$$

Then, the mean or expected value (\rightarrow I/1.12.1) of X is

$$E(X) = \frac{1}{2}(a + b) . \quad (2)$$

Proof: The expected value (\rightarrow I/1.12.1) is the probability-weighted average over all possible values:

$$E(X) = \int_{\mathcal{X}} x \cdot f_X(x) \, dx . \quad (3)$$

With the probability density function of the continuous uniform distribution (\rightarrow II/3.1.3), this becomes:

$$\begin{aligned} E(X) &= \int_a^b x \cdot \frac{1}{b - a} \, dx \\ &= \left[\frac{1}{2} \frac{x^2}{b - a} \right]_a^b \\ &= \frac{1}{2} \frac{b^2 - a^2}{b - a} \\ &= \frac{1}{2} \frac{(b + a)(b - a)}{b - a} \\ &= \frac{1}{2}(a + b) . \end{aligned} \quad (4)$$

■

3.1.7 Median

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a continuous uniform distribution (\rightarrow II/3.1.1):

$$X \sim \mathcal{U}(a, b) . \quad (1)$$

Then, the median (\rightarrow I/1.18.1) of X is

$$\text{median}(X) = \frac{1}{2}(a + b) . \quad (2)$$

Proof: The median (\rightarrow I/1.18.1) is the value at which the cumulative distribution function (\rightarrow I/1.8.1) is $1/2$:

$$F_X(\text{median}(X)) = \frac{1}{2} . \quad (3)$$

The cumulative distribution function of the continuous uniform distribution (\rightarrow II/3.1.4) is

$$F_X(x) = \begin{cases} 0 , & \text{if } x < a \\ \frac{x-a}{b-a} , & \text{if } a \leq x \leq b \\ 1 , & \text{if } x > b . \end{cases} \quad (4)$$

Thus, the inverse CDF (\rightarrow II/3.1.5) is

$$x = bp + a(1 - p) . \quad (5)$$

Setting $p = 1/2$, we obtain:

$$\text{median}(X) = b \cdot \frac{1}{2} + a \cdot \left(1 - \frac{1}{2}\right) = \frac{1}{2}(a + b) . \quad (6)$$

■

3.1.8 Mode

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a continuous uniform distribution (\rightarrow II/3.1.1):

$$X \sim \mathcal{U}(a, b) . \quad (1)$$

Then, the mode (\rightarrow I/1.18.3) of X is

$$\text{mode}(X) \in [a, b] . \quad (2)$$

Proof: The mode (\rightarrow I/1.18.3) is the value which maximizes the probability density function (\rightarrow I/1.7.1):

$$\text{mode}(X) = \arg \max_x f_X(x) . \quad (3)$$

The probability density function of the continuous uniform distribution (\rightarrow II/3.1.3) is:

$$f_X(x) = \begin{cases} \frac{1}{b-a}, & \text{if } a \leq x \leq b \\ 0, & \text{otherwise.} \end{cases} \quad (4)$$

Since the PDF attains its only non-zero value whenever $a \leq x \leq b$,

$$\max_x f_X(x) = \frac{1}{b-a}, \quad (5)$$

any value in the interval $[a, b]$ may be considered the mode of X .

■

3.1.9 Variance

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a continuous uniform distribution (\rightarrow II/3.1.1):

$$X \sim \mathcal{U}(a, b). \quad (1)$$

Then, the variance (\rightarrow I/1.13.1) of X is

$$\text{Var}(X) = \frac{1}{12}(b-a)^2. \quad (2)$$

Proof: The variance (\rightarrow I/1.13.1) is the probability-weighted average of the squared deviation from the mean (\rightarrow I/1.12.1):

$$\text{Var}(X) = \int_{\mathbb{R}} (x - \text{E}(X))^2 \cdot f_X(x) \, dx. \quad (3)$$

With the expected value (\rightarrow II/3.1.6) and probability density function (\rightarrow II/3.1.3) of the continuous uniform distribution, this reads:

$$\begin{aligned}
\text{Var}(X) &= \int_a^b \left(x - \frac{1}{2}(a+b) \right)^2 \cdot \frac{1}{b-a} dx \\
&= \frac{1}{b-a} \cdot \int_a^b \left(x - \frac{a+b}{2} \right)^2 dx \\
&= \frac{1}{b-a} \cdot \left[\frac{1}{3} \left(x - \frac{a+b}{2} \right)^3 \right]_a^b \\
&= \frac{1}{3(b-a)} \cdot \left[\left(\frac{2x - (a+b)}{2} \right)^3 \right]_a^b \\
&= \frac{1}{3(b-a)} \cdot \left[\frac{1}{8} (2x - a - b)^3 \right]_a^b \\
&= \frac{1}{24(b-a)} \cdot [(2x - a - b)^3]_a^b \\
&= \frac{1}{24(b-a)} \cdot [(2b - a - b)^3 - (2a - a - b)^3] \\
&= \frac{1}{24(b-a)} \cdot [(b-a)^3 - (a-b)^3] \\
&= \frac{1}{24(b-a)} \cdot [(b-a)^3 + (-1)^3(a-b)^3] \\
&= \frac{1}{24(b-a)} \cdot [(b-a)^3 + (b-a)^3] \\
&= \frac{2(b-a)^3}{24(b-a)} \\
&= \frac{1}{12} (b-a)^2 .
\end{aligned} \tag{4}$$

■

3.1.10 Differential entropy

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a continuous uniform distribution (\rightarrow II/3.1.1):

$$X \sim \mathcal{U}(a, b) . \tag{1}$$

Then, the differential entropy (\rightarrow I/2.2.1) of X is

$$h(X) = \ln(b-a) . \tag{2}$$

Proof: The differential entropy (\rightarrow I/2.2.1) of a random variable is defined as

$$h(X) = - \int_{\mathcal{X}} p(x) \log_b p(x) dx . \tag{3}$$

To measure $h(X)$ in nats, we set $b = e$, such that

$$h(X) = - \int_{\mathcal{X}} p(x) \ln p(x) dx . \quad (4)$$

With the probability density function of the continuous uniform distribution (\rightarrow II/3.1.3), the differential entropy of X is:

$$\begin{aligned} h(X) &= - \int_a^b \frac{1}{b-a} \ln \left(\frac{1}{b-a} \right) dx \\ &= \frac{1}{b-a} \cdot \int_a^b \ln(b-a) dx \\ &= \frac{1}{b-a} \cdot [x \cdot \ln(b-a)]_a^b \\ &= \frac{1}{b-a} \cdot [b \cdot \ln(b-a) - a \cdot \ln(b-a)] \\ &= \frac{1}{b-a} (b-a) \ln(b-a) \\ &= \ln(b-a) . \end{aligned} \quad (5)$$

■

3.1.11 Kullback-Leibler divergence

Theorem: Let X be a random variable (\rightarrow I/1.2.2). Assume two continuous uniform distributions (\rightarrow II/3.1.1) P and Q specifying the probability distribution of X as

$$\begin{aligned} P : X &\sim \mathcal{U}(a_1, b_1) \\ Q : X &\sim \mathcal{U}(a_2, b_2) . \end{aligned} \quad (1)$$

Then, the Kullback-Leibler divergence (\rightarrow I/2.5.1) of P from Q is given by

$$\text{KL}[P || Q] = \ln \frac{b_2 - a_2}{b_1 - a_1} . \quad (2)$$

Proof: The KL divergence for a continuous random variable (\rightarrow I/2.5.1) is given by

$$\text{KL}[P || Q] = \int_{\mathcal{X}} p(x) \ln \frac{p(x)}{q(x)} dx . \quad (3)$$

This means that the KL divergence of P from Q is only defined, if for all $x \in \mathcal{X}$, $q(x) = 0$ implies $p(x) = 0$. Thus, $\text{KL}[P || Q]$ only exists, if $a_2 \leq a_1$ and $b_1 \leq b_2$, i.e. if P only places non-zero probability where Q also places non-zero probability, such that $q(x)$ is not zero for any $x \in \mathcal{X}$ where $p(x)$ is positive.

If this requirement is fulfilled, we can write

$$\text{KL}[P || Q] = \int_{-\infty}^{a_1} p(x) \ln \frac{p(x)}{q(x)} dx + \int_{a_1}^{b_1} p(x) \ln \frac{p(x)}{q(x)} dx + \int_{b_1}^{+\infty} p(x) \ln \frac{p(x)}{q(x)} dx \quad (4)$$

and because $p(x) = 0$ for any $x < a_1$ and any $x > b_1$, we have

$$\text{KL}[P || Q] = \int_{-\infty}^{a_1} 0 \cdot \ln \frac{0}{q(x)} dx + \int_{a_1}^{b_1} p(x) \ln \frac{p(x)}{q(x)} dx + \int_{b_1}^{+\infty} 0 \cdot \ln \frac{0}{q(x)} dx . \quad (5)$$

Now, $(0 \cdot \ln 0)$ is taken to be zero by convention (\rightarrow I/2.1.1), such that

$$\text{KL}[P || Q] = \int_{a_1}^{b_1} p(x) \ln \frac{p(x)}{q(x)} dx \quad (6)$$

and we can use the probability density function of the continuous uniform distribution (\rightarrow II/3.1.3) to evaluate:

$$\begin{aligned} \text{KL}[P || Q] &= \int_{a_1}^{b_1} \frac{1}{b_1 - a_1} \ln \frac{\frac{1}{b_1 - a_1}}{\frac{1}{b_2 - a_2}} dx \\ &= \frac{1}{b_1 - a_1} \ln \frac{b_2 - a_2}{b_1 - a_1} \int_{a_1}^{b_1} dx \\ &= \frac{1}{b_1 - a_1} \ln \frac{b_2 - a_2}{b_1 - a_1} [x]_{a_1}^{b_1} \\ &= \frac{1}{b_1 - a_1} \ln \frac{b_2 - a_2}{b_1 - a_1} (b_1 - a_1) \\ &= \ln \frac{b_2 - a_2}{b_1 - a_1} . \end{aligned} \quad (7)$$

■

3.1.12 Maximum entropy distribution

Theorem: The continuous uniform distribution (\rightarrow II/3.1.1) maximizes differential entropy (\rightarrow I/2.2.1) for a random variable (\rightarrow I/1.2.2) with a fixed range.

Proof: Without loss of generality, let us assume that the random variable X is in the following range: $a \leq X \leq b$.

Let $g(x)$ be the probability density function (\rightarrow I/1.7.1) of a continuous uniform distribution (\rightarrow II/3.1.1) with minimum a and maximum b and let $f(x)$ be an arbitrary probability density function (\rightarrow I/1.7.1) defined on the same support $\mathcal{X} = [a, b]$.

For a random variable (\rightarrow I/1.2.2) X with set of possible values \mathcal{X} and probability density function (\rightarrow I/1.7.1) $p(x)$, the differential entropy (\rightarrow I/2.2.1) is defined as:

$$h(X) = - \int_{\mathcal{X}} p(x) \log p(x) dx \quad (1)$$

Consider the Kullback-Leibler divergence (\rightarrow I/2.5.1) of distribution $f(x)$ from distribution $g(x)$ which is non-negative (\rightarrow I/2.5.2):

$$\begin{aligned} 0 \leq \text{KL}[f||g] &= \int_{\mathcal{X}} f(x) \log \frac{f(x)}{g(x)} dx \\ &= \int_{\mathcal{X}} f(x) \log f(x) dx - \int_{\mathcal{X}} f(x) \log g(x) dx \\ &\stackrel{(1)}{=} -h[f(x)] - \int_{\mathcal{X}} f(x) \log g(x) dx . \end{aligned} \quad (2)$$

By plugging the probability density function of the continuous uniform distribution (\rightarrow II/3.1.3) into the second term, we obtain:

$$\begin{aligned} \int_{\mathcal{X}} f(x) \log g(x) dx &= \int_{\mathcal{X}} f(x) \log \frac{1}{b-a} dx \\ &= \log \frac{1}{b-a} \int_{\mathcal{X}} f(x) dx \\ &= -\log(b-a) . \end{aligned} \quad (3)$$

This is actually the negative of the differential entropy of the continuous uniform distribution (\rightarrow II/3.1.10), such that:

$$\int_{\mathcal{X}} f(x) \log g(x) dx = -h[\mathcal{U}(a, b)] = -h[g(x)] . \quad (4)$$

Combining (2) with (4), we can show that

$$\begin{aligned} 0 &\leq \text{KL}[f||g] \\ 0 &\leq -h[f(x)] - (-h[g(x)]) \\ h[g(x)] &\geq h[f(x)] \end{aligned} \quad (5)$$

which means that the differential entropy (\rightarrow I/2.2.1) of the continuous uniform distribution (\rightarrow II/3.1.1) $\mathcal{U}(a, b)$ will be larger than or equal to any other distribution (\rightarrow I/1.5.1) defined in the same range. ■

Sources:

- Wikipedia (2023): “Maximum entropy probability distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2023-08-25; URL: https://en.wikipedia.org/wiki/Maximum_entropy_probability_distribution#Uniform_and_pieewise_uniform_distributions.

3.2 Normal distribution

3.2.1 Definition

Definition: Let X be a random variable (\rightarrow I/1.2.2). Then, X is said to be normally distributed with mean μ and variance σ^2 (or, standard deviation σ)

$$X \sim \mathcal{N}(\mu, \sigma^2) , \quad (1)$$

if and only if its probability density function (\rightarrow I/1.7.1) is given by

$$\mathcal{N}(x; \mu, \sigma^2) = \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp \left[-\frac{1}{2} \left(\frac{x - \mu}{\sigma} \right)^2 \right] \quad (2)$$

where $\mu \in \mathbb{R}$ and $\sigma^2 > 0$.

Sources:

- Wikipedia (2020): “Normal distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-01-27; URL: https://en.wikipedia.org/wiki/Normal_distribution.

3.2.2 Special case of multivariate normal distribution

Theorem: The normal distribution (\rightarrow II/3.2.1) is a special case of the multivariate normal distribution (\rightarrow II/4.1.1) with number of variables $n = 1$, i.e. random vector (\rightarrow I/1.2.3) $x \in \mathbb{R}$, mean $\mu \in \mathbb{R}$ and covariance matrix $\Sigma = \sigma^2$.

Proof: The probability density function of the multivariate normal distribution (\rightarrow II/4.1.4) is

$$\mathcal{N}(x; \mu, \Sigma) = \frac{1}{\sqrt{(2\pi)^n |\Sigma|}} \cdot \exp \left[-\frac{1}{2} (x - \mu)^T \Sigma^{-1} (x - \mu) \right] . \quad (1)$$

Setting $n = 1$, such that $x, \mu \in \mathbb{R}$, and $\Sigma = \sigma^2$, we obtain

$$\begin{aligned} \mathcal{N}(x; \mu, \sigma^2) &= \frac{1}{\sqrt{(2\pi)^1 |\sigma^2|}} \cdot \exp \left[-\frac{1}{2} (x - \mu)^T (\sigma^2)^{-1} (x - \mu) \right] \\ &= \frac{1}{\sqrt{(2\pi) \sigma^2}} \cdot \exp \left[-\frac{1}{2 \sigma^2} (x - \mu)^2 \right] \\ &= \frac{1}{\sqrt{2\pi} \sigma} \cdot \exp \left[-\frac{1}{2} \left(\frac{x - \mu}{\sigma} \right)^2 \right] \end{aligned} \quad (2)$$

which is equivalent to the probability density function of the normal distribution (\rightarrow II/3.2.10). ■

Sources:

- Wikipedia (2022): “Multivariate normal distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-08-19; URL: https://en.wikipedia.org/wiki/Multivariate_normal_distribution.

3.2.3 Standard normal distribution

Definition: Let X be a random variable (\rightarrow I/1.2.2). Then, X is said to be standard normally distributed, if X follows a normal distribution (\rightarrow II/3.2.1) with mean $\mu = 0$ and variance $\sigma^2 = 1$:

$$X \sim \mathcal{N}(0, 1) . \quad (1)$$

Sources:

- Wikipedia (2020): “Normal distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-05-26; URL: https://en.wikipedia.org/wiki/Normal_distribution#Standard_normal_distribution.

3.2.4 Relationship to standard normal distribution

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a normal distribution (\rightarrow II/3.2.1) with mean μ and variance σ^2 :

$$X \sim \mathcal{N}(\mu, \sigma^2) . \quad (1)$$

Then, the quantity $Z = (X - \mu)/\sigma$ will have a standard normal distribution (\rightarrow II/3.2.3) with mean 0 and variance 1:

$$Z = \frac{X - \mu}{\sigma} \sim \mathcal{N}(0, 1) . \quad (2)$$

Proof: Note that Z is a function of X

$$Z = g(X) = \frac{X - \mu}{\sigma} \quad (3)$$

with the inverse function

$$X = g^{-1}(Z) = \sigma Z + \mu . \quad (4)$$

Because σ is positive, $g(X)$ is strictly increasing and we can calculate the cumulative distribution function of a strictly increasing function (\rightarrow I/1.8.3) as

$$F_Y(y) = \begin{cases} 0 , & \text{if } y < \min(\mathcal{Y}) \\ F_X(g^{-1}(y)) , & \text{if } y \in \mathcal{Y} \\ 1 , & \text{if } y > \max(\mathcal{Y}) . \end{cases} \quad (5)$$

The cumulative distribution function of the normally distributed (\rightarrow II/3.2.12) X is

$$F_X(x) = \int_{-\infty}^x \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp \left[-\frac{1}{2} \left(\frac{t - \mu}{\sigma} \right)^2 \right] dt . \quad (6)$$

Applying (5) to (6), we have:

$$\begin{aligned} F_Z(z) &\stackrel{(5)}{=} F_X(g^{-1}(z)) \\ &\stackrel{(6)}{=} \int_{-\infty}^{\sigma z + \mu} \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp \left[-\frac{1}{2} \left(\frac{t - \mu}{\sigma} \right)^2 \right] dt . \end{aligned} \quad (7)$$

Substituting $s = (t - \mu)/\sigma$, such that $t = \sigma s + \mu$, we obtain

$$\begin{aligned} F_Z(z) &= \int_{(-\infty - \mu)/\sigma}^{(\sigma z + \mu - \mu)/\sigma} \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp \left[-\frac{1}{2} \left(\frac{(\sigma s + \mu) - \mu}{\sigma} \right)^2 \right] d(\sigma s + \mu) \\ &= \int_{-\infty}^z \frac{\sigma}{\sqrt{2\pi}\sigma} \cdot \exp \left[-\frac{1}{2} s^2 \right] ds \\ &= \int_{-\infty}^z \frac{1}{\sqrt{2\pi}} \cdot \exp \left[-\frac{1}{2} s^2 \right] ds \end{aligned} \quad (8)$$

which is the cumulative distribution function (\rightarrow I/1.8.1) of the standard normal distribution (\rightarrow II/3.2.3).

■

3.2.5 Relationship to standard normal distribution

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a normal distribution (\rightarrow II/3.2.1) with mean μ and variance σ^2 :

$$X \sim \mathcal{N}(\mu, \sigma^2) . \quad (1)$$

Then, the quantity $Z = (X - \mu)/\sigma$ will have a standard normal distribution (\rightarrow II/3.2.3) with mean 0 and variance 1:

$$Z = \frac{X - \mu}{\sigma} \sim \mathcal{N}(0, 1) . \quad (2)$$

Proof: Note that Z is a function of X

$$Z = g(X) = \frac{X - \mu}{\sigma} \quad (3)$$

with the inverse function

$$X = g^{-1}(Z) = \sigma Z + \mu . \quad (4)$$

Because σ is positive, $g(X)$ is strictly increasing and we can calculate the probability density function of a strictly increasing function (\rightarrow I/1.7.3) as

$$f_Y(y) = \begin{cases} f_X(g^{-1}(y)) \frac{dg^{-1}(y)}{dy} , & \text{if } y \in \mathcal{Y} \\ 0 , & \text{if } y \notin \mathcal{Y} \end{cases} \quad (5)$$

where $\mathcal{Y} = \{y = g(x) : x \in \mathcal{X}\}$. With the probability density function of the normal distribution (\rightarrow II/3.2.10), we have

$$\begin{aligned} f_Z(z) &= \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp \left[-\frac{1}{2} \left(\frac{g^{-1}(z) - \mu}{\sigma} \right)^2 \right] \cdot \frac{dg^{-1}(z)}{dz} \\ &= \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp \left[-\frac{1}{2} \left(\frac{(\sigma z + \mu) - \mu}{\sigma} \right)^2 \right] \cdot \frac{d(\sigma z + \mu)}{dz} \\ &= \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp \left[-\frac{1}{2} z^2 \right] \cdot \sigma \\ &= \frac{1}{\sqrt{2\pi}} \cdot \exp \left[-\frac{1}{2} z^2 \right] \end{aligned} \quad (6)$$

which is the probability density function (\rightarrow I/1.7.1) of the standard normal distribution (\rightarrow II/3.2.3). ■

3.2.6 Relationship to standard normal distribution

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a normal distribution (\rightarrow II/3.2.1) with mean μ and variance σ^2 :

$$X \sim \mathcal{N}(\mu, \sigma^2) . \quad (1)$$

Then, the quantity $Z = (X - \mu)/\sigma$ will have a standard normal distribution (\rightarrow II/3.2.3) with mean 0 and variance 1:

$$Z = \frac{X - \mu}{\sigma} \sim \mathcal{N}(0, 1) . \quad (2)$$

Proof: The linear transformation theorem for multivariate normal distribution (\rightarrow II/4.1.14) states

$$x \sim \mathcal{N}(\mu, \Sigma) \Rightarrow y = Ax + b \sim \mathcal{N}(A\mu + b, A\Sigma A^T) \quad (3)$$

where x is an $n \times 1$ random vector (\rightarrow I/1.2.3) following a multivariate normal distribution (\rightarrow II/4.1.1) with mean μ and covariance Σ , A is an $m \times n$ matrix and b is an $m \times 1$ vector. Note that

$$Z = \frac{X - \mu}{\sigma} = \frac{X}{\sigma} - \frac{\mu}{\sigma} \quad (4)$$

is a special case of (3) with $x = X$, $\mu = \mu$, $\Sigma = \sigma^2$, $A = 1/\sigma$ and $b = \mu/\sigma$. Applying theorem (3) to Z as a function of X , we have

$$X \sim \mathcal{N}(\mu, \sigma^2) \Rightarrow Z = \frac{X}{\sigma} - \frac{\mu}{\sigma} \sim \mathcal{N}\left(\frac{\mu}{\sigma} - \frac{\mu}{\sigma}, \frac{1}{\sigma} \cdot \sigma^2 \cdot \frac{1}{\sigma}\right) \quad (5)$$

which results in the distribution:

$$Z \sim \mathcal{N}(0, 1) . \quad (6)$$

■

3.2.7 Relationship to chi-squared distribution

Theorem: Let X_1, \dots, X_n be independent (\rightarrow I/1.3.6) random variables (\rightarrow I/1.2.2) where each of them is following a normal distribution (\rightarrow II/3.2.1) with mean μ and variance σ^2 :

$$X_i \sim \mathcal{N}(\mu, \sigma^2) \quad \text{for } i = 1, \dots, n . \quad (1)$$

Define the sample mean (\rightarrow I/1.12.2)

$$\bar{X} = \frac{1}{n} \sum_{i=1}^n X_i \quad (2)$$

and the unbiased sample variance (\rightarrow I/1.13.2)

$$s^2 = \frac{1}{n-1} \sum_{i=1}^n (X_i - \bar{X})^2 . \quad (3)$$

Then, the sampling distribution (\rightarrow I/1.5.6) of the sample variance is given by a chi-squared distribution (\rightarrow II/3.7.1) with $n - 1$ degrees of freedom:

$$V = (n-1) \frac{s^2}{\sigma^2} \sim \chi^2(n-1) . \quad (4)$$

Proof: Consider the random variable (\rightarrow I/1.2.2) U_i defined as

$$U_i = \frac{X_i - \mu}{\sigma} \quad (5)$$

which follows a standard normal distribution (\rightarrow II/3.2.4)

$$U_i \sim \mathcal{N}(0, 1) . \quad (6)$$

Then, the sum of squared random variables U_i can be rewritten as

$$\begin{aligned} \sum_{i=1}^n U_i^2 &= \sum_{i=1}^n \left(\frac{X_i - \mu}{\sigma} \right)^2 \\ &= \sum_{i=1}^n \left(\frac{(X_i - \bar{X}) + (\bar{X} - \mu)}{\sigma} \right)^2 \\ &= \sum_{i=1}^n \frac{(X_i - \bar{X})^2}{\sigma^2} + \sum_{i=1}^n \frac{(\bar{X} - \mu)^2}{\sigma^2} + 2 \sum_{i=1}^n \frac{(X_i - \bar{X})(\bar{X} - \mu)}{\sigma^2} \\ &= \sum_{i=1}^n \left(\frac{X_i - \bar{X}}{\sigma} \right)^2 + \sum_{i=1}^n \left(\frac{\bar{X} - \mu}{\sigma} \right)^2 + 2 \frac{(\bar{X} - \mu)}{\sigma^2} \sum_{i=1}^n (X_i - \bar{X}) . \end{aligned} \quad (7)$$

Because the following sum is zero

$$\begin{aligned} \sum_{i=1}^n (X_i - \bar{X}) &= \sum_{i=1}^n X_i - n\bar{X} \\ &= \sum_{i=1}^n X_i - n \cdot \frac{1}{n} \sum_{i=1}^n X_i \\ &= \sum_{i=1}^n X_i - \sum_{i=1}^n X_i \\ &= 0 , \end{aligned} \quad (8)$$

the third term disappears, i.e.

$$\sum_{i=1}^n U_i^2 = \sum_{i=1}^n \left(\frac{X_i - \bar{X}}{\sigma} \right)^2 + \sum_{i=1}^n \left(\frac{\bar{X} - \mu}{\sigma} \right)^2 . \quad (9)$$

Cochran's theorem states that, if a sum of squared standard normal (\rightarrow II/3.2.3) random variables (\rightarrow I/1.2.2) can be written as a sum of squared forms

$$\begin{aligned} \sum_{i=1}^n U_i^2 &= \sum_{j=1}^m Q_j \quad \text{where} \quad Q_j = \sum_{k=1}^n \sum_{l=1}^n U_k B_{kl}^{(j)} U_l \\ &\quad \text{with} \quad \sum_{j=1}^m B^{(j)} = I_n \\ &\quad \text{and} \quad r_j = \text{rank}(B^{(j)}) , \end{aligned} \quad (10)$$

then the terms Q_j are independent (\rightarrow I/1.3.6) and each term Q_j follows a chi-squared distribution (\rightarrow II/3.7.1) with r_j degrees of freedom:

$$Q_j \sim \chi^2(r_j) . \quad (11)$$

We observe that (9) can be represented as

$$\begin{aligned} \sum_{i=1}^n U_i^2 &= \sum_{i=1}^n \left(\frac{X_i - \bar{X}}{\sigma} \right)^2 + \sum_{i=1}^n \left(\frac{\bar{X} - \mu}{\sigma} \right)^2 \\ &= Q_1 + Q_2 = \sum_{i=1}^n \left(U_i - \frac{1}{n} \sum_{j=1}^n U_j \right)^2 + \frac{1}{n} \left(\sum_{i=1}^n U_i \right)^2 \end{aligned} \quad (12)$$

where, with the $n \times n$ matrix of ones J_n , the matrices $B^{(j)}$ are

$$B^{(1)} = I_n - \frac{J_n}{n} \quad \text{and} \quad B^{(2)} = \frac{J_n}{n} . \quad (13)$$

Because all columns of $B^{(2)}$ are identical, it has rank $r_2 = 1$. Because the n columns of $B^{(1)}$ add up to zero, it has rank $r_1 = n - 1$. Thus, the conditions of Cochran's theorem are met and the squared form

$$Q_1 = \sum_{i=1}^n \left(\frac{X_i - \bar{X}}{\sigma} \right)^2 = (n-1) \frac{1}{\sigma^2} \frac{1}{n-1} \sum_{i=1}^n (X_i - \bar{X})^2 = (n-1) \frac{s^2}{\sigma^2} \quad (14)$$

follows a chi-squared distribution (\rightarrow II/3.7.1) with $n - 1$ degrees of freedom:

$$(n-1) \frac{s^2}{\sigma^2} \sim \chi^2(n-1) . \quad (15)$$

■

Sources:

- Glen-b (2014): "Why is the sampling distribution of variance a chi-squared distribution?"; in: *StackExchange CrossValidated*, retrieved on 2021-05-20; URL: <https://stats.stackexchange.com/questions/121662/why-is-the-sampling-distribution-of-variance-a-chi-squared-distribution>.
- Wikipedia (2021): "Cochran's theorem"; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-05-20; URL: https://en.wikipedia.org/wiki/Cochran%27s_theorem#Sample_mean_and_sample_variance.

3.2.8 Relationship to t-distribution

Theorem: Let X_1, \dots, X_n be independent (\rightarrow I/1.3.6) random variables (\rightarrow I/1.2.2) where each of them is following a normal distribution (\rightarrow II/3.2.1) with mean μ and variance σ^2 :

$$X_i \sim \mathcal{N}(\mu, \sigma^2) \quad \text{for } i = 1, \dots, n . \quad (1)$$

Define the sample mean (\rightarrow I/1.12.2)

$$\bar{X} = \frac{1}{n} \sum_{i=1}^n X_i \quad (2)$$

and the unbiased sample variance (\rightarrow I/1.13.2)

$$s^2 = \frac{1}{n-1} \sum_{i=1}^n (X_i - \bar{X})^2 . \quad (3)$$

Then, subtracting μ from the sample mean (\rightarrow I/1.12.1), dividing by the sample standard deviation (\rightarrow I/1.19.1) and multiplying with \sqrt{n} results in a quantity that follows a t-distribution (\rightarrow II/3.3.1) with $n - 1$ degrees of freedom:

$$t = \sqrt{n} \frac{\bar{X} - \mu}{s} \sim t(n-1) . \quad (4)$$

Proof: Note that \bar{X} is a linear combination of X_1, \dots, X_n :

$$\bar{X} = \frac{1}{n}X_1 + \dots + \frac{1}{n}X_n . \quad (5)$$

Because the linear combination of independent normal random variables is also normally distributed (\rightarrow II/3.2.26), we have:

$$\bar{X} \sim \mathcal{N}\left(\frac{1}{n}n\mu, \left(\frac{1}{n}\right)^2 n\sigma^2\right) = \mathcal{N}(\mu, \sigma^2/n) . \quad (6)$$

Let $Z = \sqrt{n}(\bar{X} - \mu)/\sigma$. Because Z is a linear transformation (\rightarrow II/4.1.14) of \bar{X} , it also follows a normal distribution:

$$Z = \sqrt{n} \frac{\bar{X} - \mu}{\sigma} \sim \mathcal{N}\left(\frac{\sqrt{n}}{\sigma}(\mu - \mu), \left(\frac{\sqrt{n}}{\sigma}\right)^2 \sigma^2/n\right) = \mathcal{N}(0, 1) . \quad (7)$$

Let $V = (n-1)s^2/\sigma^2$. We know that this function of the sample variance follows a chi-squared distribution (\rightarrow II/3.2.7) with $n - 1$ degrees of freedom:

$$V = (n-1) \frac{s^2}{\sigma^2} \sim \chi^2(n-1) . \quad (8)$$

Observe that t is the ratio of a standard normal random variable (\rightarrow II/3.2.3) and the square root of a chi-squared random variable (\rightarrow II/3.7.1), divided by its degrees of freedom:

$$t = \sqrt{n} \frac{\bar{X} - \mu}{s} = \frac{\sqrt{n} \frac{\bar{X} - \mu}{\sigma}}{\sqrt{(n-1) \frac{s^2}{\sigma^2} / (n-1)}} = \frac{Z}{\sqrt{V/(n-1)}} . \quad (9)$$

Thus, by definition of the t-distribution (\rightarrow II/3.3.1), this ratio follows a t-distribution with $n - 1$ degrees of freedom:

$$t \sim t(n-1) . \quad (10)$$

Sources:

- Wikipedia (2021): “Student’s t-distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-05-27; URL: https://en.wikipedia.org/wiki/Student%27s_t-distribution#Characterization.
- Wikipedia (2021): “Normal distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-05-27; URL: https://en.wikipedia.org/wiki/Normal_distribution#Operations_on_multiple_independent_normal_variables.

3.2.9 Gaussian integral

Theorem: The definite integral of $\exp[-x^2]$ from $-\infty$ to $+\infty$ is equal to the square root of π :

$$\int_{-\infty}^{+\infty} \exp[-x^2] \, dx = \sqrt{\pi} . \quad (1)$$

Proof: Let

$$I = \int_0^{\infty} \exp[-x^2] \, dx \quad (2)$$

and

$$I_P = \int_0^P \exp[-x^2] \, dx = \int_0^P \exp[-y^2] \, dy . \quad (3)$$

Then, we have

$$\lim_{P \rightarrow \infty} I_P = I \quad (4)$$

and

$$\lim_{P \rightarrow \infty} I_P^2 = I^2 . \quad (5)$$

Moreover, we can write

$$\begin{aligned} I_P^2 &\stackrel{(3)}{=} \left(\int_0^P \exp[-x^2] \, dx \right) \left(\int_0^P \exp[-y^2] \, dy \right) \\ &= \int_0^P \int_0^P \exp[-(x^2 + y^2)] \, dx \, dy \\ &= \iint_{S_P} \exp[-(x^2 + y^2)] \, dx \, dy \end{aligned} \quad (6)$$

where S_P is the square with corners $(0, 0)$, $(0, P)$, (P, P) and $(P, 0)$. For this integral, we can write down the following inequality

$$\iint_{C_1} \exp[-(x^2 + y^2)] \, dx \, dy \leq I_P^2 \leq \iint_{C_2} \exp[-(x^2 + y^2)] \, dx \, dy \quad (7)$$

where C_1 and C_2 are the regions in the first quadrant bounded by circles with center at $(0, 0)$ and going through the points $(0, P)$ and (P, P) , respectively. The radii of these two circles are $r_1 = \sqrt{P^2} = P$ and $r_2 = \sqrt{2P^2} = P\sqrt{2}$, such that we can rewrite equation (7) using polar coordinates as

$$\int_0^{\frac{\pi}{2}} \int_0^{r_1} \exp[-r^2] \, r \, dr \, d\theta \leq I_P^2 \leq \int_0^{\frac{\pi}{2}} \int_0^{r_2} \exp[-r^2] \, r \, dr \, d\theta . \quad (8)$$

Solving the definite integrals yields:

$$\begin{aligned}
\int_0^{\frac{\pi}{2}} \int_0^{r_1} \exp[-r^2] r \, dr \, d\theta &\leq I_P^2 \leq \int_0^{\frac{\pi}{2}} \int_0^{r_2} \exp[-r^2] r \, dr \, d\theta \\
\int_0^{\frac{\pi}{2}} \left[-\frac{1}{2} \exp[-r^2] \right]_0^{r_1} d\theta &\leq I_P^2 \leq \int_0^{\frac{\pi}{2}} \left[-\frac{1}{2} \exp[-r^2] \right]_0^{r_2} d\theta \\
-\frac{1}{2} \int_0^{\frac{\pi}{2}} (\exp[-r_1^2] - 1) \, d\theta &\leq I_P^2 \leq -\frac{1}{2} \int_0^{\frac{\pi}{2}} (\exp[-r_2^2] - 1) \, d\theta \\
-\frac{1}{2} [(\exp[-r_1^2] - 1) \theta]_0^{\frac{\pi}{2}} &\leq I_P^2 \leq -\frac{1}{2} [(\exp[-r_2^2] - 1) \theta]_0^{\frac{\pi}{2}} \\
\frac{1}{2} (1 - \exp[-r_1^2]) \frac{\pi}{2} &\leq I_P^2 \leq \frac{1}{2} (1 - \exp[-r_2^2]) \frac{\pi}{2} \\
\frac{\pi}{4} (1 - \exp[-P^2]) &\leq I_P^2 \leq \frac{\pi}{4} (1 - \exp[-2P^2])
\end{aligned} \tag{9}$$

Calculating the limit for $P \rightarrow \infty$, we obtain

$$\begin{aligned}
\lim_{P \rightarrow \infty} \frac{\pi}{4} (1 - \exp[-P^2]) &\leq \lim_{P \rightarrow \infty} I_P^2 \leq \lim_{P \rightarrow \infty} \frac{\pi}{4} (1 - \exp[-2P^2]) \\
\frac{\pi}{4} &\leq I^2 \leq \frac{\pi}{4},
\end{aligned} \tag{10}$$

such that we have a preliminary result for I :

$$I^2 = \frac{\pi}{4} \quad \Rightarrow \quad I = \frac{\sqrt{\pi}}{2}. \tag{11}$$

Because the integrand in (1) is an even function, we can calculate the final result as follows:

$$\begin{aligned}
\int_{-\infty}^{+\infty} \exp[-x^2] \, dx &= 2 \int_0^{\infty} \exp[-x^2] \, dx \\
&\stackrel{(11)}{=} 2 \frac{\sqrt{\pi}}{2} \\
&= \sqrt{\pi}.
\end{aligned} \tag{12}$$

■

Sources:

- ProofWiki (2020): “Gaussian Integral”; in: *ProofWiki*, retrieved on 2020-11-25; URL: https://proofwiki.org/wiki/Gaussian_Integral.
- ProofWiki (2020): “Integral to Infinity of Exponential of minus t squared”; in: *ProofWiki*, retrieved on 2020-11-25; URL: https://proofwiki.org/wiki/Integral_to_Infinity_of_Exponential_of_-t%5E2.

3.2.10 Probability density function

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a normal distribution (\rightarrow II/3.2.1):

$$X \sim \mathcal{N}(\mu, \sigma^2). \tag{1}$$

Then, the probability density function (\rightarrow I/1.7.1) of X is

$$f_X(x) = \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp \left[-\frac{1}{2} \left(\frac{x-\mu}{\sigma} \right)^2 \right] . \quad (2)$$

Proof: This follows directly from the definition of the normal distribution (\rightarrow II/3.2.1). ■

3.2.11 Moment-generating function

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a normal distribution (\rightarrow II/3.2.1):

$$X \sim \mathcal{N}(\mu, \sigma^2) . \quad (1)$$

Then, the moment-generating function (\rightarrow I/1.9.1) of X is

$$M_X(t) = \exp \left[\mu t + \frac{1}{2} \sigma^2 t^2 \right] . \quad (2)$$

Proof: The probability density function of the normal distribution (\rightarrow II/3.2.10) is

$$f_X(x) = \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp \left[-\frac{1}{2} \left(\frac{x-\mu}{\sigma} \right)^2 \right] \quad (3)$$

and the moment-generating function (\rightarrow I/1.9.1) is defined as

$$M_X(t) = \mathbb{E} [e^{tX}] . \quad (4)$$

Using the expected value for continuous random variables (\rightarrow I/1.12.1), the moment-generating function of X therefore is

$$\begin{aligned} M_X(t) &= \int_{-\infty}^{+\infty} \exp[tx] \cdot \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp \left[-\frac{1}{2} \left(\frac{x-\mu}{\sigma} \right)^2 \right] dx \\ &= \frac{1}{\sqrt{2\pi}\sigma} \int_{-\infty}^{+\infty} \exp \left[tx - \frac{1}{2} \left(\frac{x-\mu}{\sigma} \right)^2 \right] dx . \end{aligned} \quad (5)$$

Substituting $u = (x - \mu)/(\sqrt{2}\sigma)$, i.e. $x = \sqrt{2}\sigma u + \mu$, we have

$$\begin{aligned}
M_X(t) &= \frac{1}{\sqrt{2\pi}\sigma} \int_{(-\infty-\mu)/(\sqrt{2}\sigma)}^{(+\infty-\mu)/(\sqrt{2}\sigma)} \exp \left[t \left(\sqrt{2}\sigma u + \mu \right) - \frac{1}{2} \left(\frac{\sqrt{2}\sigma u + \mu - \mu}{\sigma} \right)^2 \right] d \left(\sqrt{2}\sigma u + \mu \right) \\
&= \frac{\sqrt{2}\sigma}{\sqrt{2\pi}\sigma} \int_{-\infty}^{+\infty} \exp \left[\left(\sqrt{2}\sigma u + \mu \right) t - u^2 \right] du \\
&= \frac{\exp(\mu t)}{\sqrt{\pi}} \int_{-\infty}^{+\infty} \exp \left[\sqrt{2}\sigma u t - u^2 \right] du \\
&= \frac{\exp(\mu t)}{\sqrt{\pi}} \int_{-\infty}^{+\infty} \exp \left[- \left(u^2 - \sqrt{2}\sigma u t \right) \right] du \\
&= \frac{\exp(\mu t)}{\sqrt{\pi}} \int_{-\infty}^{+\infty} \exp \left[- \left(u - \frac{\sqrt{2}}{2}\sigma t \right)^2 + \frac{1}{2}\sigma^2 t^2 \right] du \\
&= \frac{\exp \left[\mu t + \frac{1}{2}\sigma^2 t^2 \right]}{\sqrt{\pi}} \int_{-\infty}^{+\infty} \exp \left[- \left(u - \frac{\sqrt{2}}{2}\sigma t \right)^2 \right] du
\end{aligned} \tag{6}$$

Now substituting $v = u - \sqrt{2}/2 \sigma t$, i.e. $u = v + \sqrt{2}/2 \sigma t$, we have

$$\begin{aligned}
M_X(t) &= \frac{\exp \left[\mu t + \frac{1}{2}\sigma^2 t^2 \right]}{\sqrt{\pi}} \int_{-\infty - \sqrt{2}/2 \sigma t}^{+\infty - \sqrt{2}/2 \sigma t} \exp \left[-v^2 \right] d \left(v + \sqrt{2}/2 \sigma t \right) \\
&= \frac{\exp \left[\mu t + \frac{1}{2}\sigma^2 t^2 \right]}{\sqrt{\pi}} \int_{-\infty}^{+\infty} \exp \left[-v^2 \right] dv .
\end{aligned} \tag{7}$$

With the Gaussian integral (\rightarrow II/3.2.9)

$$\int_{-\infty}^{+\infty} \exp \left[-x^2 \right] dx = \sqrt{\pi} , \tag{8}$$

this finally becomes

$$M_X(t) = \exp \left[\mu t + \frac{1}{2}\sigma^2 t^2 \right] . \tag{9}$$

■

Sources:

- ProofWiki (2020): “Moment Generating Function of Gaussian Distribution”; in: *ProofWiki*, retrieved on 2020-03-03; URL: https://proofwiki.org/wiki/Moment_Generating_Function_of_Gaussian_Distribution.

3.2.12 Cumulative distribution function

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a normal distribution (\rightarrow II/3.2.1):

$$X \sim \mathcal{N}(\mu, \sigma^2) . \tag{1}$$

Then, the cumulative distribution function (\rightarrow I/1.8.1) of X is

$$F_X(x) = \frac{1}{2} \left[1 + \operatorname{erf} \left(\frac{x - \mu}{\sqrt{2}\sigma} \right) \right] \quad (2)$$

where $\operatorname{erf}(x)$ is the error function defined as

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x \exp(-t^2) dt . \quad (3)$$

Proof: The probability density function of the normal distribution (\rightarrow II/3.2.10) is:

$$f_X(x) = \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp \left[-\frac{1}{2} \left(\frac{x - \mu}{\sigma} \right)^2 \right] . \quad (4)$$

Thus, the cumulative distribution function (\rightarrow I/1.8.1) is:

$$\begin{aligned} F_X(x) &= \int_{-\infty}^x \mathcal{N}(z; \mu, \sigma^2) dz \\ &= \int_{-\infty}^x \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp \left[-\frac{1}{2} \left(\frac{z - \mu}{\sigma} \right)^2 \right] dz \\ &= \frac{1}{\sqrt{2\pi}\sigma} \int_{-\infty}^x \exp \left[-\left(\frac{z - \mu}{\sqrt{2}\sigma} \right)^2 \right] dz . \end{aligned} \quad (5)$$

Substituting $t = (z - \mu)/(\sqrt{2}\sigma)$, i.e. $z = \sqrt{2}\sigma t + \mu$, this becomes:

$$\begin{aligned} F_X(x) &= \frac{1}{\sqrt{2\pi}\sigma} \int_{(-\infty - \mu)/(\sqrt{2}\sigma)}^{(x - \mu)/(\sqrt{2}\sigma)} \exp(-t^2) d(\sqrt{2}\sigma t + \mu) \\ &= \frac{\sqrt{2}\sigma}{\sqrt{2\pi}\sigma} \int_{-\infty}^{\frac{x - \mu}{\sqrt{2}\sigma}} \exp(-t^2) dt \\ &= \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\frac{x - \mu}{\sqrt{2}\sigma}} \exp(-t^2) dt \\ &= \frac{1}{\sqrt{\pi}} \int_{-\infty}^0 \exp(-t^2) dt + \frac{1}{\sqrt{\pi}} \int_0^{\frac{x - \mu}{\sqrt{2}\sigma}} \exp(-t^2) dt \\ &= \frac{1}{\sqrt{\pi}} \int_0^{\infty} \exp(-t^2) dt + \frac{1}{\sqrt{\pi}} \int_0^{\frac{x - \mu}{\sqrt{2}\sigma}} \exp(-t^2) dt . \end{aligned} \quad (6)$$

Applying (3) to (6), we have:

$$\begin{aligned} F_X(x) &= \frac{1}{2} \lim_{x \rightarrow \infty} \operatorname{erf}(x) + \frac{1}{2} \operatorname{erf} \left(\frac{x - \mu}{\sqrt{2}\sigma} \right) \\ &= \frac{1}{2} + \frac{1}{2} \operatorname{erf} \left(\frac{x - \mu}{\sqrt{2}\sigma} \right) \\ &= \frac{1}{2} \left[1 + \operatorname{erf} \left(\frac{x - \mu}{\sqrt{2}\sigma} \right) \right] . \end{aligned} \quad (7)$$

Sources:

- Wikipedia (2020): “Normal distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-03-20; URL: https://en.wikipedia.org/wiki/Normal_distribution#Cumulative_distribution_function.
- Wikipedia (2020): “Error function”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-03-20; URL: https://en.wikipedia.org/wiki/Error_function.

3.2.13 Cumulative distribution function without error function

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a normal distribution (\rightarrow II/3.2.1):

$$X \sim \mathcal{N}(\mu, \sigma^2). \quad (1)$$

Then, the cumulative distribution function (\rightarrow I/1.8.1) of X can be expressed as

$$F_X(x) = \Phi_{\mu, \sigma}(x) = \varphi\left(\frac{x - \mu}{\sigma}\right) \cdot \sum_{i=1}^{\infty} \frac{\left(\frac{x - \mu}{\sigma}\right)^{2i-1}}{(2i-1)!!} + \frac{1}{2} \quad (2)$$

where $\varphi(x)$ is the probability density function (\rightarrow I/1.7.1) of the standard normal distribution (\rightarrow II/3.2.3) and $n!!$ is a double factorial.

Proof:

1) First, consider the standard normal distribution (\rightarrow II/3.2.3) $\mathcal{N}(0, 1)$ which has the probability density function (\rightarrow II/3.2.10)

$$\varphi(x) = \frac{1}{\sqrt{2\pi}} \cdot e^{-\frac{1}{2}x^2}. \quad (3)$$

Let $T(x)$ be the indefinite integral of this function. It can be obtained using infinitely repeated integration by parts as follows:

$$\begin{aligned} T(x) &= \int \varphi(x) \, dx \\ &= \int \frac{1}{\sqrt{2\pi}} \cdot e^{-\frac{1}{2}x^2} \, dx \\ &= \frac{1}{\sqrt{2\pi}} \int 1 \cdot e^{-\frac{1}{2}x^2} \, dx \\ &= \frac{1}{\sqrt{2\pi}} \cdot \left[x \cdot e^{-\frac{1}{2}x^2} + \int x^2 \cdot e^{-\frac{1}{2}x^2} \, dx \right] \\ &= \frac{1}{\sqrt{2\pi}} \cdot \left[x \cdot e^{-\frac{1}{2}x^2} + \left[\frac{1}{3}x^3 \cdot e^{-\frac{1}{2}x^2} + \int \frac{1}{3}x^4 \cdot e^{-\frac{1}{2}x^2} \, dx \right] \right] \\ &= \frac{1}{\sqrt{2\pi}} \cdot \left[x \cdot e^{-\frac{1}{2}x^2} + \left[\frac{1}{3}x^3 \cdot e^{-\frac{1}{2}x^2} + \left[\frac{1}{15}x^5 \cdot e^{-\frac{1}{2}x^2} + \int \frac{1}{15}x^6 \cdot e^{-\frac{1}{2}x^2} \, dx \right] \right] \right] \\ &= \dots \\ &= \frac{1}{\sqrt{2\pi}} \cdot \left[\sum_{i=1}^n \left(\frac{x^{2i-1}}{(2i-1)!!} \cdot e^{-\frac{1}{2}x^2} \right) + \int \left(\frac{x^{2n}}{(2n-1)!!} \cdot e^{-\frac{1}{2}x^2} \right) \, dx \right] \\ &= \frac{1}{\sqrt{2\pi}} \cdot \left[\sum_{i=1}^{\infty} \left(\frac{x^{2i-1}}{(2i-1)!!} \cdot e^{-\frac{1}{2}x^2} \right) + \lim_{n \rightarrow \infty} \int \left(\frac{x^{2n}}{(2n-1)!!} \cdot e^{-\frac{1}{2}x^2} \right) \, dx \right]. \end{aligned} \quad (4)$$

Since $(2n - 1)!!$ grows faster than x^{2n} , it holds that

$$\frac{1}{\sqrt{2\pi}} \cdot \lim_{n \rightarrow \infty} \int \left(\frac{x^{2n}}{(2n - 1)!!} \cdot e^{-\frac{1}{2}x^2} \right) dx = \int 0 dx = c \quad (5)$$

for constant c , such that the indefinite integral becomes

$$\begin{aligned} T(x) &= \frac{1}{\sqrt{2\pi}} \cdot \sum_{i=1}^{\infty} \left(\frac{x^{2i-1}}{(2i - 1)!!} \cdot e^{-\frac{1}{2}x^2} \right) + c \\ &= \frac{1}{\sqrt{2\pi}} \cdot e^{-\frac{1}{2}x^2} \cdot \sum_{i=1}^{\infty} \frac{x^{2i-1}}{(2i - 1)!!} + c \\ &\stackrel{(3)}{=} \varphi(x) \cdot \sum_{i=1}^{\infty} \frac{x^{2i-1}}{(2i - 1)!!} + c. \end{aligned} \quad (6)$$

2) Next, let $\Phi(x)$ be the cumulative distribution function (\rightarrow I/1.8.1) of the standard normal distribution (\rightarrow II/3.2.3):

$$\Phi(x) = \int_{-\infty}^x \varphi(x) dx. \quad (7)$$

It can be obtained by matching $T(0)$ to $\Phi(0)$ which is $1/2$, because the standard normal distribution is symmetric around zero:

$$\begin{aligned} T(0) &= \varphi(0) \cdot \sum_{i=1}^{\infty} \frac{0^{2i-1}}{(2i - 1)!!} + c = \frac{1}{2} = \Phi(0) \\ &\Leftrightarrow c = \frac{1}{2} \\ \Rightarrow \Phi(x) &= \varphi(x) \cdot \sum_{i=1}^{\infty} \frac{x^{2i-1}}{(2i - 1)!!} + \frac{1}{2}. \end{aligned} \quad (8)$$

3) Finally, the cumulative distribution functions (\rightarrow I/1.8.1) of the standard normal distribution (\rightarrow II/3.2.3) and the general normal distribution (\rightarrow II/3.2.1) are related to each other (\rightarrow II/3.2.4) as

$$\Phi_{\mu,\sigma}(x) = \Phi\left(\frac{x - \mu}{\sigma}\right). \quad (9)$$

Combining (9) with (8), we have:

$$\Phi_{\mu,\sigma}(x) = \varphi\left(\frac{x - \mu}{\sigma}\right) \cdot \sum_{i=1}^{\infty} \frac{\left(\frac{x - \mu}{\sigma}\right)^{2i-1}}{(2i - 1)!!} + \frac{1}{2}. \quad (10)$$

■

Sources:

- Soch J (2015): “Solution for the Indefinite Integral of the Standard Normal Probability Density Function”; in: *arXiv stat.OT*, 1512.04858; URL: <https://arxiv.org/abs/1512.04858>.
- Wikipedia (2020): “Normal distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-03-20; URL: https://en.wikipedia.org/wiki/Normal_distribution#Cumulative_distribution_function.

3.2.14 Probability of being within standard deviations from mean

Theorem: (also called “68-95-99.7 rule”) Let X be a random variable (\rightarrow I/1.2.2) following a normal distribution (\rightarrow II/3.2.1) with mean (\rightarrow I/1.12.1) μ and variance (\rightarrow I/1.13.1) σ^2 . Then, about 68%, 95% and 99.7% of the values of X will fall within 1, 2 and 3 standard deviations (\rightarrow I/1.19.1) from the mean (\rightarrow I/1.12.1), respectively:

$$\begin{aligned}\Pr(\mu - 1\sigma \leq X \leq \mu + 1\sigma) &\approx 68\% \\ \Pr(\mu - 2\sigma \leq X \leq \mu + 2\sigma) &\approx 95\% \\ \Pr(\mu - 3\sigma \leq X \leq \mu + 3\sigma) &\approx 99.7\% .\end{aligned}\tag{1}$$

Proof: The cumulative distribution function of a normally distributed (\rightarrow II/3.2.12) random variable X is

$$F_X(x) = \frac{1}{2} \left[1 + \operatorname{erf} \left(\frac{x - \mu}{\sqrt{2}\sigma} \right) \right]\tag{2}$$

where $\operatorname{erf}(x)$ is the error function defined as

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x \exp(-t^2) dt\tag{3}$$

which exhibits a point-symmetry property:

$$\operatorname{erf}(-x) = -\operatorname{erf}(x) .\tag{4}$$

Thus, the probability that X falls between $\mu - a \cdot \sigma$ and $\mu + a \cdot \sigma$ is equal to:

$$\begin{aligned}p(a) &= \Pr(\mu - a\sigma \leq X \leq \mu + a\sigma) \\ &= F_X(\mu + a\sigma) - F_X(\mu - a\sigma) \\ &\stackrel{(2)}{=} \frac{1}{2} \left[1 + \operatorname{erf} \left(\frac{\mu + a\sigma - \mu}{\sqrt{2}\sigma} \right) \right] - \frac{1}{2} \left[1 + \operatorname{erf} \left(\frac{\mu - a\sigma - \mu}{\sqrt{2}\sigma} \right) \right] \\ &= \frac{1}{2} \left[\operatorname{erf} \left(\frac{\mu + a\sigma - \mu}{\sqrt{2}\sigma} \right) - \operatorname{erf} \left(\frac{\mu - a\sigma - \mu}{\sqrt{2}\sigma} \right) \right] \\ &= \frac{1}{2} \left[\operatorname{erf} \left(\frac{a}{\sqrt{2}} \right) - \operatorname{erf} \left(-\frac{a}{\sqrt{2}} \right) \right] \\ &\stackrel{(4)}{=} \frac{1}{2} \left[\operatorname{erf} \left(\frac{a}{\sqrt{2}} \right) + \operatorname{erf} \left(\frac{a}{\sqrt{2}} \right) \right] \\ &= \operatorname{erf} \left(\frac{a}{\sqrt{2}} \right)\end{aligned}\tag{5}$$

With that, we can use numerical implementations of the error function to calculate:

$$\begin{aligned}\Pr(\mu - 1\sigma \leq X \leq \mu + 1\sigma) &= p(1) = 68.27\% \\ \Pr(\mu - 2\sigma \leq X \leq \mu + 2\sigma) &= p(2) = 95.45\% \\ \Pr(\mu - 3\sigma \leq X \leq \mu + 3\sigma) &= p(3) = 99.73\% .\end{aligned}\tag{6}$$

**Sources:**

- Wikipedia (2022): “68-95-99.7 rule”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-05.08; URL: https://en.wikipedia.org/wiki/68%E2%80%939395%E2%80%9399.7_rule.

3.2.15 Quantile function

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a normal distributions (\rightarrow II/3.2.1):

$$X \sim \mathcal{N}(\mu, \sigma^2) . \quad (1)$$

Then, the quantile function (\rightarrow I/1.11.1) of X is

$$Q_X(p) = \sqrt{2}\sigma \cdot \operatorname{erf}^{-1}(2p - 1) + \mu \quad (2)$$

where $\operatorname{erf}^{-1}(x)$ is the inverse error function.

Proof: The cumulative distribution function of the normal distribution (\rightarrow II/3.2.12) is:

$$F_X(x) = \frac{1}{2} \left[1 + \operatorname{erf} \left(\frac{x - \mu}{\sqrt{2}\sigma} \right) \right] . \quad (3)$$

Because the cumulative distribution function (CDF) is strictly monotonically increasing, the quantile function is equal to the inverse of the CDF (\rightarrow I/1.11.2):

$$Q_X(p) = F_X^{-1}(x) . \quad (4)$$

This can be derived by rearranging equation (3):

$$\begin{aligned} p &= \frac{1}{2} \left[1 + \operatorname{erf} \left(\frac{x - \mu}{\sqrt{2}\sigma} \right) \right] \\ 2p - 1 &= \operatorname{erf} \left(\frac{x - \mu}{\sqrt{2}\sigma} \right) \\ \operatorname{erf}^{-1}(2p - 1) &= \frac{x - \mu}{\sqrt{2}\sigma} \\ x &= \sqrt{2}\sigma \cdot \operatorname{erf}^{-1}(2p - 1) + \mu . \end{aligned} \quad (5)$$

**Sources:**

- Wikipedia (2020): “Normal distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-03-20; URL: https://en.wikipedia.org/wiki/Normal_distribution#Quantile_function.

3.2.16 Mean

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a normal distribution (\rightarrow II/3.2.1):

$$X \sim \mathcal{N}(\mu, \sigma^2) . \quad (1)$$

Then, the mean or expected value (\rightarrow I/1.12.1) of X is

$$E(X) = \mu . \quad (2)$$

Proof: The expected value (\rightarrow I/1.12.1) is the probability-weighted average over all possible values:

$$E(X) = \int_{\mathcal{X}} x \cdot f_X(x) dx . \quad (3)$$

With the probability density function of the normal distribution (\rightarrow II/3.2.10), this reads:

$$\begin{aligned} E(X) &= \int_{-\infty}^{+\infty} x \cdot \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp \left[-\frac{1}{2} \left(\frac{x-\mu}{\sigma} \right)^2 \right] dx \\ &= \frac{1}{\sqrt{2\pi}\sigma} \int_{-\infty}^{+\infty} x \cdot \exp \left[-\frac{1}{2} \left(\frac{x-\mu}{\sigma} \right)^2 \right] dx . \end{aligned} \quad (4)$$

Substituting $z = x - \mu$, we have:

$$\begin{aligned} E(X) &= \frac{1}{\sqrt{2\pi}\sigma} \int_{-\infty-\mu}^{+\infty-\mu} (z + \mu) \cdot \exp \left[-\frac{1}{2} \left(\frac{z}{\sigma} \right)^2 \right] d(z + \mu) \\ &= \frac{1}{\sqrt{2\pi}\sigma} \int_{-\infty}^{+\infty} (z + \mu) \cdot \exp \left[-\frac{1}{2} \left(\frac{z}{\sigma} \right)^2 \right] dz \\ &= \frac{1}{\sqrt{2\pi}\sigma} \left(\int_{-\infty}^{+\infty} z \cdot \exp \left[-\frac{1}{2} \left(\frac{z}{\sigma} \right)^2 \right] dz + \mu \int_{-\infty}^{+\infty} \exp \left[-\frac{1}{2} \left(\frac{z}{\sigma} \right)^2 \right] dz \right) \\ &= \frac{1}{\sqrt{2\pi}\sigma} \left(\int_{-\infty}^{+\infty} z \cdot \exp \left[-\frac{1}{2\sigma^2} \cdot z^2 \right] dz + \mu \int_{-\infty}^{+\infty} \exp \left[-\frac{1}{2\sigma^2} \cdot z^2 \right] dz \right) . \end{aligned} \quad (5)$$

The general antiderivatives are

$$\begin{aligned} \int x \cdot \exp [-ax^2] dx &= -\frac{1}{2a} \cdot \exp [-ax^2] \\ \int \exp [-ax^2] dx &= \frac{1}{2} \sqrt{\frac{\pi}{a}} \cdot \operatorname{erf} [\sqrt{a}x] \end{aligned} \quad (6)$$

where $\operatorname{erf}(x)$ is the error function. Using this, the integrals can be calculated as:

$$\begin{aligned} E(X) &= \frac{1}{\sqrt{2\pi}\sigma} \left(\left[-\sigma^2 \cdot \exp \left[-\frac{1}{2\sigma^2} \cdot z^2 \right] \right]_{-\infty}^{+\infty} + \mu \left[\sqrt{\frac{\pi}{2}} \sigma \cdot \operatorname{erf} \left[\frac{1}{\sqrt{2}\sigma} z \right] \right]_{-\infty}^{+\infty} \right) \\ &= \frac{1}{\sqrt{2\pi}\sigma} \left(\left(\lim_{z \rightarrow +\infty} \left(-\sigma^2 \cdot \exp \left[-\frac{1}{2\sigma^2} \cdot z^2 \right] \right) - \lim_{z \rightarrow -\infty} \left(-\sigma^2 \cdot \exp \left[-\frac{1}{2\sigma^2} \cdot z^2 \right] \right) \right) \right. \\ &\quad \left. + \mu \left(\lim_{z \rightarrow +\infty} \left(\sqrt{\frac{\pi}{2}} \sigma \cdot \operatorname{erf} \left[\frac{1}{\sqrt{2}\sigma} z \right] \right) - \lim_{z \rightarrow -\infty} \left(\sqrt{\frac{\pi}{2}} \sigma \cdot \operatorname{erf} \left[\frac{1}{\sqrt{2}\sigma} z \right] \right) \right) \right) \\ &= \frac{1}{\sqrt{2\pi}\sigma} \left([0 - 0] + \mu \left[\sqrt{\frac{\pi}{2}} \sigma - \left(-\sqrt{\frac{\pi}{2}} \sigma \right) \right] \right) \\ &= \frac{1}{\sqrt{2\pi}\sigma} \cdot \mu \cdot 2\sqrt{\frac{\pi}{2}} \sigma \\ &= \mu . \end{aligned} \quad (7)$$

**Sources:**

- Papadopoulos, Alecos (2013): “How to derive the mean and variance of Gaussian random variable?”; in: *StackExchange Mathematics*, retrieved on 2020-01-09; URL: <https://math.stackexchange.com/questions/518281/how-to-derive-the-mean-and-variance-of-a-gaussian-random-variable>.

3.2.17 Median

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a normal distribution (\rightarrow II/3.2.1):

$$X \sim \mathcal{N}(\mu, \sigma^2) . \quad (1)$$

Then, the median (\rightarrow I/1.18.1) of X is

$$\text{median}(X) = \mu . \quad (2)$$

Proof: The median (\rightarrow I/1.18.1) is the value at which the cumulative distribution function (\rightarrow I/1.8.1) is $1/2$:

$$F_X(\text{median}(X)) = \frac{1}{2} . \quad (3)$$

The cumulative distribution function of the normal distribution (\rightarrow II/3.2.12) is

$$F_X(x) = \frac{1}{2} \left[1 + \text{erf} \left(\frac{x - \mu}{\sqrt{2}\sigma} \right) \right] \quad (4)$$

where $\text{erf}(x)$ is the error function. Thus, the inverse CDF is

$$x = \sqrt{2}\sigma \cdot \text{erf}^{-1}(2p - 1) + \mu \quad (5)$$

where $\text{erf}^{-1}(x)$ is the inverse error function. Setting $p = 1/2$, we obtain:

$$\text{median}(X) = \sqrt{2}\sigma \cdot \text{erf}^{-1}(0) + \mu = \mu . \quad (6)$$

**3.2.18 Mode**

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a normal distribution (\rightarrow II/3.2.1):

$$X \sim \mathcal{N}(\mu, \sigma^2) . \quad (1)$$

Then, the mode (\rightarrow I/1.18.3) of X is

$$\text{mode}(X) = \mu . \quad (2)$$

Proof: The mode (\rightarrow I/1.18.3) is the value which maximizes the probability density function (\rightarrow I/1.7.1):

$$\text{mode}(X) = \arg \max_x f_X(x) . \quad (3)$$

The probability density function of the normal distribution (\rightarrow II/3.2.10) is:

$$f_X(x) = \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp \left[-\frac{1}{2} \left(\frac{x - \mu}{\sigma} \right)^2 \right] . \quad (4)$$

The first two derivatives of this function are:

$$f'_X(x) = \frac{df_X(x)}{dx} = \frac{1}{\sqrt{2\pi}\sigma^3} \cdot (-x + \mu) \cdot \exp \left[-\frac{1}{2} \left(\frac{x - \mu}{\sigma} \right)^2 \right] \quad (5)$$

$$f''_X(x) = \frac{d^2f_X(x)}{dx^2} = -\frac{1}{\sqrt{2\pi}\sigma^3} \cdot \exp \left[-\frac{1}{2} \left(\frac{x - \mu}{\sigma} \right)^2 \right] + \frac{1}{\sqrt{2\pi}\sigma^5} \cdot (-x + \mu)^2 \cdot \exp \left[-\frac{1}{2} \left(\frac{x - \mu}{\sigma} \right)^2 \right] . \quad (6)$$

We now calculate the root of the first derivative (5):

$$\begin{aligned} f'_X(x) = 0 &= \frac{1}{\sqrt{2\pi}\sigma^3} \cdot (-x + \mu) \cdot \exp \left[-\frac{1}{2} \left(\frac{x - \mu}{\sigma} \right)^2 \right] \\ 0 &= -x + \mu \\ x &= \mu . \end{aligned} \quad (7)$$

By plugging this value into the second derivative (6),

$$\begin{aligned} f''_X(\mu) &= -\frac{1}{\sqrt{2\pi}\sigma^3} \cdot \exp(0) + \frac{1}{\sqrt{2\pi}\sigma^5} \cdot (0)^2 \cdot \exp(0) \\ &= -\frac{1}{\sqrt{2\pi}\sigma^3} < 0 , \end{aligned} \quad (8)$$

we confirm that it is in fact a maximum which shows that

$$\text{mode}(X) = \mu . \quad (9)$$

■

3.2.19 Variance

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a normal distribution (\rightarrow II/3.2.1):

$$X \sim \mathcal{N}(\mu, \sigma^2) . \quad (1)$$

Then, the variance (\rightarrow I/1.13.1) of X is

$$\text{Var}(X) = \sigma^2 . \quad (2)$$

Proof: The variance (\rightarrow I/1.13.1) is the probability-weighted average of the squared deviation from the mean (\rightarrow I/1.12.1):

$$\text{Var}(X) = \int_{\mathbb{R}} (x - E(X))^2 \cdot f_X(x) dx . \quad (3)$$

With the expected value (\rightarrow II/3.2.16) and probability density function (\rightarrow II/3.2.10) of the normal distribution, this reads:

$$\begin{aligned}\text{Var}(X) &= \int_{-\infty}^{+\infty} (x - \mu)^2 \cdot \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp \left[-\frac{1}{2} \left(\frac{x - \mu}{\sigma} \right)^2 \right] dx \\ &= \frac{1}{\sqrt{2\pi}\sigma} \int_{-\infty}^{+\infty} (x - \mu)^2 \cdot \exp \left[-\frac{1}{2} \left(\frac{x - \mu}{\sigma} \right)^2 \right] dx .\end{aligned}\quad (4)$$

Substituting $z = x - \mu$, we have:

$$\begin{aligned}\text{Var}(X) &= \frac{1}{\sqrt{2\pi}\sigma} \int_{-\infty-\mu}^{+\infty-\mu} z^2 \cdot \exp \left[-\frac{1}{2} \left(\frac{z}{\sigma} \right)^2 \right] d(z + \mu) \\ &= \frac{1}{\sqrt{2\pi}\sigma} \int_{-\infty}^{+\infty} z^2 \cdot \exp \left[-\frac{1}{2} \left(\frac{z}{\sigma} \right)^2 \right] dz .\end{aligned}\quad (5)$$

Now substituting $z = \sqrt{2}\sigma x$, we have:

$$\begin{aligned}\text{Var}(X) &= \frac{1}{\sqrt{2\pi}\sigma} \int_{-\infty}^{+\infty} (\sqrt{2}\sigma x)^2 \cdot \exp \left[-\frac{1}{2} \left(\frac{\sqrt{2}\sigma x}{\sigma} \right)^2 \right] d(\sqrt{2}\sigma x) \\ &= \frac{1}{\sqrt{2\pi}\sigma} \cdot 2\sigma^2 \cdot \sqrt{2}\sigma \int_{-\infty}^{+\infty} x^2 \cdot \exp [-x^2] dx \\ &= \frac{2\sigma^2}{\sqrt{\pi}} \int_{-\infty}^{+\infty} x^2 \cdot e^{-x^2} dx .\end{aligned}\quad (6)$$

Since the integrand is symmetric with respect to $x = 0$, we can write:

$$\text{Var}(X) = \frac{4\sigma^2}{\sqrt{\pi}} \int_0^{\infty} x^2 \cdot e^{-x^2} dx .\quad (7)$$

If we define $z = x^2$, then $x = \sqrt{z}$ and $dx = 1/2 z^{-1/2} dz$. Substituting this into the integral

$$\text{Var}(X) = \frac{4\sigma^2}{\sqrt{\pi}} \int_0^{\infty} z \cdot e^{-z} \cdot \frac{1}{2} z^{-1/2} dz = \frac{2\sigma^2}{\sqrt{\pi}} \int_0^{\infty} z^{\frac{3}{2}-1} \cdot e^{-z} dz\quad (8)$$

and using the definition of the gamma function

$$\Gamma(x) = \int_0^{\infty} z^{x-1} \cdot e^{-z} dz ,\quad (9)$$

we can finally show that

$$\text{Var}(X) = \frac{2\sigma^2}{\sqrt{\pi}} \cdot \Gamma\left(\frac{3}{2}\right) = \frac{2\sigma^2}{\sqrt{\pi}} \cdot \frac{\sqrt{\pi}}{2} = \sigma^2 .\quad (10)$$

■

Sources:

- Papadopoulos, Alecos (2013): “How to derive the mean and variance of Gaussian random variable?”; in: *StackExchange Mathematics*, retrieved on 2020-01-09; URL: <https://math.stackexchange.com/questions/518281/how-to-derive-the-mean-and-variance-of-a-gaussian-random-variable>.
- Wikipedia (2025): “Particular values of the gamma function”; in: *Wikipedia, the free encyclopedia*, retrieved on 2025-12-19; URL: https://en.wikipedia.org/wiki/Particular_values_of_the_gamma_function#Integers_and_half-integers.

3.2.20 Full width at half maximum

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a normal distribution (\rightarrow II/3.2.1):

$$X \sim \mathcal{N}(\mu, \sigma^2) . \quad (1)$$

Then, the full width at half maximum (\rightarrow I/1.19.4) (FWHM) of X is

$$\text{FWHM}(X) = 2\sqrt{2 \ln 2} \sigma . \quad (2)$$

Proof: The probability density function of the normal distribution (\rightarrow II/3.2.10) is

$$f_X(x) = \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp \left[-\frac{1}{2} \left(\frac{x - \mu}{\sigma} \right)^2 \right] \quad (3)$$

and the mode of the normal distribution (\rightarrow II/3.2.18) is

$$\text{mode}(X) = \mu , \quad (4)$$

such that

$$f_{\max} = f_X(\text{mode}(X)) \stackrel{(4)}{=} f_X(\mu) \stackrel{(3)}{=} \frac{1}{\sqrt{2\pi}\sigma} . \quad (5)$$

The FWHM bounds satisfy the equation (\rightarrow I/1.19.4)

$$f_X(x_{\text{FWHM}}) = \frac{1}{2} f_{\max} \stackrel{(5)}{=} \frac{1}{2\sqrt{2\pi}\sigma} . \quad (6)$$

Using (3), we can develop this equation as follows:

$$\begin{aligned}
\frac{1}{\sqrt{2\pi}\sigma} \cdot \exp \left[-\frac{1}{2} \left(\frac{x_{\text{FWHM}} - \mu}{\sigma} \right)^2 \right] &= \frac{1}{2\sqrt{2\pi}\sigma} \\
\exp \left[-\frac{1}{2} \left(\frac{x_{\text{FWHM}} - \mu}{\sigma} \right)^2 \right] &= \frac{1}{2} \\
-\frac{1}{2} \left(\frac{x_{\text{FWHM}} - \mu}{\sigma} \right)^2 &= \ln \frac{1}{2} \\
\left(\frac{x_{\text{FWHM}} - \mu}{\sigma} \right)^2 &= -2 \ln \frac{1}{2} \\
\frac{x_{\text{FWHM}} - \mu}{\sigma} &= \pm \sqrt{2 \ln 2} \\
x_{\text{FWHM}} - \mu &= \pm \sqrt{2 \ln 2} \sigma \\
x_{\text{FWHM}} &= \pm \sqrt{2 \ln 2} \sigma + \mu .
\end{aligned} \tag{7}$$

This implies the following two solutions for x_{FWHM}

$$\begin{aligned}
x_1 &= \mu - \sqrt{2 \ln 2} \sigma \\
x_2 &= \mu + \sqrt{2 \ln 2} \sigma ,
\end{aligned} \tag{8}$$

such that the full width at half maximum (\rightarrow I/1.19.4) of X is

$$\begin{aligned}
\text{FWHM}(X) &= \Delta x = x_2 - x_1 \\
&\stackrel{(8)}{=} \left(\mu + \sqrt{2 \ln 2} \sigma \right) - \left(\mu - \sqrt{2 \ln 2} \sigma \right) \\
&= 2\sqrt{2 \ln 2} \sigma .
\end{aligned} \tag{9}$$

■

Sources:

- Wikipedia (2020): “Full width at half maximum”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-08-19; URL: https://en.wikipedia.org/wiki/Full_width_at_half_maximum.

3.2.21 Extreme points

Theorem: The probability density function (\rightarrow I/1.7.1) of the normal distribution (\rightarrow II/3.2.1) with mean μ and variance σ^2 has a maximum at $x = \mu$ and no other extrema. Consequently, the normal distribution (\rightarrow II/3.2.1) is a unimodal probability distribution (\rightarrow I/1.5.5).

Proof: The probability density function of the normal distribution (\rightarrow II/3.2.10) is:

$$f_X(x) = \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp \left[-\frac{1}{2} \left(\frac{x - \mu}{\sigma} \right)^2 \right] . \tag{1}$$

The first two derivatives of this function (\rightarrow II/3.2.18) are:

$$f'_X(x) = \frac{df_X(x)}{dx} = \frac{1}{\sqrt{2\pi}\sigma^3} \cdot (-x + \mu) \cdot \exp \left[-\frac{1}{2} \left(\frac{x - \mu}{\sigma} \right)^2 \right] \quad (2)$$

$$f''_X(x) = \frac{d^2f_X(x)}{dx^2} = -\frac{1}{\sqrt{2\pi}\sigma^3} \cdot \exp \left[-\frac{1}{2} \left(\frac{x - \mu}{\sigma} \right)^2 \right] + \frac{1}{\sqrt{2\pi}\sigma^5} \cdot (-x + \mu)^2 \cdot \exp \left[-\frac{1}{2} \left(\frac{x - \mu}{\sigma} \right)^2 \right] \quad (3)$$

The first derivative is zero, if and only if

$$-x + \mu = 0 \quad \Leftrightarrow \quad x = \mu \quad (4)$$

Since the second derivative is negative at this value

$$f''_X(\mu) = -\frac{1}{\sqrt{2\pi}\sigma^3} < 0, \quad (5)$$

there is a maximum at $x = \mu$. From (2), it can be seen that $f'_X(x)$ is positive for $x < \mu$ and negative for $x > \mu$. Thus, there are no further extrema and $\mathcal{N}(\mu, \sigma^2)$ is unimodal (\rightarrow II/3.2.18). ■

Sources:

- Wikipedia (2021): “Normal distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-08-25; URL: https://en.wikipedia.org/wiki/Normal_distribution#Symmetries_and_derivatives.

3.2.22 Inflection points

Theorem: The probability density function (\rightarrow I/1.7.1) of the normal distribution (\rightarrow II/3.2.1) with mean μ and variance σ^2 has two inflection points at $x = \mu - \sigma$ and $x = \mu + \sigma$, i.e. exactly one standard deviation (\rightarrow I/1.19.1) away from the expected value (\rightarrow I/1.12.1).

Proof: The probability density function of the normal distribution (\rightarrow II/3.2.10) is:

$$f_X(x) = \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp \left[-\frac{1}{2} \left(\frac{x - \mu}{\sigma} \right)^2 \right] \quad (1)$$

The first three derivatives of this function are:

$$f'_X(x) = \frac{df_X(x)}{dx} = \frac{1}{\sqrt{2\pi}\sigma} \cdot \left(-\frac{x - \mu}{\sigma^2} \right) \cdot \exp \left[-\frac{1}{2} \left(\frac{x - \mu}{\sigma} \right)^2 \right] \quad (2)$$

$$\begin{aligned} f''_X(x) &= \frac{d^2f_X(x)}{dx^2} = \frac{1}{\sqrt{2\pi}\sigma} \cdot \left(-\frac{1}{\sigma^2} \right) \cdot \exp \left[-\frac{1}{2} \left(\frac{x - \mu}{\sigma} \right)^2 \right] + \frac{1}{\sqrt{2\pi}\sigma} \cdot \left(\frac{x - \mu}{\sigma^2} \right)^2 \cdot \exp \left[-\frac{1}{2} \left(\frac{x - \mu}{\sigma} \right)^2 \right] \\ &= \frac{1}{\sqrt{2\pi}\sigma} \cdot \left[\left(\frac{x - \mu}{\sigma^2} \right)^2 - \frac{1}{\sigma^2} \right] \cdot \exp \left[-\frac{1}{2} \left(\frac{x - \mu}{\sigma} \right)^2 \right] \end{aligned} \quad (3)$$

$$\begin{aligned}
f_X'''(x) &= \frac{d^3 f_X(x)}{dx^3} = \frac{1}{\sqrt{2\pi}\sigma} \cdot \left[\frac{2}{\sigma^2} \left(\frac{x-\mu}{\sigma^2} \right) \right] \cdot \exp \left[-\frac{1}{2} \left(\frac{x-\mu}{\sigma} \right)^2 \right] - \frac{1}{\sqrt{2\pi}\sigma} \cdot \left[\left(\frac{x-\mu}{\sigma^2} \right)^2 - \frac{1}{\sigma^2} \right] \cdot \left(\frac{x-\mu}{\sigma^2} \right) \\
&= \frac{1}{\sqrt{2\pi}\sigma} \cdot \left[-\left(\frac{x-\mu}{\sigma^2} \right)^3 + 3 \left(\frac{x-\mu}{\sigma^4} \right) \right] \cdot \exp \left[-\frac{1}{2} \left(\frac{x-\mu}{\sigma} \right)^2 \right].
\end{aligned} \tag{4}$$

The second derivative is zero, if and only if

$$\begin{aligned}
0 &= \left[\left(\frac{x-\mu}{\sigma^2} \right)^2 - \frac{1}{\sigma^2} \right] \\
0 &= \frac{x^2}{\sigma^4} - \frac{2\mu x}{\sigma^4} + \frac{\mu^2}{\sigma^4} - \frac{1}{\sigma^2} \\
0 &= x^2 - 2\mu x + (\mu^2 - \sigma^2) \\
x_{1/2} &= -\frac{-2\mu}{2} \pm \sqrt{\left(\frac{-2\mu}{2} \right)^2 - (\mu^2 - \sigma^2)} \\
x_{1/2} &= \mu \pm \sqrt{\mu^2 - \mu^2 + \sigma^2} \\
x_{1/2} &= \mu \pm \sigma.
\end{aligned} \tag{5}$$

Since the third derivative is non-zero at this value

$$\begin{aligned}
f_X'''(\mu \pm \sigma) &= \frac{1}{\sqrt{2\pi}\sigma} \cdot \left[-\left(\frac{\pm\sigma}{\sigma^2} \right)^3 + 3 \left(\frac{\pm\sigma}{\sigma^4} \right) \right] \cdot \exp \left[-\frac{1}{2} \left(\frac{\pm\sigma}{\sigma} \right)^2 \right] \\
&= \frac{1}{\sqrt{2\pi}\sigma} \cdot \left(\pm \frac{2}{\sigma^3} \right) \cdot \exp \left(-\frac{1}{2} \right) \neq 0,
\end{aligned} \tag{6}$$

there are inflection points at $x_{1/2} = \mu \pm \sigma$. Because μ is the mean and σ^2 is the variance of a normal distribution (\rightarrow II/3.2.1), these points are exactly one standard deviation (\rightarrow I/1.19.1) away from the mean.

■

Sources:

- Wikipedia (2021): “Normal distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-08-25; URL: https://en.wikipedia.org/wiki/Normal_distribution#Symmetries_and_derivatives.

3.2.23 Differential entropy

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a normal distribution (\rightarrow II/3.2.1):

$$X \sim \mathcal{N}(\mu, \sigma^2). \tag{1}$$

Then, the differential entropy (\rightarrow I/2.2.1) of X is

$$h(X) = \frac{1}{2} \ln(2\pi\sigma^2 e) . \quad (2)$$

Proof: The differential entropy (\rightarrow I/2.2.1) of a random variable is defined as

$$h(X) = - \int_{\mathcal{X}} p(x) \log_b p(x) dx . \quad (3)$$

To measure $h(X)$ in nats, we set $b = e$, such that (\rightarrow I/1.12.1)

$$h(X) = -E[\ln p(x)] . \quad (4)$$

With the probability density function of the normal distribution (\rightarrow II/3.2.10), the differential entropy of X is:

$$\begin{aligned} h(X) &= -E \left[\ln \left(\frac{1}{\sqrt{2\pi}\sigma} \cdot \exp \left[-\frac{1}{2} \left(\frac{x-\mu}{\sigma} \right)^2 \right] \right) \right] \\ &= -E \left[-\frac{1}{2} \ln(2\pi\sigma^2) - \frac{1}{2} \left(\frac{x-\mu}{\sigma} \right)^2 \right] \\ &= \frac{1}{2} \ln(2\pi\sigma^2) + \frac{1}{2} E \left[\left(\frac{x-\mu}{\sigma} \right)^2 \right] \\ &= \frac{1}{2} \ln(2\pi\sigma^2) + \frac{1}{2} \cdot \frac{1}{\sigma^2} \cdot E[(x-\mu)^2] . \end{aligned} \quad (5)$$

Note that $E[(x-\mu)^2]$ corresponds to the variance (\rightarrow I/1.21.8) of X and the variance of the normal distribution (\rightarrow II/3.2.19) is σ^2 . Thus, we can proceed:

$$\begin{aligned} h(X) &= \frac{1}{2} \ln(2\pi\sigma^2) + \frac{1}{2} \cdot \frac{1}{\sigma^2} \cdot \sigma^2 \\ &= \frac{1}{2} \ln(2\pi\sigma^2) + \frac{1}{2} \\ &= \frac{1}{2} \ln(2\pi\sigma^2 e) . \end{aligned} \quad (6)$$

■

Sources:

- Wang, Peng-Hua (2012): “Differential Entropy”; in: *National Taipei University*; URL: <https://web.ntpu.edu.tw/~phwang/teaching/2012s/IT/slides/chap08.pdf>.

3.2.24 Kullback-Leibler divergence

Theorem: Let X be a random variable (\rightarrow I/1.2.2). Assume two normal distributions (\rightarrow II/3.2.1) P and Q specifying the probability distribution of X as

$$\begin{aligned} P : X &\sim \mathcal{N}(\mu_1, \sigma_1^2) \\ Q : X &\sim \mathcal{N}(\mu_2, \sigma_2^2) . \end{aligned} \quad (1)$$

Then, the Kullback-Leibler divergence (\rightarrow I/2.5.1) of P from Q is given by

$$\text{KL}[P \parallel Q] = \frac{1}{2} \left[\frac{(\mu_2 - \mu_1)^2}{\sigma_2^2} + \frac{\sigma_1^2}{\sigma_2^2} - \ln \frac{\sigma_1^2}{\sigma_2^2} - 1 \right]. \quad (2)$$

Proof: The KL divergence for a continuous random variable (\rightarrow I/2.5.1) is given by

$$\text{KL}[P \parallel Q] = \int_{\mathcal{X}} p(x) \ln \frac{p(x)}{q(x)} dx \quad (3)$$

which, applied to the normal distributions (\rightarrow II/3.2.1) in (1), yields

$$\begin{aligned} \text{KL}[P \parallel Q] &= \int_{-\infty}^{+\infty} \mathcal{N}(x; \mu_1, \sigma_1^2) \ln \frac{\mathcal{N}(x; \mu_1, \sigma_1^2)}{\mathcal{N}(x; \mu_2, \sigma_2^2)} dx \\ &= \left\langle \ln \frac{\mathcal{N}(x; \mu_1, \sigma_1^2)}{\mathcal{N}(x; \mu_2, \sigma_2^2)} \right\rangle_{p(x)}. \end{aligned} \quad (4)$$

Using the probability density function of the normal distribution (\rightarrow II/3.2.10), this becomes:

$$\begin{aligned} \text{KL}[P \parallel Q] &= \left\langle \ln \frac{\frac{1}{\sqrt{2\pi}\sigma_1} \cdot \exp \left[-\frac{1}{2} \left(\frac{x-\mu_1}{\sigma_1} \right)^2 \right]}{\frac{1}{\sqrt{2\pi}\sigma_2} \cdot \exp \left[-\frac{1}{2} \left(\frac{x-\mu_2}{\sigma_2} \right)^2 \right]} \right\rangle_{p(x)} \\ &= \left\langle \ln \left(\sqrt{\frac{\sigma_2^2}{\sigma_1^2}} \cdot \exp \left[-\frac{1}{2} \left(\frac{x-\mu_1}{\sigma_1} \right)^2 + \frac{1}{2} \left(\frac{x-\mu_2}{\sigma_2} \right)^2 \right] \right) \right\rangle_{p(x)} \\ &= \left\langle \frac{1}{2} \ln \frac{\sigma_2^2}{\sigma_1^2} - \frac{1}{2} \left(\frac{x-\mu_1}{\sigma_1} \right)^2 + \frac{1}{2} \left(\frac{x-\mu_2}{\sigma_2} \right)^2 \right\rangle_{p(x)} \\ &= \frac{1}{2} \left\langle - \left(\frac{x-\mu_1}{\sigma_1} \right)^2 + \left(\frac{x-\mu_2}{\sigma_2} \right)^2 - \ln \frac{\sigma_1^2}{\sigma_2^2} \right\rangle_{p(x)} \\ &= \frac{1}{2} \left\langle - \frac{(x-\mu_1)^2}{\sigma_1^2} + \frac{x^2 - 2\mu_2 x + \mu_2^2}{\sigma_2^2} - \ln \frac{\sigma_1^2}{\sigma_2^2} \right\rangle_{p(x)}. \end{aligned} \quad (5)$$

Because the expected value (\rightarrow I/1.12.1) is a linear operator (\rightarrow I/1.12.5), the expectation can be moved into the sum:

$$\begin{aligned} \text{KL}[P \parallel Q] &= \frac{1}{2} \left[- \frac{\langle (x-\mu_1)^2 \rangle}{\sigma_1^2} + \frac{\langle x^2 - 2\mu_2 x + \mu_2^2 \rangle}{\sigma_2^2} - \left\langle \ln \frac{\sigma_1^2}{\sigma_2^2} \right\rangle \right] \\ &= \frac{1}{2} \left[- \frac{\langle (x-\mu_1)^2 \rangle}{\sigma_1^2} + \frac{\langle x^2 \rangle - \langle 2\mu_2 x \rangle + \langle \mu_2^2 \rangle}{\sigma_2^2} - \ln \frac{\sigma_1^2}{\sigma_2^2} \right]. \end{aligned} \quad (6)$$

The first expectation corresponds to the variance (\rightarrow I/1.13.1)

$$\langle (X - \mu)^2 \rangle = \text{E}[(X - \text{E}(X))^2] = \text{Var}(X) \quad (7)$$

and the variance of a normally distributed random variable (\rightarrow II/3.2.19) is

$$X \sim \mathcal{N}(\mu, \sigma^2) \quad \Rightarrow \quad \text{Var}(X) = \sigma^2. \quad (8)$$

Additionally applying the raw moments of the normal distribution (\rightarrow II/3.2.11)

$$X \sim \mathcal{N}(\mu, \sigma^2) \quad \Rightarrow \quad \langle x \rangle = \mu \quad \text{and} \quad \langle x^2 \rangle = \mu^2 + \sigma^2, \quad (9)$$

the Kullback-Leibler divergence in (6) becomes

$$\begin{aligned} \text{KL}[P \parallel Q] &= \frac{1}{2} \left[-\frac{\sigma_1^2}{\sigma_2^2} + \frac{\mu_1^2 + \sigma_1^2 - 2\mu_2\mu_1 + \mu_2^2}{\sigma_2^2} - \ln \frac{\sigma_1^2}{\sigma_2^2} \right] \\ &= \frac{1}{2} \left[\frac{\mu_1^2 - 2\mu_1\mu_2 + \mu_2^2}{\sigma_2^2} + \frac{\sigma_1^2}{\sigma_2^2} - \ln \frac{\sigma_1^2}{\sigma_2^2} - 1 \right] \\ &= \frac{1}{2} \left[\frac{(\mu_1 - \mu_2)^2}{\sigma_2^2} + \frac{\sigma_1^2}{\sigma_2^2} - \ln \frac{\sigma_1^2}{\sigma_2^2} - 1 \right] \end{aligned} \quad (10)$$

which is equivalent to (2). ■

3.2.25 Maximum entropy distribution

Theorem: The normal distribution (\rightarrow II/3.2.1) maximizes differential entropy (\rightarrow I/2.2.1) for a random variable (\rightarrow I/1.2.2) with fixed variance (\rightarrow I/1.13.1).

Proof: For a random variable (\rightarrow I/1.2.2) X with set of possible values \mathcal{X} and probability density function (\rightarrow I/1.7.1) $p(x)$, the differential entropy (\rightarrow I/2.2.1) is defined as:

$$h(X) = - \int_{\mathcal{X}} p(x) \log p(x) \, dx. \quad (1)$$

Let $g(x)$ be the probability density function (\rightarrow I/1.7.1) of a normal distribution (\rightarrow II/3.2.1) with mean (\rightarrow I/1.12.1) μ and variance (\rightarrow I/1.13.1) σ^2 and let $f(x)$ be an arbitrary probability density function (\rightarrow I/1.7.1) with the same variance (\rightarrow I/1.13.1). Since differential entropy (\rightarrow I/2.2.1) is translation-invariant (\rightarrow I/2.2.3), we can assume that $f(x)$ has the same mean as $g(x)$.

Consider the Kullback-Leibler divergence (\rightarrow I/2.5.1) of distribution $f(x)$ from distribution $g(x)$ which is non-negative (\rightarrow I/2.5.2):

$$\begin{aligned} 0 \leq \text{KL}[f \parallel g] &= \int_{\mathcal{X}} f(x) \log \frac{f(x)}{g(x)} \, dx \\ &= \int_{\mathcal{X}} f(x) \log f(x) \, dx - \int_{\mathcal{X}} f(x) \log g(x) \, dx \\ &\stackrel{(1)}{=} -h[f(x)] - \int_{\mathcal{X}} f(x) \log g(x) \, dx. \end{aligned} \quad (2)$$

By plugging the probability density function of the normal distribution (\rightarrow II/3.2.10) into the second term, we obtain:

$$\begin{aligned}
\int_{\mathcal{X}} f(x) \log g(x) \, dx &= \int_{\mathcal{X}} f(x) \log \left(\frac{1}{\sqrt{2\pi}\sigma} \cdot \exp \left[-\frac{1}{2} \left(\frac{x-\mu}{\sigma} \right)^2 \right] \right) \, dx \\
&= \int_{\mathcal{X}} f(x) \log \left(\frac{1}{\sqrt{2\pi}\sigma^2} \right) \, dx + \int_{\mathcal{X}} f(x) \log \left(\exp \left[-\frac{(x-\mu)^2}{2\sigma^2} \right] \right) \, dx \quad (3) \\
&= -\frac{1}{2} \log(2\pi\sigma^2) \int_{\mathcal{X}} f(x) \, dx - \frac{\log(e)}{2\sigma^2} \int_{\mathcal{X}} f(x)(x-\mu)^2 \, dx .
\end{aligned}$$

Because the entire integral over a probability density function is one (\rightarrow I/1.7.1) and the second central moment is equal to the variance (\rightarrow I/1.21.8), we have:

$$\begin{aligned}
\int_{\mathcal{X}} f(x) \log g(x) \, dx &= -\frac{1}{2} \log(2\pi\sigma^2) - \frac{\log(e)\sigma^2}{2\sigma^2} \\
&= -\frac{1}{2} [\log(2\pi\sigma^2) + \log(e)] \quad (4) \\
&= -\frac{1}{2} \log(2\pi\sigma^2 e) .
\end{aligned}$$

This is actually the negative of the differential entropy of the normal distribution (\rightarrow II/3.2.23), such that:

$$\int_{\mathcal{X}} f(x) \log g(x) \, dx = -h[\mathcal{N}(\mu, \sigma^2)] = -h[g(x)] . \quad (5)$$

Combining (2) with (5), we can show that

$$\begin{aligned}
0 &\leq \text{KL}[f||g] \\
0 &\leq -h[f(x)] - (-h[g(x)]) \quad (6) \\
h[g(x)] &\geq h[f(x)]
\end{aligned}$$

which means that the differential entropy (\rightarrow I/2.2.1) of the normal distribution (\rightarrow II/3.2.1) $\mathcal{N}(\mu, \sigma^2)$ will be larger than or equal to any other distribution (\rightarrow I/1.5.1) with the same variance (\rightarrow I/1.13.1) σ^2 . ■

Sources:

- Wikipedia (2021): “Differential entropy”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-08-25; URL: https://en.wikipedia.org/wiki/Differential_entropy#Maximization_in_the_normal_distribution.

3.2.26 Linear combination of independent normals

Theorem: Let X_1, \dots, X_n be independent (\rightarrow I/1.3.6) normally distributed (\rightarrow II/3.2.1) random variables (\rightarrow I/1.2.2) with means (\rightarrow I/1.12.1) μ_1, \dots, μ_n and variances (\rightarrow I/1.13.1) $\sigma_1^2, \dots, \sigma_n^2$:

$$X_i \sim \mathcal{N}(\mu_i, \sigma_i^2) \quad \text{for } i = 1, \dots, n . \quad (1)$$

Then, any linear combination of those random variables

$$Y = \sum_{i=1}^n a_i X_i \quad \text{where} \quad a_1, \dots, a_n \in \mathbb{R} \quad (2)$$

also follows a normal distribution

$$Y \sim \mathcal{N} \left(\sum_{i=1}^n a_i \mu_i, \sum_{i=1}^n a_i^2 \sigma_i^2 \right) \quad (3)$$

with mean and variance which are functions of the individual means and variances.

Proof: A set of n independent normal random variables X_1, \dots, X_n is equivalent (\rightarrow II/4.1.17) to an n -dimensional random vector (\rightarrow I/1.2.3) x following a multivariate normal distribution (\rightarrow II/4.1.1) with a diagonal covariance matrix (\rightarrow I/1.16.1). Therefore, we can write

$$X_i \sim \mathcal{N}(\mu_i, \sigma_i^2), \quad i = 1, \dots, n \quad \Rightarrow \quad x = \begin{bmatrix} X_1 \\ \vdots \\ X_n \end{bmatrix} \sim \mathcal{N}(\mu, \Sigma) \quad (4)$$

with mean vector and covariance matrix

$$\mu = \begin{bmatrix} \mu_1 \\ \vdots \\ \mu_n \end{bmatrix} \quad \text{and} \quad \Sigma = \begin{bmatrix} \sigma_1^2 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \sigma_n^2 \end{bmatrix} = \text{diag}([\sigma_1^2, \dots, \sigma_n^2]) \quad (5)$$

Thus, we can apply the linear transformation theorem for the multivariate normal distribution (\rightarrow II/4.1.14)

$$x \sim \mathcal{N}(\mu, \Sigma) \quad \Rightarrow \quad y = Ax + b \sim \mathcal{N}(A\mu + b, A\Sigma A^T) \quad (6)$$

with the constant matrix and vector

$$A = [a_1, \dots, a_n] \quad \text{and} \quad b = 0 \quad (7)$$

This implies the following distribution for the linear combination given by equation (2):

$$Y = Ax + b \sim \mathcal{N}(A\mu, A\Sigma A^T) \quad (8)$$

Finally, we note that

$$\begin{aligned} A\mu &= [a_1, \dots, a_n] \begin{bmatrix} \mu_1 \\ \vdots \\ \mu_n \end{bmatrix} = \sum_{i=1}^n a_i \mu_i \quad \text{and} \\ A\Sigma A^T &= [a_1, \dots, a_n] \begin{bmatrix} \sigma_1^2 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \sigma_n^2 \end{bmatrix} \begin{bmatrix} a_1 \\ \vdots \\ a_n \end{bmatrix} = \sum_{i=1}^n a_i^2 \sigma_i^2. \end{aligned} \quad (9)$$



3.2.27 Normal and uncorrelated does not imply independent

Theorem: Consider two random variables (\rightarrow I/1.2.2) X and Y . If each of them is normally distributed (\rightarrow II/3.2.1) and both are uncorrelated (\rightarrow I/1.17.1), then X and Y are not necessarily independent (\rightarrow I/1.3.6).

Proof: As an example, let V follow a Bernoulli distribution (\rightarrow II/1.2.1) with success probability (\rightarrow II/1.2.1) $1/2$ and let W be defined as a transformation of V :

$$\begin{aligned} V &\sim \text{Bern}\left(\frac{1}{2}\right) \\ W &= 2V - 1 . \end{aligned} \tag{1}$$

By definition of the Bernoulli distribution (\rightarrow II/1.2.1), it follows that

$$p(V = 0) = p(V = 1) = \frac{1}{2} \quad \Rightarrow \quad p(W = -1) = p(W = +1) = \frac{1}{2} . \tag{2}$$

Moreover, let X follow a standard normal distribution (\rightarrow II/3.2.3) and let Y be defined as a combination of X and W :

$$\begin{aligned} X &\sim \mathcal{N}(0, 1) \\ Y &= WX . \end{aligned} \tag{3}$$

Then, by the nature of the random variable (\rightarrow I/1.2.2) W , it follows that

$$p(W = -1) = p(W = +1) = \frac{1}{2} \quad \Rightarrow \quad p(Y = -X) = p(Y = +X) = \frac{1}{2} . \tag{4}$$

Since the negative of a standard normal (\rightarrow II/3.2.3) random variable is also standard normally distributed (\rightarrow II/3.2.26),

$$X \sim \mathcal{N}(0, 1) \quad \Rightarrow \quad -X \sim \mathcal{N}(0, 1) , \tag{5}$$

we can calculate the probability density function (\rightarrow I/1.7.1) belonging to the mixture distribution of Y as follows:

$$\begin{aligned} p(y) &= p(y|Y = -X) \cdot p(Y = -X) + p(y|Y = +X) \cdot p(Y = +X) \\ &\stackrel{(4)}{=} \mathcal{N}(y; 0, 1) \cdot \frac{1}{2} + \mathcal{N}(y; 0, 1) \cdot \frac{1}{2} \\ &= \mathcal{N}(y; 0, 1) \end{aligned} \tag{6}$$

where we have used the law of marginal probability (\rightarrow I/1.3.3) in the first line and $\mathcal{N}(x; \mu, \sigma^2)$ denotes the probability density function of the normal distribution (\rightarrow II/3.2.10). Thus, Y is also standard normally distributed (\rightarrow II/3.2.3):

$$Y \sim \mathcal{N}(0, 1) . \tag{7}$$

This means that both X and Y have expected value zero:

$$E(X) = E(Y) = 0 . \quad (8)$$

With that, we can start to work out the covariance of X and Y :

$$\begin{aligned} \text{Cov}(X, Y) &= E[(X - E(X))(Y - E(Y))] \\ &\stackrel{(8)}{=} E[XY] \\ &\stackrel{(3)}{=} E[XWX] \\ &= E[WX^2] . \end{aligned} \quad (9)$$

Since W and X are independent (\rightarrow I/1.3.6) by construction, their expected values factorize (\rightarrow I/1.12.7):

$$\begin{aligned} \text{Cov}(X, Y) &= E[W] \cdot E[X^2] \\ &= ((-1) \cdot p(W = -1) + (+1) \cdot p(W = +1)) \cdot E[X^2] \\ &\stackrel{(2)}{=} \left((-1) \cdot \frac{1}{2} + (+1) \cdot \frac{1}{2} \right) \cdot E[X^2] \\ &= 0 \cdot E[X^2] \\ &= 0 . \end{aligned} \quad (10)$$

Thus, X and Y are uncorrelated (\rightarrow I/1.17.1):

$$\text{Corr}(X, Y) = \frac{\text{Cov}(X, Y)}{\sqrt{\text{Var}(X)}\sqrt{\text{Var}(Y)}} = 0 . \quad (11)$$

Yet, X and Y are not independent (\rightarrow I/1.3.6), since the marginal density (\rightarrow I/1.5.3) of Y is

$$p(y) = \mathcal{N}(y; 0, 1) , \quad (12)$$

but the conditional density (\rightarrow I/1.5.4) of Y given X is

$$p(y|x) = \begin{cases} 1/2 , & \text{if } y = -x \\ 1/2 , & \text{if } y = +x \\ 0 , & \text{otherwise} \end{cases} , \quad (13)$$

thus violating the behavior of probability under independence (\rightarrow I/1.3.9):

$$p(Y) \neq p(Y|X) . \quad (14)$$

Therefore, X and Y defined by (3) and (1) constitute an example for two random variables (\rightarrow I/1.2.2) that are normally distributed (\rightarrow II/3.2.1) and uncorrelated (\rightarrow I/1.17.1), but not independent (\rightarrow I/1.3.6).

■

Sources:

- Wikipedia (2024): “Misconceptions about the normal distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2024-10-04; URL: https://en.wikipedia.org/wiki/Misconceptions_about_the_normal_distribution#A_symmetric_example.

3.2.28 Marginally normal does not imply jointly normal

Theorem: Consider two random variables (\rightarrow I/1.2.2) X and Y . If the marginal distribution (\rightarrow I/1.5.3) of each of them is a normal distribution (\rightarrow II/3.2.1), then the joint distribution (\rightarrow I/1.5.2) X and Y is not necessarily a (multivariate) normal distribution (\rightarrow II/4.1.1).

Proof: Consider the example used to show that normally distributed and uncorrelated does not imply independent (\rightarrow II/3.2.27). This is characterized by the random variables (\rightarrow I/1.2.2)

$$\begin{aligned} V &\sim \text{Bern}\left(\frac{1}{2}\right) \\ W &= 2V - 1 . \end{aligned} \tag{1}$$

and

$$\begin{aligned} X &\sim \mathcal{N}(0, 1) \\ Y &= WX . \end{aligned} \tag{2}$$

Under these conditions, it can be shown that (\rightarrow II/3.2.27)

$$X \sim \mathcal{N}(0, 1) \quad \text{and} \quad Y \sim \mathcal{N}(0, 1) . \tag{3}$$

The linear transformation theorem for the multivariate normal distribution (\rightarrow II/4.1.14)

$$x \sim \mathcal{N}(\mu, \Sigma) \quad \Rightarrow \quad y = Ax + b \sim \mathcal{N}(A\mu + b, A\Sigma A^T) \tag{4}$$

implies that, for bivariate normal random variables (\rightarrow II/4.2.1) X_1 and X_2 ,

$$\begin{bmatrix} X_1 \\ X_2 \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}, \begin{bmatrix} \sigma_1^2 & \sigma_{12} \\ \sigma_{12} & \sigma_2^2 \end{bmatrix}\right) . \tag{5}$$

any linear combination of X_1 and X_2 with non-zero coefficients

$$Z = aX_1 + bX_2, \quad a \neq 0, \quad b \neq 0 \tag{6}$$

follows a univariate normal distribution (\rightarrow II/4.2.6):

$$Z \sim \mathcal{N}(a\mu_1 + b\mu_2, a^2\sigma_1^2 + 2ab\sigma_{12} + b^2\sigma_2^2) . \tag{7}$$

Consider the sum of X and Y defined by (2):

$$Z = X + Y = aX + bY \quad \text{with} \quad a = b = 1 . \tag{8}$$

If X and Y were bivariate normally distributed (\rightarrow II/4.2.1), then this sum should be univariate normally distributed (\rightarrow II/3.2.1). However, this sum cannot be normally distributed, since

$$\Pr(X + Y = 0) = \frac{1}{2} \quad \text{and} \quad \Pr(X + Y = 2X) = \frac{1}{2} , \tag{9}$$

because

$$Y = \begin{cases} X, & \text{with probability } 1/2 \\ -X, & \text{with probability } 1/2 \end{cases}. \quad (10)$$

Thus, X and Y are not following a bivariate normal distribution (\rightarrow II/4.2.1). Therefore, X and Y defined by (2) and (1) constitute an example for two random variables (\rightarrow I/1.2.2) that are marginally normal (\rightarrow II/3.2.1), but not jointly normal (\rightarrow II/4.1.1). ■

Sources:

- Wikipedia (2024): “Misconceptions about the normal distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2024-10-11; URL: https://en.wikipedia.org/wiki/Misconceptions_about_the_normal_distribution#A_symmetric_example.

3.3 t-distribution

3.3.1 Definition

Definition: Let Z and V be independent (\rightarrow I/1.3.6) random variables (\rightarrow I/1.2.2) following a standard normal distribution (\rightarrow II/3.2.3) and a chi-squared distribution (\rightarrow II/3.7.1) with ν degrees of freedom (\rightarrow I/1.5.12), respectively:

$$\begin{aligned} Z &\sim \mathcal{N}(0, 1) \\ V &\sim \chi^2(\nu). \end{aligned} \quad (1)$$

Then, the ratio of Z to the square root of V , divided by the respective degrees of freedom, is said to be t -distributed with degrees of freedom ν :

$$Y = \frac{Z}{\sqrt{V/\nu}} \sim t(\nu). \quad (2)$$

The t -distribution is also called “Student’s t -distribution”, after William S. Gosset a.k.a. “Student”.

Sources:

- Wikipedia (2021): “Student’s t -distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-04-21; URL: https://en.wikipedia.org/wiki/Student%27s_t-distribution#Characterization.

3.3.2 Special case of multivariate t -distribution

Theorem: The t -distribution (\rightarrow II/3.3.1) is a special case of the multivariate t -distribution (\rightarrow II/4.3.1) with number of variables $n = 1$, i.e. random vector (\rightarrow I/1.2.3) $x \in \mathbb{R}$, mean $\mu = 0$ and covariance matrix $\Sigma = 1$.

Proof: The probability density function of the multivariate t -distribution (\rightarrow II/4.3.2) is

$$t(x; \mu, \Sigma, \nu) = \sqrt{\frac{1}{(\nu\pi)^n |\Sigma|}} \frac{\Gamma([\nu + n]/2)}{\Gamma(\nu/2)} \left[1 + \frac{1}{\nu} (x - \mu)^T \Sigma^{-1} (x - \mu) \right]^{-(\nu+n)/2}. \quad (1)$$

Setting $n = 1$, such that $x \in \mathbb{R}$, as well as $\mu = 0$ and $\Sigma = 1$, we obtain

$$\begin{aligned}
t(x; 0, 1, \nu) &= \sqrt{\frac{1}{(\nu\pi)^1|1|}} \frac{\Gamma([\nu+1]/2)}{\Gamma(\nu/2)} \left[1 + \frac{1}{\nu}(x-0)^T 1^{-1}(x-0) \right]^{-(\nu+1)/2} \\
&= \sqrt{\frac{1}{\nu\pi}} \frac{\Gamma([\nu+1]/2)}{\Gamma(\nu/2)} \left[1 + \frac{x^2}{\nu} \right]^{-(\nu+1)/2} \\
&= \frac{1}{\sqrt{\nu\pi}} \cdot \frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})} \cdot \left[1 + \frac{x^2}{\nu} \right]^{-\frac{\nu+1}{2}} .
\end{aligned} \tag{2}$$

which is equivalent to the probability density function of the t-distribution (\rightarrow II/3.3.5).

■

Sources:

- Wikipedia (2022): “Multivariate t-distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-08-25; URL: https://en.wikipedia.org/wiki/Multivariate_t-distribution#Derivation.

3.3.3 Non-standardized t-distribution

Definition: Let X be a random variable (\rightarrow I/1.2.2) following a Student’s t-distribution (\rightarrow II/3.3.1) with ν degrees of freedom. Then, the random variable (\rightarrow I/1.2.2)

$$Y = \sigma X + \mu \tag{1}$$

is said to follow a non-standardized t-distribution with non-centrality μ , scale σ^2 and degrees of freedom ν :

$$Y \sim \text{nst}(\mu, \sigma^2, \nu) . \tag{2}$$

Sources:

- Wikipedia (2021): “Student’s t-distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-05-20; URL: https://en.wikipedia.org/wiki/Student's_t-distribution#Generalized_Student's_t-distribution.

3.3.4 Relationship to non-standardized t-distribution

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a non-standardized t-distribution (\rightarrow II/3.3.3) with mean μ , scale σ^2 and degrees of freedom ν :

$$X \sim \text{nst}(\mu, \sigma^2, \nu) . \tag{1}$$

Then, subtracting the mean and dividing by the square root of the scale results in a random variable (\rightarrow I/1.2.2) following a t-distribution (\rightarrow II/3.3.1) with degrees of freedom ν :

$$Y = \frac{X - \mu}{\sigma} \sim t(\nu) . \tag{2}$$

Proof: The non-standardized t-distribution is a special case of the multivariate t-distribution (\rightarrow II/4.3.1) in which the mean vector and scale matrix are scalars:

$$X \sim \text{nst}(\mu, \sigma^2, \nu) \Rightarrow X \sim t(\mu, \sigma^2, \nu). \quad (3)$$

Therefore, we can apply the linear transformation theorem for the multivariate t-distribution for an n -dimensional random vector x :

$$x \sim t(\mu, \Sigma, \nu) \Rightarrow y = Ax + b \sim t(A\mu + b, A\Sigma A^T, \nu). \quad (4)$$

Comparing with equation (2), we have $A = 1/\sigma$, $b = -\mu/\sigma$ and the variable Y is distributed as:

$$\begin{aligned} Y &= \frac{X - \mu}{\sigma} = \frac{X}{\sigma} - \frac{\mu}{\sigma} \\ &\sim t\left(\frac{\mu}{\sigma} - \frac{\mu}{\sigma}, \left(\frac{1}{\sigma}\right)^2 \sigma^2, \nu\right) \\ &= t(0, 1, \nu). \end{aligned} \quad (5)$$

Plugging $\mu = 0$, $\Sigma = 1$ and $n = 1$ into the probability density function of the multivariate t-distribution (\rightarrow II/4.3.2),

$$p(x) = \sqrt{\frac{1}{(\nu\pi)^n |\Sigma|}} \frac{\Gamma([\nu + n]/2)}{\Gamma(\nu/2)} \left[1 + \frac{1}{\nu} (x - \mu)^T \Sigma^{-1} (x - \mu) \right], \quad (6)$$

we get

$$p(x) = \sqrt{\frac{1}{\nu\pi}} \frac{\Gamma([\nu + 1]/2)}{\Gamma(\nu/2)} \left[1 + \frac{x^2}{\nu} \right] \quad (7)$$

which is the probability density function of Student's t-distribution (\rightarrow II/3.3.5) with ν degrees of freedom. ■

3.3.5 Probability density function

Theorem: Let T be a random variable (\rightarrow I/1.2.2) following a t-distribution (\rightarrow II/3.3.1):

$$T \sim t(\nu). \quad (1)$$

Then, the probability density function (\rightarrow I/1.7.1) of T is

$$f_T(t) = \frac{\Gamma\left(\frac{\nu+1}{2}\right)}{\Gamma\left(\frac{\nu}{2}\right) \cdot \sqrt{\nu\pi}} \cdot \left(\frac{t^2}{\nu} + 1\right)^{-\frac{\nu+1}{2}}. \quad (2)$$

Proof: A t-distributed random variable (\rightarrow II/3.3.1) is defined as the ratio of a standard normal random variable (\rightarrow II/3.2.3) and the square root of a chi-squared random variable (\rightarrow II/3.7.1), divided by its degrees of freedom (\rightarrow I/1.5.12)

$$X \sim \mathcal{N}(0, 1), Y \sim \chi^2(\nu) \Rightarrow T = \frac{X}{\sqrt{Y/\nu}} \sim t(\nu) \quad (3)$$

where X and Y are independent of each other (\rightarrow I/1.3.6).

The probability density function (\rightarrow II/3.2.10) of the standard normal distribution (\rightarrow II/3.2.3) is

$$f_X(x) = \frac{1}{\sqrt{2\pi}} \cdot e^{-\frac{x^2}{2}} \quad (4)$$

and the probability density function of the chi-squared distribution (\rightarrow II/3.7.4) is

$$f_Y(y) = \frac{1}{\Gamma\left(\frac{\nu}{2}\right) \cdot 2^{\nu/2}} \cdot y^{\frac{\nu}{2}-1} \cdot e^{-\frac{y}{2}}. \quad (5)$$

Define the random variables T and W as functions of X and Y

$$\begin{aligned} T &= X \cdot \sqrt{\frac{\nu}{Y}} \\ W &= Y, \end{aligned} \quad (6)$$

such that the inverse functions X and Y in terms of T and W are

$$\begin{aligned} X &= T \cdot \sqrt{\frac{W}{\nu}} \\ Y &= W. \end{aligned} \quad (7)$$

This implies the following Jacobian matrix and determinant:

$$\begin{aligned} J &= \begin{bmatrix} \frac{dX}{dT} & \frac{dX}{dW} \\ \frac{dY}{dT} & \frac{dY}{dW} \end{bmatrix} = \begin{bmatrix} \sqrt{\frac{W}{\nu}} & \frac{T}{2\nu\sqrt{W/\nu}} \\ 0 & 1 \end{bmatrix} \\ |J| &= \sqrt{\frac{W}{\nu}}. \end{aligned} \quad (8)$$

Because X and Y are independent (\rightarrow I/1.3.6), the joint density (\rightarrow I/1.5.2) of X and Y is equal to the product (\rightarrow I/1.3.9) of the marginal densities (\rightarrow I/1.5.3):

$$f_{X,Y}(x, y) = f_X(x) \cdot f_Y(y). \quad (9)$$

With the probability density function of an invertible function (\rightarrow I/1.7.5), the joint density (\rightarrow I/1.5.2) of T and W can be derived as:

$$f_{T,W}(t, w) = f_{X,Y}(x, y) \cdot |J|. \quad (10)$$

Substituting (7) into (4) and (5), and then with (8) into (10), we get:

$$\begin{aligned} f_{T,W}(t, w) &= f_X\left(t \cdot \sqrt{\frac{w}{\nu}}\right) \cdot f_Y(w) \cdot |J| \\ &= \frac{1}{\sqrt{2\pi}} \cdot e^{-\frac{\left(t \cdot \sqrt{\frac{w}{\nu}}\right)^2}{2}} \cdot \frac{1}{\Gamma\left(\frac{\nu}{2}\right) \cdot 2^{\nu/2}} \cdot w^{\frac{\nu}{2}-1} \cdot e^{-\frac{w}{2}} \cdot \sqrt{\frac{w}{\nu}} \\ &= \frac{1}{\sqrt{2\pi\nu} \cdot \Gamma\left(\frac{\nu}{2}\right) \cdot 2^{\nu/2}} \cdot w^{\frac{\nu+1}{2}-1} \cdot e^{-\frac{w}{2}\left(\frac{t^2}{\nu}+1\right)}. \end{aligned} \quad (11)$$

The marginal density (\rightarrow I/1.5.3) of T can now be obtained by integrating out (\rightarrow I/1.3.3) W :

$$\begin{aligned}
 f_T(t) &= \int_0^\infty f_{T,W}(t, w) \, dw \\
 &= \frac{1}{\sqrt{2\pi\nu} \cdot \Gamma\left(\frac{\nu}{2}\right) \cdot 2^{\nu/2}} \cdot \int_0^\infty w^{\frac{\nu+1}{2}-1} \cdot \exp\left[-\frac{1}{2}\left(\frac{t^2}{\nu} + 1\right)w\right] \, dw \\
 &= \frac{1}{\sqrt{2\pi\nu} \cdot \Gamma\left(\frac{\nu}{2}\right) \cdot 2^{\nu/2}} \cdot \frac{\Gamma\left(\frac{\nu+1}{2}\right)}{\left[\frac{1}{2}\left(\frac{t^2}{\nu} + 1\right)\right]^{(\nu+1)/2}} \cdot \int_0^\infty \frac{\left[\frac{1}{2}\left(\frac{t^2}{\nu} + 1\right)\right]^{(\nu+1)/2}}{\Gamma\left(\frac{\nu+1}{2}\right)} \cdot w^{\frac{\nu+1}{2}-1} \cdot \exp\left[-\frac{1}{2}\left(\frac{t^2}{\nu} + 1\right)w\right] \, dw
 \end{aligned} \tag{12}$$

At this point, we can recognize that the integrand is equal to the probability density function of a gamma distribution (\rightarrow II/3.4.7) with

$$a = \frac{\nu+1}{2} \quad \text{and} \quad b = \frac{1}{2}\left(\frac{t^2}{\nu} + 1\right), \tag{13}$$

and because a probability density function integrates to one (\rightarrow I/1.7.1), we finally have:

$$\begin{aligned}
 f_T(t) &= \frac{1}{\sqrt{2\pi\nu} \cdot \Gamma\left(\frac{\nu}{2}\right) \cdot 2^{\nu/2}} \cdot \frac{\Gamma\left(\frac{\nu+1}{2}\right)}{\left[\frac{1}{2}\left(\frac{t^2}{\nu} + 1\right)\right]^{(\nu+1)/2}} \\
 &= \frac{\Gamma\left(\frac{\nu+1}{2}\right)}{\Gamma\left(\frac{\nu}{2}\right) \cdot \sqrt{\nu\pi}} \cdot \left(\frac{t^2}{\nu} + 1\right)^{-\frac{\nu+1}{2}}.
 \end{aligned} \tag{14}$$

■

Sources:

- Computation Empire (2021): “Student’s t Distribution: Derivation of PDF”; in: *You Tube*, retrieved on 2021-10-11; URL: <https://www.youtube.com/watch?v=6BraaGEVRY8>.

3.4 Gamma distribution

3.4.1 Definition

Definition: Let X be a random variable (\rightarrow I/1.2.2). Then, X is said to follow a gamma distribution with shape (\rightarrow I/1.5.11) a and rate (\rightarrow I/1.5.10) b

$$X \sim \text{Gam}(a, b), \tag{1}$$

if and only if its probability density function (\rightarrow I/1.7.1) is given by

$$\text{Gam}(x; a, b) = \frac{b^a}{\Gamma(a)} x^{a-1} \exp[-bx], \quad x > 0 \tag{2}$$

where $a > 0$ and $b > 0$, $\Gamma(x)$ is the gamma function and the density is zero, if $x \leq 0$.

Sources:

- Koch, Karl-Rudolf (2007): “Gamma Distribution”; in: *Introduction to Bayesian Statistics*, Springer, Berlin/Heidelberg, 2007, p. 47, eq. 2.172; URL: <https://www.springer.com/de/book/9783540727231>; DOI: 10.1007/978-3-540-72726-2.

3.4.2 Special case of Wishart distribution

Theorem: The gamma distribution (\rightarrow II/3.4.1) is a special case of the Wishart distribution (\rightarrow II/5.2.1) where the number of columns of the random matrix (\rightarrow I/1.2.4) is $p = 1$.

Proof: Let X be a $p \times p$ positive-definite symmetric matrix, such that X follows a Wishart distribution (\rightarrow II/5.2.1):

$$Y \sim \mathcal{W}(V, n) . \quad (1)$$

Then, Y is described by the probability density function

$$p(Y) = \frac{1}{\Gamma_p\left(\frac{n}{2}\right)} \cdot \frac{1}{\sqrt{2^{np}|V|^n}} \cdot |X|^{(n-p-1)/2} \cdot \exp\left[-\frac{1}{2}\text{tr}(V^{-1}X)\right] \quad (2)$$

where $|A|$ is a matrix determinant, A^{-1} is a matrix inverse and $\Gamma_p(x)$ is the multivariate gamma function of order p . If $p = 1$, then $\Gamma_p(x) = \Gamma(x)$ is the ordinary gamma function, $x = X$ and $v = V$ are real numbers. Thus, the probability density function (\rightarrow I/1.7.1) of x can be developed as

$$\begin{aligned} p(x) &= \frac{1}{\Gamma\left(\frac{n}{2}\right)} \cdot \frac{1}{\sqrt{2^n v^n}} \cdot x^{(n-2)/2} \cdot \exp\left[-\frac{1}{2}\text{tr}(v^{-1}x)\right] \\ &= \frac{(2v)^{-n/2}}{\Gamma\left(\frac{n}{2}\right)} \cdot x^{n/2-1} \cdot \exp\left[-\frac{1}{2v}x\right] \end{aligned} \quad (3)$$

Finally, substituting $a = \frac{n}{2}$ and $b = \frac{1}{2v}$, we get

$$p(x) = \frac{b^a}{\Gamma(a)} x^{a-1} \exp[-bx] \quad (4)$$

which is the probability density function of the gamma distribution (\rightarrow II/3.4.7). ■

3.4.3 Standard gamma distribution

Definition: Let X be a random variable (\rightarrow I/1.2.2). Then, X is said to have a standard gamma distribution, if X follows a gamma distribution (\rightarrow II/3.4.1) with shape $a > 0$ and rate $b = 1$:

$$X \sim \text{Gam}(a, 1) . \quad (1)$$

Sources:

- JoramSoch (2017): “Gamma-distributed random numbers”; in: *MACS – a new SPM toolbox for model assessment, comparison and selection*, retrieved on 2020-05-26; URL: https://github.com/JoramSoch/MACS/blob/master/MD_gamrnd.m; DOI: 10.5281/zenodo.845404.
- NIST/SEMATECH (2012): “Gamma distribution”; in: *e-Handbook of Statistical Methods*, ch. 1.3.6.6.11; URL: <https://www.itl.nist.gov/div898/handbook/eda/section3/eda366b.htm>; DOI: 10.18434/M

3.4.4 Relationship to standard gamma distribution

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a gamma distribution (\rightarrow II/3.4.1) with shape a and rate b :

$$X \sim \text{Gam}(a, b) . \quad (1)$$

Then, the quantity $Y = bX$ will have a standard gamma distribution (\rightarrow II/3.4.3) with shape a and rate 1:

$$Y = bX \sim \text{Gam}(a, 1) . \quad (2)$$

Proof: Note that Y is a function of X

$$Y = g(X) = bX \quad (3)$$

with the inverse function

$$X = g^{-1}(Y) = \frac{1}{b}Y . \quad (4)$$

Because b must be positive, $g(X)$ is strictly increasing and we can calculate the cumulative distribution function of a strictly increasing function (\rightarrow I/1.8.3) as

$$F_Y(y) = \begin{cases} 0 , & \text{if } y < \min(\mathcal{Y}) \\ F_X(g^{-1}(y)) , & \text{if } y \in \mathcal{Y} \\ 1 , & \text{if } y > \max(\mathcal{Y}) . \end{cases} \quad (5)$$

The cumulative distribution function of the gamma-distributed (\rightarrow II/3.4.9) X is

$$F_X(x) = \int_{-\infty}^x \frac{b^a}{\Gamma(a)} t^{a-1} \exp[-bt] dt . \quad (6)$$

Applying (5) to (6), we have:

$$\begin{aligned} F_Y(y) &\stackrel{(5)}{=} F_X(g^{-1}(y)) \\ &\stackrel{(6)}{=} \int_{-\infty}^{y/b} \frac{b^a}{\Gamma(a)} t^{a-1} \exp[-bt] dt . \end{aligned} \quad (7)$$

Substituting $s = bt$, such that $t = s/b$, we obtain

$$\begin{aligned} F_Y(y) &= \int_{-\infty}^{b(y/b)} \frac{b^a}{\Gamma(a)} \left(\frac{s}{b}\right)^{a-1} \exp\left[-b\left(\frac{s}{b}\right)\right] d\left(\frac{s}{b}\right) \\ &= \int_{-\infty}^y \frac{b^a}{\Gamma(a)} \frac{1}{b^{a-1}b} s^{a-1} \exp[-s] ds \\ &= \int_{-\infty}^y \frac{1}{\Gamma(a)} s^{a-1} \exp[-s] ds \end{aligned} \quad (8)$$

which is the cumulative distribution function (\rightarrow I/1.8.1) of the standard gamma distribution (\rightarrow II/3.4.3).

■

3.4.5 Relationship to standard gamma distribution

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a gamma distribution (\rightarrow II/3.4.1) with shape a and rate b :

$$X \sim \text{Gam}(a, b) . \quad (1)$$

Then, the quantity $Y = bX$ will have a standard gamma distribution (\rightarrow II/3.4.3) with shape a and rate 1:

$$Y = bX \sim \text{Gam}(a, 1) . \quad (2)$$

Proof: Note that Y is a function of X

$$Y = g(X) = bX \quad (3)$$

with the inverse function

$$X = g^{-1}(Y) = \frac{1}{b}Y . \quad (4)$$

Because b must be positive, $g(X)$ is strictly increasing and we can calculate the probability density function of a strictly increasing function (\rightarrow I/1.7.3) as

$$f_Y(y) = \begin{cases} f_X(g^{-1}(y)) \frac{dg^{-1}(y)}{dy} , & \text{if } y \in \mathcal{Y} \\ 0 , & \text{if } y \notin \mathcal{Y} \end{cases} \quad (5)$$

where $\mathcal{Y} = \{y = g(x) : x \in \mathcal{X}\}$. With the probability density function of the gamma distribution (\rightarrow II/3.4.7), we have

$$\begin{aligned} f_Y(y) &= \frac{b^a}{\Gamma(a)} [g^{-1}(y)]^{a-1} \exp[-b g^{-1}(y)] \cdot \frac{dg^{-1}(y)}{dy} \\ &= \frac{b^a}{\Gamma(a)} \left(\frac{1}{b}y\right)^{a-1} \exp\left[-b\left(\frac{1}{b}y\right)\right] \cdot \frac{d\left(\frac{1}{b}y\right)}{dy} \\ &= \frac{b^a}{\Gamma(a)} \frac{1}{b^{a-1}} y^{a-1} \exp[-y] \cdot \frac{1}{b} \\ &= \frac{1}{\Gamma(a)} y^{a-1} \exp[-y] \end{aligned} \quad (6)$$

which is the probability density function (\rightarrow I/1.7.1) of the standard gamma distribution (\rightarrow II/3.4.3). ■

3.4.6 Scaling of a gamma random variable

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a gamma distribution (\rightarrow II/3.4.1) with shape a and rate b :

$$X \sim \text{Gam}(a, b) . \quad (1)$$

Then, the quantity $Y = cX$ will also be gamma-distributed with shape a and rate b/c :

$$Y = cX \sim \text{Gam}\left(a, \frac{b}{c}\right). \quad (2)$$

Proof: Note that Y is a function of X

$$Y = g(X) = cX \quad (3)$$

with the inverse function

$$X = g^{-1}(Y) = \frac{1}{c}Y. \quad (4)$$

Because the parameters of a gamma distribution are positive (\rightarrow II/3.4.1), c must also be positive. Thus, $g(X)$ is strictly increasing and we can calculate the probability density function of a strictly increasing function (\rightarrow I/1.7.3) as

$$f_Y(y) = \begin{cases} f_X(g^{-1}(y)) \frac{dg^{-1}(y)}{dy}, & \text{if } y \in \mathcal{Y} \\ 0, & \text{if } y \notin \mathcal{Y} \end{cases} \quad (5)$$

The probability density function of the gamma-distributed (\rightarrow II/3.4.7) X is

$$f_X(x) = \frac{b^a}{\Gamma(a)} x^{a-1} \exp[-bx]. \quad (6)$$

Applying (5) to (6), we have:

$$\begin{aligned} f_Y(y) &= \frac{b^a}{\Gamma(a)} [g^{-1}(y)]^{a-1} \exp[-bg^{-1}(y)] \frac{dg^{-1}(y)}{dy} \\ &= \frac{b^a}{\Gamma(a)} \left(\frac{1}{c}y\right)^{a-1} \exp\left[-b\left(\frac{1}{c}y\right)\right] \frac{d\left(\frac{1}{c}y\right)}{dy} \\ &= \frac{b^a}{\Gamma(a)} \left(\frac{1}{c}\right)^a \left(\frac{1}{c}\right)^{-1} y^{a-1} \exp\left[-\frac{b}{c}y\right] \frac{1}{c} \\ &= \frac{(b/c)^a}{\Gamma(a)} y^{a-1} \exp\left[-\frac{b}{c}y\right] \end{aligned} \quad (7)$$

which is the probability density function (\rightarrow I/1.7.1) of a gamma distribution (\rightarrow II/3.4.1) with shape a and rate b/c . ■

3.4.7 Probability density function

Theorem: Let X be a positive random variable (\rightarrow I/1.2.2) following a gamma distribution (\rightarrow II/3.4.1):

$$X \sim \text{Gam}(a, b). \quad (1)$$

Then, the probability density function (\rightarrow I/1.7.1) of X is

$$f_X(x) = \frac{b^a}{\Gamma(a)} x^{a-1} \exp[-bx] . \quad (2)$$

Proof: This follows directly from the definition of the gamma distribution (\rightarrow II/3.4.1). ■

3.4.8 Moment-generating function

Theorem: Let X follow a gamma distribution (\rightarrow II/3.4.1):

$$X \sim \text{Gam}(a, b) . \quad (1)$$

Then, the moment-generating function (\rightarrow I/1.9.1) of X is

$$M_X(t) = \left(1 - \frac{t}{b}\right)^{-a} . \quad (2)$$

Proof: The moment-generating function of a random variable (\rightarrow I/1.9.1) X is defined as:

$$M_X(t) = \mathbb{E} [e^{tX}] , \quad t \in \mathbb{R} . \quad (3)$$

Applying the law of the unconscious statistician (\rightarrow I/1.12.9), we have:

$$M_X(t) = \int_{\mathbb{R}} e^{tx} \cdot f_X(x) dx . \quad (4)$$

With the probability density function of the gamma distribution (\rightarrow II/3.4.7), we have:

$$M_X(t) = \int_{\mathbb{R}} \exp[tx] \cdot \frac{b^a}{\Gamma(a)} x^{a-1} \exp[-bx] dx . \quad (5)$$

Now we summarize the two exponential functions inside the integral:

$$\begin{aligned} M_X(t) &= \int_{\mathbb{R}} \frac{b^a}{\Gamma(a)} x^{a-1} \exp[-(b-t)x] dx \\ &= \int_{\mathbb{R}} \frac{(b-t)^a}{(b-t)^a} \cdot \frac{b^a}{\Gamma(a)} x^{a-1} \exp[-(b-t)x] dx \\ &= \int_{\mathbb{R}} \frac{b^a}{(b-t)^a} \cdot \frac{(b-t)^a}{\Gamma(a)} x^{a-1} \exp[-(b-t)x] dx \\ &= \left(\frac{b}{b-t}\right)^a \int_{\mathbb{R}} \frac{(b-t)^a}{\Gamma(a)} x^{a-1} \exp[-(b-t)x] dx . \end{aligned} \quad (6)$$

The integrand is equal to the probability density function of a gamma distribution (\rightarrow II/3.4.7):

$$M_X(t) = \left(\frac{b}{b-t}\right)^a \int_{\mathbb{R}} \text{Gam}(x; a, b-t) dx . \quad (7)$$

Because the entire probability density integrates to one (\rightarrow I/1.7.1), we finally have:

$$M_X(t) = \left(\frac{b}{b-t}\right)^a = \left(\frac{b-t}{b}\right)^{-a} = \left(\frac{b}{b} - \frac{t}{b}\right)^{-a} = \left(1 - \frac{t}{b}\right)^{-a} . \quad (8)$$
■

3.4.9 Cumulative distribution function

Theorem: Let X be a positive random variable (\rightarrow I/1.2.2) following a gamma distribution (\rightarrow II/3.4.1):

$$X \sim \text{Gam}(a, b) . \quad (1)$$

Then, the cumulative distribution function (\rightarrow I/1.8.1) of X is

$$F_X(x) = \frac{\gamma(a, bx)}{\Gamma(a)} \quad (2)$$

where $\Gamma(x)$ is the gamma function and $\gamma(s, x)$ is the lower incomplete gamma function.

Proof: The probability density function of the gamma distribution (\rightarrow II/3.4.7) is:

$$f_X(x) = \frac{b^a}{\Gamma(a)} x^{a-1} \exp[-bx] . \quad (3)$$

Thus, the cumulative distribution function (\rightarrow I/1.8.1) is:

$$\begin{aligned} F_X(x) &= \int_0^x \text{Gam}(z; a, b) dz \\ &= \int_0^x \frac{b^a}{\Gamma(a)} z^{a-1} \exp[-bz] dz \\ &= \frac{b^a}{\Gamma(a)} \int_0^x z^{a-1} \exp[-bz] dz . \end{aligned} \quad (4)$$

Substituting $t = bz$, i.e. $z = t/b$, this becomes:

$$\begin{aligned} F_X(x) &= \frac{b^a}{\Gamma(a)} \int_{b \cdot 0}^{bx} \left(\frac{t}{b}\right)^{a-1} \exp\left[-b\left(\frac{t}{b}\right)\right] d\left(\frac{t}{b}\right) \\ &= \frac{b^a}{\Gamma(a)} \cdot \frac{1}{b^{a-1}} \cdot \frac{1}{b} \int_0^{bx} t^{a-1} \exp[-t] dt \\ &= \frac{1}{\Gamma(a)} \int_0^{bx} t^{a-1} \exp[-t] dt . \end{aligned} \quad (5)$$

With the definition of the lower incomplete gamma function

$$\gamma(s, x) = \int_0^x t^{s-1} \exp[-t] dt , \quad (6)$$

we arrive at the final result given by equation (2):

$$F_X(x) = \frac{\gamma(a, bx)}{\Gamma(a)} . \quad (7)$$

■

Sources:

- Wikipedia (2020): “Incomplete gamma function”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-10-29; URL: https://en.wikipedia.org/wiki/Incomplete_gamma_function#Definition.

3.4.10 Quantile function

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a gamma distribution (\rightarrow II/3.4.1):

$$X \sim \text{Gam}(a, b) . \quad (1)$$

Then, the quantile function (\rightarrow I/1.11.1) of X is

$$Q_X(p) = \begin{cases} -\infty , & \text{if } p = 0 \\ \gamma^{-1}(a, \Gamma(a) \cdot p)/b , & \text{if } p > 0 \end{cases} \quad (2)$$

where $\gamma^{-1}(s, y)$ is the inverse of the lower incomplete gamma function $\gamma(s, x)$

Proof: The cumulative distribution function of the gamma distribution (\rightarrow II/3.4.9) is:

$$F_X(x) = \begin{cases} 0 , & \text{if } x < 0 \\ \frac{\gamma(a, bx)}{\Gamma(a)} , & \text{if } x \geq 0 . \end{cases} \quad (3)$$

The quantile function (\rightarrow I/1.11.1) $Q_X(p)$ is defined as the smallest x , such that $F_X(x) = p$:

$$Q_X(p) = \min \{x \in \mathbb{R} \mid F_X(x) = p\} . \quad (4)$$

Thus, we have $Q_X(p) = -\infty$, if $p = 0$. When $p > 0$, it holds that (\rightarrow I/1.11.2)

$$Q_X(p) = F_X^{-1}(x) . \quad (5)$$

This can be derived by rearranging equation (3):

$$\begin{aligned} p &= \frac{\gamma(a, bx)}{\Gamma(a)} \\ \Gamma(a) \cdot p &= \gamma(a, bx) \\ \gamma^{-1}(a, \Gamma(a) \cdot p) &= bx \\ x &= \frac{\gamma^{-1}(a, \Gamma(a) \cdot p)}{b} . \end{aligned} \quad (6)$$

■

Sources:

- Wikipedia (2020): “Incomplete gamma function”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-11-19; URL: https://en.wikipedia.org/wiki/Incomplete_gamma_function#Definition.

3.4.11 Mean

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a gamma distribution (\rightarrow II/3.4.1):

$$X \sim \text{Gam}(a, b) . \quad (1)$$

Then, the mean or expected value (\rightarrow I/1.12.1) of X is

$$E(X) = \frac{a}{b} . \quad (2)$$

Proof: The expected value (\rightarrow I/1.12.1) is the probability-weighted average over all possible values:

$$E(X) = \int_{\mathcal{X}} x \cdot f_X(x) dx . \quad (3)$$

With the probability density function of the gamma distribution (\rightarrow II/3.4.7), this reads:

$$\begin{aligned} E(X) &= \int_0^\infty x \cdot \frac{b^a}{\Gamma(a)} x^{a-1} \exp[-bx] dx \\ &= \int_0^\infty \frac{b^a}{\Gamma(a)} x^{(a+1)-1} \exp[-bx] dx \\ &= \int_0^\infty \frac{1}{b} \cdot \frac{b^{a+1}}{\Gamma(a)} x^{(a+1)-1} \exp[-bx] dx . \end{aligned} \quad (4)$$

Employing the relation $\Gamma(x+1) = \Gamma(x) \cdot x$, we have

$$E(X) = \int_0^\infty \frac{a}{b} \cdot \frac{b^{a+1}}{\Gamma(a+1)} x^{(a+1)-1} \exp[-bx] dx \quad (5)$$

and again using the density of the gamma distribution (\rightarrow II/3.4.7), we get

$$\begin{aligned} E(X) &= \frac{a}{b} \int_0^\infty \text{Gam}(x; a+1, b) dx \\ &= \frac{a}{b} . \end{aligned} \quad (6)$$

■

Sources:

- Turlapaty, Anish (2013): “Gamma random variable: mean & variance”; in: *YouTube*, retrieved on 2020-05-19; URL: <https://www.youtube.com/watch?v=Sy4wP-Y2dmA>.

3.4.12 Median

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a gamma distribution (\rightarrow II/3.4.1):

$$X \sim \text{Gam}(a, b) . \quad (1)$$

Then, the median (\rightarrow I/1.18.1) of X is

$$\text{median}(X) = \frac{1}{b} \gamma_a^{-1} \left(\frac{\Gamma(a)}{2} \right) \quad (2)$$

where $\Gamma(x)$ is the gamma function and $\gamma_s^{-1}(y)$ is the inverse function of the lower incomplete gamma function $\gamma(s, x)$ in which the first argument is s .

Proof: The median (\rightarrow I/1.18.1) is the value at which the cumulative distribution function (\rightarrow I/1.8.1) is 1/2:

$$F_X(\text{median}(X)) = \frac{1}{2} . \quad (3)$$

The cumulative distribution function of the gamma distribution (\rightarrow II/3.4.9) is

$$F_X(x) = \frac{\gamma(a, bx)}{\Gamma(a)} \quad (4)$$

where the lower incomplete gamma function $\gamma(s, x)$ is given by

$$\gamma(s, x) = \int_0^x t^{s-1} \exp(-t) dt . \quad (5)$$

Thus, the inverse CDF, i.e. the quantile function (\rightarrow I/1.11.1), is

$$x = \frac{1}{b} \gamma_a^{-1}(p\Gamma(a)) \quad (6)$$

where $\gamma_a^{-1}(y)$ is the inverse function of $\gamma(a, x)$. Setting $p = 1/2$, we obtain:

$$\text{median}(X) = \frac{1}{b} \gamma_a^{-1} \left(\frac{\Gamma(a)}{2} \right) . \quad (7)$$

■

Sources:

- Wikipedia (2025): “Gamma distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2025-10-24; URL: https://en.wikipedia.org/wiki/Gamma_distribution#Median_approximations_and_bounds.

3.4.13 Mode

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a gamma distribution (\rightarrow II/3.4.1):

$$X \sim \text{Gam}(a, b) . \quad (1)$$

Then, the mode (\rightarrow I/1.18.3) of X is

$$\text{mode}(X) = \begin{cases} \frac{a-1}{b} , & \text{if } a \geq 1 \\ 0 , & \text{if } a < 1 . \end{cases} \quad (2)$$

Proof: The mode (\rightarrow I/1.18.3) is the value which maximizes the probability density function (\rightarrow I/1.7.1):

$$\text{mode}(X) = \arg \max_x f_X(x) . \quad (3)$$

The probability density function of the gamma distribution (\rightarrow II/3.4.7) is:

$$f_X(x) = \frac{b^a}{\Gamma(a)} x^{a-1} \exp[-bx] . \quad (4)$$

The first two derivatives of this function are:

$$\begin{aligned} f'_X(x) &= \frac{df_X(x)}{dx} = \frac{b^a}{\Gamma(a)} (-bx^{a-1} \exp[-bx] + (a-1)x^{a-2} \exp[-bx]) \\ &= \frac{b^a}{\Gamma(a)} x^{a-1} \exp[-bx] \left(\frac{a-1}{x} - b \right) \end{aligned} \quad (5)$$

$$\begin{aligned}
f_X''(x) &= \frac{d^2 f_X(x)}{dx^2} = \frac{b^a}{\Gamma(a)} x^{a-1} \exp[-bx] \left(-\frac{a-1}{x^2} \right) + \frac{b^a}{\Gamma(a)} x^{a-1} \exp[-bx] \left(\frac{a-1}{x} - b \right)^2 \\
&= \frac{b^a}{\Gamma(a)} x^{a-1} \exp[-bx] \left(\left(\frac{a-1}{x} - b \right)^2 - \frac{a-1}{x^2} \right).
\end{aligned} \tag{6}$$

We now calculate the root of the first derivative (5):

$$\begin{aligned}
f_X'(x) = 0 &= \frac{b^a}{\Gamma(a)} x^{a-1} \exp[-bx] \left(\frac{a-1}{x} - b \right) \\
&\Leftrightarrow \\
0 &= \frac{a-1}{x} - b \\
bx &= a-1 \\
x &= \frac{a-1}{b}.
\end{aligned} \tag{7}$$

By plugging this value into the second derivative (6), we find:

$$\begin{aligned}
f_X''\left(\frac{a-1}{b}\right) &= \frac{b^a}{\Gamma(a)} \left(\frac{a-1}{b}\right)^{a-1} \exp\left[-b\left(\frac{a-1}{b}\right)\right] \left(\left(\frac{a-1}{\frac{a-1}{b}} - b \right)^2 - \frac{a-1}{\left(\frac{a-1}{b}\right)^2} \right) \\
&= \frac{b^a}{\Gamma(a)} \left(\frac{a-1}{b}\right)^{a-1} \exp[-(a-1)] \left((b-b)^2 - \frac{b^2}{a-1} \right) \\
&= \frac{b^a}{\Gamma(a)} \left(\frac{a-1}{b}\right)^{a-1} \exp[-(a-1)] \left(-\frac{b^2}{a-1} \right).
\end{aligned} \tag{8}$$

Thus, if $a \geq 1$, then $f_X'((a-1)/b)$ is negative, such that $f_X(x)$ reaches its maximum at $x = (a-1)/b$. However, if $a < 1$, this value is negative and not in the support of the random variable (\rightarrow II/3.4.1) X . In this case, the mode of X is 0, since $f_X(x)$ tends towards infinity at $x = 0$:

$$\begin{aligned}
\lim_{\substack{x \rightarrow 0 \\ a < 1}} f_X(x) &= \lim_{\substack{x \rightarrow 0 \\ a < 1}} \frac{b^a}{\Gamma(a)} x^{a-1} \exp[-bx] \\
&= \frac{b^a}{\Gamma(a)} \lim_{\substack{x \rightarrow 0 \\ a < 1}} x^{a-1} = \infty.
\end{aligned} \tag{9}$$

■

3.4.14 Variance

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a gamma distribution (\rightarrow II/3.4.1):

$$X \sim \text{Gam}(a, b). \tag{1}$$

Then, the variance (\rightarrow I/1.13.1) of X is

$$\text{Var}(X) = \frac{a}{b^2} . \quad (2)$$

Proof: The variance (\rightarrow I/1.13.1) can be expressed in terms of expected values (\rightarrow I/1.13.4) as

$$\text{Var}(X) = E(X^2) - E(X)^2 . \quad (3)$$

The expected value of a gamma random variable (\rightarrow II/3.4.11) is

$$E(X) = \frac{a}{b} . \quad (4)$$

With the probability density function of the gamma distribution (\rightarrow II/3.4.7), the expected value of a squared gamma random variable is

$$\begin{aligned} E(X^2) &= \int_0^\infty x^2 \cdot \frac{b^a}{\Gamma(a)} x^{a-1} \exp[-bx] dx \\ &= \int_0^\infty \frac{b^a}{\Gamma(a)} x^{(a+2)-1} \exp[-bx] dx \\ &= \int_0^\infty \frac{1}{b^2} \cdot \frac{b^{a+2}}{\Gamma(a)} x^{(a+2)-1} \exp[-bx] dx . \end{aligned} \quad (5)$$

Twice-applying the relation $\Gamma(x+1) = \Gamma(x) \cdot x$, we have

$$E(X^2) = \int_0^\infty \frac{a(a+1)}{b^2} \cdot \frac{b^{a+2}}{\Gamma(a+2)} x^{(a+2)-1} \exp[-bx] dx \quad (6)$$

and again using the density of the gamma distribution (\rightarrow II/3.4.7), we get

$$\begin{aligned} E(X^2) &= \frac{a(a+1)}{b^2} \int_0^\infty \text{Gam}(x; a+2, b) dx \\ &= \frac{a^2 + a}{b^2} . \end{aligned} \quad (7)$$

Plugging (7) and (4) into (3), the variance of a gamma random variable finally becomes

$$\begin{aligned} \text{Var}(X) &= \frac{a^2 + a}{b^2} - \left(\frac{a}{b}\right)^2 \\ &= \frac{a}{b^2} . \end{aligned} \quad (8)$$

■

Sources:

- Turlapaty, Anish (2013): “Gamma random variable: mean & variance”; in: *YouTube*, retrieved on 2020-05-19; URL: <https://www.youtube.com/watch?v=Sy4wP-Y2dmA>.

3.4.15 Logarithmic expectation

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a gamma distribution (\rightarrow II/3.4.1):

$$X \sim \text{Gam}(a, b) . \quad (1)$$

Then, the expectation (\rightarrow I/1.12.1) of the natural logarithm of X is

$$\mathbb{E}(\ln X) = \psi(a) - \ln(b) \quad (2)$$

where $\psi(x)$ is the digamma function.

Proof: Let $Y = \ln(X)$, such that $\mathbb{E}(Y) = \mathbb{E}(\ln X)$ and consider the special case that $b = 1$. In this case, the probability density function of the gamma distribution (\rightarrow II/3.4.7) is

$$f_X(x) = \frac{1}{\Gamma(a)} x^{a-1} \exp[-x] . \quad (3)$$

Multiplying this function with dx , we obtain

$$f_X(x) dx = \frac{1}{\Gamma(a)} x^a \exp[-x] \frac{dx}{x} . \quad (4)$$

Substituting $y = \ln x$, i.e. $x = e^y$, such that $dx/dy = x$, i.e. $dx/x = dy$, we get

$$\begin{aligned} f_Y(y) dy &= \frac{1}{\Gamma(a)} (e^y)^a \exp[-e^y] dy \\ &= \frac{1}{\Gamma(a)} \exp[ay - e^y] dy . \end{aligned} \quad (5)$$

Because $f_Y(y)$ integrates to one, we have

$$\begin{aligned} 1 &= \int_{\mathbb{R}} f_Y(y) dy \\ 1 &= \int_{\mathbb{R}} \frac{1}{\Gamma(a)} \exp[ay - e^y] dy \\ \Gamma(a) &= \int_{\mathbb{R}} \exp[ay - e^y] dy . \end{aligned} \quad (6)$$

Note that the integrand in (6) is differentiable with respect to a :

$$\begin{aligned} \frac{d}{da} \exp[ay - e^y] dy &= y \exp[ay - e^y] dy \\ &\stackrel{(5)}{=} \Gamma(a) y f_Y(y) dy . \end{aligned} \quad (7)$$

Now we can calculate the expected value of $Y = \ln(X)$:

$$\begin{aligned}
E(Y) &= \int_{\mathbb{R}} y f_Y(y) dy \\
&\stackrel{(7)}{=} \frac{1}{\Gamma(a)} \int_{\mathbb{R}} \frac{d}{da} \exp[ay - e^y] dy \\
&= \frac{1}{\Gamma(a)} \frac{d}{da} \int_{\mathbb{R}} \exp[ay - e^y] dy \\
&\stackrel{(6)}{=} \frac{1}{\Gamma(a)} \frac{d}{da} \Gamma(a) \\
&= \frac{\Gamma'(a)}{\Gamma(a)} .
\end{aligned} \tag{8}$$

Using the derivative of a logarithmized function

$$\frac{d}{dx} \ln f(x) = \frac{f'(x)}{f(x)} \tag{9}$$

and the definition of the digamma function

$$\psi(x) = \frac{d}{dx} \ln \Gamma(x) , \tag{10}$$

we have

$$E(Y) = \psi(a) . \tag{11}$$

Finally, noting that $1/b$ acts as a scaling parameter (\rightarrow II/3.4.4) on a gamma-distributed (\rightarrow II/3.4.1) random variable (\rightarrow I/1.2.2),

$$X \sim \text{Gam}(a, 1) \quad \Rightarrow \quad \frac{1}{b} X \sim \text{Gam}(a, b) , \tag{12}$$

and that a scaling parameter acts additively on the logarithmic expectation of a random variable,

$$E[\ln(cX)] = E[\ln(X) + \ln(c)] = E[\ln(X)] + \ln(c) , \tag{13}$$

it follows that

$$X \sim \text{Gam}(a, b) \quad \Rightarrow \quad E(\ln X) = \psi(a) - \ln(b) . \tag{14}$$

■

Sources:

- whuber (2018): “What is the expected value of the logarithm of Gamma distribution?”; in: *StackExchange CrossValidated*, retrieved on 2020-05-25; URL: <https://stats.stackexchange.com/questions/370880/what-is-the-expected-value-of-the-logarithm-of-gamma-distribution>.

3.4.16 Expectation of $x \ln x$

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a gamma distribution (\rightarrow II/3.4.1):

$$X \sim \text{Gam}(a, b) . \quad (1)$$

Then, the mean or expected value (\rightarrow I/1.12.1) of $(X \cdot \ln X)$ is

$$\mathbb{E}(X \ln X) = \frac{a}{b} [\psi(a+1) - \ln(b)] . \quad (2)$$

Proof: With the definition of the expected value (\rightarrow I/1.12.1), the law of the unconscious statistician (\rightarrow I/1.12.9) and the probability density function of the gamma distribution (\rightarrow II/3.4.7), we have:

$$\begin{aligned} \mathbb{E}(X \ln X) &= \int_0^\infty x \ln x \cdot \frac{b^a}{\Gamma(a)} x^{a-1} \exp[-bx] dx \\ &= \frac{1}{\Gamma(a)} \int_0^\infty \ln x \cdot \frac{b^{a+1}}{b} x^a \exp[-bx] dx \\ &= \frac{\Gamma(a+1)}{\Gamma(a)b} \int_0^\infty \ln x \cdot \frac{b^{a+1}}{\Gamma(a+1)} x^{(a+1)-1} \exp[-bx] dx \end{aligned} \quad (3)$$

The integral now corresponds to the logarithmic expectation of a gamma distribution (\rightarrow II/3.4.15) with shape $a+1$ and rate b

$$\mathbb{E}(\ln Y) \quad \text{where} \quad Y \sim \text{Gam}(a+1, b) \quad (4)$$

which is given by (\rightarrow II/3.4.15)

$$\mathbb{E}(\ln Y) = \psi(a+1) - \ln(b) \quad (5)$$

where $\psi(x)$ is the digamma function. Additionally employing the relation

$$\Gamma(x+1) = \Gamma(x) \cdot x \quad \Leftrightarrow \quad \frac{\Gamma(x+1)}{\Gamma(x)} = x , \quad (6)$$

the expression in equation (3) develops into:

$$\mathbb{E}(X \ln X) = \frac{a}{b} [\psi(a+1) - \ln(b)] . \quad (7)$$

■

Sources:

- gunes (2020): “What is the expected value of $x \log(x)$ of the gamma distribution?”; in: *StackExchange CrossValidated*, retrieved on 2020-10-15; URL: <https://stats.stackexchange.com/questions/457357/what-is-the-expected-value-of-x-logx-of-the-gamma-distribution>.

3.4.17 Differential entropy

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a gamma distribution (\rightarrow II/3.4.1):

$$X \sim \text{Gam}(a, b) \quad (1)$$

Then, the differential entropy (\rightarrow I/2.2.1) of X in nats is

$$h(X) = a + \ln \Gamma(a) + (1 - a) \cdot \psi(a) + \ln b . \quad (2)$$

Proof: The differential entropy (\rightarrow I/2.2.1) of a random variable is defined as

$$h(X) = - \int_{\mathcal{X}} p(x) \log_b p(x) dx . \quad (3)$$

To measure $h(X)$ in nats, we set $b = e$, such that (\rightarrow I/1.12.1)

$$h(X) = -E[\ln p(x)] . \quad (4)$$

With the probability density function of the gamma distribution (\rightarrow II/3.4.7), the differential entropy of X is:

$$\begin{aligned} h(X) &= -E \left[\ln \left(\frac{b^a}{\Gamma(a)} x^{a-1} \exp[-bx] \right) \right] \\ &= -E[a \cdot \ln b - \ln \Gamma(a) + (a-1) \ln x - bx] \\ &= -a \cdot \ln b + \ln \Gamma(a) - (a-1) \cdot E(\ln x) + b \cdot E(x) . \end{aligned} \quad (5)$$

Using the mean (\rightarrow II/3.4.11) and logarithmic expectation (\rightarrow II/3.4.15) of the gamma distribution (\rightarrow II/3.4.1)

$$X \sim \text{Gam}(a, b) \quad \Rightarrow \quad E(X) = \frac{a}{b} \quad \text{and} \quad E(\ln X) = \psi(a) - \ln(b) , \quad (6)$$

the differential entropy (\rightarrow I/2.2.1) of X becomes:

$$\begin{aligned} h(X) &= -a \cdot \ln b + \ln \Gamma(a) - (a-1) \cdot (\psi(a) - \ln b) + b \cdot \frac{a}{b} \\ &= -a \cdot \ln b + \ln \Gamma(a) + (1-a) \cdot \psi(a) + a \cdot \ln b - \ln b + a \\ &= a + \ln \Gamma(a) + (1-a) \cdot \psi(a) - \ln b . \end{aligned} \quad (7)$$

■

Sources:

- Wikipedia (2021): “Gamma distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-07-14; URL: https://en.wikipedia.org/wiki/Gamma_distribution#Information_entropy.

3.4.18 Kullback-Leibler divergence

Theorem: Let X be a random variable (\rightarrow I/1.2.2). Assume two gamma distributions (\rightarrow II/3.4.1) P and Q specifying the probability distribution of X as

$$\begin{aligned} P : X &\sim \text{Gam}(a_1, b_1) \\ Q : X &\sim \text{Gam}(a_2, b_2) . \end{aligned} \quad (1)$$

Then, the Kullback-Leibler divergence (\rightarrow I/2.5.1) of P from Q is given by

$$\text{KL}[P \parallel Q] = a_2 \ln \frac{b_1}{b_2} - \ln \frac{\Gamma(a_1)}{\Gamma(a_2)} + (a_1 - a_2) \psi(a_1) - (b_1 - b_2) \frac{a_1}{b_1} . \quad (2)$$

Proof: The KL divergence for a continuous random variable (\rightarrow I/2.5.1) is given by

$$\text{KL}[P \parallel Q] = \int_{\mathcal{X}} p(x) \ln \frac{p(x)}{q(x)} dx \quad (3)$$

which, applied to the gamma distributions (\rightarrow II/3.4.1) in (1), yields

$$\begin{aligned} \text{KL}[P \parallel Q] &= \int_{-\infty}^{+\infty} \text{Gam}(x; a_1, b_1) \ln \frac{\text{Gam}(x; a_1, b_1)}{\text{Gam}(x; a_2, b_2)} dx \\ &= \left\langle \ln \frac{\text{Gam}(x; a_1, b_1)}{\text{Gam}(x; a_2, b_2)} \right\rangle_{p(x)} . \end{aligned} \quad (4)$$

Using the probability density function of the gamma distribution (\rightarrow II/3.4.7), this becomes:

$$\begin{aligned} \text{KL}[P \parallel Q] &= \left\langle \ln \frac{\frac{b_1^{a_1}}{\Gamma(a_1)} x^{a_1-1} \exp[-b_1 x]}{\frac{b_2^{a_2}}{\Gamma(a_2)} x^{a_2-1} \exp[-b_2 x]} \right\rangle_{p(x)} \\ &= \left\langle \ln \left(\frac{b_1^{a_1}}{b_2^{a_2}} \cdot \frac{\Gamma(a_2)}{\Gamma(a_1)} \cdot x^{a_1-a_2} \cdot \exp[-(b_1 - b_2)x] \right) \right\rangle_{p(x)} \\ &= \langle a_1 \cdot \ln b_1 - a_2 \cdot \ln b_2 - \ln \Gamma(a_1) + \ln \Gamma(a_2) + (a_1 - a_2) \cdot \ln x - (b_1 - b_2) \cdot x \rangle_{p(x)} . \end{aligned} \quad (5)$$

Using the mean of the gamma distribution (\rightarrow II/3.4.11) and the expected value of a logarithmized gamma variate (\rightarrow II/3.4.15)

$$\begin{aligned} x \sim \text{Gam}(a, b) \quad \Rightarrow \quad \langle x \rangle &= \frac{a}{b} \quad \text{and} \\ \langle \ln x \rangle &= \psi(a) - \ln(b) , \end{aligned} \quad (6)$$

the Kullback-Leibler divergence from (5) becomes:

$$\begin{aligned} \text{KL}[P \parallel Q] &= a_1 \cdot \ln b_1 - a_2 \cdot \ln b_2 - \ln \Gamma(a_1) + \ln \Gamma(a_2) + (a_1 - a_2) \cdot (\psi(a_1) - \ln(b_1)) - (b_1 - b_2) \cdot \frac{a_1}{b_1} \\ &= a_2 \cdot \ln b_1 - a_2 \cdot \ln b_2 - \ln \Gamma(a_1) + \ln \Gamma(a_2) + (a_1 - a_2) \cdot \psi(a_1) - (b_1 - b_2) \cdot \frac{a_1}{b_1} . \end{aligned} \quad (7)$$

Finally, combining the logarithms, we get:

$$\text{KL}[P || Q] = a_2 \ln \frac{b_1}{b_2} - \ln \frac{\Gamma(a_1)}{\Gamma(a_2)} + (a_1 - a_2) \psi(a_1) - (b_1 - b_2) \frac{a_1}{b_1}. \quad (8)$$

■

Sources:

- Penny, William D. (2001): “KL-Divergences of Normal, Gamma, Dirichlet and Wishart densities”; in: *University College, London*; URL: <https://www.fil.ion.ucl.ac.uk/~wpenny/publications/densities.ps>.

3.5 Exponential distribution

3.5.1 Definition

Definition: Let X be a random variable (\rightarrow I/1.2.2). Then, X is said to be exponentially distributed with rate (or, inverse scale) λ

$$X \sim \text{Exp}(\lambda), \quad (1)$$

if and only if its probability density function (\rightarrow I/1.7.1) is given by

$$\text{Exp}(x; \lambda) = \lambda \exp[-\lambda x], \quad x \geq 0 \quad (2)$$

where $\lambda > 0$, and the density is zero, if $x < 0$.

Sources:

- Wikipedia (2020): “Exponential distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-02-08; URL: https://en.wikipedia.org/wiki/Exponential_distribution#Definitions.

3.5.2 Special case of gamma distribution

Theorem: The exponential distribution (\rightarrow II/3.5.1) is a special case of the gamma distribution (\rightarrow II/3.4.1) with shape $a = 1$ and rate $b = \lambda$.

Proof: The probability density function of the gamma distribution (\rightarrow II/3.4.7) is

$$\text{Gam}(x; a, b) = \frac{b^a}{\Gamma(a)} x^{a-1} \exp[-bx]. \quad (1)$$

Setting $a = 1$ and $b = \lambda$, we obtain

$$\begin{aligned} \text{Gam}(x; 1, \lambda) &= \frac{\lambda^1}{\Gamma(1)} x^{1-1} \exp[-\lambda x] \\ &= \frac{x^0}{\Gamma(1)} \lambda \exp[-\lambda x] \\ &= \lambda \exp[-\lambda x] \end{aligned} \quad (2)$$

which is equivalent to the probability density function of the exponential distribution (\rightarrow II/3.5.3).

■

3.5.3 Probability density function

Theorem: Let X be a non-negative random variable (\rightarrow I/1.2.2) following an exponential distribution (\rightarrow II/3.5.1):

$$X \sim \text{Exp}(\lambda) . \quad (1)$$

Then, the probability density function (\rightarrow I/1.7.1) of X is

$$f_X(x) = \lambda \exp[-\lambda x] . \quad (2)$$

Proof: This follows directly from the definition of the exponential distribution (\rightarrow II/3.5.1). ■

3.5.4 Moment-generating function

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following an exponential distribution (\rightarrow II/3.5.1):

$$X \sim \text{Exp}(\lambda) . \quad (1)$$

Then, the moment generating function (\rightarrow I/1.9.1) of X is

$$M_X(t) = \frac{\lambda}{\lambda - t} \quad (2)$$

which is well-defined for $t < \lambda$.

Proof: Suppose X follows an exponential distribution (\rightarrow II/3.5.1) with rate λ ; that is, $X \sim \text{Exp}(\lambda)$. Then, the probability density function (\rightarrow II/3.5.3) is given by

$$f_X(x) = \lambda e^{-\lambda x} \quad (3)$$

and the moment-generating function (\rightarrow I/1.9.1) is defined as

$$M_X(t) = \text{E} [e^{tX}] . \quad (4)$$

Using the definition of expected value for continuous random variables (\rightarrow I/1.12.1), the moment-generating function of X is thus:

$$\begin{aligned} M_X(t) &= \int_0^{\infty} e^{tx} \cdot f_X(x) dx \\ &= \int_0^{\infty} e^{tx} \cdot \lambda e^{-\lambda x} dx \\ &= \int_0^{\infty} \lambda e^{x(t-\lambda)} dx \\ &= \frac{\lambda}{t-\lambda} e^{x(t-\lambda)} \Big|_{x=0}^{x=\infty} \\ &= \lim_{x \rightarrow \infty} \left[\frac{\lambda}{t-\lambda} e^{x(t-\lambda)} \right] - \frac{\lambda}{t-\lambda} \\ &= \frac{\lambda}{t-\lambda} \left[\lim_{x \rightarrow \infty} e^{x(t-\lambda)} - 1 \right] . \end{aligned} \quad (5)$$

Note that t cannot be equal to λ , else $M_X(t)$ is undefined. Further, if $t > \lambda$, then $\lim_{x \rightarrow \infty} e^{x(t-\lambda)} = \infty$, which implies that $M_X(t)$ diverges for $t \geq \lambda$. So, we must restrict the domain of $M_X(t)$ to $t < \lambda$. Assuming this, we can further simplify (5):

$$\begin{aligned} M_X(t) &= \frac{\lambda}{t - \lambda} \left[\lim_{x \rightarrow \infty} e^{x(t-\lambda)} - 1 \right] \\ &= \frac{\lambda}{t - \lambda} [0 - 1] \\ &= \frac{\lambda}{\lambda - t} . \end{aligned} \tag{6}$$

This completes the proof of (2). ■

3.5.5 Cumulative distribution function

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following an exponential distribution (\rightarrow II/3.5.1):

$$X \sim \text{Exp}(\lambda) . \tag{1}$$

Then, the cumulative distribution function (\rightarrow I/1.8.1) of X is

$$F_X(x) = \begin{cases} 0 , & \text{if } x < 0 \\ 1 - \exp[-\lambda x] , & \text{if } x \geq 0 . \end{cases} \tag{2}$$

Proof: The probability density function of the exponential distribution (\rightarrow II/3.5.3) is:

$$\text{Exp}(x; \lambda) = \begin{cases} 0 , & \text{if } x < 0 \\ \lambda \exp[-\lambda x] , & \text{if } x \geq 0 . \end{cases} \tag{3}$$

Thus, the cumulative distribution function (\rightarrow I/1.8.1) is:

$$F_X(x) = \int_{-\infty}^x \text{Exp}(z; \lambda) dz . \tag{4}$$

If $x < 0$, we have:

$$F_X(x) = \int_{-\infty}^x 0 dz = 0 . \tag{5}$$

If $x \geq 0$, we have using (3):

$$\begin{aligned}
F_X(x) &= \int_{-\infty}^0 \text{Exp}(z; \lambda) dz + \int_0^x \text{Exp}(z; \lambda) dz \\
&= \int_{-\infty}^0 0 dz + \int_0^x \lambda \exp[-\lambda z] dz \\
&= 0 + \lambda \left[-\frac{1}{\lambda} \exp[-\lambda z] \right]_0^x \\
&= \lambda \left[\left(-\frac{1}{\lambda} \exp[-\lambda x] \right) - \left(-\frac{1}{\lambda} \exp[-\lambda \cdot 0] \right) \right] \\
&= 1 - \exp[-\lambda x] .
\end{aligned} \tag{6}$$

■

3.5.6 Quantile function

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following an exponential distribution (\rightarrow II/3.5.1):

$$X \sim \text{Exp}(\lambda) . \tag{1}$$

Then, the quantile function (\rightarrow I/1.11.1) of X is

$$Q_X(p) = \begin{cases} -\infty , & \text{if } p = 0 \\ -\frac{\ln(1-p)}{\lambda} , & \text{if } p > 0 . \end{cases} \tag{2}$$

Proof: The cumulative distribution function of the exponential distribution (\rightarrow II/3.5.5) is:

$$F_X(x) = \begin{cases} 0 , & \text{if } x < 0 \\ 1 - \exp[-\lambda x] , & \text{if } x \geq 0 . \end{cases} \tag{3}$$

The quantile function (\rightarrow I/1.11.1) $Q_X(p)$ is defined as the smallest x , such that $F_X(x) = p$:

$$Q_X(p) = \min \{x \in \mathbb{R} \mid F_X(x) = p\} . \tag{4}$$

Thus, we have $Q_X(p) = -\infty$, if $p = 0$. When $p > 0$, it holds that (\rightarrow I/1.11.2)

$$Q_X(p) = F_X^{-1}(p) . \tag{5}$$

This can be derived by rearranging equation (3):

$$\begin{aligned}
p &= 1 - \exp[-\lambda x] \\
\exp[-\lambda x] &= 1 - p \\
-\lambda x &= \ln(1 - p) \\
x &= -\frac{\ln(1 - p)}{\lambda} .
\end{aligned} \tag{6}$$

■

3.5.7 Mean

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following an exponential distribution (\rightarrow II/3.5.1):

$$X \sim \text{Exp}(\lambda) . \quad (1)$$

Then, the mean or expected value (\rightarrow I/1.12.1) of X is

$$\text{E}(X) = \frac{1}{\lambda} . \quad (2)$$

Proof: The expected value (\rightarrow I/1.12.1) is the probability-weighted average over all possible values:

$$\text{E}(X) = \int_{\mathcal{X}} x \cdot f_X(x) \, dx . \quad (3)$$

With the probability density function of the exponential distribution (\rightarrow II/3.5.3), this reads:

$$\begin{aligned} \text{E}(X) &= \int_0^{+\infty} x \cdot \lambda \exp(-\lambda x) \, dx \\ &= \lambda \int_0^{+\infty} x \cdot \exp(-\lambda x) \, dx . \end{aligned} \quad (4)$$

Using the following anti-derivative

$$\int x \cdot \exp(-\lambda x) \, dx = \left(-\frac{1}{\lambda} x - \frac{1}{\lambda^2} \right) \exp(-\lambda x) , \quad (5)$$

the expected value becomes

$$\begin{aligned} \text{E}(X) &= \lambda \left[\left(-\frac{1}{\lambda} x - \frac{1}{\lambda^2} \right) \exp(-\lambda x) \right]_0^{+\infty} \\ &= \lambda \left[\lim_{x \rightarrow \infty} \left(-\frac{1}{\lambda} x - \frac{1}{\lambda^2} \right) \exp(-\lambda x) - \left(-\frac{1}{\lambda} \cdot 0 - \frac{1}{\lambda^2} \right) \exp(-\lambda \cdot 0) \right] \\ &= \lambda \left[0 + \frac{1}{\lambda^2} \right] \\ &= \frac{1}{\lambda} . \end{aligned} \quad (6)$$

■

Sources:

- Koch, Karl-Rudolf (2007): “Expected Value”; in: *Introduction to Bayesian Statistics*, Springer, Berlin/Heidelberg, 2007, p. 39, eq. 2.142a; URL: <https://www.springer.com/de/book/9783540727231>; DOI: 10.1007/978-3-540-72726-2.

3.5.8 Median

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following an exponential distribution (\rightarrow II/3.5.1):

$$X \sim \text{Exp}(\lambda) . \quad (1)$$

Then, the median (\rightarrow I/1.18.1) of X is

$$\text{median}(X) = \frac{\ln 2}{\lambda} . \quad (2)$$

Proof: The median (\rightarrow I/1.18.1) is the value at which the cumulative distribution function (\rightarrow I/1.8.1) is $1/2$:

$$F_X(\text{median}(X)) = \frac{1}{2} . \quad (3)$$

The cumulative distribution function of the exponential distribution (\rightarrow II/3.5.5) is

$$F_X(x) = 1 - \exp[-\lambda x], \quad x \geq 0 . \quad (4)$$

Thus, the inverse CDF is

$$x = -\frac{\ln(1-p)}{\lambda} \quad (5)$$

and setting $p = 1/2$, we obtain:

$$\text{median}(X) = -\frac{\ln(1-\frac{1}{2})}{\lambda} = \frac{\ln 2}{\lambda} . \quad (6)$$

■

3.5.9 Mode

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following an exponential distribution (\rightarrow II/3.5.1):

$$X \sim \text{Exp}(\lambda) . \quad (1)$$

Then, the mode (\rightarrow I/1.18.3) of X is

$$\text{mode}(X) = 0 . \quad (2)$$

Proof: The mode (\rightarrow I/1.18.3) is the value which maximizes the probability density function (\rightarrow I/1.7.1):

$$\text{mode}(X) = \arg \max_x f_X(x) . \quad (3)$$

The probability density function of the exponential distribution (\rightarrow II/3.5.3) is:

$$f_X(x) = \begin{cases} 0 , & \text{if } x < 0 \\ \lambda e^{-\lambda x} , & \text{if } x \geq 0 . \end{cases} \quad (4)$$

Since

$$f_X(0) = \lambda \quad (5)$$

and

$$0 < e^{-\lambda x} < 1 \quad \text{for any } x > 0, \quad (6)$$

it follows that

$$\text{mode}(X) = 0. \quad (7)$$

■

3.5.10 Variance

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following an exponential distribution (\rightarrow II/3.5.1):

$$X \sim \text{Exp}(\lambda). \quad (1)$$

Then, the variance (\rightarrow I/1.13.1) of X is

$$\text{Var}(X) = \frac{1}{\lambda^2}. \quad (2)$$

Proof: The variance (\rightarrow I/1.13.1) of a random variable is defined as

$$\text{Var}(X) = E[(X - E(X))^2] \quad (3)$$

which, partitioned into expected values (\rightarrow I/1.13.4), reads:

$$\text{Var}(X) = E[X^2] - E[X]^2. \quad (4)$$

The expected value of the exponential distribution (\rightarrow II/3.5.7) is:

$$E[X] = \frac{1}{\lambda} \quad (5)$$

The second moment $E[X^2]$ can be derived as follows:

$$\begin{aligned} E[X^2] &= \int_{-\infty}^{+\infty} x^2 \cdot f_X(x) \, dx \\ &= \int_0^{+\infty} x^2 \cdot \lambda \exp(-\lambda x) \, dx \\ &= \lambda \int_0^{+\infty} x^2 \cdot \exp(-\lambda x) \, dx \end{aligned} \quad (6)$$

Using the following anti-derivative

$$\begin{aligned}
\int_0^{+\infty} x^2 \cdot \exp(-\lambda x) dx &= \left[-\frac{1}{\lambda} x^2 \cdot \exp(-\lambda x) \right]_0^{+\infty} - \int_0^{+\infty} 2x \left(-\frac{1}{\lambda} x \cdot \exp(-\lambda x) \right) dx \\
&= \left[-\frac{1}{\lambda} x^2 \cdot \exp(-\lambda x) \right]_0^{+\infty} - \left(\left[\frac{1}{\lambda^2} 2x \cdot \exp(-\lambda x) \right]_0^{+\infty} - \int_0^{+\infty} 2 \left(\frac{1}{\lambda^2} \cdot \exp(-\lambda x) \right) dx \right) \\
&= \left[-\frac{x^2}{\lambda} \cdot \exp(-\lambda x) \right]_0^{+\infty} - \left(\left[\frac{2x}{\lambda^2} \cdot \exp(-\lambda x) \right]_0^{+\infty} - \left[-\frac{2}{\lambda^3} \cdot \exp(-\lambda x) \right]_0^{+\infty} \right) \\
&= \left[\left(-\frac{x^2}{\lambda} - \frac{2x}{\lambda^2} - \frac{2}{\lambda^3} \right) \exp(-\lambda x) \right]_0^{+\infty},
\end{aligned} \tag{7}$$

the second moment becomes

$$\begin{aligned}
E[X^2] &= \lambda \left[\left(-\frac{x^2}{\lambda} - \frac{2x}{\lambda^2} - \frac{2}{\lambda^3} \right) \exp(-\lambda x) \right]_0^{+\infty} \\
&= \lambda \left[\lim_{x \rightarrow \infty} \left(-\frac{x^2}{\lambda} - \frac{2x}{\lambda^2} - \frac{2}{\lambda^3} \right) \exp(-\lambda x) - \left(0 - 0 - \frac{2}{\lambda^3} \right) \exp(-\lambda \cdot 0) \right] \\
&= \lambda \left[0 + \frac{2}{\lambda^3} \right] \\
&= \frac{2}{\lambda^2}.
\end{aligned} \tag{8}$$

Plugging (8) and (5) into (4), we have:

$$\begin{aligned}
\text{Var}(X) &= E[X^2] - E[X]^2 \\
&= \frac{2}{\lambda^2} - \left(\frac{1}{\lambda} \right)^2 \\
&= \frac{2}{\lambda^2} - \frac{1}{\lambda^2} \\
&= \frac{1}{\lambda^2}.
\end{aligned} \tag{9}$$

■

Sources:

- Taboga, Marco (2023): “Exponential distribution”; in: *Lectures on probability theory and mathematical statistics*, retrieved on 2023-01-23; URL: <https://www.statlect.com/probability-distributions/exponential-distribution>.
- Wikipedia (2023): “Variance”; in: *Wikipedia, the free encyclopedia*, retrieved on 2023-01-23; URL: <https://en.wikipedia.org/wiki/Variance#Definition>.

3.5.11 Skewness

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following an exponential distribution (\rightarrow II/3.5.1):

$$X \sim \text{Exp}(\lambda) . \quad (1)$$

Then the skewness (\rightarrow I/1.14.1) of X is

$$\text{Skew}(X) = 2 . \quad (2)$$

Proof: To compute the skewness of X , we partition the skewness into expected values (\rightarrow I/1.14.3)

$$\text{Skew}(X) = \frac{E(X^3) - 3\mu\sigma^2 - \mu^3}{\sigma^3} \quad (3)$$

where μ and σ are the mean and standard deviation of X , respectively. Since X follows an exponential distribution (\rightarrow II/3.5.1), the mean (\rightarrow II/3.5.7) of X is given by

$$\mu = E(X) = \frac{1}{\lambda} \quad (4)$$

and the standard deviation (\rightarrow II/3.5.10) of X is given by

$$\sigma = \sqrt{\text{Var}(X)} = \sqrt{\frac{1}{\lambda^2}} = \frac{1}{\lambda} . \quad (5)$$

Substituting (4) and (5) into (3) gives:

$$\begin{aligned} \text{Skew}(X) &= \frac{E(X^3) - 3\mu\sigma^2 - \mu^3}{\sigma^3} \\ &= \frac{E(X^3)}{\sigma^3} - \frac{3\mu\sigma^2 + \mu^3}{\sigma^3} \\ &= \frac{E(X^3)}{\left(\frac{1}{\lambda}\right)^3} - \frac{3\left(\frac{1}{\lambda}\right)\left(\frac{1}{\lambda}\right)^2 + \left(\frac{1}{\lambda}\right)^3}{\left(\frac{1}{\lambda}\right)^3} \\ &= \lambda^3 \cdot E(X^3) - \frac{\frac{3}{\lambda^3} + \frac{1}{\lambda^3}}{\frac{1}{\lambda^3}} \\ &= \lambda^3 \cdot E(X^3) - 4 . \end{aligned} \quad (6)$$

Thus, the remaining work is to compute $E(X^3)$. To do this, we use the moment-generating function of the exponential distribution (\rightarrow II/3.5.4) to calculate

$$E(X^3) = M_X'''(0) \quad (7)$$

based on the relationship between raw moment and moment-generating function (\rightarrow I/1.21.2). First, we differentiate the moment-generating function of the exponential distribution (\rightarrow II/3.5.4)

$$M_X(t) = \frac{\lambda}{\lambda - t} = \lambda(\lambda - t)^{-1} \quad (8)$$

with respect to t . Using the chain rule gives:

$$\begin{aligned} M_X'(t) &= -1 \cdot \lambda(\lambda - t)^{-2} \cdot (-1) \\ &= \lambda(\lambda - t)^{-2} . \end{aligned} \quad (9)$$

We continue using the chain rule to obtain the second derivative:

$$\begin{aligned} M_X''(t) &= -2 \cdot \lambda(\lambda - t)^{-3} \cdot (-1) \\ &= 2\lambda(\lambda - t)^{-3} . \end{aligned} \tag{10}$$

Finally, one more application of the chain rule gives us the third derivative:

$$\begin{aligned} M_X'''(t) &= -3 \cdot 2\lambda(\lambda - t)^{-4} \cdot (-1) \\ &= 6\lambda(\lambda - t)^{-4} \\ &= \frac{6\lambda}{(\lambda - t)^4} . \end{aligned} \tag{11}$$

Applying (7), together with (11), yields

$$\begin{aligned} E(X^3) &= M_X'''(0) \\ &= \frac{6\lambda}{(\lambda - 0)^4} \\ &= \frac{6\lambda}{\lambda^4} \\ &= \frac{6}{\lambda^3} . \end{aligned} \tag{12}$$

We now substitute (12) into (6), giving

$$\begin{aligned} \text{Skew}(X) &= \lambda^3 \cdot E(X^3) - 4 \\ &= \lambda^3 \cdot \left(\frac{6}{\lambda^3} \right) - 4 \\ &= 6 - 4 \\ &= 2 . \end{aligned} \tag{13}$$

This completes the proof of (2). ■

3.6 Log-normal distribution

3.6.1 Definition

Definition: Let $\ln X$ be a random variable (\rightarrow I/1.2.2) following a normal distribution (\rightarrow II/3.2.1) with mean μ and variance σ^2 (or, standard deviation σ):

$$Y = \ln(X) \sim \mathcal{N}(\mu, \sigma^2) . \tag{1}$$

Then, the exponential function of Y is said to have a log-normal distribution with location parameter μ and scale parameter σ

$$X = \exp(Y) \sim \ln \mathcal{N}(\mu, \sigma^2) \tag{2}$$

where $\mu \in \mathbb{R}$ and $\sigma^2 > 0$.

Sources:

- Wikipedia (2022): “Log-normal distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-02-07; URL: https://en.wikipedia.org/wiki/Log-normal_distribution.

3.6.2 Probability density function

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a log-normal distribution (\rightarrow II/3.6.1):

$$X \sim \ln \mathcal{N}(\mu, \sigma^2) . \quad (1)$$

Then, the probability density function (\rightarrow I/1.7.1) of X is given by:

$$f_X(x) = \frac{1}{x\sigma\sqrt{2\pi}} \cdot \exp \left[-\frac{(\ln x - \mu)^2}{2\sigma^2} \right] . \quad (2)$$

Proof: A log-normally distributed random variable (\rightarrow II/3.6.1) is defined as the exponential function of a normal random variable (\rightarrow II/3.2.1):

$$Y \sim \mathcal{N}(\mu, \sigma^2) \quad \Rightarrow \quad X = \exp(Y) \sim \ln \mathcal{N}(\mu, \sigma^2) . \quad (3)$$

The probability density function of the normal distribution (\rightarrow II/3.2.10) is

$$f_Y(y) = \frac{1}{\sigma\sqrt{2\pi}} \cdot \exp \left[-\frac{(y - \mu)^2}{2\sigma^2} \right] . \quad (4)$$

Writing X as a function of Y , we have

$$X = g(Y) = \exp(Y) \quad (5)$$

with the inverse function

$$Y = g^{-1}(X) = \ln(X) . \quad (6)$$

Because the derivative of $\exp(Y)$ is always positive, $g(Y)$ is strictly increasing and we can calculate the probability density function of a strictly increasing function (\rightarrow I/1.7.3) as

$$f_X(x) = \begin{cases} f_Y(g^{-1}(x)) \frac{dg^{-1}(x)}{dx} , & \text{if } x \in \mathcal{X} \\ 0 , & \text{if } x \notin \mathcal{X} \end{cases} \quad (7)$$

where $\mathcal{X} = \{x = g(y) : y \in \mathcal{Y}\}$. With the probability density function of the normal distribution (\rightarrow II/3.2.10), we have

$$\begin{aligned}
f_X(x) &= f_Y(g^{-1}(x)) \cdot \frac{dg^{-1}(x)}{dx} \\
&= \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp \left[-\frac{1}{2} \left(\frac{g^{-1}(x) - \mu}{\sigma} \right)^2 \right] \cdot \frac{dg^{-1}(x)}{dx} \\
&= \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp \left[-\frac{1}{2} \left(\frac{(\ln x) - \mu}{\sigma} \right)^2 \right] \cdot \frac{d(\ln x)}{dx} \\
&= \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp \left[-\frac{1}{2} \left(\frac{\ln x - \mu}{\sigma} \right)^2 \right] \cdot \frac{1}{x} \\
&= \frac{1}{x\sigma\sqrt{2\pi}} \cdot \exp \left[-\frac{(\ln x - \mu)^2}{2\sigma^2} \right]
\end{aligned} \tag{8}$$

which is the probability density function (\rightarrow I/1.7.1) of the log-normal distribution (\rightarrow II/3.6.1). ■

Sources:

- Taboga, Marco (2021): “Log-normal distribution”; in: *Lectures on probability and statistics*, retrieved on 2022-02-13; URL: <https://www.statlect.com/probability-distributions/log-normal-distribution>.

3.6.3 Cumulative distribution function

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a log-normal distribution (\rightarrow II/3.6.1):

$$X \sim \ln \mathcal{N}(\mu, \sigma^2) . \tag{1}$$

Then, the cumulative distribution function (\rightarrow I/1.8.1) of X is

$$F_X(x) = \frac{1}{2} \left[1 + \operatorname{erf} \left(\frac{\ln x - \mu}{\sqrt{2}\sigma} \right) \right] \tag{2}$$

where $\operatorname{erf}(x)$ is the error function defined as

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x \exp(-t^2) dt . \tag{3}$$

Proof: The probability density function of the log-normal distribution (\rightarrow II/3.6.2) is:

$$f_X(x) = \frac{1}{x\sigma\sqrt{2\pi}} \cdot \exp \left[-\left(\frac{\ln x - \mu}{\sqrt{2}\sigma} \right)^2 \right] . \tag{4}$$

Thus, the cumulative distribution function (\rightarrow I/1.8.1) is:

$$\begin{aligned}
F_X(x) &= \int_{-\infty}^x \ln \mathcal{N}(z; \mu, \sigma^2) dz \\
&= \int_{-\infty}^x \frac{1}{z\sigma\sqrt{2\pi}} \cdot \exp \left[- \left(\frac{\ln z - \mu}{\sqrt{2}\sigma} \right)^2 \right] dz \\
&= \frac{1}{\sigma\sqrt{2\pi}} \int_{-\infty}^x \frac{1}{z} \cdot \exp \left[- \left(\frac{\ln z - \mu}{\sqrt{2}\sigma} \right)^2 \right] dz .
\end{aligned} \tag{5}$$

From this point forward, the proof is similar to the derivation of the cumulative distribution function for the normal distribution (\rightarrow II/3.2.12). Substituting $t = (\ln z - \mu)/(\sqrt{2}\sigma)$, i.e. $\ln z = \sqrt{2}\sigma t + \mu$, $z = \exp(\sqrt{2}\sigma t + \mu)$ this becomes:

$$\begin{aligned}
F_X(x) &= \frac{1}{\sigma\sqrt{2\pi}} \int_{(-\infty-\mu)/(\sqrt{2}\sigma)}^{(\ln x - \mu)/(\sqrt{2}\sigma)} \frac{1}{\exp(\sqrt{2}\sigma t + \mu)} \cdot \exp(-t^2) d \left[\exp(\sqrt{2}\sigma t + \mu) \right] \\
&= \frac{\sqrt{2}\sigma}{\sigma\sqrt{2\pi}} \int_{-\infty}^{\frac{\ln x - \mu}{\sqrt{2}\sigma}} \frac{1}{\exp(\sqrt{2}\sigma t + \mu)} \cdot \exp(-t^2) \cdot \exp(\sqrt{2}\sigma t + \mu) dt \\
&= \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\frac{\ln x - \mu}{\sqrt{2}\sigma}} \exp(-t^2) dt \\
&= \frac{1}{\sqrt{\pi}} \int_{-\infty}^0 \exp(-t^2) dt + \frac{1}{\sqrt{\pi}} \int_0^{\frac{\ln x - \mu}{\sqrt{2}\sigma}} \exp(-t^2) dt \\
&= \frac{1}{\sqrt{\pi}} \int_0^{\infty} \exp(-t^2) dt + \frac{1}{\sqrt{\pi}} \int_0^{\frac{\ln x - \mu}{\sqrt{2}\sigma}} \exp(-t^2) dt .
\end{aligned} \tag{6}$$

Applying (3) to (6), we have:

$$\begin{aligned}
F_X(x) &= \frac{1}{2} \lim_{x \rightarrow \infty} \operatorname{erf}(x) + \frac{1}{2} \operatorname{erf} \left(\frac{\ln x - \mu}{\sqrt{2}\sigma} \right) \\
&= \frac{1}{2} + \frac{1}{2} \operatorname{erf} \left(\frac{\ln x - \mu}{\sqrt{2}\sigma} \right) \\
&= \frac{1}{2} \left[1 + \operatorname{erf} \left(\frac{\ln x - \mu}{\sqrt{2}\sigma} \right) \right] .
\end{aligned} \tag{7}$$

■

Sources:

- skdhfgeq2134 (2015): “How to derive the cdf of a lognormal distribution from its pdf”; in: *StackExchange*, retrieved on 2022-06-29; URL: <https://stats.stackexchange.com/questions/151398/how-to-derive-t-151404#151404>.

3.6.4 Quantile function

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a log-normal distribution (\rightarrow II/3.6.1):

$$X \sim \ln \mathcal{N}(\mu, \sigma^2) . \tag{1}$$

Then, the quantile function (\rightarrow I/1.11.1) of X is

$$Q_X(p) = \exp(\mu + \sqrt{2}\sigma \cdot \operatorname{erf}^{-1}(2p - 1)) \quad (2)$$

where $\operatorname{erf}^{-1}(x)$ is the inverse error function.

Proof: The cumulative distribution function of the log-normal distribution (\rightarrow II/3.6.3) is:

$$F_X(x) = \frac{1}{2} \left[1 + \operatorname{erf} \left(\frac{\ln x - \mu}{\sqrt{2}\sigma} \right) \right]. \quad (3)$$

From this point forward, the proof is similar to the derivation of the quantile function for the normal distribution (\rightarrow II/3.2.15). Because the cumulative distribution function (CDF) is strictly monotonically increasing, the quantile function is equal to the inverse of the CDF (\rightarrow I/1.11.2):

$$Q_X(p) = F_X^{-1}(x). \quad (4)$$

This can be derived by rearranging equation (3):

$$\begin{aligned} p &= \frac{1}{2} \left[1 + \operatorname{erf} \left(\frac{\ln x - \mu}{\sqrt{2}\sigma} \right) \right] \\ 2p - 1 &= \operatorname{erf} \left(\frac{\ln x - \mu}{\sqrt{2}\sigma} \right) \\ \operatorname{erf}^{-1}(2p - 1) &= \frac{\ln x - \mu}{\sqrt{2}\sigma} \\ x &= \exp(\mu + \sqrt{2}\sigma \cdot \operatorname{erf}^{-1}(2p - 1)). \end{aligned} \quad (5)$$

■

Sources:

- Wikipedia (2022): “Log-normal distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-07-08; URL: https://en.wikipedia.org/wiki/Log-normal_distribution#Mode,_median,_quantiles.

3.6.5 Mean

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a log-normal distribution (\rightarrow II/3.6.1):

$$X \sim \ln \mathcal{N}(\mu, \sigma^2). \quad (1)$$

Then, the mean or expected value (\rightarrow I/1.12.1) of X is

$$\mathbb{E}(X) = \exp \left(\mu + \frac{1}{2}\sigma^2 \right). \quad (2)$$

Proof: The expected value (\rightarrow I/1.12.1) is the probability-weighted average over all possible values:

$$\mathbb{E}(X) = \int_{\mathcal{X}} x \cdot f_X(x) \, dx. \quad (3)$$

With the probability density function of the log-normal distribution (\rightarrow II/3.6.2), this is:

$$\begin{aligned}
E(X) &= \int_0^{+\infty} x \cdot \frac{1}{x\sqrt{2\pi\sigma^2}} \cdot \exp\left[-\frac{1}{2} \frac{(\ln x - \mu)^2}{\sigma^2}\right] dx \\
&= \frac{1}{\sqrt{2\pi\sigma^2}} \int_0^{+\infty} \exp\left[-\frac{1}{2} \frac{(\ln x - \mu)^2}{\sigma^2}\right] dx .
\end{aligned} \tag{4}$$

Substituting $z = \frac{\ln x - \mu}{\sigma}$, i.e. $x = \exp(\mu + \sigma z)$, we have:

$$\begin{aligned}
E(X) &= \frac{1}{\sqrt{2\pi\sigma^2}} \int_{(-\infty - \mu)/(\sigma)}^{(\ln x - \mu)/(\sigma)} \exp\left(-\frac{1}{2}z^2\right) d[\exp(\mu + \sigma z)] \\
&= \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{+\infty} \exp\left(-\frac{1}{2}z^2\right) \sigma \exp(\mu + \sigma z) dz \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \exp\left(-\frac{1}{2}z^2 + \sigma z + \mu\right) dz \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \exp\left[-\frac{1}{2}(z^2 - 2\sigma z - 2\mu)\right] dz .
\end{aligned} \tag{5}$$

Now multiplying with $\exp(\frac{1}{2}\sigma^2)$ and $\exp(-\frac{1}{2}\sigma^2)$, we have:

$$\begin{aligned}
E(X) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \exp\left[-\frac{1}{2}(z^2 - 2\sigma z + \sigma^2 - 2\mu - \sigma^2)\right] dz \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \exp\left[-\frac{1}{2}(z^2 - 2\sigma z + \sigma^2)\right] \exp\left(\mu + \frac{1}{2}\sigma^2\right) dz \\
&= \exp\left(\mu + \frac{1}{2}\sigma^2\right) \int_{-\infty}^{+\infty} \frac{1}{\sqrt{2\pi}} \exp\left[-\frac{1}{2}(z - \sigma)^2\right] dz .
\end{aligned} \tag{6}$$

The probability density function of a normal distribution (\rightarrow II/3.2.10) is given by

$$f_X(x) = \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp\left[-\frac{1}{2}\left(\frac{x - \mu}{\sigma}\right)^2\right] \tag{7}$$

and, with unit variance $\sigma^2 = 1$, this reads:

$$f_X(x) = \frac{1}{\sqrt{2\pi}} \cdot \exp\left[-\frac{1}{2}(x - \mu)^2\right] . \tag{8}$$

Using the definition of the probability density function (\rightarrow I/1.7.1), we get

$$\int_{-\infty}^{+\infty} \frac{1}{\sqrt{2\pi}} \cdot \exp\left[-\frac{1}{2}(x - \mu)^2\right] dx = 1 \tag{9}$$

and applying (9) to (6), we have:

$$E(X) = \exp\left(\mu + \frac{1}{2}\sigma^2\right) . \tag{10}$$

■

Sources:

- Taboga, Marco (2022): “Log-normal distribution”; in: *Lectures on probability theory and mathematical statistics*, retrieved on 2022-10-01; URL: <https://www.statlect.com/probability-distributions/log-normal-distribution>.

3.6.6 Median

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a log-normal distribution (\rightarrow II/3.6.1):

$$X \sim \ln \mathcal{N}(\mu, \sigma^2) . \quad (1)$$

Then, the median (\rightarrow I/1.18.1) of X is

$$\text{median}(X) = e^\mu . \quad (2)$$

Proof: The median (\rightarrow I/1.18.1) is the value at which the cumulative distribution function is $1/2$:

$$F_X(\text{median}(X)) = \frac{1}{2} . \quad (3)$$

The cumulative distribution function of the lognormal distribution (\rightarrow II/3.6.3) is

$$F_X(x) = \frac{1}{2} \left[1 + \text{erf} \left(\frac{\ln(x) - \mu}{\sigma\sqrt{2}} \right) \right] \quad (4)$$

where $\text{erf}(x)$ is the error function defined as

$$\text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x \exp(-t^2) dt . \quad (5)$$

Thus, the inverse cumulative distribution function is

$$\begin{aligned} \ln(x) &= \sigma\sqrt{2} \cdot \text{erf}^{-1}(2p - 1) + \mu \\ x &= \exp \left[\sigma\sqrt{2} \cdot \text{erf}^{-1}(2p - 1) + \mu \right] \end{aligned} \quad (6)$$

where $\text{erf}^{-1}(x)$ is the inverse error function. Setting $p = 1/2$, we obtain:

$$\begin{aligned} \ln [\text{median}(X)] &= \sigma\sqrt{2} \cdot \text{erf}^{-1}(0) + \mu \\ \text{median}(X) &= e^\mu . \end{aligned} \quad (7)$$

■

3.6.7 Mode

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a log-normal distribution (\rightarrow II/3.6.1):

$$X \sim \ln \mathcal{N}(\mu, \sigma^2) . \quad (1)$$

Then, the mode (\rightarrow I/1.18.3) of X is

$$\text{mode}(X) = e^{(\mu - \sigma^2)} . \quad (2)$$

Proof: The mode (\rightarrow I/1.18.3) is the value which maximizes the probability density function (\rightarrow I/1.7.1):

$$\text{mode}(X) = \arg \max_x f_X(x) . \quad (3)$$

The probability density function of the log-normal distribution (\rightarrow II/3.6.2) is:

$$f_X(x) = \frac{1}{x\sigma\sqrt{2\pi}} \cdot \exp \left[-\frac{(\ln x - \mu)^2}{2\sigma^2} \right] . \quad (4)$$

The first two derivatives of this function are:

$$f'_X(x) = -\frac{1}{x^2\sigma\sqrt{2\pi}} \cdot \exp \left[-\frac{(\ln x - \mu)^2}{2\sigma^2} \right] \cdot \left(1 + \frac{\ln x - \mu}{\sigma^2} \right) \quad (5)$$

$$\begin{aligned} f''_X(x) &= \frac{1}{\sqrt{2\pi}\sigma^2 x^3} \cdot \exp \left[-\frac{(\ln x - \mu)^2}{2\sigma^2} \right] \cdot (\ln x - \mu) \cdot \left(1 + \frac{\ln x - \mu}{\sigma^2} \right) \\ &+ \frac{\sqrt{2}}{\sqrt{\pi}x^3} \cdot \exp \left[-\frac{(\ln x - \mu)^2}{2\sigma^2} \right] \cdot \left(1 + \frac{\ln x - \mu}{\sigma^2} \right) \\ &- \frac{1}{\sqrt{2\pi}\sigma^2 x^3} \cdot \exp \left[-\frac{(\ln x - \mu)^2}{2\sigma^2} \right] . \end{aligned} \quad (6)$$

We now calculate the root of the first derivative (5):

$$\begin{aligned} f'_X(x) = 0 &= -\frac{1}{x^2\sigma\sqrt{2\pi}} \cdot \exp \left[-\frac{(\ln x - \mu)^2}{2\sigma^2} \right] \cdot \left(1 + \frac{\ln x - \mu}{\sigma^2} \right) \\ -1 &= \frac{\ln x - \mu}{\sigma^2} \\ x &= e^{(\mu - \sigma^2)} . \end{aligned} \quad (7)$$

By plugging this value into the second derivative (6),

$$\begin{aligned} f''_X(e^{(\mu - \sigma^2)}) &= \frac{1}{\sqrt{2\pi}\sigma^2(e^{(\mu - \sigma^2)})^3} \cdot \exp \left[-\frac{\sigma^2}{2} \right] \cdot (\sigma^2) \cdot (0) \\ &+ \frac{\sqrt{2}}{\sqrt{\pi}(e^{(\mu - \sigma^2)})^3} \cdot \exp \left[-\frac{\sigma^2}{2} \right] \cdot (0) \\ &- \frac{1}{\sqrt{2\pi}\sigma^2(e^{(\mu - \sigma^2)})^3} \cdot \exp \left[-\frac{\sigma^2}{2} \right] \\ &= -\frac{1}{\sqrt{2\pi}\sigma^2(e^{(\mu - \sigma^2)})^3} \cdot \exp \left[-\frac{\sigma^2}{2} \right] < 0 , \end{aligned} \quad (8)$$

we confirm that it is a maximum, showing that

$$\text{mode}(X) = e^{(\mu - \sigma^2)} . \quad (9)$$

■

Sources:

- Wikipedia (2022): “Log-normal distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-02-12; URL: https://en.wikipedia.org/wiki/Log-normal_distribution#Mode.
- Mdoc (2015): “Mode of lognormal distribution”; in: *Mathematics Stack Exchange*, retrieved on 2022-02-12; URL: <https://math.stackexchange.com/questions/1321221/mode-of-lognormal-distribution/1321626>.

3.6.8 Variance

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a log-normal distribution (\rightarrow II/3.6.1):

$$X \sim \ln \mathcal{N}(\mu, \sigma^2). \quad (1)$$

Then, the variance (\rightarrow I/1.13.1) of X is

$$\text{Var}(X) = \exp(2\mu + 2\sigma^2) - \exp(2\mu + \sigma^2) . \quad (2)$$

Proof: The variance (\rightarrow I/1.13.1) of a random variable is defined as

$$\text{Var}(X) = \text{E}[(X - \text{E}(X))^2] \quad (3)$$

which, partitioned into expected values (\rightarrow I/1.13.4), reads:

$$\text{Var}(X) = \text{E}[X^2] - \text{E}[X]^2 . \quad (4)$$

The expected value of the log-normal distribution (\rightarrow II/3.6.5) is:

$$\text{E}[X] = \exp\left(\mu + \frac{1}{2}\sigma^2\right) \quad (5)$$

The second moment $\text{E}[X^2]$ can be derived as follows:

$$\begin{aligned} \text{E}[X^2] &= \int_{-\infty}^{+\infty} x^2 \cdot f_X(x) \, dx \\ &= \int_0^{+\infty} x^2 \cdot \frac{1}{x\sqrt{2\pi\sigma^2}} \cdot \exp\left[-\frac{1}{2} \frac{(\ln x - \mu)^2}{\sigma^2}\right] \, dx \\ &= \frac{1}{\sqrt{2\pi\sigma^2}} \int_0^{+\infty} x \cdot \exp\left[-\frac{1}{2} \frac{(\ln x - \mu)^2}{\sigma^2}\right] \, dx \end{aligned} \quad (6)$$

Substituting $z = \frac{\ln x - \mu}{\sigma}$, i.e. $x = \exp(\mu + \sigma z)$, we have:

$$\begin{aligned}
E[X^2] &= \frac{1}{\sqrt{2\pi\sigma^2}} \int_{(-\infty-\mu)/(\sigma)}^{(\ln x - \mu)/(\sigma)} \exp(\mu + \sigma z) \exp\left(-\frac{1}{2}z^2\right) d[\exp(\mu + \sigma z)] \\
&= \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{+\infty} \exp\left(-\frac{1}{2}z^2\right) \sigma \exp(2\mu + 2\sigma z) dz \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \exp\left[-\frac{1}{2}(z^2 - 4\sigma z - 4\mu)\right] dz
\end{aligned} \tag{7}$$

Now multiplying the integrand by $\exp(2\sigma^2)$ and $\exp(-2\sigma^2)$, this becomes:

$$\begin{aligned}
E[X^2] &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \exp\left[-\frac{1}{2}(z^2 - 4\sigma z + 4\sigma^2 - 4\sigma^2 - 4\mu)\right] dz \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \exp\left[-\frac{1}{2}(z^2 - 4\sigma z + 4\sigma^2)\right] \exp(2\sigma^2 + 2\mu) dz \\
&= \exp(2\sigma^2 + 2\mu) \int_{-\infty}^{+\infty} \frac{1}{\sqrt{2\pi}} \exp\left[-\frac{1}{2}(z - 2\sigma)^2\right] dz
\end{aligned} \tag{8}$$

The probability density function of a normal distribution (\rightarrow II/3.2.10) is given by

$$f_X(x) = \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp\left[-\frac{1}{2}\left(\frac{x - \mu}{\sigma}\right)^2\right] \tag{9}$$

and, with $\mu = 2\sigma$ and unit variance, this reads:

$$f_X(x) = \frac{1}{\sqrt{2\pi}} \cdot \exp\left[-\frac{1}{2}(x - 2\sigma)^2\right]. \tag{10}$$

Using the definition of the probability density function (\rightarrow I/1.7.1), we get

$$\int_{-\infty}^{+\infty} \frac{1}{\sqrt{2\pi}} \cdot \exp\left[-\frac{1}{2}(x - 2\sigma)^2\right] dx = 1 \tag{11}$$

and applying (11) to (8), we have:

$$E[X]^2 = \exp(2\sigma^2 + 2\mu). \tag{12}$$

Finally, plugging (12) and (5) into (4), we have:

$$\begin{aligned}
\text{Var}(X) &= E[X^2] - E[X]^2 \\
&= \exp(2\sigma^2 + 2\mu) - \left[\exp\left(\mu + \frac{1}{2}\sigma^2\right)\right]^2 \\
&= \exp(2\sigma^2 + 2\mu) - \exp(2\mu + \sigma^2).
\end{aligned} \tag{13}$$

Sources:

- Taboga, Marco (2022): “Log-normal distribution”; in: *Lectures on probability theory and mathematical statistics*, retrieved on 2022-10-01; URL: <https://www.statlect.com/probability-distributions/log-normal-distribution>.
- Wikipedia (2022): “Variance”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-10-01; URL: <https://en.wikipedia.org/wiki/Variance#Definition>.

3.6.9 Product of independent log-normals

Theorem: Let X_1, \dots, X_n be independent (\rightarrow I/1.3.6) random variables (\rightarrow I/1.2.2) following log-normal distributions (\rightarrow II/3.6.1):

$$X_i \sim \ln \mathcal{N}(\mu_i, \sigma_i^2), \quad i = 1, \dots, n. \quad (1)$$

Then, the product of these random variables also follows a log-normal distribution (\rightarrow II/3.6.1)

$$Z = \prod_{i=1}^n X_i \sim \mathcal{N}(\mu, \sigma^2) \quad (2)$$

where the log-normal (\rightarrow II/3.6.1) parameters are given by

$$\mu = \sum_{i=1}^n \mu_i \quad \text{and} \quad \sigma^2 = \sum_{i=1}^n \sigma_i^2. \quad (3)$$

Proof: A random variable follows a log-normal distribution, if and only if its natural logarithm follows a normal distribution (\rightarrow II/3.6.1):

$$X \sim \ln \mathcal{N}(\mu, \sigma^2) \quad \Leftrightarrow \quad \ln X \sim \mathcal{N}(\mu, \sigma^2). \quad (4)$$

Thus, from (1), we have

$$Y_i = \ln X_i \sim \mathcal{N}(\mu_i, \sigma_i^2) \quad (5)$$

and from (2), we have

$$\ln Z = \ln \left(\prod_{i=1}^n X_i \right) = \sum_{i=1}^n \ln X_i = \sum_{i=1}^n Y_i. \quad (6)$$

This means that the logarithm of the product of independent log-normal (\rightarrow II/3.6.1) random variables is a sum of independent normal (\rightarrow II/3.2.1) random variables. Because any linear combination of independent normal random variables is again normally distributed (\rightarrow II/3.2.26), this sum follows a normal distribution. Combining this with (6) and (5), we have:

$$\ln Z = \sum_{i=1}^n Y_i \sim \mathcal{N} \left(\sum_{i=1}^n \mu_i, \sum_{i=1}^n \sigma_i^2 \right). \quad (7)$$

If a random variable follows a normal distribution, then its exponential follows a log-normal distribution with the same parameters (\rightarrow II/3.6.1):

$$Y \sim \mathcal{N}(\mu, \sigma^2) \quad \Leftrightarrow \quad \exp(Y) \sim \ln \mathcal{N}(\mu, \sigma^2). \quad (8)$$

Thus, from (7), we have

$$Z = \exp(\ln Z) \sim \ln \mathcal{N} \left(\sum_{i=1}^n \mu_i, \sum_{i=1}^n \sigma_i^2 \right) \quad (9)$$

which is equivalent to (2) and (3). ■

Sources:

- drhab (2018): “If X_i is a log-normal r.v., show product of all X_i is also a log-normal r.v.”; in: *StackExchange Mathematics*, retrieved on 2024-11-15; URL: <https://math.stackexchange.com/a/2838307/480910>.

3.6.10 Geometric mean of independent log-normals

Theorem: Let X_1, \dots, X_n be independent (\rightarrow I/1.3.6) random variables (\rightarrow I/1.2.2) following log-normal distributions (\rightarrow II/3.6.1):

$$X_i \sim \ln \mathcal{N}(\mu_i, \sigma_i^2), \quad i = 1, \dots, n. \quad (1)$$

Then, the geometric mean of these random variables also follows a log-normal distribution (\rightarrow II/3.6.1):

$$Z = \sqrt[n]{\prod_{i=1}^n X_i} \sim \mathcal{N}(\mu, \sigma^2) \quad (2)$$

where the log-normal (\rightarrow II/3.6.1) parameters are given by

$$\mu = \frac{1}{n} \sum_{i=1}^n \mu_i \quad \text{and} \quad \sigma^2 = \frac{1}{n^2} \sum_{i=1}^n \sigma_i^2. \quad (3)$$

Proof: A random variable follows a log-normal distribution, if and only if its natural logarithm follows a normal distribution (\rightarrow II/3.6.1):

$$X \sim \ln \mathcal{N}(\mu, \sigma^2) \quad \Leftrightarrow \quad \ln X \sim \mathcal{N}(\mu, \sigma^2). \quad (4)$$

Thus, from (1), we have

$$Y_i = \ln X_i \sim \mathcal{N}(\mu_i, \sigma_i^2) \quad (5)$$

and from (2), we have

$$\ln Z = \ln \left(\sqrt[n]{\prod_{i=1}^n X_i} \right) = \frac{1}{n} \sum_{i=1}^n \ln X_i = \frac{1}{n} \sum_{i=1}^n Y_i. \quad (6)$$

This means that the logarithm of the geometric mean of independent log-normal (\rightarrow II/3.6.1) random variables is the arithmetic mean of independent normal (\rightarrow II/3.2.1) random variables. This average, like any linear combination of independent normal random variables, is again normally distributed (\rightarrow II/3.2.26). Thus, combining (6) and (5), we have:

$$\ln Z = \frac{1}{n} \sum_{i=1}^n Y_i \sim \mathcal{N} \left(\frac{1}{n} \sum_{i=1}^n \mu_i, \frac{1}{n^2} \sum_{i=1}^n \sigma_i^2 \right). \quad (7)$$

If a random variable [follows a normal distribution, then its exponential follows a log-normal distribution with the same parameters]:

$$Y \sim \mathcal{N}(\mu, \sigma^2) \quad \Leftrightarrow \quad \exp(Y) \sim \ln \mathcal{N}(\mu, \sigma^2). \quad (8)$$

Thus, from (7), we have

$$Z = \exp(\ln Z) \sim \ln \mathcal{N} \left(\frac{1}{n} \sum_{i=1}^n \mu_i, \frac{1}{n^2} \sum_{i=1}^n \sigma_i^2 \right) \quad (9)$$

which is equivalent to (2) and (3). ■

Sources:

- Probability Fact (2022): “The geometric mean of independent log-normal random variables has a log-normal distribution”; in: *X*, retrieved on 2024-11-22; URL: <https://x.com/ProbFact/status/1592989704646848512>.

3.7 Chi-squared distribution

3.7.1 Definition

Definition: Let X_1, \dots, X_k be independent (\rightarrow I/1.3.6) random variables (\rightarrow I/1.2.2) where each of them is following a standard normal distribution (\rightarrow II/3.2.3):

$$X_i \sim \mathcal{N}(0, 1) \quad \text{for } i = 1, \dots, n. \quad (1)$$

Then, the sum of their squares follows a chi-squared distribution with k degrees of freedom:

$$Y = \sum_{i=1}^k X_i^2 \sim \chi^2(k) \quad \text{where } k > 0. \quad (2)$$

The probability density function of the chi-squared distribution (\rightarrow II/3.7.4) with k degrees of freedom is

$$\chi^2(x; k) = \frac{1}{2^{k/2} \Gamma(k/2)} x^{k/2-1} \exp[-x/2] \quad (3)$$

where $k > 0$ and the density is zero, if $x \leq 0$.

Sources:

- Wikipedia (2020): “Chi-square distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-10-12; URL: https://en.wikipedia.org/wiki/Chi-square_distribution#Definitions.
- Robert V. Hogg, Joseph W. McKean, Allen T. Craig (2018): “The Chi-Squared-Distribution”; in: *Introduction to Mathematical Statistics*, Pearson, Boston, 2019, p. 178, eq. 3.3.7; URL: <https://www.pearson.com/store/p/introduction-to-mathematical-statistics/P100000843744>.

3.7.2 Special case of gamma distribution

Theorem: The chi-squared distribution (\rightarrow II/3.7.1) with k degrees of freedom is a special case of the gamma distribution (\rightarrow II/3.4.1) with shape $k/2$ and rate $1/2$:

$$X \sim \text{Gam} \left(\frac{k}{2}, \frac{1}{2} \right) \quad \Rightarrow \quad X \sim \chi^2(k). \quad (1)$$

Proof: The probability density function of the gamma distribution (\rightarrow II/3.4.7) for $x > 0$, where α is the shape parameter and β is the rate parameter, is as follows:

$$\text{Gam}(x; \alpha, \beta) = \frac{\beta^\alpha}{\Gamma(\alpha)} x^{\alpha-1} \exp[-\beta x] \quad (2)$$

If we let $\alpha = k/2$ and $\beta = 1/2$, we obtain

$$\text{Gam}\left(x; \frac{k}{2}, \frac{1}{2}\right) = \frac{x^{k/2-1} \exp[-x/2]}{\Gamma(k/2) 2^{k/2}} = \frac{1}{2^{k/2} \Gamma(k/2)} x^{k/2-1} \exp[-x/2] \quad (3)$$

which is equivalent to the probability density function of the chi-squared distribution (\rightarrow II/3.7.4). ■

3.7.3 Special case of gamma distribution

Theorem: The chi-squared distribution (\rightarrow II/3.7.1) with $n \in \mathbb{Z}^*$ degrees of freedom (\rightarrow I/1.5.12) is a special case of the gamma distribution (\rightarrow II/3.4.1) with parameters (\rightarrow I/1.5.7) $\alpha = \frac{n}{2}$, $\beta = \frac{1}{2}$ and support $t < \frac{1}{2}$.

Proof: The moment-generating function (\rightarrow I/1.9.1) of a gamma random variable (\rightarrow II/3.4.1) $X \sim \text{Gam}(\alpha, \beta)$ is

$$M_X(t) = \left(1 - \frac{t}{\beta}\right)^{-\alpha}, \quad t < \beta, \quad \beta > 0. \quad (1)$$

The moment-generating function (\rightarrow I/1.9.1) of the a chi-squared random variable (\rightarrow II/3.7.1) $Y \sim \chi_n^2$ with n degrees of freedom is

$$M_Y(t) = (1 - 2t)^{-n/2}, \quad t < \frac{1}{2}. \quad (2)$$

If there is a random variable (\rightarrow I/1.2.2) $X \sim \text{Gam}\left(\frac{n}{2}, \frac{1}{2}\right)$, then

$$M_X(t) = \left(1 - \frac{t}{\frac{1}{2}}\right)^{-(n/2)} = (1 - 2t)^{-n/2} = M_Y(t) \quad \text{for } t < \frac{1}{2} \quad (3)$$

“If the moment-generating function exists for t in an open interval containing zero, it uniquely determines the probability distribution.” (Rice, 2007, p. 155) Both moment-generating functions (1) and (2) satisfy this condition. Specifically, $M_X(t)$ is defined for $t < \frac{1}{2}$, and for $M_Y(t)$, we have $t < \beta$ with $\beta > 0$; both of these intervals contain 0.

By the uniqueness of the moment-generating function, the chi-squared distribution with n degrees of freedom is a special case of the gamma distribution with parameters $\alpha = \frac{n}{2}$ and $\beta = \frac{1}{2}$ and support $t < \frac{1}{2}$. This completes the proof. ■

Sources:

- John Rice (2007): “The Moment-Generating Function”; in: *Mathematical Statistics, Third Edition*, p. 155 and p. A2; URL: <https://korivernon.com/documents/MathematicalStatisticsandDataAnalysis3ed.pdf>.
- Irene Vrbik (2025): “MGF of a Gamma and Chi square”; in: *Stat 205*; URL: <https://irene.vrbik.ok.ubc.ca/quarto/stat205/lectures/proofs/mgf-gamma.html>.

- Wikipedia (2025): “Chi-squared distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2025-12-26; URL: https://en.wikipedia.org/wiki/Chi-squared_distribution.
- Wikipedia (2025): “Gamma distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2025-12-26; URL: https://en.wikipedia.org/wiki/Gamma_distribution.

3.7.4 Probability density function

Theorem: Let Y be a random variable (\rightarrow I/1.2.2) following a chi-squared distribution (\rightarrow II/3.7.1):

$$Y \sim \chi^2(k) . \quad (1)$$

Then, the probability density function (\rightarrow I/1.7.1) of Y is

$$f_Y(y) = \frac{1}{2^{k/2} \Gamma(k/2)} y^{k/2-1} \exp[-y/2] . \quad (2)$$

Proof: A chi-square-distributed random variable (\rightarrow II/3.7.1) with k degrees of freedom is defined as the sum of k squared standard normal random variables (\rightarrow II/3.2.3):

$$X_1, \dots, X_k \sim \mathcal{N}(0, 1) \quad \Rightarrow \quad Y = \sum_{i=1}^k X_i^2 \sim \chi^2(k) . \quad (3)$$

Let x_1, \dots, x_k be values of X_1, \dots, X_k and consider $x = (x_1, \dots, x_k)$ to be a point in k -dimensional space. Define

$$y = \sum_{i=1}^k x_i^2 \quad (4)$$

and let $f_Y(y)$ and $F_Y(y)$ be the probability density function (\rightarrow I/1.7.1) and cumulative distribution function (\rightarrow I/1.8.1) of Y . Because the PDF is the first derivative of the CDF (\rightarrow I/1.7.7), we can write:

$$F_Y(y) = \frac{F_Y(y)}{dy} dy = f_Y(y) dy . \quad (5)$$

Then, the cumulative distribution function (\rightarrow I/1.8.1) of Y can be expressed as

$$f_Y(y) dy = \int_V \prod_{i=1}^k (\mathcal{N}(x_i; 0, 1) dx_i) \quad (6)$$

where $\mathcal{N}(x_i; 0, 1)$ is the probability density function (\rightarrow I/1.7.1) of the standard normal distribution (\rightarrow II/3.2.3) and V is the elemental shell volume at $y(x)$, which is proportional to the $(k-1)$ -dimensional surface in k -space for which equation (4) is fulfilled. Using the probability density function of the normal distribution (\rightarrow II/3.2.10), equation (6) can be developed as follows:

$$\begin{aligned}
f_Y(y) dy &= \int_V \prod_{i=1}^k \left(\frac{1}{\sqrt{2\pi}} \cdot \exp \left[-\frac{1}{2} x_i^2 \right] dx_i \right) \\
&= \int_V \frac{\exp \left[-\frac{1}{2} (x_1^2 + \dots + x_k^2) \right]}{(2\pi)^{k/2}} dx_1 \dots dx_k \\
&= \frac{1}{(2\pi)^{k/2}} \int_V \exp \left[-\frac{y}{2} \right] dx_1 \dots dx_k .
\end{aligned} \tag{7}$$

Because y is constant within the set V , it can be moved out of the integral:

$$f_Y(y) dy = \frac{\exp[-y/2]}{(2\pi)^{k/2}} \int_V dx_1 \dots dx_k . \tag{8}$$

Now, the integral is simply the surface area of the $(k-1)$ -dimensional sphere with radius $r = \sqrt{y}$, which is

$$A = 2r^{k-1} \frac{\pi^{k/2}}{\Gamma(k/2)} , \tag{9}$$

times the infinitesimal thickness of the sphere, which is

$$\frac{dr}{dy} = \frac{1}{2} y^{-1/2} \Leftrightarrow dr = \frac{dy}{2y^{1/2}} . \tag{10}$$

Substituting (9) and (10) into (8), we have:

$$\begin{aligned}
f_Y(y) dy &= \frac{\exp[-y/2]}{(2\pi)^{k/2}} \cdot A dr \\
&= \frac{\exp[-y/2]}{(2\pi)^{k/2}} \cdot 2r^{k-1} \frac{\pi^{k/2}}{\Gamma(k/2)} \cdot \frac{dy}{2y^{1/2}} \\
&= \frac{1}{2^{k/2} \Gamma(k/2)} \cdot \frac{2\sqrt{y}^{k-1}}{2\sqrt{y}} \cdot \exp[-y/2] dy \\
&= \frac{1}{2^{k/2} \Gamma(k/2)} \cdot y^{\frac{k}{2}-1} \cdot \exp \left[-\frac{y}{2} \right] dy .
\end{aligned} \tag{11}$$

From this, we get the final result in (2):

$$f_Y(y) = \frac{1}{2^{k/2} \Gamma(k/2)} y^{k/2-1} \exp[-y/2] . \tag{12}$$

■

Sources:

- Wikipedia (2020): “Proofs related to chi-squared distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-11-25; URL: https://en.wikipedia.org/wiki/Proofs_related_to_chi-squared_distribution#Derivation_of_the_pdf_for_k_degrees_of_freedom.
- Wikipedia (2020): “n-sphere”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-11-25; URL: https://en.wikipedia.org/wiki/N-sphere#Volume_and_surface_area.

3.7.5 Raw moments

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a chi-squared distribution (\rightarrow II/3.7.1) with k degrees of freedom:

$$X \sim \chi^2(k) . \quad (1)$$

Then, if $m > -k/2$, the raw moment (\rightarrow I/1.21.3) $E(X^m)$ exists and is equal to:

$$E(X^m) = 2^m \frac{\Gamma(\frac{k}{2} + m)}{\Gamma(\frac{k}{2})} . \quad (2)$$

Proof: Combining the definition of the raw moment (\rightarrow I/1.21.3) with the probability density function of the chi-squared distribution (\rightarrow II/3.7.4), we have:

$$\begin{aligned} E(X^m) &= \int_0^\infty x^m \frac{1}{2^{k/2} \Gamma(\frac{k}{2})} x^{k/2-1} \exp[-x/2] dx \\ &= \frac{1}{2^{k/2} \Gamma(\frac{k}{2})} \int_0^\infty x^{(k/2)+m-1} \exp[-x/2] dx . \end{aligned} \quad (3)$$

Now, we substitute $u = x/2$, such that $x = 2u$. As a result, we obtain:

$$\begin{aligned} E(X^m) &= \frac{1}{2^{k/2} \Gamma(\frac{k}{2})} \int_0^\infty 2^{(k/2)+m-1} u^{(k/2)+m-1} \exp[-u] d(2u) \\ &= \frac{2^{(k/2)+m}}{2^{k/2} \Gamma(\frac{k}{2})} \int_0^\infty u^{(k/2)+m-1} \exp[-u] du \\ &= \frac{2^m}{\Gamma(\frac{k}{2})} \int_0^\infty u^{(k/2)+m-1} \exp[-u] du . \end{aligned} \quad (4)$$

With the definition of the gamma function as

$$\Gamma(x) = \int_0^\infty t^{x-1} e^{-t} dt, \quad x > 0 , \quad (5)$$

this leads to the desired result when $m > -k/2$. Observe that, if m is a non-negative integer, then $m > -k/2$ is always true. Therefore, all moments (\rightarrow I/1.21.1) of a chi-squared distribution (\rightarrow II/3.7.1) exist and the m -th raw moment is given by the equation above. ■

Sources:

- Robert V. Hogg, Joseph W. McKean, Allen T. Craig (2018): “The 2-Distribution”; in: *Introduction to Mathematical Statistics*, Pearson, Boston, 2019, p. 179, eq. 3.3.8; URL: <https://www.pearson.com/store/p/introduction-to-mathematical-statistics/P100000843744>.

3.8 F-distribution

3.8.1 Definition

Definition: Let X_1 and X_2 be independent (\rightarrow I/1.3.6) random variables (\rightarrow I/1.2.2) following a chi-squared distribution (\rightarrow II/3.7.1) with ν_1 and ν_2 degrees of freedom (\rightarrow I/1.5.12), respectively:

$$\begin{aligned} X_1 &\sim \chi^2(\nu_1) \\ X_2 &\sim \chi^2(\nu_2) . \end{aligned} \quad (1)$$

Then, the ratio of X_1 to X_2 , divided by their respective degrees of freedom, is said to be F -distributed with numerator degrees of freedom ν_1 and denominator degrees of freedom ν_2 :

$$Y = \frac{X_1/\nu_1}{X_2/\nu_2} \sim F(\nu_1, \nu_2) \quad \text{where } \nu_1, \nu_2 > 0 . \quad (2)$$

The F -distribution is also called “Snedecor’s F -distribution” or “Fisher–Snedecor distribution”, after Ronald A. Fisher and George W. Snedecor.

Sources:

- Wikipedia (2021): “F-distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-04-21; URL: <https://en.wikipedia.org/wiki/F-distribution#Characterization>.

3.8.2 Probability density function

Theorem: Let F be a random variable (\rightarrow I/1.2.2) following an F -distribution (\rightarrow II/3.8.1):

$$F \sim F(u, v) . \quad (1)$$

Then, the probability density function (\rightarrow I/1.7.1) of F is

$$f_F(f) = \frac{\Gamma\left(\frac{u+v}{2}\right)}{\Gamma\left(\frac{u}{2}\right) \cdot \Gamma\left(\frac{v}{2}\right)} \cdot \left(\frac{u}{v}\right)^{\frac{u}{2}} \cdot f^{\frac{u}{2}-1} \cdot \left(\frac{u}{v}f + 1\right)^{-\frac{u+v}{2}} . \quad (2)$$

Proof: An F -distributed random variable (\rightarrow II/3.8.1) is defined as the ratio of two chi-squared random variables (\rightarrow II/3.7.1), divided by their degrees of freedom (\rightarrow I/1.5.12)

$$X \sim \chi^2(u), Y \sim \chi^2(v) \quad \Rightarrow \quad F = \frac{X/u}{Y/v} \sim F(u, v) \quad (3)$$

where X and Y are independent of each other (\rightarrow I/1.3.6).

The probability density function of the chi-squared distribution (\rightarrow II/3.7.4) is

$$f_X(x) = \frac{1}{\Gamma\left(\frac{u}{2}\right) \cdot 2^{u/2}} \cdot x^{\frac{u}{2}-1} \cdot e^{-\frac{x}{2}} . \quad (4)$$

Define the random variables F and W as functions of X and Y

$$\begin{aligned} F &= \frac{X/u}{Y/v} \\ W &= Y , \end{aligned} \quad (5)$$

such that the inverse functions X and Y in terms of F and W are

$$\begin{aligned} X &= \frac{u}{v}FW \\ Y &= W. \end{aligned} \quad (6)$$

This implies the following Jacobian matrix and determinant:

$$\begin{aligned} J &= \begin{bmatrix} \frac{dX}{dF} & \frac{dX}{dW} \\ \frac{dY}{dF} & \frac{dY}{dW} \end{bmatrix} = \begin{bmatrix} \frac{u}{v}W & \frac{u}{v}F \\ 0 & 1 \end{bmatrix} \\ |J| &= \frac{u}{v}W. \end{aligned} \quad (7)$$

Because X and Y are independent (\rightarrow I/1.3.6), the joint density (\rightarrow I/1.5.2) of X and Y is equal to the product (\rightarrow I/1.3.9) of the marginal densities (\rightarrow I/1.5.3):

$$f_{X,Y}(x, y) = f_X(x) \cdot f_Y(y). \quad (8)$$

With the probability density function of an invertible function (\rightarrow I/1.7.5), the joint density (\rightarrow I/1.5.2) of F and W can be derived as:

$$f_{F,W}(f, w) = f_{X,Y}(x, y) \cdot |J|. \quad (9)$$

Substituting (6) into (4), and then with (7) into (9), we get:

$$\begin{aligned} f_{F,W}(f, w) &= f_X\left(\frac{u}{v}fw\right) \cdot f_Y(w) \cdot |J| \\ &= \frac{1}{\Gamma\left(\frac{u}{2}\right) \cdot 2^{u/2}} \cdot \left(\frac{u}{v}fw\right)^{\frac{u}{2}-1} \cdot e^{-\frac{1}{2}\left(\frac{u}{v}fw\right)} \cdot \frac{1}{\Gamma\left(\frac{v}{2}\right) \cdot 2^{v/2}} \cdot w^{\frac{v}{2}-1} \cdot e^{-\frac{w}{2}} \cdot \frac{u}{v}w \\ &= \frac{\left(\frac{u}{v}\right)^{\frac{u}{2}} \cdot f^{\frac{u}{2}-1}}{\Gamma\left(\frac{u}{2}\right) \cdot \Gamma\left(\frac{v}{2}\right) \cdot 2^{(u+v)/2}} \cdot w^{\frac{u+v}{2}-1} \cdot e^{-\frac{w}{2}\left(\frac{u}{v}f+1\right)}. \end{aligned} \quad (10)$$

The marginal density (\rightarrow I/1.5.3) of F can now be obtained by integrating out (\rightarrow I/1.3.3) W :

$$\begin{aligned} f_F(f) &= \int_0^\infty f_{F,W}(f, w) dw \\ &= \frac{\left(\frac{u}{v}\right)^{\frac{u}{2}} \cdot f^{\frac{u}{2}-1}}{\Gamma\left(\frac{u}{2}\right) \cdot \Gamma\left(\frac{v}{2}\right) \cdot 2^{(u+v)/2}} \cdot \int_0^\infty w^{\frac{u+v}{2}-1} \cdot \exp\left[-\frac{1}{2}\left(\frac{u}{v}f+1\right)w\right] dw \\ &= \frac{\left(\frac{u}{v}\right)^{\frac{u}{2}} \cdot f^{\frac{u}{2}-1}}{\Gamma\left(\frac{u}{2}\right) \cdot \Gamma\left(\frac{v}{2}\right) \cdot 2^{(u+v)/2}} \cdot \frac{\Gamma\left(\frac{u+v}{2}\right)}{\left[\frac{1}{2}\left(\frac{u}{v}f+1\right)\right]^{(u+v)/2}} \cdot \int_0^\infty \frac{\left[\frac{1}{2}\left(\frac{u}{v}f+1\right)\right]^{(u+v)/2}}{\Gamma\left(\frac{u+v}{2}\right)} \cdot w^{\frac{u+v}{2}-1} \cdot \exp\left[-\frac{1}{2}\left(\frac{u}{v}f+1\right)w\right] dw \end{aligned} \quad (11)$$

At this point, we can recognize that the integrand is equal to the probability density function of a gamma distribution (\rightarrow II/3.4.7) with

$$a = \frac{u+v}{2} \quad \text{and} \quad b = \frac{1}{2}\left(\frac{u}{v}f+1\right), \quad (12)$$

and because a probability density function integrates to one (\rightarrow I/1.7.1), we finally have:

$$\begin{aligned} f_F(f) &= \frac{\left(\frac{u}{v}\right)^{\frac{u}{2}} \cdot f^{\frac{u}{2}-1}}{\Gamma\left(\frac{u}{2}\right) \cdot \Gamma\left(\frac{v}{2}\right) \cdot 2^{(u+v)/2}} \cdot \frac{\Gamma\left(\frac{u+v}{2}\right)}{\left[\frac{1}{2}\left(\frac{u}{v}f + 1\right)\right]^{(u+v)/2}} \\ &= \frac{\Gamma\left(\frac{u+v}{2}\right)}{\Gamma\left(\frac{u}{2}\right) \cdot \Gamma\left(\frac{v}{2}\right)} \cdot \left(\frac{u}{v}\right)^{\frac{u}{2}} \cdot f^{\frac{u}{2}-1} \cdot \left(\frac{u}{v}f + 1\right)^{-\frac{u+v}{2}}. \end{aligned} \quad (13)$$

■

Sources:

- statisticsmatt (2018): “Statistical Distributions: Derive the F Distribution”; in: *YouTube*, retrieved on 2021-10-11; URL: <https://www.youtube.com/watch?v=AmHiOKYmHkI>.

3.9 Beta distribution

3.9.1 Definition

Definition: Let X be a random variable (\rightarrow I/1.2.2). Then, X is said to follow a beta distribution with shape parameters α and β

$$X \sim \text{Bet}(\alpha, \beta), \quad (1)$$

if and only if its probability density function (\rightarrow I/1.7.1) is given by

$$\text{Bet}(x; \alpha, \beta) = \frac{1}{B(\alpha, \beta)} x^{\alpha-1} (1-x)^{\beta-1} \quad (2)$$

where $\alpha > 0$ and $\beta > 0$, $B(x, y)$ is the beta function and the density is zero, if $x \notin [0, 1]$.

Sources:

- Wikipedia (2020): “Beta distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-05-10; URL: https://en.wikipedia.org/wiki/Beta_distribution#Definitions.

3.9.2 Special case of Dirichlet distribution

Theorem: The beta distribution (\rightarrow II/3.9.1) with shape parameters α and β is a special case of the Dirichlet distribution (\rightarrow II/2.2.1) with concentration parameters $\alpha_1 = \alpha$ and $\alpha_2 = \beta$:

$$X \sim \text{Dir}([\alpha, \beta]) \quad \Rightarrow \quad X \sim \text{Bet}(\alpha, \beta). \quad (1)$$

Proof: The probability density function of the Dirichlet distribution (\rightarrow II/4.5.2), where x is a $1 \times k$ vector with $x_i \in [0, 1]$ for $i = 1, \dots, k$, is as follows:

$$\text{Dir}(x; [\alpha_1, \dots, \alpha_k]) = \frac{\Gamma\left(\sum_{i=1}^k \alpha_i\right)}{\prod_{i=1}^k \Gamma(\alpha_i)} \prod_{i=1}^k x_i^{\alpha_i-1}. \quad (2)$$

If we let $k = 2$, $\alpha_1 = \alpha$ and $\alpha_2 = \beta$, we obtain

$$\text{Dir}(x; [\alpha, \beta]) = \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha) \Gamma(\beta)} x_1^{\alpha-1} x_2^{\beta-1} . \quad (3)$$

Applying the beta function $B(x, y) = \Gamma(x)\Gamma(y)/\Gamma(x+y)$, we have

$$\text{Dir}(x; [\alpha, \beta]) = \frac{1}{B(\alpha, \beta)} x_1^{\alpha-1} x_2^{\beta-1} . \quad (4)$$

Recognizing that $\sum_{i=1}^k x_i = 1$, such that $x_2 = 1 - x_1$, we get

$$\text{Dir}(x; [\alpha, \beta]) = \frac{1}{B(\alpha, \beta)} x_1^{\alpha-1} (1 - x_1)^{\beta-1} \quad (5)$$

which is equivalent to the probability density function of the beta distribution (\rightarrow II/3.9.5). ■

3.9.3 Relationship to chi-squared distribution

Theorem: Let X and Y be independent (\rightarrow I/1.3.6) random variables (\rightarrow I/1.2.2) following chi-squared distributions (\rightarrow II/3.7.1):

$$X \sim \chi^2(m) \quad \text{and} \quad Y \sim \chi^2(n) . \quad (1)$$

Then, the quantity $X/(X+Y)$ follows a beta distribution (\rightarrow II/3.9.1):

$$\frac{X}{X+Y} \sim \text{Bet} \left(\frac{m}{2}, \frac{n}{2} \right) . \quad (2)$$

Proof: The probability density function of the chi-squared distribution (\rightarrow II/3.7.4) is

$$X \sim \chi^2(u) \quad \Rightarrow \quad f_X(x) = \frac{1}{\Gamma\left(\frac{u}{2}\right) \cdot 2^{u/2}} \cdot x^{\frac{u}{2}-1} \cdot e^{-\frac{x}{2}} . \quad (3)$$

Define the random variables Z and W as functions of X and Y

$$\begin{aligned} Z &= \frac{X}{X+Y} \\ W &= Y , \end{aligned} \quad (4)$$

such that the inverse functions X and Y in terms of Z and W are

$$\begin{aligned} X &= \frac{ZW}{1-Z} \\ Y &= W . \end{aligned} \quad (5)$$

This implies the following Jacobian matrix and determinant:

$$\begin{aligned} J &= \begin{bmatrix} \frac{dX}{dZ} & \frac{dX}{dW} \\ \frac{dY}{dZ} & \frac{dY}{dW} \end{bmatrix} = \begin{bmatrix} \frac{W}{(1-Z)^2} & \frac{Z}{1-Z} \\ 0 & 1 \end{bmatrix} \\ |J| &= \frac{W}{(1-Z)^2} . \end{aligned} \quad (6)$$

Because X and Y are independent (\rightarrow I/1.3.6), the joint density (\rightarrow I/1.5.2) of X and Y is equal to the product (\rightarrow I/1.3.9) of the marginal densities (\rightarrow I/1.5.3):

$$f_{X,Y}(x, y) = f_X(x) \cdot f_Y(y) . \quad (7)$$

With the probability density function of an invertible function (\rightarrow I/1.7.5), the joint density (\rightarrow I/1.5.2) of Z and W can be derived as:

$$f_{Z,W}(z, w) = f_{X,Y}(x, y) \cdot |J| . \quad (8)$$

Substituting (5) into (3), and then with (6) into (8), we get:

$$\begin{aligned} f_{Z,W}(z, w) &= f_X\left(\frac{zw}{1-z}\right) \cdot f_Y(w) \cdot |J| \\ &= \frac{1}{\Gamma\left(\frac{m}{2}\right) \cdot 2^{m/2}} \cdot \left(\frac{zw}{1-z}\right)^{\frac{m}{2}-1} \cdot e^{-\frac{1}{2}\left(\frac{zw}{1-z}\right)} \cdot \frac{1}{\Gamma\left(\frac{n}{2}\right) \cdot 2^{n/2}} \cdot w^{\frac{n}{2}-1} \cdot e^{-\frac{w}{2}} \cdot \frac{w}{(1-z)^2} \\ &= \frac{1}{\Gamma\left(\frac{m}{2}\right) \Gamma\left(\frac{n}{2}\right) \cdot 2^{m/2} 2^{n/2}} \cdot \left(\frac{z}{1-z}\right)^{\frac{m}{2}-1} \left(\frac{1}{(1-z)}\right)^2 \cdot w^{\frac{m}{2}+\frac{n}{2}-1} e^{-\frac{1}{2}\left(\frac{zw}{1-z} + \frac{w(1-z)}{1-z}\right)} \\ &= \frac{1}{\Gamma\left(\frac{m}{2}\right) \Gamma\left(\frac{n}{2}\right) \cdot 2^{(m+n)/2}} \cdot z^{\frac{m}{2}-1} \cdot (1-z)^{-\frac{m}{2}-1} \cdot w^{\frac{m+n}{2}-1} \cdot e^{-\frac{1}{2}\left(\frac{w}{1-z}\right)} . \end{aligned} \quad (9)$$

The marginal density (\rightarrow I/1.5.3) of Z can now be obtained by integrating out (\rightarrow I/1.3.3) W :

$$\begin{aligned} f_Z(z) &= \int_0^\infty f_{Z,W}(z, w) dw \\ &= \frac{1}{\Gamma\left(\frac{m}{2}\right) \Gamma\left(\frac{n}{2}\right) \cdot 2^{(m+n)/2}} \cdot z^{\frac{m}{2}-1} \cdot (1-z)^{-\frac{m}{2}-1} \cdot \int_0^\infty w^{\frac{m+n}{2}-1} \cdot e^{-\frac{1}{2}\left(\frac{w}{1-z}\right)} dw \\ &= \frac{1}{\Gamma\left(\frac{m}{2}\right) \Gamma\left(\frac{n}{2}\right) \cdot 2^{(m+n)/2}} \cdot z^{\frac{m}{2}-1} \cdot (1-z)^{-\frac{m}{2}-1} \cdot \frac{\Gamma\left(\frac{m+n}{2}\right)}{\left(\frac{1}{2(1-z)}\right)^{\frac{m+n}{2}}} \\ &\quad \int_0^\infty \frac{\left(\frac{1}{2(1-z)}\right)^{\frac{m+n}{2}}}{\Gamma\left(\frac{m+n}{2}\right)} \cdot w^{\frac{m+n}{2}-1} \cdot e^{-\frac{1}{2(1-z)}w} dw . \end{aligned} \quad (10)$$

At this point, we can recognize that the integrand is equal to the probability density function of a gamma distribution (\rightarrow II/3.4.7) with

$$a = \frac{m+n}{2} \quad \text{and} \quad b = \frac{1}{2(1-z)} , \quad (11)$$

and because a probability density function integrates to one (\rightarrow I/1.7.1), we have:

$$\begin{aligned}
f_Z(z) &= \frac{1}{\Gamma\left(\frac{m}{2}\right) \Gamma\left(\frac{n}{2}\right) \cdot 2^{(m+n)/2}} \cdot z^{\frac{m}{2}-1} \cdot (1-z)^{-\frac{m}{2}-1} \cdot \frac{\Gamma\left(\frac{m+n}{2}\right)}{\left(\frac{1}{2(1-z)}\right)^{\frac{m+n}{2}}} \\
&= \frac{\Gamma\left(\frac{m+n}{2}\right) \cdot 2^{(m+n)/2}}{\Gamma\left(\frac{m}{2}\right) \Gamma\left(\frac{n}{2}\right) \cdot 2^{(m+n)/2}} \cdot z^{\frac{m}{2}-1} \cdot (1-z)^{-\frac{m}{2}+\frac{m+n}{2}-1} \\
&= \frac{\Gamma\left(\frac{m+n}{2}\right)}{\Gamma\left(\frac{m}{2}\right) \Gamma\left(\frac{n}{2}\right)} \cdot z^{\frac{m}{2}-1} \cdot (1-z)^{\frac{n}{2}-1}.
\end{aligned} \tag{12}$$

With the definition of the beta function (\rightarrow II/3.9.8), this becomes

$$f_Z(z) = \frac{1}{B\left(\frac{m}{2}, \frac{n}{2}\right)} \cdot z^{\frac{m}{2}-1} \cdot (1-z)^{\frac{n}{2}-1} \tag{13}$$

which is the probability density function of the beta distribution (\rightarrow II/3.9.5) with parameters

$$\alpha = \frac{m}{2} \quad \text{and} \quad \beta = \frac{n}{2}, \tag{14}$$

such that

$$Z \sim \text{Bet}\left(\frac{m}{2}, \frac{n}{2}\right). \tag{15}$$

Sources:

- Probability Fact (2021): “If $X \sim \text{chisq}(m)$ and $Y \sim \text{chisq}(n)$ are independent”; in: *Twitter*, retrieved on 2022-10-17; URL: <https://twitter.com/ProbFact/status/1450492787854647300>.

3.9.4 Relationship to F-distribution

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following an F-distribution (\rightarrow II/3.8.1):

$$X \sim F(d_1, d_2). \tag{1}$$

Then, the quantity

$$Y = \frac{d_1 X / d_2}{1 + d_1 X / d_2} = \frac{d_1 X}{d_2 + d_1 X} \tag{2}$$

follows a beta distribution (\rightarrow II/3.9.1):

$$Y \sim \text{Bet}\left(\frac{d_1}{2}, \frac{d_2}{2}\right). \tag{3}$$

Proof: We denote $Y = g(X)$. The first derivative of the g is:

$$\begin{aligned}
\frac{dg(x)}{dx} &= \frac{d}{dx} \left(\frac{d_1 x}{d_2 + d_1 x} \right) \\
&= \frac{d_1 d_2 + d_1^2 x - d_1^2 x}{(d_2 + d_1 x)^2} \\
&= \frac{d_1 d_2}{(d_2 + d_1 x)^2}.
\end{aligned} \tag{4}$$

This derivative is positive for all $x \geq 0$, such that Y is a strictly increasing function of X . This means we can derive the distribution of Y by applying the probability density function of a strictly increasing function of a continuous random variable (\rightarrow I/1.7.3):

$$f_Y(y) = \begin{cases} f_X(g^{-1}(y)) \frac{dg^{-1}(y)}{dy}, & \text{if } y \in \mathcal{Y} \\ 0, & \text{if } y \notin \mathcal{Y}. \end{cases} \quad (5)$$

where $\mathcal{Y} = \{y = g(x) : x \in \mathcal{X}\}$. Because $g : \mathbb{R}_{\geq 0} \rightarrow [0, 1]$, we have $\mathcal{X} = \mathbb{R}_{\geq 0}$ and $\mathcal{Y} = [0, 1]$, such that

$$f_Y(y) = 0 \quad \text{for } y \notin [0, 1]. \quad (6)$$

The inverse function of g is:

$$\begin{aligned} g(x) = y &= \frac{d_1 x}{d_2 + d_1 x} \\ d_2 y + d_1 x y &= d_1 x \\ d_1 x - d_1 x y &= d_2 y \\ x(d_1 - d_1 y) &= d_2 y \\ x &= \frac{d_2 y}{d_1 - d_1 y} = g^{-1}(y). \end{aligned} \quad (7)$$

The derivative of g^{-1} with respect to y is:

$$\begin{aligned} \frac{dg^{-1}(y)}{dy} &= \frac{d}{dy} \left(\frac{d_2 y}{d_1 - d_1 y} \right) \\ &= \frac{d_1 d_2 + d_1 d_2 y - (-d_1 d_2 y)}{(d_1 - d_1 y)^2} \\ &= \frac{d_1 d_2}{d_1^2 - 2d_1^2 y + d_1^2 y^2} \\ &= \frac{d_2}{d_1 - 2d_1 y + d_1 y^2} \\ &= \frac{d_2}{d_1(1 - 2y + y^2)} \\ &= \frac{d_2}{d_1} \cdot \frac{1}{(1 - y)^2}. \end{aligned} \quad (8)$$

The probability density function of the F-distribution (\rightarrow II/3.8.2) with degrees of freedom (\rightarrow I/1.5.12) d_1 and d_2 is:

$$f_X(x) = \frac{\Gamma\left(\frac{d_1 + d_2}{2}\right)}{\Gamma\left(\frac{d_1}{2}\right) \cdot \Gamma\left(\frac{d_2}{2}\right)} \cdot \left(\frac{d_1}{d_2}\right)^{\frac{d_1}{2}} \cdot x^{\frac{d_1}{2} - 1} \cdot \left(\frac{d_1}{d_2} x + 1\right)^{-\frac{d_2 + d_2}{2}}. \quad (9)$$

With that, we have everything that we need to derive the distribution of Y for $y \in \mathcal{Y}$. Combining (5), (9), (7) and (8), $f_Y(y)$ for $y \in [0, 1]$ becomes:

$$\begin{aligned}
f_Y(y) &= f_X(g^{-1}(y)) \frac{dg^{-1}(y)}{dy} \\
&= \frac{\Gamma\left(\frac{d_1+d_2}{2}\right)}{\Gamma\left(\frac{d_1}{2}\right) \cdot \Gamma\left(\frac{d_2}{2}\right)} \cdot \left(\frac{d_1}{d_2}\right)^{\frac{d_1}{2}} \cdot \left(\frac{d_2 y}{d_1 - d_1 y}\right)^{\frac{d_1}{2}-1} \cdot \left(\frac{d_1}{d_2} \left(\frac{d_2 y}{d_1 - d_1 y}\right) + 1\right)^{-\frac{d_1+d_2}{2}} \cdot \\
&\quad \left(\frac{d_2}{d_1} \cdot \frac{1}{(1-y)^2}\right) \\
&= \frac{1}{B\left(\frac{d_1}{2}, \frac{d_2}{2}\right)} \cdot \left(\frac{d_1}{d_2}\right)^{\frac{d_1}{2}} \cdot d_2^{\frac{d_1}{2}-1} \cdot y^{\frac{d_1}{2}-1} \cdot d_1^{-\left(\frac{d_1}{2}-1\right)} \cdot (1-y)^{-\left(\frac{d_1}{2}-1\right)} \cdot \\
&\quad \left(\frac{d_1}{d_2} \left(\frac{d_2 y}{d_1 - d_1 y}\right) + 1\right)^{-\frac{d_1+d_2}{2}} \cdot \left(\frac{d_2}{d_1} \cdot \frac{1}{(1-y)^2}\right) \\
&= \frac{1}{B\left(\frac{d_1}{2}, \frac{d_2}{2}\right)} \cdot \left(\frac{d_1}{d_2}\right) \cdot \left(\frac{d_2}{d_1}\right) \cdot y^{\frac{d_1}{2}-1} \cdot (1-y)^{-\frac{d_1}{2}+1} \cdot (1-y)^{-2} \cdot \\
&\quad \left(\frac{d_1 d_2 y}{d_2(d_1 - d_1 y)} + \frac{d_2(d_1 - d_1 y)}{d_2(d_1 - d_1 y)}\right)^{-\frac{d_1+d_2}{2}} \\
&= \frac{1}{B\left(\frac{d_1}{2}, \frac{d_2}{2}\right)} \cdot y^{\frac{d_1}{2}-1} \cdot (1-y)^{-\frac{d_1}{2}-1} \cdot \left(\frac{d_1 d_2}{d_2(d_1 - d_1 y)}\right)^{-\frac{d_1+d_2}{2}} \\
&= \frac{1}{B\left(\frac{d_1}{2}, \frac{d_2}{2}\right)} \cdot y^{\frac{d_1}{2}-1} \cdot (1-y)^{-\frac{d_1}{2}-1} \cdot \left(\frac{1}{1-y}\right)^{-\frac{d_1+d_2}{2}} \\
&= \frac{1}{B\left(\frac{d_1}{2}, \frac{d_2}{2}\right)} \cdot y^{\frac{d_1}{2}-1} \cdot (1-y)^{-\frac{d_1}{2}-1} \cdot (1-y)^{\frac{d_1+d_2}{2}} \\
&= \frac{1}{B\left(\frac{d_1}{2}, \frac{d_2}{2}\right)} \cdot y^{\frac{d_1}{2}-1} \cdot (1-y)^{\frac{d_2}{2}-1} .
\end{aligned} \tag{10}$$

This is the probability density function of the beta distribution (\rightarrow II/3.9.5) with parameters

$$\alpha = \frac{d_1}{2} \quad \text{and} \quad \beta = \frac{d_2}{2} , \tag{11}$$

such that

$$Y \sim \text{Bet}\left(\frac{d_1}{2}, \frac{d_2}{2}\right) . \tag{12}$$

■

Sources:

- Wikipedia (2025): “F-distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2025-04-04; URL: https://en.wikipedia.org/wiki/F-distribution#Related_distributions.
- Wikipedia (2025): “Beta distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2025-04-04; URL: https://en.wikipedia.org/wiki/Beta_distribution#Related_distributions.

3.9.5 Probability density function

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a beta distribution (\rightarrow II/3.9.1):

$$X \sim \text{Bet}(\alpha, \beta) . \quad (1)$$

Then, the probability density function (\rightarrow I/1.7.1) of X is

$$f_X(x) = \frac{1}{\text{B}(\alpha, \beta)} x^{\alpha-1} (1-x)^{\beta-1} . \quad (2)$$

Proof: This follows directly from the definition of the beta distribution (\rightarrow II/3.9.1). ■

3.9.6 Moment-generating function

Theorem: Let X be a positive random variable (\rightarrow I/1.2.2) following a beta distribution (\rightarrow II/3.4.1):

$$X \sim \text{Bet}(\alpha, \beta) . \quad (1)$$

Then, the moment-generating function (\rightarrow I/1.9.1) of X is

$$M_X(t) = 1 + \sum_{n=1}^{\infty} \left(\prod_{m=0}^{n-1} \frac{\alpha + m}{\alpha + \beta + m} \right) \frac{t^n}{n!} . \quad (2)$$

Proof: The probability density function of the beta distribution (\rightarrow II/3.9.5) is

$$f_X(x) = \frac{1}{\text{B}(\alpha, \beta)} x^{\alpha-1} (1-x)^{\beta-1} \quad (3)$$

and the moment-generating function (\rightarrow I/1.9.1) is defined as

$$M_X(t) = \text{E} [e^{tX}] . \quad (4)$$

Using the expected value for continuous random variables (\rightarrow I/1.12.1), the moment-generating function of X therefore is

$$\begin{aligned} M_X(t) &= \int_0^1 \exp[tx] \cdot \frac{1}{\text{B}(\alpha, \beta)} x^{\alpha-1} (1-x)^{\beta-1} dx \\ &= \frac{1}{\text{B}(\alpha, \beta)} \int_0^1 e^{tx} x^{\alpha-1} (1-x)^{\beta-1} dx . \end{aligned} \quad (5)$$

With the relationship between beta function and gamma function

$$\text{B}(\alpha, \beta) = \frac{\Gamma(\alpha) \Gamma(\beta)}{\Gamma(\alpha + \beta)} \quad (6)$$

and the integral representation of the confluent hypergeometric function (Kummer's function of the first kind)

$${}_1F_1(a, b, z) = \frac{\Gamma(b)}{\Gamma(a) \Gamma(b-a)} \int_0^1 e^{zu} u^{a-1} (1-u)^{(b-a)-1} du , \quad (7)$$

the moment-generating function can be written as

$$M_X(t) = {}_1F_1(\alpha, \alpha + \beta, t) . \quad (8)$$

Note that the series equation for the confluent hypergeometric function (Kummer's function of the first kind) is

$${}_1F_1(a, b, z) = \sum_{n=0}^{\infty} \frac{a^{\bar{n}}}{b^{\bar{n}}} \frac{z^n}{n!} \quad (9)$$

where $m^{\bar{n}}$ is the rising factorial

$$m^{\bar{n}} = \prod_{i=0}^{n-1} (m + i) , \quad (10)$$

so that the moment-generating function can be written as

$$M_X(t) = \sum_{n=0}^{\infty} \frac{\alpha^{\bar{n}}}{(\alpha + \beta)^{\bar{n}}} \frac{t^n}{n!} . \quad (11)$$

Applying the rising factorial equation (10) and using $m^{\bar{0}} = x^0 = 0! = 1$, we finally have:

$$M_X(t) = 1 + \sum_{n=1}^{\infty} \left(\prod_{m=0}^{n-1} \frac{\alpha + m}{\alpha + \beta + m} \right) \frac{t^n}{n!} . \quad (12)$$

■

Sources:

- Wikipedia (2020): “Beta distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-11-25; URL: https://en.wikipedia.org/wiki/Beta_distribution#Moment_generating_function.
- Wikipedia (2020): “Confluent hypergeometric function”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-11-25; URL: https://en.wikipedia.org/wiki/Confluent_hypergeometric_function#Kummer's_equation.

3.9.7 Cumulative distribution function

Theorem: Let X be a positive random variable (\rightarrow I/1.2.2) following a beta distribution (\rightarrow II/3.4.1):

$$X \sim \text{Bet}(\alpha, \beta) . \quad (1)$$

Then, the cumulative distribution function (\rightarrow I/1.8.1) of X is

$$F_X(x) = \frac{B(x; \alpha, \beta)}{B(\alpha, \beta)} \quad (2)$$

where $B(a, b)$ is the beta function and $B(x; a, b)$ is the incomplete gamma function.

Proof: The probability density function of the beta distribution (\rightarrow II/3.9.5) is:

$$f_X(x) = \frac{1}{B(\alpha, \beta)} x^{\alpha-1} (1-x)^{\beta-1} . \quad (3)$$

Thus, the cumulative distribution function (\rightarrow I/1.8.1) is:

$$\begin{aligned} F_X(x) &= \int_0^x \text{Bet}(z; \alpha, \beta) \, dz \\ &= \int_0^x \frac{1}{B(\alpha, \beta)} z^{\alpha-1} (1-z)^{\beta-1} \, dz \\ &= \frac{1}{B(\alpha, \beta)} \int_0^x z^{\alpha-1} (1-z)^{\beta-1} \, dz . \end{aligned} \quad (4)$$

With the definition of the incomplete beta function

$$B(x; a, b) = \int_0^x t^{a-1} (1-t)^{b-1} \, dt , \quad (5)$$

we arrive at the final result given by equation (2):

$$F_X(x) = \frac{B(x; \alpha, \beta)}{B(\alpha, \beta)} . \quad (6)$$

■

Sources:

- Wikipedia (2020): “Beta distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-11-19; URL: https://en.wikipedia.org/wiki/Beta_distribution#Cumulative_distribution_function.
- Wikipedia (2020): “Beta function”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-11-19; URL: https://en.wikipedia.org/wiki/Beta_function#Incomplete_beta_function.

3.9.8 Mean

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a beta distribution (\rightarrow II/3.9.1):

$$X \sim \text{Bet}(\alpha, \beta) . \quad (1)$$

Then, the mean or expected value (\rightarrow I/1.12.1) of X is

$$E(X) = \frac{\alpha}{\alpha + \beta} . \quad (2)$$

Proof: The expected value (\rightarrow I/1.12.1) is the probability-weighted average over all possible values:

$$E(X) = \int_{\mathcal{X}} x \cdot f_X(x) \, dx . \quad (3)$$

The probability density function of the beta distribution (\rightarrow II/3.9.5) is

$$f_X(x) = \frac{1}{B(\alpha, \beta)} x^{\alpha-1} (1-x)^{\beta-1}, \quad 0 \leq x \leq 1 \quad (4)$$

where the beta function is given by a ratio gamma functions:

$$B(\alpha, \beta) = \frac{\Gamma(\alpha) \cdot \Gamma(\beta)}{\Gamma(\alpha + \beta)} . \quad (5)$$

Combining (3), (4) and (5), we have:

$$\begin{aligned}
E(X) &= \int_0^1 x \cdot \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha) \cdot \Gamma(\beta)} x^{\alpha-1} (1-x)^{\beta-1} dx \\
&= \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)} \cdot \frac{\Gamma(\alpha + 1)}{\Gamma(\alpha + 1 + \beta)} \int_0^1 \frac{\Gamma(\alpha + 1 + \beta)}{\Gamma(\alpha + 1) \cdot \Gamma(\beta)} x^{(\alpha+1)-1} (1-x)^{\beta-1} dx .
\end{aligned} \tag{6}$$

Employing the relation $\Gamma(x + 1) = \Gamma(x) \cdot x$, we have

$$\begin{aligned}
E(X) &= \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)} \cdot \frac{\alpha \cdot \Gamma(\alpha)}{(\alpha + \beta) \cdot \Gamma(\alpha + \beta)} \int_0^1 \frac{\Gamma(\alpha + 1 + \beta)}{\Gamma(\alpha + 1) \cdot \Gamma(\beta)} x^{(\alpha+1)-1} (1-x)^{\beta-1} dx \\
&= \frac{\alpha}{\alpha + \beta} \int_0^1 \frac{\Gamma(\alpha + 1 + \beta)}{\Gamma(\alpha + 1) \cdot \Gamma(\beta)} x^{(\alpha+1)-1} (1-x)^{\beta-1} dx
\end{aligned} \tag{7}$$

and again using the density of the beta distribution (\rightarrow II/3.9.5), we get

$$\begin{aligned}
E(X) &= \frac{\alpha}{\alpha + \beta} \int_0^1 \text{Bet}(x; \alpha + 1, \beta) dx \\
&= \frac{\alpha}{\alpha + \beta} .
\end{aligned} \tag{8}$$

■

Sources:

- Boer Commander (2020): “Beta Distribution Mean and Variance Proof”; in: *YouTube*, retrieved on 2021-04-29; URL: <https://www.youtube.com/watch?v=3OgCcnpZtZ8>.

3.9.9 Median

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a beta distribution (\rightarrow II/3.9.1):

$$X \sim \text{Bet}(\alpha, \beta) . \tag{1}$$

Then, the median (\rightarrow I/1.18.1) of X is

$$\text{median}(X) = B_{\alpha, \beta}^{-1} \left(\frac{B(\alpha, \beta)}{2} \right) = I_{1/2}^{-1}(\alpha, \beta) \tag{2}$$

where $B(a, b)$ is the beta function, $B_{a, b}^{-1}(y)$ is the inverse function of the incomplete beta function $B(x; a, b)$ and $I_y^{-1}(a, b)$ is the inverse function of the regularized incomplete beta function.

Proof: The median (\rightarrow I/1.18.1) is the value at which the cumulative distribution function (\rightarrow I/1.8.1) is 1/2:

$$F_X(\text{median}(X)) = \frac{1}{2} . \tag{3}$$

The cumulative distribution function of the beta distribution (\rightarrow II/3.9.7) is

$$F_X(x) = \frac{B(x; \alpha, \beta)}{B(\alpha, \beta)} \tag{4}$$

where the incomplete beta function $B(x; a, b)$ is given by

$$B(x; a, b) = \int_0^x t^{a-1} (1-t)^{b-1} dt . \quad (5)$$

Thus, the inverse CDF, i.e. the quantile function (\rightarrow I/1.11.1), is

$$x = B_{\alpha, \beta}^{-1}(p B(\alpha, \beta)) \quad (6)$$

where $B_{a,b}^{-1}(y)$ is the inverse function of $B(x; a, b)$. Setting $p = 1/2$, we obtain:

$$\text{median}(X) = B_{\alpha, \beta}^{-1} \left(\frac{B(\alpha, \beta)}{2} \right) . \quad (7)$$

Alternatively, the cumulative distribution function may be written as

$$F_X(x) = I_x(a, b) \quad (8)$$

using the regularized incomplete beta function

$$I_x(a, b) = \frac{B(x; \alpha, \beta)}{B(\alpha, \beta)} \quad (9)$$

in which case the inverse CDF is

$$x = I_p^{-1}(a, b) , \quad (10)$$

such that the median becomes

$$\text{median}(X) = I_{1/2}^{-1}(\alpha, \beta) . \quad (11)$$

■

Sources:

- Wikipedia (2025): “Beta distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2025-10-24; URL: https://en.wikipedia.org/wiki/Beta_distribution#Median.

3.9.10 Mode

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a beta distribution (\rightarrow II/3.9.1):

$$X \sim \text{Bet}(\alpha, \beta) . \quad (1)$$

Then, the mode (\rightarrow I/1.18.3) of X is

$$\text{mode}(X) \in \begin{cases} \{0, 1\} , & \text{if } \alpha < 1 \text{ and } \beta < 1 \\ [0, 1] , & \text{if } \alpha = 1 \text{ and } \beta = 1 \end{cases} \quad (2)$$

and

$$\text{mode}(X) = \begin{cases} 0 \text{ or } 1 , & \text{if } \alpha < 1 \text{ or } \beta < 1 \text{ (but not } \alpha < 1 \text{ and } \beta < 1) \\ \frac{\alpha-1}{\alpha+\beta-2} , & \text{if } \alpha \geq 1 \text{ and } \beta \geq 1 \text{ (but not } \alpha = 1 \text{ and } \beta = 1) . \end{cases} \quad (3)$$

Proof: The mode (\rightarrow I/1.18.3) is the value which maximizes the probability density function (\rightarrow I/1.7.1):

$$\text{mode}(X) = \arg \max_x f_X(x) . \quad (4)$$

The probability density function of the beta distribution (\rightarrow II/3.9.5) is:

$$f_X(x) = \frac{1}{B(\alpha, \beta)} x^{\alpha-1} (1-x)^{\beta-1} . \quad (5)$$

1) If $\alpha < 1$, then 0 is the mode, since

$$\lim_{\substack{x \rightarrow 0 \\ \alpha < 1}} f_X(x) = \infty , \quad \text{because} \quad \lim_{x \rightarrow 0} x^{\alpha-1} = \infty \quad \text{for} \quad \alpha < 1 , \quad (6)$$

and if $\beta < 1$, then 1 is the mode, since

$$\lim_{\substack{x \rightarrow 1 \\ \beta < 1}} f_X(x) = \infty , \quad \text{because} \quad \lim_{x \rightarrow 1} (1-x)^{\beta-1} = \infty \quad \text{for} \quad \beta < 1 . \quad (7)$$

2) If both $\alpha < 1$ and $\beta < 1$, then

$$\lim_{x \rightarrow 0} f_X(x) = \infty \quad \text{and} \quad \lim_{x \rightarrow 1} f_X(x) = \infty , \quad (8)$$

so any value from the set $\{0, 1\}$ may be considered the mode.

3) If both $\alpha = 1$ and $\beta = 1$, then

$$\begin{aligned} f_X(x) &= \frac{1}{B(1, 1)} x^{1-1} (1-x)^{1-1} \\ &= \frac{\Gamma(2)}{\Gamma(1)\Gamma(1)} x^0 (1-x)^0 \\ &= 1 = \text{const.} , \end{aligned} \quad (9)$$

i.e. the distribution becomes equivalent to the (standard) continuous uniform distribution (\rightarrow II/3.1.1) with parameters $a = 0$ and $b = 1$ which has a constant probability density function (\rightarrow II/3.1.3). Thus, any value from the interval $[0, 1]$ may be considered the mode (\rightarrow II/3.1.8).

4) For the remaining cases, we must analyze the probability density function. The first two derivatives of this function are:

$$\begin{aligned} f'_X(x) &= \frac{df_X(x)}{dx} = \frac{1}{B(\alpha, \beta)} [-(\beta-1)x^{\alpha-1}(1-x)^{\beta-2} + (\alpha-1)x^{\alpha-2}(1-x)^{\beta-1}] \\ &= \frac{1}{B(\alpha, \beta)} [(\alpha-1)x^{\alpha-2}(1-x)^{\beta-1} - (\beta-1)x^{\alpha-1}(1-x)^{\beta-2}] \end{aligned} \quad (10)$$

$$\begin{aligned} f''_X(x) &= \frac{d^2 f_X(x)}{dx^2} = \frac{1}{B(\alpha, \beta)} [(\alpha-1)((\alpha-2)x^{\alpha-3}(1-x)^{\beta-1} - (\beta-1)x^{\alpha-2}(1-x)^{\beta-2}) - \\ &\quad (\beta-1)((\alpha-1)x^{\alpha-2}(1-x)^{\beta-2} - (\beta-2)x^{\alpha-1}(1-x)^{\beta-3})] \\ &= \frac{1}{B(\alpha, \beta)} [(\alpha-1)(\alpha-2)x^{\alpha-3}(1-x)^{\beta-1} - 2(\alpha-1)(\beta-1)x^{\alpha-2}(1-x)^{\beta-2} + \\ &\quad (\beta-1)(\beta-2)x^{\alpha-1}(1-x)^{\beta-3}] . \end{aligned} \quad (11)$$

We now calculate the root of the first derivative (10):

$$\begin{aligned}
 f'_X(x) = 0 &= \frac{1}{B(\alpha, \beta)} [(\alpha - 1)x^{\alpha-2}(1-x)^{\beta-1} - (\beta - 1)x^{\alpha-1}(1-x)^{\beta-2}] \\
 &\Leftrightarrow \\
 (\beta - 1)x^{\alpha-1}(1-x)^{\beta-2} &= (\alpha - 1)x^{\alpha-2}(1-x)^{\beta-1} \\
 (\beta - 1)x &= (\alpha - 1)(1-x) \\
 x[(\beta - 1) + (\alpha - 1)] &= \alpha - 1 \\
 x &= \frac{\alpha - 1}{\alpha + \beta - 2}.
 \end{aligned} \tag{12}$$

Note that for this quantity, we have

$$\begin{aligned}
 \frac{\alpha - 1}{\alpha + \beta - 2} &< 0, \quad \text{if } \alpha < 1 \quad \text{and} \quad \beta > 2 - \alpha \\
 \frac{\alpha - 1}{\alpha + \beta - 2} &> 1, \quad \text{if } \beta < 1 \quad \text{and} \quad \alpha > 2 - \beta.
 \end{aligned} \tag{13}$$

Also note that the following holds:

$$1 - x = 1 - \frac{\alpha - 1}{\alpha + \beta - 2} = \frac{\alpha + \beta - 2}{\alpha + \beta - 2} - \frac{\alpha - 1}{\alpha + \beta - 2} = \frac{\beta - 1}{\alpha + \beta - 2}. \tag{14}$$

By plugging x and $1 - x$ into the second derivative (11), we find:

$$\begin{aligned}
 f''_X\left(\frac{\alpha - 1}{\alpha + \beta - 2}\right) &= \frac{1}{B(\alpha, \beta)} \left[(\alpha - 1)(\alpha - 2) \left(\frac{\alpha - 1}{\alpha + \beta - 2}\right)^{\alpha-3} \left(\frac{\beta - 1}{\alpha + \beta - 2}\right)^{\beta-1} - \right. \\
 &\quad 2(\alpha - 1)(\beta - 1) \left(\frac{\alpha - 1}{\alpha + \beta - 2}\right)^{\alpha-2} \left(\frac{\beta - 1}{\alpha + \beta - 2}\right)^{\beta-2} + \\
 &\quad \left. (\beta - 1)(\beta - 2) \left(\frac{\alpha - 1}{\alpha + \beta - 2}\right)^{\alpha-1} \left(\frac{\beta - 1}{\alpha + \beta - 2}\right)^{\beta-3} \right].
 \end{aligned} \tag{15}$$

Multiplying with factors which are certainly positive, we can focus on those parts of the second derivative which determine its sign:

$$\begin{aligned}
 \frac{f''_X(x) \cdot B(\alpha, \beta)}{\left(\frac{\alpha-1}{\alpha+\beta-2}\right)^{\alpha-3} \cdot \left(\frac{\beta-1}{\alpha+\beta-2}\right)^{\beta-3}} &= (\alpha - 1)(\alpha - 2) \left(\frac{\beta - 1}{\alpha + \beta - 2}\right)^2 - \\
 &\quad 2(\alpha - 1)(\beta - 1) \left(\frac{\alpha - 1}{\alpha + \beta - 2}\right) \left(\frac{\beta - 1}{\alpha + \beta - 2}\right) + \\
 &\quad (\beta - 1)(\beta - 2) \left(\frac{\alpha - 1}{\alpha + \beta - 2}\right)^2.
 \end{aligned} \tag{16}$$

Further multiplying with or dividing by terms which are necessarily positive and thus do not change the sign of the function value, we get:

$$\begin{aligned}
\frac{f_X''(x) \cdot B(\alpha, \beta)}{\left(\frac{\alpha-1}{\alpha+\beta-2}\right)^{\alpha-3} \cdot \left(\frac{\beta-1}{\alpha+\beta-2}\right)^{\beta-3}} \cdot \frac{(\alpha+\beta-2)^2}{(\alpha-1)(\beta-1)} &= (\alpha-2)(\beta-1) - 2(\alpha-1)(\beta-1) + (\alpha-1)(\beta-2) \\
&= (\alpha-1)[(\beta-2) - (\beta-1)] + (\beta-1)[(\alpha-1) - (\alpha-2)] \\
&= -(\alpha-1) - (\beta-1) \\
&< 0, \quad \text{if } \alpha > 1 \quad \text{and} \quad \beta > 1.
\end{aligned} \tag{17}$$

Thus, $f'_X(x)$ is negative for $x = \frac{\alpha-1}{\alpha+\beta-2}$, demonstrating that this is a maximum. To summarize:

- If $\alpha < 1$ and $\beta < 1$, then $f_X(x)$ diverges at both ends and both values from the set $\{0, 1\}$ can be seen as the mode of X .
- If $\alpha < 1$ or $\beta < 1$ (but not $\alpha < 1$ and $\beta < 1$), then the mode of X is 0 or 1, because $f_X(x)$ tends towards infinity at $x = 0$ or $x = 1$.
- If $\alpha = 1$ and $\beta = 1$, then $f_X(x)$ is constant and any value in the interval $[0, 1]$ can be seen as the mode of X .
- If $\alpha \geq 1$ and $\beta \geq 1$ (but not $\alpha = 1$ and $\beta = 1$), then $0 < x = \frac{\alpha-1}{\alpha+\beta-2} < 1$ and $f'_X(x) = 0$ and $f'_X(x) < 0$, such that $f_X(x)$ reaches its maximum at $\frac{\alpha-1}{\alpha+\beta-2} = \text{mode}(X)$.

■

Sources:

- Wikipedia (2025): “Beta distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2025-10-24; URL: https://en.wikipedia.org/wiki/Beta_distribution#Mode.

3.9.11 Variance

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a beta distribution (\rightarrow II/3.9.1):

$$X \sim \text{Bet}(\alpha, \beta). \tag{1}$$

Then, the variance (\rightarrow I/1.13.1) of X is

$$\text{Var}(X) = \frac{\alpha\beta}{(\alpha+\beta+1) \cdot (\alpha+\beta)^2}. \tag{2}$$

Proof: The variance (\rightarrow I/1.13.1) can be expressed in terms of expected values (\rightarrow I/1.13.4) as

$$\text{Var}(X) = E(X^2) - E(X)^2. \tag{3}$$

The expected value of a beta random variable (\rightarrow II/3.9.8) is

$$E(X) = \frac{\alpha}{\alpha+\beta}. \tag{4}$$

The probability density function of the beta distribution (\rightarrow II/3.9.5) is

$$f_X(x) = \frac{1}{B(\alpha, \beta)} x^{\alpha-1} (1-x)^{\beta-1}, \quad 0 \leq x \leq 1 \tag{5}$$

where the beta function is given by a ratio gamma functions:

$$B(\alpha, \beta) = \frac{\Gamma(\alpha) \cdot \Gamma(\beta)}{\Gamma(\alpha + \beta)} . \quad (6)$$

Therefore, the expected value of a squared beta random variable becomes

$$\begin{aligned} E(X^2) &= \int_0^1 x^2 \cdot \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha) \cdot \Gamma(\beta)} x^{\alpha-1} (1-x)^{\beta-1} dx \\ &= \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)} \cdot \frac{\Gamma(\alpha + 2)}{\Gamma(\alpha + 2 + \beta)} \int_0^1 \frac{\Gamma(\alpha + 2 + \beta)}{\Gamma(\alpha + 2) \cdot \Gamma(\beta)} x^{(\alpha+2)-1} (1-x)^{\beta-1} dx . \end{aligned} \quad (7)$$

Twice-applying the relation $\Gamma(x + 1) = \Gamma(x) \cdot x$, we have

$$\begin{aligned} E(X^2) &= \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)} \cdot \frac{(\alpha + 1) \cdot \alpha \cdot \Gamma(\alpha)}{(\alpha + \beta + 1) \cdot (\alpha + \beta) \cdot \Gamma(\alpha + \beta)} \int_0^1 \frac{\Gamma(\alpha + 2 + \beta)}{\Gamma(\alpha + 2) \cdot \Gamma(\beta)} x^{(\alpha+2)-1} (1-x)^{\beta-1} dx \\ &= \frac{(\alpha + 1) \cdot \alpha}{(\alpha + \beta + 1) \cdot (\alpha + \beta)} \int_0^1 \frac{\Gamma(\alpha + 2 + \beta)}{\Gamma(\alpha + 2) \cdot \Gamma(\beta)} x^{(\alpha+2)-1} (1-x)^{\beta-1} dx \end{aligned} \quad (8)$$

and again using the density of the beta distribution (\rightarrow II/3.9.5), we get

$$\begin{aligned} E(X^2) &= \frac{(\alpha + 1) \cdot \alpha}{(\alpha + \beta + 1) \cdot (\alpha + \beta)} \int_0^1 \text{Bet}(x; \alpha + 2, \beta) dx \\ &= \frac{(\alpha + 1) \cdot \alpha}{(\alpha + \beta + 1) \cdot (\alpha + \beta)} . \end{aligned} \quad (9)$$

Plugging (9) and (4) into (3), the variance of a beta random variable finally becomes

$$\begin{aligned} \text{Var}(X) &= \frac{(\alpha + 1) \cdot \alpha}{(\alpha + \beta + 1) \cdot (\alpha + \beta)} - \left(\frac{\alpha}{\alpha + \beta} \right)^2 \\ &= \frac{(\alpha^2 + \alpha) \cdot (\alpha + \beta)}{(\alpha + \beta + 1) \cdot (\alpha + \beta)^2} - \frac{\alpha^2 \cdot (\alpha + \beta + 1)}{(\alpha + \beta + 1) \cdot (\alpha + \beta)^2} \\ &= \frac{(\alpha^3 + \alpha^2\beta + \alpha^2 + \alpha\beta) - (\alpha^3 + \alpha^2\beta + \alpha^2)}{(\alpha + \beta + 1) \cdot (\alpha + \beta)^2} \\ &= \frac{\alpha\beta}{(\alpha + \beta + 1) \cdot (\alpha + \beta)^2} . \end{aligned} \quad (10)$$

■

Sources:

- Boer Commander (2020): “Beta Distribution Mean and Variance Proof”; in: *YouTube*, retrieved on 2021-04-29; URL: <https://www.youtube.com/watch?v=3OgCcnPZtZ8>.

3.10 Wald distribution

3.10.1 Definition

Definition: Let X be a random variable (\rightarrow I/1.2.2). Then, X is said to follow a Wald distribution with drift rate γ and threshold α

$$X \sim \text{Wald}(\gamma, \alpha), \quad (1)$$

if and only if its probability density function (\rightarrow I/1.7.1) is given by

$$\text{Wald}(x; \gamma, \alpha) = \frac{\alpha}{\sqrt{2\pi x^3}} \exp\left(-\frac{(\alpha - \gamma x)^2}{2x}\right) \quad (2)$$

where $\gamma > 0$, $\alpha > 0$, and the density is zero if $x \leq 0$.

Sources:

- Anders, R., Alario, F.-X., and van Maanen, L. (2016): “The Shifted Wald Distribution for Response Time Data Analysis”; in: *Psychological Methods*, vol. 21, no. 3, pp. 309-327; URL: <https://dx.doi.org/10.1037/met0000066>; DOI: 10.1037/met0000066.

3.10.2 Probability density function

Theorem: Let X be a positive random variable (\rightarrow I/1.2.2) following a Wald distribution (\rightarrow II/3.10.1):

$$X \sim \text{Wald}(\gamma, \alpha). \quad (1)$$

Then, the probability density function (\rightarrow I/1.7.1) of X is

$$f_X(x) = \frac{\alpha}{\sqrt{2\pi x^3}} \exp\left(-\frac{(\alpha - \gamma x)^2}{2x}\right). \quad (2)$$

Proof: This follows directly from the definition of the Wald distribution (\rightarrow II/3.10.1). ■

3.10.3 Moment-generating function

Theorem: Let X be a positive random variable (\rightarrow I/1.2.2) following a Wald distribution (\rightarrow II/3.10.1):

$$X \sim \text{Wald}(\gamma, \alpha). \quad (1)$$

Then, the moment-generating function (\rightarrow I/1.9.1) of X is

$$M_X(t) = \exp\left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)}\right]. \quad (2)$$

Proof: The probability density function of the Wald distribution (\rightarrow II/3.10.2) is

$$f_X(x) = \frac{\alpha}{\sqrt{2\pi x^3}} \exp\left(-\frac{(\alpha - \gamma x)^2}{2x}\right) \quad (3)$$

and the moment-generating function (\rightarrow I/1.9.1) is defined as

$$M_X(t) = \mathbb{E}\left[e^{tX}\right]. \quad (4)$$

Using the definition of expected value for continuous random variables (\rightarrow I/1.12.1), the moment-generating function of X therefore is

$$\begin{aligned} M_X(t) &= \int_0^\infty e^{tx} \cdot \frac{\alpha}{\sqrt{2\pi x^3}} \cdot \exp\left[-\frac{(\alpha - \gamma x)^2}{2x}\right] dx \\ &= \frac{\alpha}{\sqrt{2\pi}} \int_0^\infty x^{-3/2} \cdot \exp\left[tx - \frac{(\alpha - \gamma x)^2}{2x}\right] dx. \end{aligned} \quad (5)$$

To evaluate this integral, we will need two identities about modified Bessel functions of the second kind¹, denoted K_p . The function K_p (for $p \in \mathbb{R}$) is one of the two linearly independent solutions of the differential equation

$$x^2 \frac{d^2 y}{dx^2} + x \frac{dy}{dx} - (x^2 + p^2)y = 0. \quad (6)$$

The first of these identities² gives an explicit solution for $K_{-1/2}$:

$$K_{-1/2}(x) = \sqrt{\frac{\pi}{2x}} e^{-x}. \quad (7)$$

The second of these identities³ gives an integral representation of K_p :

$$K_p(\sqrt{ab}) = \frac{1}{2} \left(\frac{a}{b}\right)^{p/2} \int_0^\infty x^{p-1} \cdot \exp\left[-\frac{1}{2} \left(ax + \frac{b}{x}\right)\right] dx. \quad (8)$$

Starting from (5), we can expand the binomial term and rearrange the moment generating function into the following form:

$$\begin{aligned} M_X(t) &= \frac{\alpha}{\sqrt{2\pi}} \int_0^\infty x^{-3/2} \cdot \exp\left[tx - \frac{\alpha^2}{2x} + \alpha\gamma - \frac{\gamma^2 x}{2}\right] dx \\ &= \frac{\alpha}{\sqrt{2\pi}} \cdot e^{\alpha\gamma} \int_0^\infty x^{-3/2} \cdot \exp\left[\left(t - \frac{\gamma^2}{2}\right)x - \frac{\alpha^2}{2x}\right] dx \\ &= \frac{\alpha}{\sqrt{2\pi}} \cdot e^{\alpha\gamma} \int_0^\infty x^{-3/2} \cdot \exp\left[-\frac{1}{2}(\gamma^2 - 2t)x - \frac{1}{2} \cdot \frac{\alpha^2}{x}\right] dx. \end{aligned} \quad (9)$$

The integral now has the form of the integral in (8) with $p = -1/2$, $a = \gamma^2 - 2t$, and $b = \alpha^2$. This allows us to write the moment-generating function in terms of the modified Bessel function $K_{-1/2}$:

$$M_X(t) = \frac{\alpha}{\sqrt{2\pi}} \cdot e^{\alpha\gamma} \cdot 2 \left(\frac{\gamma^2 - 2t}{\alpha^2}\right)^{1/4} \cdot K_{-1/2}\left(\sqrt{\alpha^2(\gamma^2 - 2t)}\right). \quad (10)$$

Combining with (7) and simplifying gives

¹<https://dlmf.nist.gov/10.25>

²<https://dlmf.nist.gov/10.39.2>

³<https://dlmf.nist.gov/10.32.10>

$$\begin{aligned}
M_X(t) &= \frac{\alpha}{\sqrt{2\pi}} \cdot e^{\alpha\gamma} \cdot 2 \left(\frac{\gamma^2 - 2t}{\alpha^2} \right)^{1/4} \cdot \sqrt{\frac{\pi}{2\sqrt{\alpha^2(\gamma^2 - 2t)}}} \cdot \exp \left[-\sqrt{\alpha^2(\gamma^2 - 2t)} \right] \\
&= \frac{\alpha}{\sqrt{2} \cdot \sqrt{\pi}} \cdot e^{\alpha\gamma} \cdot 2 \cdot \frac{(\gamma^2 - 2t)^{1/4}}{\sqrt{\alpha}} \cdot \frac{\sqrt{\pi}}{\sqrt{2} \cdot \sqrt{\alpha} \cdot (\gamma^2 - 2t)^{1/4}} \cdot \exp \left[-\sqrt{\alpha^2(\gamma^2 - 2t)} \right] \quad (11) \\
&= e^{\alpha\gamma} \cdot \exp \left[-\sqrt{\alpha^2(\gamma^2 - 2t)} \right] \\
&= \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)} \right].
\end{aligned}$$

This finishes the proof of (2). ■

Sources:

- Siegrist, K. (2020): “The Wald Distribution”; in: *Random: Probability, Mathematical Statistics, Stochastic Processes*, retrieved on 2020-09-13; URL: <https://www.randomservices.org/random/special/Wald.html>.
- National Institute of Standards and Technology (2020): “NIST Digital Library of Mathematical Functions”, retrieved on 2020-09-13; URL: <https://dlmf.nist.gov>.

3.10.4 Mean

Theorem: Let X be a positive random variable (\rightarrow I/1.2.2) following a Wald distribution (\rightarrow II/3.10.1):

$$X \sim \text{Wald}(\gamma, \alpha). \quad (1)$$

Then, the mean or expected value (\rightarrow I/1.12.1) of X is

$$E(X) = \frac{\alpha}{\gamma}. \quad (2)$$

Proof: The mean or expected value $E(X)$ is the first moment (\rightarrow I/1.21.1) of X , so we can use (\rightarrow I/1.21.2) the moment-generating function of the Wald distribution (\rightarrow II/3.10.3) to calculate

$$E(X) = M'_X(0). \quad (3)$$

First we differentiate

$$M_X(t) = \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)} \right] \quad (4)$$

with respect to t . Using the chain rule gives

$$\begin{aligned}
M'_X(t) &= \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)} \right] \cdot -\frac{1}{2} (\alpha^2(\gamma^2 - 2t))^{-1/2} \cdot -2\alpha^2 \\
&= \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)} \right] \cdot \frac{\alpha^2}{\sqrt{\alpha^2(\gamma^2 - 2t)}}.
\end{aligned} \quad (5)$$

Evaluating (5) at $t = 0$ gives the desired result:

$$\begin{aligned}
M'_X(0) &= \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2(0))} \right] \cdot \frac{\alpha^2}{\sqrt{\alpha^2(\gamma^2 - 2(0))}} \\
&= \exp \left[\alpha\gamma - \sqrt{\alpha^2 \cdot \gamma^2} \right] \cdot \frac{\alpha^2}{\sqrt{\alpha^2 \cdot \gamma^2}} \\
&= \exp[0] \cdot \frac{\alpha^2}{\alpha\gamma} \\
&= \frac{\alpha}{\gamma} .
\end{aligned} \tag{6}$$

■

3.10.5 Variance

Theorem: Let X be a positive random variable (\rightarrow I/1.2.2) following a Wald distribution (\rightarrow II/3.10.1):

$$X \sim \text{Wald}(\gamma, \alpha) . \tag{1}$$

Then, the variance (\rightarrow I/1.13.1) of X is

$$\text{Var}(X) = \frac{\alpha}{\gamma^3} . \tag{2}$$

Proof: To compute the variance of X , we partition the variance into expected values (\rightarrow I/1.13.4):

$$\text{Var}(X) = E(X^2) - E(X)^2. \tag{3}$$

We then use the moment-generating function of the Wald distribution (\rightarrow II/3.10.3) to calculate

$$E(X^2) = M''_X(0) . \tag{4}$$

First we differentiate

$$M_X(t) = \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)} \right] \tag{5}$$

with respect to t . Using the chain rule gives

$$\begin{aligned}
M'_X(t) &= \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)} \right] \cdot -\frac{1}{2} (\alpha^2(\gamma^2 - 2t))^{-1/2} \cdot -2\alpha^2 \\
&= \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)} \right] \cdot \frac{\alpha^2}{\sqrt{\alpha^2(\gamma^2 - 2t)}} \\
&= \alpha \cdot \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)} \right] \cdot (\gamma^2 - 2t)^{-1/2} .
\end{aligned} \tag{6}$$

Now we use the product rule to obtain the second derivative:

$$\begin{aligned}
M_X''(t) &= \alpha \cdot \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)} \right] \cdot (\gamma^2 - 2t)^{-1/2} \cdot -\frac{1}{2} (\alpha^2(\gamma^2 - 2t))^{-1/2} \cdot -2\alpha^2 \\
&\quad + \alpha \cdot \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)} \right] \cdot -\frac{1}{2} (\gamma^2 - 2t)^{-3/2} \cdot -2 \\
&= \alpha^2 \cdot \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)} \right] \cdot (\gamma^2 - 2t)^{-1} \\
&\quad + \alpha \cdot \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)} \right] \cdot (\gamma^2 - 2t)^{-3/2} \\
&= \alpha \cdot \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)} \right] \left[\frac{\alpha}{\gamma^2 - 2t} + \frac{1}{\sqrt{(\gamma^2 - 2t)^3}} \right].
\end{aligned} \tag{7}$$

Applying (4) yields

$$\begin{aligned}
E(X^2) &= M_X''(0) \\
&= \alpha \cdot \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2(0))} \right] \left[\frac{\alpha}{\gamma^2 - 2(0)} + \frac{1}{\sqrt{(\gamma^2 - 2(0))^3}} \right] \\
&= \alpha \cdot \exp [\alpha\gamma - \alpha\gamma] \cdot \left[\frac{\alpha}{\gamma^2} + \frac{1}{\gamma^3} \right] \\
&= \frac{\alpha^2}{\gamma^2} + \frac{\alpha}{\gamma^3}.
\end{aligned} \tag{8}$$

Since the mean of a Wald distribution (\rightarrow II/3.10.4) is given by $E(X) = \alpha/\gamma$, we can apply (3) to show

$$\begin{aligned}
\text{Var}(X) &= E(X^2) - E(X)^2 \\
&= \frac{\alpha^2}{\gamma^2} + \frac{\alpha}{\gamma^3} - \left(\frac{\alpha}{\gamma} \right)^2 \\
&= \frac{\alpha}{\gamma^3}
\end{aligned} \tag{9}$$

which completes the proof of (2). ■

3.10.6 Skewness

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following a Wald distribution (\rightarrow II/3.10.1):

$$X \sim \text{Wald}(\gamma, \alpha). \tag{1}$$

Then the skewness (\rightarrow I/1.14.1) of X is

$$\text{Skew}(X) = \frac{3}{\sqrt{\alpha\gamma}}. \tag{2}$$

Proof: To compute the skewness of X , we partition the skewness into expected values (\rightarrow I/1.14.3):

$$\text{Skew}(X) = \frac{E(X^3) - 3\mu\sigma^2 - \mu^3}{\sigma^3}, \quad (3)$$

where μ and σ are the mean and standard deviation of X , respectively. Since X follows a Wald distribution, the mean (\rightarrow II/3.10.4) of X is given by

$$\mu = E(X) = \frac{\alpha}{\gamma} \quad (4)$$

and the standard deviation (\rightarrow II/3.10.5) of X is given by

$$\sigma = \sqrt{\text{Var}(X)} = \sqrt{\frac{\alpha}{\gamma^3}}. \quad (5)$$

Substituting (4) and (5) into (3) gives:

$$\begin{aligned} \text{Skew}(X) &= \frac{E(X^3) - 3\mu\sigma^2 - \mu^3}{\sigma^3} \\ &= \frac{E(X^3) - 3\left(\frac{\alpha}{\gamma}\right)\left(\frac{\alpha}{\gamma^3}\right) - \left(\frac{\alpha}{\gamma}\right)^3}{\left(\sqrt{\frac{\alpha}{\gamma^3}}\right)^3} \\ &= \frac{\gamma^{9/2}}{\alpha^{3/2}} \left[E(X^3) - \frac{3\alpha^2}{\gamma^4} - \frac{\alpha^3}{\gamma^3} \right]. \end{aligned} \quad (6)$$

Thus, the remaining work is to compute $E(X^3)$. To do this, we use the moment-generating function of the Wald distribution (\rightarrow II/3.10.3) to calculate

$$E(X^3) = M_X'''(0) \quad (7)$$

based on the relationship between raw moment and moment-generating function (\rightarrow I/1.21.2). First, we differentiate the moment-generating function

$$M_X(t) = \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)} \right] \quad (8)$$

with respect to t . Using the chain rule, we have:

$$\begin{aligned} M_X'(t) &= \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)} \right] \cdot -\frac{1}{2} (\alpha^2(\gamma^2 - 2t))^{-1/2} \cdot -2\alpha^2 \\ &= \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)} \right] \cdot \frac{\alpha^2}{\sqrt{\alpha^2(\gamma^2 - 2t)}} \\ &= \alpha \cdot \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)} \right] \cdot (\gamma^2 - 2t)^{-1/2}. \end{aligned} \quad (9)$$

Now we use the product rule to obtain the second derivative:

$$\begin{aligned}
M_X''(t) &= \alpha \cdot \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)} \right] \cdot (\gamma^2 - 2t)^{-1/2} \cdot -\frac{1}{2} (\alpha^2(\gamma^2 - 2t))^{-1/2} \cdot -2\alpha^2 \\
&\quad + \alpha \cdot \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)} \right] \cdot -\frac{1}{2} (\gamma^2 - 2t)^{-3/2} \cdot -2 \\
&= \alpha^2 \cdot \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)} \right] \cdot (\gamma^2 - 2t)^{-1} \\
&\quad + \alpha \cdot \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)} \right] \cdot (\gamma^2 - 2t)^{-3/2} \\
&= \frac{\alpha^2}{\gamma^2 - 2t} \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)} \right] + \frac{\alpha}{(\gamma^2 - 2t)^{3/2}} \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)} \right] .
\end{aligned} \tag{10}$$

Finally, one more application of the chain rule will give us the third derivative. To start, we will decompose the second derivative obtained in (10) as

$$M''(t) = f(t) + g(t) \tag{11}$$

where

$$f(t) = \frac{\alpha^2}{\gamma^2 - 2t} \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)} \right] \tag{12}$$

and

$$g(t) = \frac{\alpha}{(\gamma^2 - 2t)^{3/2}} \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)} \right] . \tag{13}$$

With this decomposition, $M_X'(t) = f'(t) + g'(t)$. Applying the product rule to f gives:

$$\begin{aligned}
f'(t) &= 2\alpha^2(\gamma^2 - 2t)^{-2} \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)} \right] \\
&\quad + \alpha^2(\gamma^2 - 2t)^{-1} \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)} \right] \cdot -\frac{1}{2} [\alpha^2(\gamma^2 - 2t)]^{-1/2} \cdot -2\alpha^2 \\
&= \frac{2\alpha^2}{(\gamma^2 - 2t)^2} \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)} \right] \\
&\quad + \frac{\alpha^3}{(\gamma^2 - 2t)^{3/2}} \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)} \right] .
\end{aligned} \tag{14}$$

Similarly, applying the product rule to g gives:

$$\begin{aligned}
g'(t) &= -\frac{3}{2}\alpha(\gamma^2 - 2t)^{-5/2}(-2) \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)} \right] \\
&\quad + \alpha(\gamma^2 - 2t)^{-3/2} \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)} \right] \cdot -\frac{1}{2} [\alpha^2(\gamma^2 - 2t)]^{-1/2} \cdot -2\alpha^2 \\
&= \frac{3\alpha}{(\gamma^2 - 2t)^{5/2}} \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)} \right] \\
&\quad + \frac{\alpha^2}{(\gamma^2 - 2t)^2} \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)} \right] .
\end{aligned} \tag{15}$$

Applying (7), together with (14) and (15), yields

$$\begin{aligned}
E(X^3) &= M_X'''(0) \\
&= f'(0) + g'(0) \\
&= \left[\frac{2\alpha^2}{\gamma^4} + \frac{\alpha^3}{\gamma^3} \right] + \left[\frac{3\alpha}{\gamma^5} + \frac{\alpha^2}{\gamma^4} \right] \\
&= \frac{3\alpha^2}{\gamma^4} + \frac{\alpha^3}{\gamma^3} + \frac{3\alpha}{\gamma^5} .
\end{aligned} \tag{16}$$

We now substitute (16) into (6), giving

$$\begin{aligned}
\text{Skew}(X) &= \frac{\gamma^{9/2}}{\alpha^{3/2}} \left[E(X^3) - \frac{3\alpha^2}{\gamma^4} - \frac{\alpha^3}{\gamma^3} \right] \\
&= \frac{\gamma^{9/2}}{\alpha^{3/2}} \left[\frac{3\alpha^2}{\gamma^4} + \frac{\alpha^3}{\gamma^3} + \frac{3\alpha}{\gamma^5} - \frac{3\alpha^2}{\gamma^4} - \frac{\alpha^3}{\gamma^3} \right] \\
&= \frac{\gamma^{9/2}}{\alpha^{3/2}} \cdot \frac{3\alpha}{\gamma^5} \\
&= \frac{3}{\alpha^{1/2} \cdot \gamma^{1/2}} \\
&= \frac{3}{\sqrt{\alpha\gamma}} .
\end{aligned} \tag{17}$$

This completes the proof of (2). ■

3.10.7 Method of moments

Theorem: Let $y = \{y_1, \dots, y_n\}$ be a set of observed data independent and identically distributed (\rightarrow I/1.2.8) according to a Wald distribution (\rightarrow II/3.10.1) with drift rate γ and threshold α :

$$y_i \sim \text{Wald}(\gamma, \alpha), \quad i = 1, \dots, n . \tag{1}$$

Then, the method-of-moments estimates (\rightarrow I/4.1.8) for the parameters γ and α are given by

$$\begin{aligned}
\hat{\gamma} &= \sqrt{\frac{\bar{y}}{\bar{v}}} \\
\hat{\alpha} &= \sqrt{\frac{\bar{y}^3}{\bar{v}}}
\end{aligned} \tag{2}$$

where \bar{y} is the sample mean (\rightarrow I/1.12.2) and \bar{v} is the unbiased sample variance (\rightarrow I/1.13.2):

$$\begin{aligned}
\bar{y} &= \frac{1}{n} \sum_{i=1}^n y_i \\
\bar{v} &= \frac{1}{n-1} \sum_{i=1}^n (y_i - \bar{y})^2 .
\end{aligned} \tag{3}$$

Proof: The mean (\rightarrow II/3.10.4) and variance (\rightarrow II/3.10.5) of the Wald distribution (\rightarrow II/3.10.1) in terms of the parameters γ and α are given by

$$\begin{aligned} E(X) &= \frac{\alpha}{\gamma} \\ \text{Var}(X) &= \frac{\alpha}{\gamma^3} . \end{aligned} \tag{4}$$

Thus, matching the moments (\rightarrow I/4.1.8) requires us to solve the following system of equations for γ and α :

$$\begin{aligned} \bar{y} &= \frac{\alpha}{\gamma} \\ \bar{v} &= \frac{\alpha}{\gamma^3} . \end{aligned} \tag{5}$$

To this end, our first step is to express the second equation of (5) as follows:

$$\begin{aligned} \bar{v} &= \frac{\alpha}{\gamma^3} \\ &= \frac{\alpha}{\gamma} \cdot \gamma^{-2} \\ &= \bar{y} \cdot \gamma^{-2} . \end{aligned} \tag{6}$$

Rearranging (6) gives

$$\gamma^2 = \frac{\bar{y}}{\bar{v}} , \tag{7}$$

or equivalently,

$$\gamma = \sqrt{\frac{\bar{y}}{\bar{v}}} . \tag{8}$$

Our final step is to solve the first equation of (5) for α and substitute (8) for γ :

$$\begin{aligned} \alpha &= \bar{y} \cdot \gamma \\ &= \bar{y} \cdot \sqrt{\frac{\bar{y}}{\bar{v}}} \\ &= \sqrt{\bar{y}^2} \cdot \sqrt{\frac{\bar{y}}{\bar{v}}} \\ &= \sqrt{\frac{\bar{y}^3}{\bar{v}}} . \end{aligned} \tag{9}$$

Together, (8) and (9) constitute the method-of-moment estimates of γ and α .

■

3.11 ex-Gaussian distribution

3.11.1 Definition

Definition: Let A be a random variable (\rightarrow I/1.2.2) that is normally distributed (\rightarrow II/3.2.1) with mean μ and variance σ^2 , and let B be a random variable that is exponentially distributed (\rightarrow II/3.5.1) with rate λ . Suppose further that A and B are independent (\rightarrow I/1.3.6). Then the sum $X = A + B$ is said to have an exponentially-modified Gaussian (i.e., ex-Gaussian) distribution, with parameters μ , σ , and λ ; that is,

$$X \sim \text{ex-Gaussian}(\mu, \sigma, \lambda), \quad (1)$$

where $\mu \in \mathbb{R}$, $\sigma > 0$, and $\lambda > 0$.

Sources:

- Luce, R. D. (1986): “Response Times: Their Role in Inferring Elementary Mental Organization”, 35-36; URL: <https://global.oup.com/academic/product/response-times-9780195036428>.

3.11.2 Probability density function

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following an ex-Gaussian distribution (\rightarrow II/3.11.1):

$$X \sim \text{ex-Gaussian}(\mu, \sigma, \lambda). \quad (1)$$

Then the probability density function (\rightarrow I/1.7.1) of X is

$$f_X(t) = \frac{\lambda}{\sqrt{2\pi}} \exp \left[\frac{\lambda^2 \sigma^2}{2} - \lambda(t - \mu) \right] \cdot \int_{-\infty}^{\frac{t-\mu}{\sigma} - \lambda\sigma} \exp \left[-\frac{1}{2}y^2 \right] dy. \quad (2)$$

Proof: Suppose X follows an ex-Gaussian distribution (\rightarrow II/3.11.1). Then $X = A + B$, where A and B are independent (\rightarrow I/1.3.6), A is normally distributed (\rightarrow II/3.2.1) with mean (\rightarrow II/3.2.16) μ and variance (\rightarrow II/3.2.19) σ^2 , and B is exponentially distributed (\rightarrow II/3.5.1) with rate λ . Then, the probability density function (\rightarrow II/3.2.10) for A is given by

$$f_A(t) = \frac{1}{\sigma\sqrt{2\pi}} \exp \left[-\frac{1}{2} \left(\frac{t - \mu}{\sigma} \right)^2 \right], \quad (3)$$

and the probability density function (\rightarrow II/3.5.3) for B is given by

$$f_B(t) = \begin{cases} \lambda \exp[-\lambda t], & \text{if } t \geq 0 \\ 0, & \text{if } t < 0. \end{cases} \quad (4)$$

Thus, the probability density function for the sum (\rightarrow I/1.7.2) $X = A + B$ is given by taking the convolution of f_A and f_B :

$$\begin{aligned}
f_X(t) &= \int_{-\infty}^{\infty} f_A(x) f_B(t-x) dx \\
&= \int_{-\infty}^t f_A(x) f_B(t-x) dx + \int_t^{\infty} f_A(x) f_B(t-x) dx \\
&= \int_{-\infty}^t f_A(x) f_B(t-x) dx ,
\end{aligned} \tag{5}$$

which follows from the fact that $f_B(t-x) = 0$ for $x > t$. From here, we substitute the expressions (3) and (4) for the probability density functions f_A and f_B in (5):

$$\begin{aligned}
f_X(t) &= \int_{-\infty}^t \frac{1}{\sigma\sqrt{2\pi}} \exp \left[-\frac{1}{2} \left(\frac{x-\mu}{\sigma} \right)^2 \right] \cdot \lambda \exp[-\lambda(t-x)] dx \\
&= \frac{\lambda}{\sigma\sqrt{2\pi}} \int_{-\infty}^t \exp \left[-\frac{1}{2} \left(\frac{x-\mu}{\sigma} \right)^2 \right] \cdot \exp[-\lambda t + \lambda x] dx \\
&= \frac{\lambda}{\sigma\sqrt{2\pi}} \int_{-\infty}^t \exp \left[-\frac{1}{2} \left(\frac{x-\mu}{\sigma} \right)^2 \right] \cdot \exp[-\lambda t] \cdot \exp[\lambda x] dx \\
&= \frac{\lambda \exp[-\lambda t]}{\sigma\sqrt{2\pi}} \int_{-\infty}^t \exp \left[-\frac{1}{2} \left(\frac{x-\mu}{\sigma} \right)^2 + \lambda x \right] dx .
\end{aligned} \tag{6}$$

We can further simplify the integrand with a substitution; to this end, let

$$y = g(x) = \frac{x-\mu}{\sigma} - \lambda\sigma \tag{7}$$

This gives the following three identities:

$$\frac{dy}{dx} = \frac{1}{\sigma} , \quad \text{or equivalently,} \quad dx = \sigma dy , \tag{8}$$

$$\frac{x-\mu}{\sigma} = y + \lambda\sigma , \quad \text{and} \tag{9}$$

$$x = y\sigma + \lambda\sigma^2 + \mu . \tag{10}$$

Substituting these identities into (6) gives

$$\begin{aligned}
f_X(t) &= \frac{\lambda \exp[-\lambda t]}{\sigma \sqrt{2\pi}} \int_{-\infty}^{g(t)} \exp \left[-\frac{1}{2}(y + \lambda\sigma)^2 + \lambda(y\sigma + \lambda\sigma^2 + \mu) \right] \sigma dy \\
&= \frac{\lambda \exp[-\lambda t]}{\sigma \sqrt{2\pi}} \int_{-\infty}^{\frac{x-\mu}{\sigma} + \lambda\sigma} \exp \left[-\frac{1}{2}(y^2 + 2y\lambda\sigma + \lambda^2\sigma^2) + \lambda y\sigma + \lambda^2\sigma^2 + \lambda\mu \right] dy \\
&= \frac{\lambda \exp[-\lambda t]}{\sqrt{2\pi}} \int_{-\infty}^{\frac{x-\mu}{\sigma} + \lambda\sigma} \exp \left[-\frac{1}{2}y^2 - y\lambda\sigma - \frac{\lambda^2\sigma^2}{2} + \lambda y\sigma + \lambda^2\sigma^2 + \lambda\mu \right] dy \\
&= \frac{\lambda \exp[-\lambda t]}{\sqrt{2\pi}} \int_{-\infty}^{\frac{x-\mu}{\sigma} + \lambda\sigma} \exp \left[-\frac{1}{2}y^2 \right] \cdot \exp \left[\frac{\lambda^2\sigma^2}{2} + \lambda\mu \right] dy \\
&= \frac{\lambda \exp[-\lambda t]}{\sqrt{2\pi}} \cdot \exp \left[\frac{\lambda^2\sigma^2}{2} + \lambda\mu \right] \int_{-\infty}^{\frac{x-\mu}{\sigma} + \lambda\sigma} \exp \left[-\frac{1}{2}y^2 \right] \cdot dy \\
&= \frac{\lambda}{\sqrt{2\pi}} \cdot \exp \left[-\lambda t + \frac{\lambda^2\sigma^2}{2} + \lambda\mu \right] \int_{-\infty}^{\frac{x-\mu}{\sigma} + \lambda\sigma} \exp \left[-\frac{1}{2}y^2 \right] \cdot dy \\
&= \frac{\lambda}{\sqrt{2\pi}} \cdot \exp \left[\frac{\lambda^2\sigma^2}{2} - \lambda(t - \mu) \right] \int_{-\infty}^{\frac{x-\mu}{\sigma} + \lambda\sigma} \exp \left[-\frac{1}{2}y^2 \right] \cdot dy .
\end{aligned} \tag{11}$$

This finishes the proof of (2). ■

3.11.3 Moment-generating function

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following an ex-Gaussian distribution (\rightarrow II/3.11.1):

$$X \sim \text{ex-Gaussian}(\mu, \sigma, \lambda) . \tag{1}$$

Then, the moment generating function (\rightarrow I/1.9.1) of X is

$$M_X(t) = \left(\frac{\lambda}{\lambda - t} \right) \exp \left[\mu t + \frac{1}{2} \sigma^2 t^2 \right] . \tag{2}$$

Proof: Suppose X follows an ex-Gaussian distribution (\rightarrow II/3.11.1). Then, $X = A + B$ where A and B are independent (\rightarrow I/1.3.6), A is normally distributed (\rightarrow II/3.2.1) with mean (\rightarrow II/3.2.16) μ and variance (\rightarrow II/3.2.19) σ^2 , and B is exponentially distributed (\rightarrow II/3.5.1) with rate λ . Then the moment generating function (\rightarrow II/3.2.11) for A is given by

$$M_A(t) = \exp \left[\mu t + \frac{1}{2} \sigma^2 t^2 \right] \tag{3}$$

and the moment generating function (\rightarrow II/3.5.4) for B is given by

$$M_B(t) = \frac{\lambda}{\lambda - t} . \tag{4}$$

By definition, X is a linear combination of independent random variables A and B , so the moment generating function (\rightarrow I/1.9.5) of X is the product of $M_A(t)$ and $M_B(t)$. That is,

$$\begin{aligned}
M_X(t) &= M_A(t) \cdot M_B(t) \\
&= \exp \left[\mu t + \frac{1}{2} \sigma^2 t^2 \right] \cdot \left(\frac{\lambda}{\lambda - t} \right) \\
&= \left(\frac{\lambda}{\lambda - t} \right) \exp \left[\mu t + \frac{1}{2} \sigma^2 t^2 \right] .
\end{aligned} \tag{5}$$

This finishes the proof of (2). ■

3.11.4 Mean

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following an ex-Gaussian distribution (\rightarrow II/3.11.1):

$$X \sim \text{ex-Gaussian}(\mu, \sigma, \lambda) . \tag{1}$$

Then, the mean or expected value (\rightarrow I/1.12.1) of X is

$$E(X) = \mu + \frac{1}{\lambda} . \tag{2}$$

Proof: The mean or expected value $E(X)$ is the first raw moment (\rightarrow I/1.21.1) of X , so we can use (\rightarrow I/1.21.2) the moment-generating function of the ex-Gaussian distribution (\rightarrow II/3.11.3) to calculate

$$E(X) = M'_X(0) . \tag{3}$$

First, we differentiate

$$M_X(t) = \left(\frac{\lambda}{\lambda - t} \right) \exp \left[\mu t + \frac{1}{2} \sigma^2 t^2 \right] \tag{4}$$

with respect to t . Using the product rule and chain rule gives:

$$\begin{aligned}
M'_X(t) &= \frac{\lambda}{(\lambda - t)^2} \exp \left[\mu t + \frac{1}{2} \sigma^2 t^2 \right] + \left(\frac{\lambda}{\lambda - t} \right) \exp \left[\mu t + \frac{1}{2} \sigma^2 t^2 \right] (\mu + \sigma^2 t) \\
&= \left(\frac{\lambda}{\lambda - t} \right) \cdot \exp \left[\mu t + \frac{1}{2} \sigma^2 t^2 \right] \cdot \left[\frac{1}{\lambda - t} + \mu + \sigma^2 t \right] .
\end{aligned} \tag{5}$$

Evaluating (5) at $t = 0$ gives the desired result:

$$\begin{aligned}
M'_X(0) &= \left(\frac{\lambda}{\lambda - 0} \right) \cdot \exp \left[\mu \cdot 0 + \frac{1}{2} \sigma^2 \cdot 0^2 \right] \cdot \left[\frac{1}{\lambda - 0} + \mu + \sigma^2 \cdot 0 \right] \\
&= 1 \cdot 1 \cdot \left[\frac{1}{\lambda} + \mu \right] \\
&= \mu + \frac{1}{\lambda} .
\end{aligned} \tag{6}$$

■

3.11.5 Variance

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following an ex-Gaussian distribution (\rightarrow II/3.11.1):

$$X \sim \text{ex-Gaussian}(\mu, \sigma, \lambda) . \quad (1)$$

Then, the variance (\rightarrow I/1.13.1) of X is

$$\text{Var}(X) = \sigma^2 + \frac{1}{\lambda^2} . \quad (2)$$

Proof: To compute the variance of X , we partition the variance into expected values (\rightarrow I/1.13.4):

$$\text{Var}(X) = E(X^2) - E(X)^2 . \quad (3)$$

We then use the moment-generating function of the ex-Gaussian distribution (\rightarrow II/3.11.3) to calculate

$$E(X^2) = M_X''(0) \quad (4)$$

based on the relationship between raw moment and moment-generating function (\rightarrow I/1.21.2). First, we differentiate

$$M_X(t) = \left(\frac{\lambda}{\lambda - t} \right) \exp \left[\mu t + \frac{1}{2} \sigma^2 t^2 \right] \quad (5)$$

with respect to t . Using the product rule and chain rule gives:

$$\begin{aligned} M_X'(t) &= \frac{\lambda}{(\lambda - t)^2} \exp \left[\mu t + \frac{1}{2} \sigma^2 t^2 \right] + \left(\frac{\lambda}{\lambda - t} \right) \exp \left[\mu t + \frac{1}{2} \sigma^2 t^2 \right] (\mu + \sigma^2 t) \\ &= \left(\frac{\lambda}{\lambda - t} \right) \cdot \exp \left[\mu t + \frac{1}{2} \sigma^2 t^2 \right] \cdot \left[\frac{1}{\lambda - t} + \mu + \sigma^2 t \right] \\ &= M_X(t) \cdot \left[\frac{1}{\lambda - t} + \mu + \sigma^2 t \right] . \end{aligned} \quad (6)$$

We now use the product rule to obtain the second derivative:

$$\begin{aligned} M_X''(t) &= M_X'(t) \cdot \left[\frac{1}{\lambda - t} + \mu + \sigma^2 t \right] + M_X(t) \cdot \left[\frac{1}{(\lambda - t)^2} + \sigma^2 \right] \\ &\stackrel{(6)}{=} M_X(t) \cdot \left[\frac{1}{\lambda - t} + \mu + \sigma^2 t \right]^2 + M_X(t) \cdot \left[\frac{1}{(\lambda - t)^2} + \sigma^2 \right] \\ &= M_X(t) \cdot \left[\left(\frac{1}{\lambda - t} + \mu + \sigma^2 t \right)^2 + \frac{1}{(\lambda - t)^2} + \sigma^2 \right] \\ &= \left(\frac{\lambda}{\lambda - t} \right) \cdot \exp \left[\mu t + \frac{1}{2} \sigma^2 t^2 \right] \cdot \left[\left(\frac{1}{\lambda - t} + \mu + \sigma^2 t \right)^2 + \frac{1}{(\lambda - t)^2} + \sigma^2 \right] \end{aligned} \quad (7)$$

Applying (4) yields

$$\begin{aligned}
E(X^2) &= M_X''(0) \\
&= \left(\frac{\lambda}{\lambda - 0} \right) \cdot \exp \left[\mu \cdot 0 + \frac{1}{2} \sigma^2 \cdot 0^2 \right] \cdot \left[\left(\frac{1}{\lambda - 0} + \mu + \sigma^2 \cdot 0 \right)^2 + \frac{1}{(\lambda - 0)^2} + \sigma^2 \right] \\
&= 1 \cdot 1 \cdot \left[\left(\frac{1}{\lambda} + \mu \right)^2 + \frac{1}{\lambda^2} + \sigma^2 \right] \\
&= \frac{1}{\lambda^2} + \frac{2\mu}{\lambda} + \mu^2 + \frac{1}{\lambda^2} + \sigma^2 \\
&= \frac{2}{\lambda^2} + \frac{2\mu}{\lambda} + \mu^2 + \sigma^2 .
\end{aligned} \tag{8}$$

Since the mean of an ex-Gaussian distribution (\rightarrow II/3.11.4) is given by

$$E(X) = \mu + \frac{1}{\lambda} , \tag{9}$$

we can apply (3) to show

$$\begin{aligned}
\text{Var}(X) &= E(X^2) - E(X)^2 \\
&= \left[\frac{2}{\lambda^2} + \frac{2\mu}{\lambda} + \mu^2 + \sigma^2 \right] - \left(\mu + \frac{1}{\lambda} \right)^2 \\
&= \frac{2}{\lambda^2} + \frac{2\mu}{\lambda} + \mu^2 + \sigma^2 - \mu^2 - \frac{2\mu}{\lambda} - \frac{1}{\lambda^2} \\
&= \sigma^2 + \frac{1}{\lambda^2} .
\end{aligned} \tag{10}$$

This completes the proof of (2). ■

3.11.6 Skewness

Theorem: Let X be a random variable (\rightarrow I/1.2.2) following an ex-Gaussian distribution (\rightarrow II/3.11.1):

$$X \sim \text{ex-Gaussian}(\mu, \sigma, \lambda) . \tag{1}$$

Then the skewness (\rightarrow I/1.14.1) of X is

$$\text{Skew}(X) = \frac{2}{\lambda^3 \left(\sigma^2 + \frac{1}{\lambda^2} \right)^{\frac{3}{2}}} . \tag{2}$$

Proof:

To compute the skewness of X , we partition the skewness into expected values (\rightarrow I/1.14.3):

$$\text{Skew}(X) = \frac{E(X^3) - 3\mu\sigma^2 - \mu^3}{\sigma^3} , \tag{3}$$

where μ and σ are the mean and standard deviation of X , respectively. To prevent confusion between the labels used for the ex-Gaussian parameters in (1) and the mean and standard deviation of X , we rewrite (3) as

$$\text{Skew}(X) = \frac{E(X^3) - 3 \cdot E(X) \cdot \text{Var}(X) - E(X)^3}{\text{Var}(X)^{\frac{3}{2}}}. \quad (4)$$

Since X follows an ex-Gaussian distribution (\rightarrow II/3.11.1), the mean (\rightarrow II/3.11.4) of X is given by

$$E(X) = \mu + \frac{1}{\lambda} \quad (5)$$

and the variance (\rightarrow II/3.11.5) of X is given by

$$\text{Var}(X) = \sigma^2 + \frac{1}{\lambda^2}. \quad (6)$$

Thus, the primary work is to compute $E(X^3)$. To do this, we use the moment-generating function of the ex-Gaussian distribution (\rightarrow II/3.11.3) to calculate

$$E(X^3) = M_X'''(0) \quad (7)$$

based on the relationship between raw moment and moment-generating function (\rightarrow I/1.21.2).

First, we differentiate the moment-generating function of the ex-Gaussian distribution (\rightarrow II/3.11.3)

$$M_X(t) = \left(\frac{\lambda}{\lambda - t} \right) \exp \left[\mu t + \frac{1}{2} \sigma^2 t^2 \right] \quad (8)$$

with respect to t . Using the product rule and chain rule, we have:

$$\begin{aligned} M_X'(t) &= \frac{\lambda}{(\lambda - t)^2} \exp \left[\mu t + \frac{1}{2} \sigma^2 t^2 \right] + \left(\frac{\lambda}{\lambda - t} \right) \exp \left[\mu t + \frac{1}{2} \sigma^2 t^2 \right] (\mu + \sigma^2 t) \\ &= \left(\frac{\lambda}{\lambda - t} \right) \cdot \exp \left[\mu t + \frac{1}{2} \sigma^2 t^2 \right] \cdot \left[\frac{1}{\lambda - t} + \mu + \sigma^2 t \right] \\ &= M_X(t) \cdot \left[\frac{1}{\lambda - t} + \mu + \sigma^2 t \right]. \end{aligned} \quad (9)$$

We then use the product rule to obtain the second derivative:

$$\begin{aligned} M_X''(t) &= M_X'(t) \cdot \left[\frac{1}{\lambda - t} + \mu + \sigma^2 t \right] + M_X(t) \cdot \left[\frac{1}{(\lambda - t)^2} + \sigma^2 \right] \\ &= M_X(t) \cdot \left[\frac{1}{\lambda - t} + \mu + \sigma^2 t \right]^2 + M_X(t) \cdot \left[\frac{1}{(\lambda - t)^2} + \sigma^2 \right] \\ &= M_X(t) \cdot \left[\left(\frac{1}{\lambda - t} + \mu + \sigma^2 t \right)^2 + \frac{1}{(\lambda - t)^2} + \sigma^2 \right]. \end{aligned} \quad (10)$$

Finally, we use the product rule and chain rule to obtain the third derivative:

$$M_X'''(t) = M_X'(t) \left[\left(\frac{1}{\lambda - t} + \mu + \sigma^2 t \right)^2 + \frac{1}{(\lambda - t)^2} + \sigma^2 \right] + M_X(t) \left[2 \left(\frac{1}{\lambda - t} + \mu + \sigma^2 t \right) \left(\frac{1}{(\lambda - t)^2} + \sigma^2 \right) + \frac{1}{(\lambda - t)^3} \right] \quad (11)$$

Applying (7), together with (11), yields:

$$\begin{aligned}
E(X^3) &= M_X'''(0) \\
&= M_X'(0) \left[\left(\frac{1}{\lambda} + \mu \right)^2 + \frac{1}{\lambda^2} + \sigma^2 \right] + M_X(0) \left[2 \left(\frac{1}{\lambda} + \mu \right) \left(\frac{1}{\lambda^2} + \sigma^2 \right) + \frac{2}{\lambda^3} \right] \\
&= \left(\mu + \frac{1}{\lambda} \right) \left(\frac{1}{\lambda^2} + \frac{2\mu}{\lambda} + \mu^2 + \frac{1}{\lambda^2} + \sigma^2 \right) + \left(\frac{2}{\lambda^3} + \frac{2\sigma^2}{\lambda} + \frac{2\mu}{\lambda^2} + 2\mu\sigma^2 + \frac{2}{\lambda^3} \right) \\
&= \left(\mu + \frac{1}{\lambda} \right) \left(\frac{2}{\lambda^2} + \frac{2\mu}{\lambda} + \mu^2 + \sigma^2 \right) + \left(\frac{4}{\lambda^3} + \frac{2\sigma^2}{\lambda} + \frac{2\mu}{\lambda^2} + 2\mu\sigma^2 \right) \\
&= \frac{2\mu}{\lambda^2} + \frac{2\mu^2}{\lambda} + \mu^3 + \mu\sigma^2 + \frac{2}{\lambda^3} + \frac{2\mu}{\lambda^2} + \frac{\mu^2}{\lambda} + \frac{\sigma^2}{\lambda} + \frac{4}{\lambda^3} + \frac{2\sigma^2}{\lambda} + \frac{2\mu}{\lambda^2} + 2\mu\sigma^2 \\
&= \frac{6\mu}{\lambda^2} + \frac{6}{\lambda^3} + \frac{3\mu^2 + 3\sigma^2}{\lambda} + 3\mu\sigma^2 + \mu^3.
\end{aligned} \tag{12}$$

We now substitute (12), (5), and (6) into the numerator of (4), giving

$$\begin{aligned}
E(X^3) - 3 \cdot E(X) \cdot \text{Var}(X) - E(X)^3 &= \left(\frac{6\mu}{\lambda^2} + \frac{6}{\lambda^3} + \frac{3\mu^2 + 3\sigma^2}{\lambda} + 3\mu\sigma^2 + \mu^3 \right) - 3 \left(\mu + \frac{1}{\lambda} \right) \left(\sigma^2 + \frac{1}{\lambda^2} \right) - \left(\mu + \frac{1}{\lambda} \right)^3 \\
&= \frac{6\mu}{\lambda^2} + \frac{6}{\lambda^3} + \frac{3\mu^2 + 3\sigma^2}{\lambda} + 3\mu\sigma^2 + \mu^3 - 3\mu\sigma^2 - \frac{3\mu}{\lambda^2} - \frac{3\sigma^2}{\lambda} - \frac{3}{\lambda^3} - \mu^3 - \frac{3}{\lambda} \\
&= \frac{2}{\lambda^3}.
\end{aligned} \tag{13}$$

Thus, we have:

$$\begin{aligned}
\text{Skew}(X) &= \frac{E(X^3) - 3 \cdot E(X) \cdot \text{Var}(X) - E(X)^3}{\text{Var}(X)^{\frac{3}{2}}} \\
&= \frac{\frac{2}{\lambda^3}}{\left(\sigma^2 + \frac{1}{\lambda^2} \right)^{\frac{3}{2}}} \\
&= \frac{2}{\lambda^3 \left(\sigma^2 + \frac{1}{\lambda^2} \right)^{\frac{3}{2}}}.
\end{aligned} \tag{14}$$

This completes the proof of (2). ■

3.11.7 Method of moments

Theorem: Let $y = \{y_1, \dots, y_n\}$ be a set of observed data independent and identically distributed (\rightarrow I/1.2.8) according to an ex-Gaussian distribution (\rightarrow II/3.11.1) with parameters μ , σ , and λ :

$$y_i \sim \text{ex-Gaussian}(\mu, \sigma, \lambda), \quad i = 1, \dots, n. \tag{1}$$

Then, the method-of-moments estimates (\rightarrow I/4.1.8) for the parameters μ , σ , and λ are given by

$$\begin{aligned}
\hat{\mu} &= \bar{y} - \sqrt[3]{\frac{\bar{s} \cdot \bar{v}^{3/2}}{2}} \\
\hat{\sigma} &= \sqrt{\bar{v} \cdot \left(1 - \sqrt[3]{\frac{\bar{s}^2}{4}}\right)} \\
\hat{\lambda} &= \sqrt[3]{\frac{2}{\bar{s} \cdot \bar{v}^{3/2}}} ,
\end{aligned} \tag{2}$$

where \bar{y} is the sample mean (\rightarrow I/1.12.2), \bar{v} is the sample variance (\rightarrow I/1.13.2) and \bar{s} is the sample skewness (\rightarrow I/1.14.2)

$$\begin{aligned}
\bar{y} &= \frac{1}{n} \sum_{i=1}^n y_i \\
\bar{v} &= \frac{1}{n-1} \sum_{i=1}^n (y_i - \bar{y})^2 \\
\bar{s} &= \frac{\frac{1}{n} \sum_{i=1}^n (y_i - \bar{y})^3}{\left[\frac{1}{n} \sum_{i=1}^n (y_i - \bar{y})^2\right]^{3/2}} .
\end{aligned} \tag{3}$$

Proof: The mean (\rightarrow II/3.11.4), variance (\rightarrow II/3.11.5), and skewness (\rightarrow II/3.11.6) of the ex-Gaussian distribution (\rightarrow II/3.11.1) in terms of the parameters μ , σ , and λ are given by

$$\begin{aligned}
E(X) &= \mu + \frac{1}{\lambda} \\
\text{Var}(X) &= \sigma^2 + \frac{1}{\lambda^2} \\
\text{Skew}(X) &= \frac{2}{\lambda^3 \left(\sigma^2 + \frac{1}{\lambda^2}\right)^{3/2}} .
\end{aligned} \tag{4}$$

Thus, matching the moments (\rightarrow I/4.1.8) requires us to solve the following system of equations for μ , σ , and λ :

$$\begin{aligned}
\bar{y} &= \mu + \frac{1}{\lambda} \\
\bar{v} &= \sigma^2 + \frac{1}{\lambda^2} \\
\bar{s} &= \frac{2}{\lambda^3 \left(\sigma^2 + \frac{1}{\lambda^2}\right)^{3/2}} .
\end{aligned} \tag{5}$$

To this end, our first step is to substitute the second equation of (5) into the third equation:

$$\begin{aligned}
\bar{s} &= \frac{2}{\lambda^3 \left(\sigma^2 + \frac{1}{\lambda^2}\right)^{3/2}} \\
&= \frac{2}{\lambda^3 \cdot \bar{v}^{3/2}} .
\end{aligned} \tag{6}$$

Re-expressing (6) in terms of λ^3 and taking the cube root gives:

$$\lambda = \sqrt[3]{\frac{2}{\bar{s} \cdot \bar{v}^{3/2}}} . \quad (7)$$

Next, we solve the first equation of (5) for μ and substitute (7):

$$\begin{aligned} \mu &= \bar{y} - \frac{1}{\lambda} \\ &= \bar{y} - \sqrt[3]{\frac{\bar{s} \cdot \bar{v}^{3/2}}{2}} . \end{aligned} \quad (8)$$

Finally, we solve the second equation of (5) for σ :

$$\sigma^2 = \bar{v} - \frac{1}{\lambda^2} . \quad (9)$$

Taking the square root gives and substituting (7) gives:

$$\begin{aligned} \sigma &= \sqrt{\bar{v} - \frac{1}{\lambda^2}} \\ &= \sqrt{\bar{v} - \left(\sqrt[3]{\frac{\bar{s} \cdot \bar{v}^{3/2}}{2}} \right)^2} \\ &= \sqrt{\bar{v} - \bar{v} \cdot \sqrt[3]{\frac{\bar{s}^2}{4}}} \\ &= \sqrt{\bar{v} \cdot \left(1 - \sqrt[3]{\frac{\bar{s}^2}{4}} \right)} . \end{aligned} \quad (10)$$

Together, (8), (10), and (7) constitute the method-of-moment estimates of μ , σ , and λ .

■

4 Multivariate continuous distributions

4.1 Multivariate normal distribution

4.1.1 Definition

Definition: Let X be an n -dimensional random vector (\rightarrow I/1.2.3). Then, X is said to be multivariate normally distributed with mean μ and covariance Σ

$$X \sim \mathcal{N}(\mu, \Sigma), \quad (1)$$

if and only if its probability density function (\rightarrow I/1.7.1) is given by

$$\mathcal{N}(x; \mu, \Sigma) = \frac{1}{\sqrt{(2\pi)^n |\Sigma|}} \cdot \exp \left[-\frac{1}{2} (x - \mu)^T \Sigma^{-1} (x - \mu) \right] \quad (2)$$

where μ is an n -dimensional real vector and Σ is an $n \times n$ positive-definite matrix.

Sources:

- Koch KR (2007): “Multivariate Normal Distribution”; in: *Introduction to Bayesian Statistics*, ch. 2.5.1, pp. 51-53, eq. 2.195; URL: <https://www.springer.com/gp/book/9783540727231>; DOI: 10.1007/978-3-540-72726-2.

4.1.2 Special case of matrix-normal distribution

Theorem: The multivariate normal distribution (\rightarrow II/4.1.1) is a special case of the matrix-normal distribution (\rightarrow II/5.1.1) with number of variables $p = 1$, i.e. random matrix (\rightarrow I/1.2.2) $X = x \in \mathbb{R}^{n \times 1}$, mean $M = \mu \in \mathbb{R}^{n \times 1}$, covariance across rows $U = \Sigma$ and covariance across columns $V = 1$.

Proof: The probability density function of the matrix-normal distribution (\rightarrow II/5.1.3) is

$$\mathcal{MN}(X; M, U, V) = \frac{1}{\sqrt{(2\pi)^{np} |V|^n |U|^p}} \cdot \exp \left[-\frac{1}{2} \text{tr} (V^{-1} (X - M)^T U^{-1} (X - M)) \right]. \quad (1)$$

Setting $p = 1$, $X = x$, $M = \mu$, $U = \Sigma$ and $V = 1$, we obtain

$$\begin{aligned} \mathcal{MN}(x; \mu, \Sigma, 1) &= \frac{1}{\sqrt{(2\pi)^n |1|^n |\Sigma|^1}} \cdot \exp \left[-\frac{1}{2} \text{tr} (1^{-1} (x - \mu)^T \Sigma^{-1} (x - \mu)) \right] \\ &= \frac{1}{\sqrt{(2\pi)^n |\Sigma|}} \cdot \exp \left[-\frac{1}{2} (x - \mu)^T \Sigma^{-1} (x - \mu) \right] \end{aligned} \quad (2)$$

which is equivalent to the probability density function of the multivariate normal distribution (\rightarrow II/4.1.4). ■

Sources:

- Wikipedia (2022): “Matrix normal distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-07-31; URL: https://en.wikipedia.org/wiki/Matrix_normal_distribution#Definition.

4.1.3 Relationship to chi-squared distribution

Theorem: Let x be an n -dimensional random vector (\rightarrow I/1.2.3) following a multivariate normal distribution (\rightarrow II/4.1.1) with zero mean (\rightarrow I/1.12.16) and arbitrary covariance matrix (\rightarrow II/4.1.8) Σ :

$$x \sim \mathcal{N}(0, \Sigma) . \quad (1)$$

Then, the quadratic form of x , weighted by Σ , follows a chi-squared distribution (\rightarrow II/3.7.1) with n degrees of freedom (\rightarrow I/1.5.12):

$$y = x^T \Sigma^{-1} x \sim \chi^2(n) . \quad (2)$$

Proof: Define a new random vector (\rightarrow I/1.2.3) z as

$$z = \Sigma^{-1/2} x . \quad (3)$$

where $\Sigma^{-1/2}$ is the matrix square root of Σ . This matrix must exist, because Σ is a covariance matrix (\rightarrow I/1.16.1) and thus positive semi-definite (\rightarrow I/1.16.5). Due to the linear transformation theorem (\rightarrow II/4.1.14), z is distributed as

$$\begin{aligned} z &\sim \mathcal{N}\left(\Sigma^{-1/2}0, \Sigma^{-1/2}\Sigma\Sigma^{-1/2T}\right) \\ &\sim \mathcal{N}\left(\Sigma^{-1/2}0, \Sigma^{-1/2}\Sigma^{1/2}\Sigma^{1/2}\Sigma^{-1/2}\right) \\ &\sim \mathcal{N}(0, I_n) , \end{aligned} \quad (4)$$

i.e. each entry of this vector follows (\rightarrow II/4.1.15) a standard normal distribution (\rightarrow II/3.2.3):

$$z_i \sim \mathcal{N}(0, 1) \quad \text{for all } i = 1, \dots, n . \quad (5)$$

We further observe that y can be represented in terms of z

$$y = x^T \Sigma^{-1} x = (x^T \Sigma^{-1/2}) (\Sigma^{-1/2} x) = z^T z , \quad (6)$$

thus z is a sum of n squared standard normally distributed (\rightarrow II/3.2.3) random variables (\rightarrow I/1.2.2)

$$y = \sum_{i=1}^n z_i^2 \quad \text{where all } z_i \sim \mathcal{N}(0, 1) \quad (7)$$

which, by definition, is chi-squared distributed (\rightarrow II/3.7.1) with n degrees of freedom:

$$y \sim \chi^2(n) . \quad (8)$$

■

Sources:

- Koch KR (2007): “Chi-Squared Distribution”; in: *Introduction to Bayesian Statistics*, ch. 2.4.5, pp. 48-49, eq. 2.180; URL: <https://www.springer.com/gp/book/9783540727231>; DOI: 10.1007/978-3-540-72726-2.

4.1.4 Probability density function

Theorem: Let X be a random vector (\rightarrow I/1.2.3) following a multivariate normal distribution (\rightarrow II/4.1.1):

$$X \sim \mathcal{N}(\mu, \Sigma) . \quad (1)$$

Then, the probability density function (\rightarrow I/1.7.1) of X is

$$f_X(x) = \frac{1}{\sqrt{(2\pi)^n |\Sigma|}} \cdot \exp \left[-\frac{1}{2} (x - \mu)^T \Sigma^{-1} (x - \mu) \right] . \quad (2)$$

Proof: This follows directly from the definition of the multivariate normal distribution (\rightarrow II/4.1.1). ■

4.1.5 Moment-generating function

Theorem: Let x follow a multivariate normal distribution (\rightarrow II/4.1.1):

$$x \sim \mathcal{N}(\mu, \Sigma) . \quad (1)$$

Then, the moment-generating function (\rightarrow I/1.9.1) of x is

$$M_x(t) = \exp \left[t^T \mu + \frac{1}{2} t^T \Sigma t \right] . \quad (2)$$

Proof: The moment-generating function of a random vector (\rightarrow I/1.9.1) X is defined as:

$$M_X(t) = \mathbb{E} \left[e^{t^T X} \right] , \quad t \in \mathbb{R}^n . \quad (3)$$

Applying the law of the unconscious statistician (\rightarrow I/1.12.9), we have:

$$M_x(t) = \int_{\mathcal{X}} e^{t^T x} \cdot f_X(x) \, dx . \quad (4)$$

With the probability density function of the multivariate normal distribution (\rightarrow II/4.1.4), we have:

$$M_x(t) = \int_{\mathbb{R}^n} \exp [t^T x] \cdot \frac{1}{\sqrt{(2\pi)^n |\Sigma|}} \cdot \exp \left[-\frac{1}{2} (x - \mu)^T \Sigma^{-1} (x - \mu) \right] \, dx . \quad (5)$$

Now we summarize the two exponential functions inside the integral:

$$\begin{aligned}
M_x(t) &= \int_{\mathbb{R}^n} \frac{1}{\sqrt{(2\pi)^n |\Sigma|}} \cdot \exp \left[-\frac{1}{2} (x - \mu)^T \Sigma^{-1} (x - \mu) + t^T x \right] dx \\
&= \int_{\mathbb{R}^n} \frac{1}{\sqrt{(2\pi)^n |\Sigma|}} \cdot \exp \left[-\frac{1}{2} (x^T \Sigma^{-1} x - 2\mu^T \Sigma^{-1} x + \mu^T \Sigma^{-1} \mu - 2t^T x) \right] dx \\
&= \int_{\mathbb{R}^n} \frac{1}{\sqrt{(2\pi)^n |\Sigma|}} \cdot \exp \left[-\frac{1}{2} (x^T \Sigma^{-1} x - 2(\mu + \Sigma t)^T \Sigma^{-1} x + \mu^T \Sigma^{-1} \mu) \right] dx \\
&= \int_{\mathbb{R}^n} \frac{1}{\sqrt{(2\pi)^n |\Sigma|}} \cdot \exp \left[-\frac{1}{2} ((x - [\mu + \Sigma t])^T \Sigma^{-1} (x - [\mu + \Sigma t]) - 2t^T \mu - t^T \Sigma t) \right] dx \\
&= \exp \left[t^T \mu + \frac{1}{2} t^T \Sigma t \right] \int_{\mathbb{R}^n} \frac{1}{\sqrt{(2\pi)^n |\Sigma|}} \cdot \exp \left[-\frac{1}{2} (x - [\mu + \Sigma t])^T \Sigma^{-1} (x - [\mu + \Sigma t]) \right] dx .
\end{aligned} \tag{6}$$

The integrand is equal to the probability density function of a multivariate normal distribution (\rightarrow II/4.1.4):

$$M_x(t) = \exp \left[t^T \mu + \frac{1}{2} t^T \Sigma t \right] \int_{\mathbb{R}^n} \mathcal{N}(x; \mu + \Sigma t, \Sigma) dx . \tag{7}$$

Because the entire probability density integrates to one (\rightarrow I/1.7.1), we finally have:

$$M_x(t) = \exp \left[t^T \mu + \frac{1}{2} t^T \Sigma t \right] . \tag{8}$$

■

4.1.6 Mean

Theorem: Let x follow a multivariate normal distribution (\rightarrow II/4.1.1):

$$x \sim \mathcal{N}(\mu, \Sigma) . \tag{1}$$

Then, the mean or expected value (\rightarrow I/1.12.1) of x is

$$E(x) = \mu . \tag{2}$$

Proof:

1) First, consider a set of independent (\rightarrow I/1.3.6) and standard normally (\rightarrow II/3.2.3) distributed random variables (\rightarrow I/1.2.2):

$$z_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, 1), \quad i = 1, \dots, n . \tag{3}$$

Then, these variables together form a multivariate normally (\rightarrow II/4.1.17) distributed random vector (\rightarrow I/1.2.3):

$$z \sim \mathcal{N}(0_n, I_n) . \tag{4}$$

By definition, the expected value of a random vector is equal to the vector of all expected values (\rightarrow I/1.12.16):

$$\mathbb{E}(z) = \mathbb{E} \left(\begin{bmatrix} z_1 \\ \vdots \\ z_n \end{bmatrix} \right) = \begin{bmatrix} \mathbb{E}(z_1) \\ \vdots \\ \mathbb{E}(z_n) \end{bmatrix} . \quad (5)$$

Because the expected value of all its entries is zero (\rightarrow II/3.2.16), the expected value of the random vector is

$$\mathbb{E}(z) = \begin{bmatrix} \mathbb{E}(z_1) \\ \vdots \\ \mathbb{E}(z_n) \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \end{bmatrix} = 0_n . \quad (6)$$

2) Next, consider an $n \times n$ matrix A solving the equation $AA^T = \Sigma$. Such a matrix exists, because Σ is defined to be positive definite (\rightarrow II/4.1.1). Then, x can be represented as a linear transformation (\rightarrow II/4.1.14) of z :

$$x = Az + \mu \sim \mathcal{N}(A0_n + \mu, AI_nA^T) = \mathcal{N}(\mu, \Sigma) . \quad (7)$$

Thus, the expected value (\rightarrow I/1.12.1) of x can be written as:

$$\mathbb{E}(x) = \mathbb{E}(Az + \mu) . \quad (8)$$

With the linearity of the expected value (\rightarrow I/1.12.5), this becomes:

$$\begin{aligned} \mathbb{E}(x) &= \mathbb{E}(Az + \mu) \\ &= \mathbb{E}(Az) + \mathbb{E}(\mu) \\ &= A \mathbb{E}(z) + \mu \\ &\stackrel{(6)}{=} A 0_n + \mu \\ &= \mu . \end{aligned} \quad (9)$$

■

Sources:

- Taboga, Marco (2021): “Multivariate normal distribution”; in: *Lectures on probability theory and mathematical statistics*, retrieved on 2022-09-15; URL: <https://www.statlect.com/probability-distributions/multivariate-normal-distribution>.

4.1.7 Mode

Theorem: Let X follow a multivariate normal distribution (\rightarrow II/4.1.1):

$$X \sim \mathcal{N}(\mu, \Sigma) . \quad (1)$$

Then, the mode (\rightarrow I/1.18.3) of X is

$$\text{mode}(X) = \mu . \quad (2)$$

Proof: The mode (\rightarrow I/1.18.3) is the value which maximizes the probability density function (\rightarrow I/1.7.1):

$$\text{mode}(X) = \arg \max_x f_X(x) . \quad (3)$$

The probability density function of the multivariate normal distribution (\rightarrow II/4.1.4) is:

$$f_X(x) = \frac{1}{\sqrt{(2\pi)^n |\Sigma|}} \cdot \exp \left[-\frac{1}{2} (x - \mu)^T \Sigma^{-1} (x - \mu) \right] . \quad (4)$$

The gradient of this function $\nabla_x f_X(x) \in \mathbb{R}^n$ is:

$$\begin{aligned} \nabla_x f_X(x) &= f_X(x) \cdot \nabla_x \left[-\frac{1}{2} (x - \mu)^T \Sigma^{-1} (x - \mu) \right] \\ &= f_X(x) \cdot \left[-\frac{1}{2} (2 \Sigma^{-1} (x - \mu)) \right] \\ &= f_X(x) \cdot [-\Sigma^{-1} (x - \mu)] . \end{aligned} \quad (5)$$

The Hessian of this function $\nabla_x^2 f_X(x) \in \mathbb{R}^{n \times n}$ is:

$$\begin{aligned} \nabla_x^2 f_X(x) &= \nabla_x f_X(x) \cdot [-\Sigma^{-1} (x - \mu)]^T + f_X(x) \cdot \nabla_x [-\Sigma^{-1} (x - \mu)] \\ &= f_X(x) \cdot [-\Sigma^{-1} (x - \mu)] [-\Sigma^{-1} (x - \mu)]^T + f_X(x) \cdot [-\Sigma^{-1}] \\ &= f_X(x) \cdot [\Sigma^{-1} (x - \mu)(x - \mu)^T \Sigma^{-1} - \Sigma^{-1}] . \end{aligned} \quad (6)$$

Setting the gradient (5) to zero, we calculate the root:

$$\begin{aligned} \nabla_x f_X(x) = 0 &= f_X(x) \cdot [-\Sigma^{-1} (x - \mu)] \\ \Leftrightarrow 0 &= -\Sigma^{-1} (x - \mu) \\ \Leftrightarrow x &= \mu . \end{aligned} \quad (7)$$

Plugging this value into the Hessian (6), we obtain:

$$\begin{aligned} \nabla_x^2 f_X(\mu) &= f_X(\mu) \cdot [\Sigma^{-1} (\mu - \mu)(\mu - \mu)^T \Sigma^{-1} - \Sigma^{-1}] \\ &= -f_X(\mu) \cdot \Sigma^{-1} . \end{aligned} \quad (8)$$

Since Σ is positive-definite (\rightarrow II/4.1.1), Σ^{-1} is also positive-definite (\rightarrow II/4.1.1) and since $f_X(\mu)$ is positive, $-f_X(\mu) \cdot \Sigma^{-1}$ is a negative-definite matrix, so that $f_X(\mu)$ is a maximum. Taken together, this shows that

$$\text{mode}(X) = \mu . \quad (9)$$

■

4.1.8 Covariance

Theorem: Let x follow a multivariate normal distribution (\rightarrow II/4.1.1):

$$x \sim \mathcal{N}(\mu, \Sigma) . \quad (1)$$

Then, the covariance matrix (\rightarrow I/1.16.1) of x is

$$\text{Cov}(x) = \Sigma . \quad (2)$$

Proof:

1) First, consider a set of independent (\rightarrow I/1.3.6) and standard normally (\rightarrow II/3.2.3) distributed random variables (\rightarrow I/1.2.2):

$$z_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, 1), \quad i = 1, \dots, n . \quad (3)$$

Then, these variables together form a multivariate normally (\rightarrow II/4.1.17) distributed random vector (\rightarrow I/1.2.3):

$$z \sim \mathcal{N}(0_n, I_n) . \quad (4)$$

Because the covariance is zero for independent random variables (\rightarrow I/1.15.6), we have

$$\text{Cov}(z_i, z_j) = 0 \quad \text{for all } i \neq j . \quad (5)$$

Moreover, as the variance of all entries of the vector is one (\rightarrow II/3.2.19), we have

$$\text{Var}(z_i) = 1 \quad \text{for all } i = 1, \dots, n . \quad (6)$$

Taking (5) and (6) together, the covariance matrix (\rightarrow I/1.16.1) of z is

$$\text{Cov}(z) = \begin{bmatrix} 1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 1 \end{bmatrix} = I_n . \quad (7)$$

2) Next, consider an $n \times n$ matrix A solving the equation $AA^T = \Sigma$. Such a matrix exists, because Σ is defined to be positive definite (\rightarrow II/4.1.1). Then, x can be represented as a linear transformation (\rightarrow II/4.1.14) of z :

$$x = Az + \mu \sim \mathcal{N}(A0_n + \mu, AI_nA^T) = \mathcal{N}(\mu, \Sigma) . \quad (8)$$

Thus, the covariance (\rightarrow I/1.15.1) of x can be written as:

$$\text{Cov}(x) = \text{Cov}(Az + \mu) . \quad (9)$$

With the invariance of the covariance matrix under addition (\rightarrow I/1.16.6)

$$\text{Cov}(x + a) = \text{Cov}(x) \quad (10)$$

and the scaling of the covariance matrix upon multiplication (\rightarrow I/1.16.7)

$$\text{Cov}(Ax) = A\text{Cov}(x)A^T , \quad (11)$$

this becomes:

$$\begin{aligned}
 \text{Cov}(x) &= \text{Cov}(Az + \mu) \\
 &\stackrel{(10)}{=} \text{Cov}(Az) \\
 &\stackrel{(11)}{=} A \text{Cov}(z) A^T \\
 &\stackrel{(7)}{=} A I_n A^T \\
 &= A A^T \\
 &= \Sigma .
 \end{aligned} \tag{12}$$

■

Sources:

- Rosenfeld, Meni (2016): “Deriving the Covariance of Multivariate Gaussian”; in: *StackExchange Mathematics*, retrieved on 2022-09-15; URL: <https://math.stackexchange.com/questions/1905977/deriving-the-covariance-of-multivariate-gaussian>.

4.1.9 Expectation of a quadratic form

Theorem: Let X follow a multivariate normal distribution (\rightarrow II/4.1.1):

$$X \sim \mathcal{N}(\mu, \Sigma) . \tag{1}$$

Then, the expectation (\rightarrow I/1.12.1) of the quadratic form $X^T A X$ is

$$\mathbb{E} [X^T A X] = \mu^T A \mu + \text{tr}(A \Sigma) \tag{2}$$

where A is an $n \times n$ matrix.

Proof: For any random vector (\rightarrow I/1.2.3) $X \in \mathbb{R}^n$, this expectation is a function of mean and covariance (\rightarrow I/1.12.17):

$$\mathbb{E} [X^T A X] = \mathbb{E}(X)^T A X + \text{tr}(A \text{Cov}(X)) . \tag{3}$$

For a multivariate normal random vector (\rightarrow II/4.1.1) $X \sim \mathcal{N}(\mu, \Sigma)$, mean (\rightarrow II/4.1.6) and covariance (\rightarrow II/4.1.8) are

$$\mathbb{E}(X) = \mu \quad \text{and} \quad \text{Cov}(X) = \Sigma . \tag{4}$$

Combing (3) with (4), we have:

$$\mathbb{E} [X^T A X] = \mu^T A \mu + \text{tr}(A \Sigma) \tag{5}$$

■

4.1.10 Differential entropy

Theorem: Let x follow a multivariate normal distribution (\rightarrow II/4.1.1)

$$x \sim \mathcal{N}(\mu, \Sigma) . \quad (1)$$

Then, the differential entropy (\rightarrow I/2.2.1) of x in nats is

$$h(x) = \frac{n}{2} \ln(2\pi) + \frac{1}{2} \ln |\Sigma| + \frac{1}{2} n . \quad (2)$$

Proof: The differential entropy (\rightarrow I/2.2.1) of a random variable is defined as

$$h(X) = - \int_{\mathcal{X}} p(x) \log_b p(x) dx . \quad (3)$$

To measure $h(X)$ in nats, we set $b = e$, such that (\rightarrow I/1.12.1)

$$h(X) = -E [\ln p(x)] . \quad (4)$$

With the probability density function of the multivariate normal distribution (\rightarrow II/4.1.4), the differential entropy of x is:

$$\begin{aligned} h(x) &= -E \left[\ln \left(\frac{1}{\sqrt{(2\pi)^n |\Sigma|}} \cdot \exp \left[-\frac{1}{2} (x - \mu)^T \Sigma^{-1} (x - \mu) \right] \right) \right] \\ &= -E \left[-\frac{n}{2} \ln(2\pi) - \frac{1}{2} \ln |\Sigma| - \frac{1}{2} (x - \mu)^T \Sigma^{-1} (x - \mu) \right] \\ &= \frac{n}{2} \ln(2\pi) + \frac{1}{2} \ln |\Sigma| + \frac{1}{2} E [(x - \mu)^T \Sigma^{-1} (x - \mu)] . \end{aligned} \quad (5)$$

The last term can be evaluated as

$$\begin{aligned} E [(x - \mu)^T \Sigma^{-1} (x - \mu)] &= E [\text{tr} ((x - \mu)^T \Sigma^{-1} (x - \mu))] \\ &= E [\text{tr} (\Sigma^{-1} (x - \mu) (x - \mu)^T)] \\ &= \text{tr} (\Sigma^{-1} E [(x - \mu) (x - \mu)^T]) \\ &= \text{tr} (\Sigma^{-1} \Sigma) \\ &= \text{tr} (I_n) \\ &= n , \end{aligned} \quad (6)$$

such that the differential entropy is

$$h(x) = \frac{n}{2} \ln(2\pi) + \frac{1}{2} \ln |\Sigma| + \frac{1}{2} n . \quad (7)$$

■

Sources:

- Kiuahn (2018): “Entropy of the multivariate Gaussian”; in: *StackExchange Mathematics*, retrieved on 2020-05-14; URL: <https://math.stackexchange.com/questions/2029707/entropy-of-the-multivariate-ga>

4.1.11 Mutual information

Theorem: Let $X \in \mathbb{R}^n$ and $Y \in \mathbb{R}^m$ be random vectors (\rightarrow I/1.2.3) that are jointly multivariate normal (\rightarrow II/4.1.1):

$$\begin{bmatrix} X \\ Y \end{bmatrix} \sim \mathcal{N} \left(\begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}, \begin{bmatrix} \Sigma_1 & \Sigma_{12} \\ \Sigma_{21} & \Sigma_2 \end{bmatrix} \right) . \quad (1)$$

Then, the mutual information (\rightarrow I/2.4.1) of X and Y is

$$I(X, Y) = \frac{1}{2} \ln \left[\frac{|\Sigma_1| |\Sigma_2|}{|\Sigma|} \right] \quad (2)$$

where $\Sigma \in \mathbb{R}^{p \times p}$ is the covariance matrix (\rightarrow I/1.16.1) of the random vector (\rightarrow I/1.2.3) $\begin{bmatrix} X \\ Y \end{bmatrix} \in \mathbb{R}^p$,

with $p = n + m$.

Proof: Mutual information can be written in terms of marginal and joint differential entropy (\rightarrow I/2.4.3):

$$I(X, Y) = h(X) + h(Y) - h(X, Y) . \quad (3)$$

The marginal distributions of the multivariate normal distribution are also multivariate normal (\rightarrow II/4.1.15)

$$\begin{bmatrix} X_1 \\ X_2 \end{bmatrix} \sim \mathcal{N} \left(\begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}, \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix} \right) \Rightarrow X_1 \sim \mathcal{N}(\mu_1, \Sigma_{11}) , \quad (4)$$

such that the marginals (\rightarrow I/1.5.3) of X and Y are:

$$X \sim \mathcal{N}(\mu_1, \Sigma_1) \quad \text{and} \quad Y \sim \mathcal{N}(\mu_2, \Sigma_2) . \quad (5)$$

The differential entropy of the multivariate normal distribution (\rightarrow II/4.1.10) is

$$h(x) = \frac{n}{2} \ln(2\pi) + \frac{1}{2} \ln |\Sigma| + \frac{1}{2} n \quad (6)$$

where $|\Sigma|$ is the determinant of Σ . Combining (3) with (6), we get:

$$\begin{aligned}
I(X, Y) &\stackrel{(3)}{=} h(X) + h(Y) - h(X, Y) \\
&\stackrel{(5)}{=} h[\mathcal{N}(\mu_1, \Sigma_1)] + h[\mathcal{N}(\mu_2, \Sigma_2)] - h[\mathcal{N}(\mu, \Sigma)] \\
&\stackrel{(6)}{=} \left[\frac{n}{2} \ln(2\pi) + \frac{1}{2} \ln |\Sigma_1| + \frac{1}{2} n \right] + \left[\frac{m}{2} \ln(2\pi) + \frac{1}{2} \ln |\Sigma_2| + \frac{1}{2} m \right] - \left[\frac{p}{2} \ln(2\pi) + \frac{1}{2} \ln |\Sigma| + \frac{1}{2} p \right] \\
&= \left(\frac{n+m-p}{2} \ln(2\pi) + \frac{1}{2} (n+m-p) \right) + \left(\frac{1}{2} \ln |\Sigma_1| + \frac{1}{2} \ln |\Sigma_2| - \frac{1}{2} \ln |\Sigma| \right) \\
&= \frac{1}{2} (\ln |\Sigma_1| + \ln |\Sigma_2| - \ln |\Sigma|) \\
&= \frac{1}{2} \ln \left[\frac{|\Sigma_1| |\Sigma_2|}{|\Sigma|} \right].
\end{aligned} \tag{7}$$

■

Sources:

- a06e (2019): “Mutual information between subsets of variables in the multivariate normal distribution”; in: *StackExchange Cross Validated*, retrieved on 2024-11-01; URL: <https://stats.stackexchange.com/a/438613/270304>.

4.1.12 Kullback-Leibler divergence

Theorem: Let x be an n -dimensional random vector (\rightarrow I/1.2.3). Assume two multivariate normal distributions (\rightarrow II/4.1.1) P and Q specifying the probability distribution of x as

$$\begin{aligned}
P : x &\sim \mathcal{N}(\mu_1, \Sigma_1) \\
Q : x &\sim \mathcal{N}(\mu_2, \Sigma_2).
\end{aligned} \tag{1}$$

Then, the Kullback-Leibler divergence (\rightarrow I/2.5.1) of P from Q is given by

$$\text{KL}[P || Q] = \frac{1}{2} \left[(\mu_2 - \mu_1)^T \Sigma_2^{-1} (\mu_2 - \mu_1) + \text{tr}(\Sigma_2^{-1} \Sigma_1) - \ln \frac{|\Sigma_1|}{|\Sigma_2|} - n \right]. \tag{2}$$

Proof: The KL divergence for a continuous random variable (\rightarrow I/2.5.1) is given by

$$\text{KL}[P || Q] = \int_{\mathcal{X}} p(x) \ln \frac{p(x)}{q(x)} dx \tag{3}$$

which, applied to the multivariate normal distributions (\rightarrow II/4.1.1) in (1), yields

$$\begin{aligned}
\text{KL}[P || Q] &= \int_{\mathbb{R}^n} \mathcal{N}(x; \mu_1, \Sigma_1) \ln \frac{\mathcal{N}(x; \mu_1, \Sigma_1)}{\mathcal{N}(x; \mu_2, \Sigma_2)} dx \\
&= \left\langle \ln \frac{\mathcal{N}(x; \mu_1, \Sigma_1)}{\mathcal{N}(x; \mu_2, \Sigma_2)} \right\rangle_{p(x)}.
\end{aligned} \tag{4}$$

Using the probability density function of the multivariate normal distribution (\rightarrow II/4.1.4), this becomes:

$$\begin{aligned}
\text{KL}[P \parallel Q] &= \left\langle \ln \frac{\frac{1}{\sqrt{(2\pi)^n |\Sigma_1|}} \cdot \exp \left[-\frac{1}{2} (x - \mu_1)^T \Sigma_1^{-1} (x - \mu_1) \right]}{\frac{1}{\sqrt{(2\pi)^n |\Sigma_2|}} \cdot \exp \left[-\frac{1}{2} (x - \mu_2)^T \Sigma_2^{-1} (x - \mu_2) \right]} \right\rangle_{p(x)} \\
&= \left\langle \frac{1}{2} \ln \frac{|\Sigma_2|}{|\Sigma_1|} - \frac{1}{2} (x - \mu_1)^T \Sigma_1^{-1} (x - \mu_1) + \frac{1}{2} (x - \mu_2)^T \Sigma_2^{-1} (x - \mu_2) \right\rangle_{p(x)} \quad (5) \\
&= \frac{1}{2} \left\langle \ln \frac{|\Sigma_2|}{|\Sigma_1|} - (x - \mu_1)^T \Sigma_1^{-1} (x - \mu_1) + (x - \mu_2)^T \Sigma_2^{-1} (x - \mu_2) \right\rangle_{p(x)}.
\end{aligned}$$

Now, using the fact that $x = \text{tr}(x)$, if a is scalar, and the trace property $\text{tr}(ABC) = \text{tr}(BCA)$, we have:

$$\begin{aligned}
\text{KL}[P \parallel Q] &= \frac{1}{2} \left\langle \ln \frac{|\Sigma_2|}{|\Sigma_1|} - \text{tr} [\Sigma_1^{-1} (x - \mu_1)(x - \mu_1)^T] + \text{tr} [\Sigma_2^{-1} (x - \mu_2)(x - \mu_2)^T] \right\rangle_{p(x)} \\
&= \frac{1}{2} \left\langle \ln \frac{|\Sigma_2|}{|\Sigma_1|} - \text{tr} [\Sigma_1^{-1} (x - \mu_1)(x - \mu_1)^T] + \text{tr} [\Sigma_2^{-1} (xx^T - 2\mu_2 x^T + \mu_2 \mu_2^T)] \right\rangle_{p(x)}. \quad (6)
\end{aligned}$$

Because trace function and expected value are both linear operators (\rightarrow I/1.12.20), the expectation can be moved inside the trace:

$$\begin{aligned}
\text{KL}[P \parallel Q] &= \frac{1}{2} \left(\ln \frac{|\Sigma_2|}{|\Sigma_1|} - \text{tr} [\Sigma_1^{-1} \langle (x - \mu_1)(x - \mu_1)^T \rangle_{p(x)}] + \text{tr} [\Sigma_2^{-1} \langle xx^T - 2\mu_2 x^T + \mu_2 \mu_2^T \rangle_{p(x)}] \right) \\
&= \frac{1}{2} \left(\ln \frac{|\Sigma_2|}{|\Sigma_1|} - \text{tr} [\Sigma_1^{-1} \langle (x - \mu_1)(x - \mu_1)^T \rangle_{p(x)}] + \text{tr} [\Sigma_2^{-1} (\langle xx^T \rangle_{p(x)} - \langle 2\mu_2 x^T \rangle_{p(x)} + \langle \mu_2 \mu_2^T \rangle_{p(x)})] \right) \quad (7)
\end{aligned}$$

Using the expectation of a linear form for the multivariate normal distribution (\rightarrow II/4.1.14)

$$x \sim \mathcal{N}(\mu, \Sigma) \quad \Rightarrow \quad \langle Ax \rangle = A\mu \quad (8)$$

and the expectation of a quadratic form for the multivariate normal distribution (\rightarrow I/1.12.17)

$$x \sim \mathcal{N}(\mu, \Sigma) \quad \Rightarrow \quad \langle x^T A x \rangle = \mu^T A \mu + \text{tr}(A \Sigma), \quad (9)$$

the Kullback-Leibler divergence from (7) becomes:

$$\begin{aligned}
\text{KL}[P \parallel Q] &= \frac{1}{2} \left(\ln \frac{|\Sigma_2|}{|\Sigma_1|} - \text{tr} [\Sigma_1^{-1} \Sigma_1] + \text{tr} [\Sigma_2^{-1} (\Sigma_1 + \mu_1 \mu_1^T - 2\mu_2 \mu_1^T + \mu_2 \mu_2^T)] \right) \\
&= \frac{1}{2} \left(\ln \frac{|\Sigma_2|}{|\Sigma_1|} - \text{tr} [I_n] + \text{tr} [\Sigma_2^{-1} \Sigma_1] + \text{tr} [\Sigma_2^{-1} (\mu_1 \mu_1^T - 2\mu_2 \mu_1^T + \mu_2 \mu_2^T)] \right) \\
&= \frac{1}{2} \left(\ln \frac{|\Sigma_2|}{|\Sigma_1|} - n + \text{tr} [\Sigma_2^{-1} \Sigma_1] + \text{tr} [\mu_1^T \Sigma_2^{-1} \mu_1 - 2\mu_1^T \Sigma_2^{-1} \mu_2 + \mu_2^T \Sigma_2^{-1} \mu_2] \right) \quad (10) \\
&= \frac{1}{2} \left[\ln \frac{|\Sigma_2|}{|\Sigma_1|} - n + \text{tr} [\Sigma_2^{-1} \Sigma_1] + (\mu_2 - \mu_1)^T \Sigma_2^{-1} (\mu_2 - \mu_1) \right].
\end{aligned}$$

Finally, rearranging the terms, we get:

$$\text{KL}[P || Q] = \frac{1}{2} \left[(\mu_2 - \mu_1)^T \Sigma_2^{-1} (\mu_2 - \mu_1) + \text{tr}(\Sigma_2^{-1} \Sigma_1) - \ln \frac{|\Sigma_1|}{|\Sigma_2|} - n \right]. \quad (11)$$

■

Sources:

- Duchi, John (2014): “Derivations for Linear Algebra and Optimization”; in: *University of California, Berkeley*; URL: http://www.eecs.berkeley.edu/~jduchi/projects/general_notes.pdf.

4.1.13 Maximum entropy distribution

Theorem: The multivariate normal distribution (\rightarrow II/4.1.1) maximizes differential entropy (\rightarrow I/2.2.1) for a random vector (\rightarrow I/1.2.3) with fixed covariance matrix (\rightarrow I/1.16.1).

Proof: For a random vector (\rightarrow I/1.2.2) X with set of possible values \mathcal{X} and probability density function (\rightarrow I/1.7.1) $p(x)$, the differential entropy (\rightarrow I/2.2.1) is defined as:

$$h(X) = - \int_{\mathcal{X}} p(x) \log p(x) dx. \quad (1)$$

Let $g(x)$ be the probability density function (\rightarrow I/1.7.1) of a multivariate normal distribution (\rightarrow II/3.2.1) with mean (\rightarrow I/1.12.1) μ and covariance (\rightarrow I/1.16.1) Σ and let $f(x)$ be an arbitrary probability density function (\rightarrow I/1.7.1) with the same covariance (\rightarrow I/1.16.1). Since differential entropy (\rightarrow I/2.2.1) is translation-invariant (\rightarrow I/2.2.3), we can assume that $f(x)$ has the same mean as $g(x)$.

Consider the Kullback-Leibler divergence (\rightarrow I/2.5.1) of distribution $f(x)$ from distribution $g(x)$ which is non-negative (\rightarrow I/2.5.2):

$$\begin{aligned} 0 \leq \text{KL}[f||g] &= \int_{\mathcal{X}} f(x) \log \frac{f(x)}{g(x)} dx \\ &= \int_{\mathcal{X}} f(x) \log f(x) dx - \int_{\mathcal{X}} f(x) \log g(x) dx \\ &\stackrel{(1)}{=} -h[f(x)] - \int_{\mathcal{X}} f(x) \log g(x) dx. \end{aligned} \quad (2)$$

By plugging the probability density function of the multivariate normal distribution (\rightarrow II/4.1.4) into the second term, we obtain:

$$\begin{aligned} \int_{\mathcal{X}} f(x) \log g(x) dx &= \int_{\mathcal{X}} f(x) \log \left(\frac{1}{\sqrt{(2\pi)^n |\Sigma|}} \cdot \exp \left[-\frac{1}{2} (x - \mu)^T \Sigma^{-1} (x - \mu) \right] \right) dx \\ &= \int_{\mathcal{X}} f(x) \log \left(\frac{1}{\sqrt{(2\pi)^n |\Sigma|}} \right) dx + \int_{\mathcal{X}} f(x) \log \left(\exp \left[-\frac{1}{2} (x - \mu)^T \Sigma^{-1} (x - \mu) \right] \right) dx \\ &= \left(-\frac{n}{2} \log(2\pi) - \frac{1}{2} \log |\Sigma| \right) \int_{\mathcal{X}} f(x) dx - \frac{1}{2} \int_{\mathcal{X}} f(x) [(x - \mu)^T \Sigma^{-1} (x - \mu)] dx. \end{aligned} \quad (3)$$

Because the entire integral over a probability density function is one (\rightarrow I/1.7.1) and with the definition of the expected value (\rightarrow I/1.12.1), this becomes:

$$\int_{\mathcal{X}} f(x) \log g(x) dx = -\frac{n}{2} \log(2\pi) - \frac{1}{2} \log |\Sigma| - \frac{1}{2} \langle (x - \mu)^T \Sigma^{-1} (x - \mu) \rangle_{f(x)} . \quad (4)$$

Using the expectation of a trace (\rightarrow I/1.12.20) and the definition of the covariance matrix (\rightarrow I/1.16.1), the second term can be developed as follows:

$$\begin{aligned} \langle (x - \mu)^T \Sigma^{-1} (x - \mu) \rangle_{f(x)} &= \langle \text{tr} [(x - \mu)^T \Sigma^{-1} (x - \mu)] \rangle_{f(x)} \\ &= \langle \text{tr} [\Sigma^{-1} (x - \mu) (x - \mu)^T] \rangle_{f(x)} \\ &= \text{tr} \left[\Sigma^{-1} \langle (x - \mu) (x - \mu)^T \rangle_{f(x)} \right] \\ &= \text{tr} [\Sigma^{-1} \Sigma] \\ &= \text{tr} [I_n] \\ &= n . \end{aligned} \quad (5)$$

Thus, the second term in (2) is equal to

$$\int_{\mathcal{X}} f(x) \log g(x) dx = -\frac{n}{2} \log(2\pi) - \frac{1}{2} \log |\Sigma| - \frac{n}{2} . \quad (6)$$

This is actually the negative of the differential entropy of the multivariate normal distribution (\rightarrow II/3.2.23), such that:

$$\int_{\mathcal{X}} f(x) \log g(x) dx = -h[\mathcal{N}(\mu, \Sigma)] = -h[g(x)] . \quad (7)$$

Combining (2) with (7), we can show that

$$\begin{aligned} 0 &\leq \text{KL}[f||g] \\ 0 &\leq -h[f(x)] - (-h[g(x)]) \\ h[g(x)] &\geq h[f(x)] \end{aligned} \quad (8)$$

which means that the differential entropy (\rightarrow I/2.2.1) of the multivariate normal distribution (\rightarrow II/4.1.1) $\mathcal{N}(\mu, \Sigma)$ will be larger than or equal to any other distribution (\rightarrow I/1.5.1) with the same covariance matrix (\rightarrow I/1.16.1) Σ . ■

Sources:

- Wikipedia (2025): “Maximum entropy probability distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2025-05-23; URL: https://en.wikipedia.org/wiki/Maximum_entropy_probability_distribution#Other_examples.

4.1.14 Linear transformation

Theorem: Let x follow a multivariate normal distribution (\rightarrow II/4.1.1):

$$x \sim \mathcal{N}(\mu, \Sigma) . \quad (1)$$

Then, any linear transformation of x is also multivariate normally distributed:

$$y = Ax + b \sim \mathcal{N}(A\mu + b, A\Sigma A^T) . \quad (2)$$

Proof: The moment-generating function of a random vector (\rightarrow I/1.9.1) x is

$$M_x(t) = \mathbb{E} \left(\exp [t^T x] \right) \quad (3)$$

and therefore the moment-generating function of the random vector y is given by

$$\begin{aligned} M_y(t) &\stackrel{(2)}{=} \mathbb{E} \left(\exp [t^T (Ax + b)] \right) \\ &= \mathbb{E} \left(\exp [t^T Ax] \cdot \exp [t^T b] \right) \\ &= \exp [t^T b] \cdot \mathbb{E} \left(\exp [t^T Ax] \right) \\ &\stackrel{(3)}{=} \exp [t^T b] \cdot M_x(A^T t) . \end{aligned} \quad (4)$$

The moment-generating function of the multivariate normal distribution (\rightarrow II/4.1.5) is

$$M_x(t) = \exp \left[t^T \mu + \frac{1}{2} t^T \Sigma t \right] \quad (5)$$

and therefore the moment-generating function of the random vector y becomes

$$\begin{aligned} M_y(t) &\stackrel{(4)}{=} \exp [t^T b] \cdot M_x(A^T t) \\ &\stackrel{(5)}{=} \exp [t^T b] \cdot \exp \left[t^T A\mu + \frac{1}{2} t^T A\Sigma A^T t \right] \\ &= \exp \left[t^T (A\mu + b) + \frac{1}{2} t^T A\Sigma A^T t \right] . \end{aligned} \quad (6)$$

Because moment-generating function and probability density function of a random variable are equivalent, this demonstrates that y is following a multivariate normal distribution with mean $A\mu + b$ and covariance $A\Sigma A^T$. ■

Sources:

- Taboga, Marco (2010): “Linear combinations of normal random variables”; in: *Lectures on probability and statistics*, retrieved on 2019-08-27; URL: <https://www.statlect.com/probability-distributions/normal-distribution-linear-combinations>.

4.1.15 Marginal distributions

Theorem: Let x follow a multivariate normal distribution (\rightarrow II/4.1.1):

$$x \sim \mathcal{N}(\mu, \Sigma) . \quad (1)$$

Then, the marginal distribution (\rightarrow I/1.5.3) of any subset vector x_s is also a multivariate normal distribution

$$x_s \sim \mathcal{N}(\mu_s, \Sigma_s) \quad (2)$$

where μ_s drops the irrelevant variables (the ones not in the subset, i.e. marginalized out) from the mean vector μ and Σ_s drops the corresponding rows and columns from the covariance matrix Σ .

Proof: Define an $m \times n$ subset matrix S such that $s_{ij} = 1$, if the j -th element in x_s corresponds to the i -th element in x , and $s_{ij} = 0$ otherwise. Then,

$$x_s = Sx \quad (3)$$

and we can apply the linear transformation theorem (\rightarrow II/4.1.14) to give

$$x_s \sim \mathcal{N}(S\mu, S\Sigma S^T). \quad (4)$$

Finally, we see that $S\mu = \mu_s$ and $S\Sigma S^T = \Sigma_s$. ■

4.1.16 Conditional distributions

Theorem: Let x follow a multivariate normal distribution (\rightarrow II/4.1.1)

$$x \sim \mathcal{N}(\mu, \Sigma). \quad (1)$$

Then, the conditional distribution (\rightarrow I/1.5.4) of any subset vector x_1 , given the complement vector x_2 , is also a multivariate normal distribution

$$x_1|x_2 \sim \mathcal{N}(\mu_{1|2}, \Sigma_{1|2}) \quad (2)$$

where the conditional mean (\rightarrow I/1.12.1) and covariance (\rightarrow I/1.15.1) are

$$\begin{aligned} \mu_{1|2} &= \mu_1 + \Sigma_{12}\Sigma_{22}^{-1}(x_2 - \mu_2) \\ \Sigma_{1|2} &= \Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21} \end{aligned} \quad (3)$$

with block-wise mean and covariance defined as

$$\begin{aligned} \mu &= \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix} \\ \Sigma &= \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix}. \end{aligned} \quad (4)$$

Proof: Without loss of generality, we assume that, in parallel to (4),

$$x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \quad (5)$$

where x_1 is an $n_1 \times 1$ vector, x_2 is an $n_2 \times 1$ vector and x is an $n_1 + n_2 = n \times 1$ vector.

By construction, the joint distribution (\rightarrow I/1.5.2) of x_1 and x_2 is:

$$x_1, x_2 \sim \mathcal{N}(\mu, \Sigma) . \quad (6)$$

Moreover, the marginal distribution (\rightarrow I/1.5.3) of x_2 follows from (\rightarrow II/4.1.15) (1) and (4) as

$$x_2 \sim \mathcal{N}(\mu_2, \Sigma_{22}) . \quad (7)$$

According to the law of conditional probability (\rightarrow I/1.3.4), it holds that

$$p(x_1|x_2) = \frac{p(x_1, x_2)}{p(x_2)} \quad (8)$$

Applying (6) and (7) to (8), we have:

$$p(x_1|x_2) = \frac{\mathcal{N}(x; \mu, \Sigma)}{\mathcal{N}(x_2; \mu_2, \Sigma_{22})} . \quad (9)$$

Using the probability density function of the multivariate normal distribution (\rightarrow II/4.1.4), this becomes:

$$\begin{aligned} p(x_1|x_2) &= \frac{1/\sqrt{(2\pi)^n|\Sigma|} \cdot \exp\left[-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)\right]}{1/\sqrt{(2\pi)^{n_2}|\Sigma_{22}|} \cdot \exp\left[-\frac{1}{2}(x_2-\mu_2)^T\Sigma_{22}^{-1}(x_2-\mu_2)\right]} \\ &= \frac{1}{\sqrt{(2\pi)^{n-n_2}}} \cdot \sqrt{\frac{|\Sigma_{22}|}{|\Sigma|}} \cdot \exp\left[-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu) + \frac{1}{2}(x_2-\mu_2)^T\Sigma_{22}^{-1}(x_2-\mu_2)\right] . \end{aligned} \quad (10)$$

Writing the inverse of Σ as

$$\Sigma^{-1} = \begin{bmatrix} \Sigma^{11} & \Sigma^{12} \\ \Sigma^{21} & \Sigma^{22} \end{bmatrix} \quad (11)$$

and applying (4) to (10), we get:

$$\begin{aligned} p(x_1|x_2) &= \frac{1}{\sqrt{(2\pi)^{n-n_2}}} \cdot \sqrt{\frac{|\Sigma_{22}|}{|\Sigma|}} \cdot \\ &\quad \exp\left[-\frac{1}{2}\left(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} - \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}\right)^T \begin{bmatrix} \Sigma^{11} & \Sigma^{12} \\ \Sigma^{21} & \Sigma^{22} \end{bmatrix} \left(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} - \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}\right) \right. \\ &\quad \left. + \frac{1}{2}(x_2 - \mu_2)^T \Sigma_{22}^{-1}(x_2 - \mu_2)\right] . \end{aligned} \quad (12)$$

Multiplying out within the exponent of (12), we have

$$\begin{aligned} p(x_1|x_2) &= \frac{1}{\sqrt{(2\pi)^{n-n_2}}} \cdot \sqrt{\frac{|\Sigma_{22}|}{|\Sigma|}} \cdot \\ &\quad \exp\left[-\frac{1}{2}\left((x_1 - \mu_1)^T \Sigma^{11}(x_1 - \mu_1) + 2(x_1 - \mu_1)^T \Sigma^{12}(x_2 - \mu_2) + (x_2 - \mu_2)^T \Sigma^{22}(x_2 - \mu_2)\right) \right. \\ &\quad \left. + \frac{1}{2}(x_2 - \mu_2)^T \Sigma_{22}^{-1}(x_2 - \mu_2)\right] \end{aligned} \quad (13)$$

where we have used the fact that $\Sigma^{21T} = \Sigma^{12}$, because Σ^{-1} is a symmetric matrix.

The inverse of a block matrix is

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix}^{-1} = \begin{bmatrix} (A - BD^{-1}C)^{-1} & -(A - BD^{-1}C)^{-1}BD^{-1} \\ -D^{-1}C(A - BD^{-1}C)^{-1} & D^{-1} + D^{-1}C(A - BD^{-1}C)^{-1}BD^{-1} \end{bmatrix}, \quad (14)$$

thus the inverse of Σ in (11) is

$$\begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix}^{-1} = \begin{bmatrix} (\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})^{-1} & -(\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})^{-1}\Sigma_{12}\Sigma_{22}^{-1} \\ -\Sigma_{22}^{-1}\Sigma_{21}(\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})^{-1} & \Sigma_{22}^{-1} + \Sigma_{22}^{-1}\Sigma_{21}(\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})^{-1}\Sigma_{12}\Sigma_{22}^{-1} \end{bmatrix}. \quad (15)$$

Plugging this into (13), we have:

$$\begin{aligned} p(x_1|x_2) &= \frac{1}{\sqrt{(2\pi)^{n-n_2}}} \cdot \sqrt{\frac{|\Sigma_{22}|}{|\Sigma|}} \cdot \\ &\exp \left[-\frac{1}{2} \left((x_1 - \mu_1)^T (\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})^{-1} (x_1 - \mu_1) - \right. \right. \\ &\quad 2(x_1 - \mu_1)^T (\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})^{-1} \Sigma_{12}\Sigma_{22}^{-1} (x_2 - \mu_2) + \\ &\quad (x_2 - \mu_2)^T [\Sigma_{22}^{-1} + \Sigma_{22}^{-1}\Sigma_{21}(\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})^{-1}\Sigma_{12}\Sigma_{22}^{-1}] (x_2 - \mu_2)) \\ &\quad \left. + \frac{1}{2} ((x_2 - \mu_2)^T \Sigma_{22}^{-1} (x_2 - \mu_2)) \right]. \end{aligned} \quad (16)$$

Eliminating some terms, we have:

$$\begin{aligned} p(x_1|x_2) &= \frac{1}{\sqrt{(2\pi)^{n-n_2}}} \cdot \sqrt{\frac{|\Sigma_{22}|}{|\Sigma|}} \cdot \\ &\exp \left[-\frac{1}{2} \left((x_1 - \mu_1)^T (\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})^{-1} (x_1 - \mu_1) - \right. \right. \\ &\quad 2(x_1 - \mu_1)^T (\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})^{-1} \Sigma_{12}\Sigma_{22}^{-1} (x_2 - \mu_2) + \\ &\quad \left. (x_2 - \mu_2)^T \Sigma_{22}^{-1} \Sigma_{21} (\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})^{-1} \Sigma_{12}\Sigma_{22}^{-1} (x_2 - \mu_2) \right). \end{aligned} \quad (17)$$

Rearranging the terms, we have

$$\begin{aligned} p(x_1|x_2) &= \frac{1}{\sqrt{(2\pi)^{n-n_2}}} \cdot \sqrt{\frac{|\Sigma_{22}|}{|\Sigma|}} \cdot \exp \left[-\frac{1}{2} \cdot \right. \\ &\quad \left. [(x_1 - \mu_1) - \Sigma_{12}\Sigma_{22}^{-1}(x_2 - \mu_2)]^T (\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})^{-1} [(x_1 - \mu_1) - \Sigma_{12}\Sigma_{22}^{-1}(x_2 - \mu_2)] \right] \\ &= \frac{1}{\sqrt{(2\pi)^{n-n_2}}} \cdot \sqrt{\frac{|\Sigma_{22}|}{|\Sigma|}} \cdot \exp \left[-\frac{1}{2} \cdot \right. \\ &\quad \left. [x_1 - (\mu_1 + \Sigma_{12}\Sigma_{22}^{-1}(x_2 - \mu_2))]^T (\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})^{-1} [x_1 - (\mu_1 + \Sigma_{12}\Sigma_{22}^{-1}(x_2 - \mu_2))] \right] \end{aligned} \quad (18)$$

where we have used the fact that $\Sigma_{21} = \Sigma_{12}^T$, because Σ is a covariance matrix (\rightarrow I/1.16.1).

The determinant of a block matrix is

$$\begin{vmatrix} A & B \\ C & D \end{vmatrix} = |D| \cdot |A - BD^{-1}C|, \quad (19)$$

such that we have for Σ that

$$\begin{vmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{vmatrix} = |\Sigma_{22}| \cdot |\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}|. \quad (20)$$

With this and $n - n_2 = n_1$, we finally arrive at

$$p(x_1|x_2) = \frac{1}{\sqrt{(2\pi)^{n_1} |\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}|}} \cdot \exp \left[-\frac{1}{2} \cdot \left[x_1 - (\mu_1 + \Sigma_{12}\Sigma_{22}^{-1}(x_2 - \mu_2)) \right]^T (\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})^{-1} \left[x_1 - (\mu_1 + \Sigma_{12}\Sigma_{22}^{-1}(x_2 - \mu_2)) \right] \right] \quad (21)$$

which is the probability density function of a multivariate normal distribution (\rightarrow II/4.1.4)

$$p(x_1|x_2) = \mathcal{N}(x_1; \mu_{1|2}, \Sigma_{1|2}) \quad (22)$$

with the mean (\rightarrow I/1.12.1) $\mu_{1|2}$ and covariance (\rightarrow I/1.15.1) $\Sigma_{1|2}$ given by (3).

■

Sources:

- Wang, Ruye (2006): “Marginal and conditional distributions of multivariate normal distribution”; in: *Computer Image Processing and Analysis*; URL: <http://fourier.eng.hmc.edu/e161/lectures/gaussianprocess/node7.html>.
- Wikipedia (2020): “Multivariate normal distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-03-20; URL: https://en.wikipedia.org/wiki/Multivariate_normal_distribution#Conditional_distributions.

4.1.17 Conditions for independence

Theorem: Let x be an n -dimensional random vector (\rightarrow I/1.2.3) following a multivariate normal distribution (\rightarrow II/4.1.1):

$$x \sim \mathcal{N}(\mu, \Sigma). \quad (1)$$

Then, the components of x are statistically independent (\rightarrow I/1.3.6), if and only if the covariance matrix (\rightarrow I/1.16.1) is a diagonal matrix:

$$p(x) = p(x_1) \cdot \dots \cdot p(x_n) \quad \Leftrightarrow \quad \Sigma = \text{diag}([\sigma_1^2, \dots, \sigma_n^2]). \quad (2)$$

Proof: The marginal distribution of one entry from a multivariate normal random vector is a univariate normal distribution (\rightarrow II/4.1.15) where mean (\rightarrow I/1.12.1) and variance (\rightarrow I/1.13.1) are equal to the corresponding entries of the mean vector and covariance matrix:

$$x \sim \mathcal{N}(\mu, \Sigma) \quad \Rightarrow \quad x_i \sim \mathcal{N}(\mu_i, \sigma_{ii}^2) . \quad (3)$$

The probability density function of the multivariate normal distribution (\rightarrow II/4.1.4) is

$$p(x) = \frac{1}{\sqrt{(2\pi)^n |\Sigma|}} \cdot \exp \left[-\frac{1}{2} (x - \mu)^T \Sigma^{-1} (x - \mu) \right] \quad (4)$$

and the probability density function of the univariate normal distribution (\rightarrow II/3.2.10) is

$$p(x_i) = \frac{1}{\sqrt{2\pi\sigma_i^2}} \cdot \exp \left[-\frac{1}{2} \left(\frac{x_i - \mu_i}{\sigma_i} \right)^2 \right] . \quad (5)$$

1) Let

$$p(x) = p(x_1) \cdot \dots \cdot p(x_n) . \quad (6)$$

Then, because the covariance is zero under independence (\rightarrow I/1.15.6), the entries of the covariance matrix are the pair-wise covariances (\rightarrow I/1.16.1) and the covariance matrix of the multivariate normal distribution (\rightarrow II/4.1.8) is equal to Σ , we have

$$\Sigma = \text{diag} ([\text{Cov}(x_1, x_1), \dots, \text{Cov}(x_n, x_n)]) . \quad (7)$$

Moreover, because the diagonal entries of the covariance matrix are the element-wise variances (\rightarrow I/1.15.5) and the variance of the univariate normal distribution (\rightarrow II/3.2.19) is equal to σ^2 and equating $\sigma^2_{_i} = \sigma^2_{_ii}$ from (3), we get

$$\Sigma = \text{diag} ([\sigma_1^2, \dots, \sigma_n^2]) . \quad (8)$$

2) Let

$$\Sigma = \text{diag} ([\sigma_1^2, \dots, \sigma_n^2]) . \quad (9)$$

Then, we have

$$\begin{aligned} p(x) &\stackrel{(4)}{=} \frac{1}{\sqrt{(2\pi)^n |\text{diag} ([\sigma_1^2, \dots, \sigma_n^2])|}} \cdot \exp \left[-\frac{1}{2} (x - \mu)^T \text{diag} ([\sigma_1^2, \dots, \sigma_n^2])^{-1} (x - \mu) \right] \\ &= \frac{1}{\sqrt{(2\pi)^n \prod_{i=1}^n \sigma_i^2}} \cdot \exp \left[-\frac{1}{2} (x - \mu)^T \text{diag} ([1/\sigma_1^2, \dots, 1/\sigma_n^2]) (x - \mu) \right] \\ &= \frac{1}{\sqrt{(2\pi)^n \prod_{i=1}^n \sigma_i^2}} \cdot \exp \left[-\frac{1}{2} \sum_{i=1}^n \frac{(x_i - \mu_i)^2}{\sigma_i^2} \right] \\ &= \prod_{i=1}^n \frac{1}{\sqrt{2\pi\sigma_i^2}} \cdot \exp \left[-\frac{1}{2} \left(\frac{x_i - \mu_i}{\sigma_i} \right)^2 \right] \end{aligned} \quad (10)$$

which implies that

$$p(x) = p(x_1) \cdot \dots \cdot p(x_n) . \quad (11)$$

■

4.1.18 Independence of products

Theorem: Let X be an n -dimensional random vector (\rightarrow I/1.2.3) following a multivariate normal distribution (\rightarrow II/4.1.1):

$$X \sim \mathcal{N}(\mu, \Sigma) \quad (1)$$

and consider two matrices $A \in \mathbb{R}^{k \times n}$ and $B \in \mathbb{R}^{l \times n}$. Then, AX and BX are independent (\rightarrow I/1.3.6), if and only if the cross-matrix product, weighted with the covariance matrix (\rightarrow II/4.1.8) is equal to the zero matrix:

$$AX \text{ and } BX \text{ ind.} \Leftrightarrow A\Sigma B^T = 0_{kl} . \quad (2)$$

Proof: Define a new random vector (\rightarrow I/1.2.3) C as

$$C = \begin{bmatrix} A \\ B \end{bmatrix} \in \mathbb{R}^{(k+l) \times n} . \quad (3)$$

Then, due to the linear transformation theorem (\rightarrow II/4.1.14), we have

$$CX = \begin{bmatrix} AX \\ BX \end{bmatrix} \sim \mathcal{N} \left(\begin{bmatrix} A\mu \\ B\mu \end{bmatrix}, C\Sigma C^T \right) \quad (4)$$

with the combined covariance matrix (\rightarrow I/1.16.1)

$$C\Sigma C^T = \begin{bmatrix} A\Sigma A^T & A\Sigma B^T \\ B\Sigma A^T & B\Sigma B^T \end{bmatrix} . \quad (5)$$

We know that the necessary and sufficient condition for two components of a multivariate normal random vector to be independent is that their entries in the covariance matrix are zero (\rightarrow II/4.1.17). Thus, AX and BX are independent (\rightarrow I/1.3.6), if and only if

$$A\Sigma B^T = (B\Sigma A^T)^T = 0_{kl} \quad (6)$$

where 0_{kl} is the $k \times l$ zero matrix. This proves the result in (2).

■

Sources:

- jld (2018): “Understanding t-test for linear regression”; in: *StackExchange CrossValidated*, retrieved on 2022-12-13; URL: <https://stats.stackexchange.com/a/344008>.

4.1.19 Drawing samples

Theorem: Let $X \in \mathbb{R}^n$ be a random vector (\rightarrow I/1.2.3) with all entries independently following a standard normal distribution (\rightarrow II/3.2.3). Moreover, let A be an $n \times n$ matrix, such that $AA^T = \Sigma$. Then, $Y = \mu + AX$ follows a multivariate normal distribution (\rightarrow II/4.1.1) with mean (\rightarrow I/1.12.16) μ and covariance (\rightarrow I/1.16.1) Σ :

$$Y = \mu + AX \sim \mathcal{N}(\mu, \Sigma) . \quad (1)$$

Proof: If all entries of X are independent and standard normally distributed (\rightarrow II/3.2.3)

$$X_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, 1) \quad \text{for all } i = 1, \dots, n , \quad (2)$$

this implies a multivariate normal distribution with diagonal covariance matrix (\rightarrow II/4.1.17):

$$X \sim \mathcal{N}(0_n, I_n) . \quad (3)$$

Thus, with the linear transformation theorem for the multivariate normal distribution (\rightarrow II/4.1.14), it follows that

$$\begin{aligned} Y = \mu + AX &\sim \mathcal{N}(A0_n + \mu, AI_nA^T) \\ &\sim \mathcal{N}(\mu, AA^T) \\ &\sim \mathcal{N}(\mu, \Sigma) . \end{aligned} \quad (4)$$

Thus, given X defined by (2), Y defined by (1) is a sample (\rightarrow I/1.1.6) from $\mathcal{N}(\mu, \Sigma)$. ■

Sources:

- Wikipedia (2025): “Multivariate normal distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2025-05-23; URL: https://en.wikipedia.org/wiki/Multivariate_normal_distribution#Drawing_values_from_the_distribution.

4.2 Bivariate normal distribution

4.2.1 Definition

Definition: Let X be an 2×1 random vector (\rightarrow I/1.2.3). Then, X is said to have a bivariate normal distribution, if X follows a multivariate normal distribution (\rightarrow II/4.1.1)

$$X \sim \mathcal{N}(\mu, \Sigma) \quad (1)$$

with means (\rightarrow I/1.12.1) μ_1 and μ_2 , variances (\rightarrow I/1.13.1) σ_1^2 and σ_2^2 and covariance (\rightarrow I/1.15.1) σ_{12} :

$$\mu = \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix} \quad \text{and} \quad \Sigma = \begin{bmatrix} \sigma_1^2 & \sigma_{12} \\ \sigma_{12} & \sigma_2^2 \end{bmatrix} . \quad (2)$$

Sources:

- Wikipedia (2023): “Multivariate normal distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2023-09-22; URL: https://en.wikipedia.org/wiki/Multivariate_normal_distribution#Bivariate_case.

4.2.2 Probability density function

Theorem: Let $X = \begin{bmatrix} X_1 \\ X_2 \end{bmatrix}$ follow a bivariate normal distribution (\rightarrow II/4.2.1):

$$X \sim \mathcal{N} \left(\mu = \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}, \Sigma = \begin{bmatrix} \sigma_1^2 & \sigma_{12} \\ \sigma_{12} & \sigma_2^2 \end{bmatrix} \right). \quad (1)$$

Then, the probability density function (\rightarrow I/1.7.1) of X is:

$$f_X(x) = \frac{1}{2\pi\sqrt{\sigma_1^2\sigma_2^2 - \sigma_{12}^2}} \cdot \exp \left[-\frac{1}{2} \frac{\sigma_2^2(x_1 - \mu_1)^2 - 2\sigma_{12}(x_1 - \mu_1)(x_2 - \mu_2) + \sigma_1^2(x_2 - \mu_2)^2}{\sigma_1^2\sigma_2^2 - \sigma_{12}^2} \right]. \quad (2)$$

Proof: The probability density function of the multivariate normal distribution (\rightarrow II/4.1.4) for an n -dimensional random vector (\rightarrow I/1.2.3) x is:

$$f_X(x) = \frac{1}{\sqrt{(2\pi)^n |\Sigma|}} \cdot \exp \left[-\frac{1}{2} (x - \mu)^T \Sigma^{-1} (x - \mu) \right]. \quad (3)$$

Plugging in $n = 2$, $\mu = \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}$ and $\Sigma = \begin{bmatrix} \sigma_1^2 & \sigma_{12} \\ \sigma_{12} & \sigma_2^2 \end{bmatrix}$, we obtain:

$$\begin{aligned} f_X(x) &= \frac{1}{\sqrt{(2\pi)^2 \left| \begin{bmatrix} \sigma_1^2 & \sigma_{12} \\ \sigma_{12} & \sigma_2^2 \end{bmatrix} \right|}} \cdot \exp \left[-\frac{1}{2} \left(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} - \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix} \right)^T \begin{bmatrix} \sigma_1^2 & \sigma_{12} \\ \sigma_{12} & \sigma_2^2 \end{bmatrix}^{-1} \left(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} - \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix} \right) \right] \\ &= \frac{1}{2\pi \left| \begin{bmatrix} \sigma_1^2 & \sigma_{12} \\ \sigma_{12} & \sigma_2^2 \end{bmatrix} \right|^{\frac{1}{2}}} \cdot \exp \left[-\frac{1}{2} \begin{bmatrix} (x_1 - \mu_1) & (x_2 - \mu_2) \end{bmatrix} \begin{bmatrix} \sigma_1^2 & \sigma_{12} \\ \sigma_{12} & \sigma_2^2 \end{bmatrix}^{-1} \begin{bmatrix} (x_1 - \mu_1) \\ (x_2 - \mu_2) \end{bmatrix} \right]. \end{aligned} \quad (4)$$

Using the determinant of a 2×2 matrix

$$\left| \begin{bmatrix} a & b \\ c & d \end{bmatrix} \right| = ad - bc \quad (5)$$

and the inverse of of a 2×2 matrix

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix}^{-1} = \frac{1}{ad - bc} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix}, \quad (6)$$

the probability density function (\rightarrow I/1.7.1) becomes:

$$\begin{aligned} f_X(x) &= \frac{1}{2\pi\sqrt{\sigma_1^2\sigma_2^2 - \sigma_{12}^2}} \cdot \exp \left[-\frac{1}{2(\sigma_1^2\sigma_2^2 - \sigma_{12}^2)} \begin{bmatrix} (x_1 - \mu_1) & (x_2 - \mu_2) \end{bmatrix} \begin{bmatrix} \sigma_2^2 & -\sigma_{12} \\ -\sigma_{12} & \sigma_1^2 \end{bmatrix} \begin{bmatrix} (x_1 - \mu_1) \\ (x_2 - \mu_2) \end{bmatrix} \right] \\ &= \frac{1}{2\pi\sqrt{\sigma_1^2\sigma_2^2 - \sigma_{12}^2}} \cdot \exp \left[-\frac{1}{2(\sigma_1^2\sigma_2^2 - \sigma_{12}^2)} \begin{bmatrix} \sigma_2^2(x_1 - \mu_1) - \sigma_{12}(x_2 - \mu_2) & \sigma_1^2(x_2 - \mu_2) - \sigma_{12}(x_1 - \mu_1) \end{bmatrix} \begin{bmatrix} (x_1 - \mu_1) \\ (x_2 - \mu_2) \end{bmatrix} \right] \\ &= \frac{1}{2\pi\sqrt{\sigma_1^2\sigma_2^2 - \sigma_{12}^2}} \cdot \exp \left[-\frac{1}{2(\sigma_1^2\sigma_2^2 - \sigma_{12}^2)} (\sigma_2^2(x_1 - \mu_1)^2 - \sigma_{12}(x_1 - \mu_1)(x_2 - \mu_2) + \sigma_1^2(x_2 - \mu_2)^2 - \sigma_{12}(x_2 - \mu_2)(x_1 - \mu_1)) \right] \\ &= \frac{1}{2\pi\sqrt{\sigma_1^2\sigma_2^2 - \sigma_{12}^2}} \cdot \exp \left[-\frac{1}{2} \frac{\sigma_2^2(x_1 - \mu_1)^2 - 2\sigma_{12}(x_1 - \mu_1)(x_2 - \mu_2) + \sigma_1^2(x_2 - \mu_2)^2}{\sigma_1^2\sigma_2^2 - \sigma_{12}^2} \right]. \end{aligned} \quad (7)$$

■

4.2.3 Probability density function in terms of correlation coefficient

Theorem: Let $X = \begin{bmatrix} X_1 \\ X_2 \end{bmatrix}$ follow a bivariate normal distribution (\rightarrow II/4.2.1):

$$X \sim \mathcal{N} \left(\mu = \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}, \Sigma = \begin{bmatrix} \sigma_1^2 & \sigma_{12} \\ \sigma_{12} & \sigma_2^2 \end{bmatrix} \right). \quad (1)$$

Then, the probability density function (\rightarrow I/1.7.1) of X is

$$f_X(x) = \frac{1}{2\pi\sigma_1\sigma_2\sqrt{1-\rho^2}} \cdot \exp \left[-\frac{1}{2(1-\rho^2)} \left(\left(\frac{x_1 - \mu_1}{\sigma_1} \right)^2 - 2\rho \frac{(x_1 - \mu_1)(x_2 - \mu_2)}{\sigma_1\sigma_2} + \left(\frac{x_2 - \mu_2}{\sigma_2} \right)^2 \right) \right] \quad (2)$$

where ρ is the correlation (\rightarrow I/1.17.1) between X_1 and X_2 .

Proof: Since X follows a special case of the multivariate normal distribution, its covariance matrix is (\rightarrow II/4.1.8)

$$\text{Cov}(X) = \Sigma = \begin{bmatrix} \sigma_1^2 & \sigma_{12} \\ \sigma_{12} & \sigma_2^2 \end{bmatrix} \quad (3)$$

and the covariance matrix can be decomposed into correlation matrix and standard deviations (\rightarrow I/1.16.8):

$$\begin{aligned}
\Sigma &= \begin{bmatrix} \sigma_1^2 & \rho \sigma_1 \sigma_2 \\ \rho \sigma_1 \sigma_2 & \sigma_2^2 \end{bmatrix} \\
&= \begin{bmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{bmatrix} \begin{bmatrix} 1 & \rho \\ \rho & 1 \end{bmatrix} \begin{bmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{bmatrix}.
\end{aligned} \tag{4}$$

The determinant of this matrix is

$$\begin{aligned}
|\Sigma| &= \left| \begin{bmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{bmatrix} \begin{bmatrix} 1 & \rho \\ \rho & 1 \end{bmatrix} \begin{bmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{bmatrix} \right| \\
&= \left| \begin{bmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{bmatrix} \right| \cdot \left| \begin{bmatrix} 1 & \rho \\ \rho & 1 \end{bmatrix} \right| \cdot \left| \begin{bmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{bmatrix} \right| \\
&= (\sigma_1 \sigma_2)(1 - \rho^2)(\sigma_1 \sigma_2) \\
&= \sigma_1^2 \sigma_2^2 (1 - \rho^2)
\end{aligned} \tag{5}$$

and the inverse of this matrix is

$$\begin{aligned}
\Sigma^{-1} &= \left(\begin{bmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{bmatrix} \begin{bmatrix} 1 & \rho \\ \rho & 1 \end{bmatrix} \begin{bmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{bmatrix} \right)^{-1} \\
&= \begin{bmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{bmatrix}^{-1} \begin{bmatrix} 1 & \rho \\ \rho & 1 \end{bmatrix}^{-1} \begin{bmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{bmatrix}^{-1} \\
&= \frac{1}{1 - \rho^2} \begin{bmatrix} 1/\sigma_1 & 0 \\ 0 & 1/\sigma_2 \end{bmatrix} \begin{bmatrix} 1 & -\rho \\ -\rho & 1 \end{bmatrix} \begin{bmatrix} 1/\sigma_1 & 0 \\ 0 & 1/\sigma_2 \end{bmatrix}.
\end{aligned} \tag{6}$$

The probability density function of the multivariate normal distribution (\rightarrow II/4.1.4) for an n -dimensional random vector (\rightarrow I/1.2.3) x is:

$$f_X(x) = \frac{1}{\sqrt{(2\pi)^n |\Sigma|}} \cdot \exp \left[-\frac{1}{2} (x - \mu)^T \Sigma^{-1} (x - \mu) \right]. \tag{7}$$

Plugging in $n = 2$, μ from (1) and Σ from (5) and (6), the probability density function becomes:

$$\begin{aligned}
f_X(x) &= \frac{1}{\sqrt{(2\pi)^2 \sigma_1^2 \sigma_2^2 (1 - \rho^2)}} \cdot \exp \left[-\frac{1}{2} \left(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} - \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix} \right)^T \frac{1}{1 - \rho^2} \begin{bmatrix} 1/\sigma_1 & 0 \\ 0 & 1/\sigma_2 \end{bmatrix} \begin{bmatrix} 1 & -\rho \\ -\rho & 1 \end{bmatrix} \begin{bmatrix} 1/\sigma_1 & 0 \\ 0 & 1/\sigma_2 \end{bmatrix} \right] \\
&= \frac{1}{2\pi \sigma_1 \sigma_2 \sqrt{1 - \rho^2}} \cdot \exp \left[-\frac{1}{2(1 - \rho^2)} \begin{bmatrix} \frac{x_1 - \mu_1}{\sigma_1} & \frac{x_2 - \mu_2}{\sigma_2} \end{bmatrix} \begin{bmatrix} 1 & -\rho \\ -\rho & 1 \end{bmatrix} \begin{bmatrix} \frac{x_1 - \mu_1}{\sigma_1} \\ \frac{x_2 - \mu_2}{\sigma_2} \end{bmatrix} \right] \\
&= \frac{1}{2\pi \sigma_1 \sigma_2 \sqrt{1 - \rho^2}} \cdot \exp \left[-\frac{1}{2(1 - \rho^2)} \left[\left(\frac{x_1 - \mu_1}{\sigma_1} - \rho \frac{x_2 - \mu_2}{\sigma_2} \right) \left(\frac{x_2 - \mu_2}{\sigma_2} - \rho \frac{x_1 - \mu_1}{\sigma_1} \right) \right] \begin{bmatrix} \frac{x_1 - \mu_1}{\sigma_1} \\ \frac{x_2 - \mu_2}{\sigma_2} \end{bmatrix} \right] \\
&= \frac{1}{2\pi \sigma_1 \sigma_2 \sqrt{1 - \rho^2}} \cdot \exp \left[-\frac{1}{2(1 - \rho^2)} \left(\left(\frac{x_1 - \mu_1}{\sigma_1} \right)^2 - 2\rho \frac{(x_1 - \mu_1)(x_2 - \mu_2)}{\sigma_1 \sigma_2} + \left(\frac{x_2 - \mu_2}{\sigma_2} \right)^2 \right) \right]. \tag{8}
\end{aligned}$$

■

Sources:

- Wikipedia (2023): “Multivariate normal distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2023-09-29; URL: https://en.wikipedia.org/wiki/Multivariate_normal_distribution#Bivariate_case.

4.2.4 Construction from standard normal distributions

Theorem: Let Y_1 and Y_2 be independent (\rightarrow I/1.3.6) random variables (\rightarrow I/1.2.2) following a standard normal distribution (\rightarrow II/3.2.3):

$$Y_1 \sim \mathcal{N}(0, 1) \quad \text{and} \quad Y_2 \sim \mathcal{N}(0, 1) \quad \text{ind.} \tag{1}$$

and define the two random variables (\rightarrow I/1.2.2) X_1 and X_2

$$\begin{aligned}
X_1 &= \sigma_1 Y_1 + \mu_1 \\
X_2 &= \sigma_2 \left(\rho Y_1 + \sqrt{1 - \rho^2} Y_2 \right) + \mu_2
\end{aligned} \tag{2}$$

where $\mu_1, \mu_2 \in \mathbb{R}$, $\sigma_1, \sigma_2 \in \mathbb{R}_{>0}$ and $\rho \in [-1, +1]$. Then, the random vector (\rightarrow I/1.2.3) with entries X_1 and X_2 follows a bivariate normal distribution (\rightarrow II/4.2.1)

$$X = \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} \sim \mathcal{N} \left(\begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}, \begin{bmatrix} \sigma_1^2 & \rho \sigma_1 \sigma_2 \\ \rho \sigma_1 \sigma_2 & \sigma_2^2 \end{bmatrix} \right) \tag{3}$$

where mean and covariance (\rightarrow II/4.2.1) are functions of the parameters μ_1 , μ_2 , σ_1 , σ_2 and ρ .

Proof: The probability density function of the standard normal distribution (\rightarrow II/3.2.10) is

$$Y \sim \mathcal{N}(0, 1) \quad \Rightarrow \quad f_Y(y) = \frac{1}{\sqrt{2\pi}} \cdot \exp \left[-\frac{1}{2} y^2 \right]. \tag{4}$$

The random variables X_1 and X_2 are functions of Y_1 and Y_2

$$\begin{aligned} X_1 &= \sigma_1 Y_1 + \mu_1 \\ X_2 &= \sigma_2 \left(\rho Y_1 + \sqrt{1 - \rho^2} Y_2 \right) + \mu_2, \end{aligned} \quad (5)$$

such that the inverse functions Y_1 and Y_2 in terms of X_1 and X_2 are

$$\begin{aligned} Y_1 &= (X_1 - \mu_1) / \sigma_1 \\ Y_2 &= [(X_2 - \mu_2) / \sigma_2 - \rho Y_1] / \sqrt{1 - \rho^2} \\ &= [(X_2 - \mu_2) / \sigma_2 - \rho (X_1 - \mu_1) / \sigma_1] / \sqrt{1 - \rho^2}. \end{aligned} \quad (6)$$

This implies the following Jacobian matrix

$$J = \begin{bmatrix} \frac{dY_1}{dX_1} & \frac{dY_1}{dX_2} \\ \frac{dY_2}{dX_1} & \frac{dY_2}{dX_2} \end{bmatrix} = \begin{bmatrix} \frac{1}{\sigma_1} & 0 \\ \frac{\rho}{\sigma_1 \sqrt{1 - \rho^2}} & \frac{1}{\sigma_2 \sqrt{1 - \rho^2}} \end{bmatrix} \quad (7)$$

and determinant of the Jacobian matrix

$$\begin{aligned} |J| &= \frac{1}{\sigma_1} \cdot \frac{1}{\sigma_2 \sqrt{1 - \rho^2}} - 0 \cdot \frac{\rho}{\sigma_1 \sqrt{1 - \rho^2}} \\ &= \frac{1}{\sigma_1 \sigma_2 \sqrt{1 - \rho^2}} \\ &= \frac{1}{\sqrt{\sigma_1^2 \sigma_2^2 (1 - \rho^2)}}. \end{aligned} \quad (8)$$

Because Y_1 and Y_2 are independent (\rightarrow I/1.3.6), the joint density (\rightarrow I/1.5.2) of Y_1 and Y_2 is equal to the product (\rightarrow I/1.3.9) of the marginal densities (\rightarrow I/1.5.3):

$$f_{Y_1, Y_2}(y_1, y_2) = f_{Y_1}(y_1) \cdot f_{Y_2}(y_2). \quad (9)$$

Substituting (4) into (9), we get:

$$\begin{aligned} f_{Y_1, Y_2}(y_1, y_2) &= \frac{1}{\sqrt{2\pi}} \exp \left[-\frac{1}{2} y_1^2 \right] \cdot \frac{1}{\sqrt{2\pi}} \exp \left[-\frac{1}{2} y_2^2 \right] \\ &= \frac{1}{\sqrt{(2\pi)^2}} \cdot \exp \left[-\frac{1}{2} (y_1^2 + y_2^2) \right]. \end{aligned} \quad (10)$$

With the probability density function of an invertible function (\rightarrow I/1.7.5), the joint density (\rightarrow I/1.5.2) of X_1 and X_2 can be derived as:

$$f_{X_1, X_2}(x_1, x_2) = f_{Y_1, Y_2}(y_1, y_2) \cdot |J|. \quad (11)$$

Substituting (10), (6) and (8) into (11), we get:

$$\begin{aligned}
f_{X_1, X_2}(x_1, x_2) &= \frac{1}{\sqrt{(2\pi)^2}} \cdot \exp \left[-\frac{1}{2} \left(\left(\frac{x_1 - \mu_1}{\sigma_1} \right)^2 + \left(\left[\frac{x_2 - \mu_2}{\sigma_2} - \rho \frac{x_1 - \mu_1}{\sigma_1} \right] / \sqrt{1 - \rho^2} \right)^2 \right) \right] \cdot \frac{1}{\sqrt{\sigma_1^2 \sigma_2^2 (1 - \rho^2)}} \\
&= \frac{1}{\sqrt{(2\pi)^2 \sigma_1^2 \sigma_2^2 (1 - \rho^2)}} \cdot \exp \left[-\frac{1}{2} \left(\left(\frac{x_1 - \mu_1}{\sigma_1} \right)^2 + \frac{1}{1 - \rho^2} \left[\left(\frac{x_2 - \mu_2}{\sigma_2} \right)^2 - 2\rho \left(\frac{x_1 - \mu_1}{\sigma_1} \right) \left(\frac{x_2 - \mu_2}{\sigma_2} \right) \right] \right) \right] \\
&= \frac{1}{2\pi \sigma_1 \sigma_2 \sqrt{1 - \rho^2}} \cdot \exp \left[-\frac{1}{2(1 - \rho^2)} \left(\left(\frac{x_1 - \mu_1}{\sigma_1} \right)^2 - 2\rho \frac{(x_1 - \mu_1)(x_2 - \mu_2)}{\sigma_1 \sigma_2} + \left(\frac{x_2 - \mu_2}{\sigma_2} \right)^2 \right) \right]
\end{aligned} \tag{12}$$

This is the probability density function of the bivariate normal distribution (\rightarrow II/4.2.3) with parameters

$$\mu = \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix} \quad \text{and} \quad \Sigma = \begin{bmatrix} \sigma_1^2 & \rho \sigma_1 \sigma_2 \\ \rho \sigma_1 \sigma_2 & \sigma_2^2 \end{bmatrix}. \tag{13}$$

Thus, it follows that

$$X \sim \mathcal{N}(\mu, \Sigma). \tag{14}$$

■

Sources:

- Ostwald, Dirk (2023): “Normalverteilungen”; in: *Allgemeines Lineares Modell*, Einheit (4), Folie 15; URL: https://www.ipsy.ovgu.de/ipsy_media/Methodenlehre+I/Sommersemester+2023/Allgemeines+Lineares+Modell/4_Normalverteilungen.pdf.
- Wikipedia (2025): “Multivariate normal distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2025-05-23; URL: https://en.wikipedia.org/wiki/Multivariate_normal_distribution#Bivariate_case.

4.2.5 Mutual information

Theorem: Let X and Y follow a bivariate normal distribution (\rightarrow II/4.2.1):

$$\begin{bmatrix} X \\ Y \end{bmatrix} \sim \mathcal{N} \left(\begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}, \begin{bmatrix} \sigma_1^2 & \sigma_{12} \\ \sigma_{12} & \sigma_2^2 \end{bmatrix} \right). \tag{1}$$

Then, the mutual information (\rightarrow I/2.4.1) of X and Y is

$$I(X, Y) = -\frac{1}{2} \ln(1 - \rho^2) \tag{2}$$

where ρ is the correlation (\rightarrow I/1.17.1) of X and Y .

Proof: Mutual information can be written in terms of marginal and joint differential entropy (\rightarrow I/2.4.3):

$$I(X, Y) = h(X) + h(Y) - h(X, Y). \tag{3}$$

The marginal distributions of the multivariate normal distribution are also multivariate normal (\rightarrow II/4.1.15)

$$\begin{bmatrix} X_1 \\ X_2 \end{bmatrix} \sim \mathcal{N} \left(\begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}, \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix} \right) \Rightarrow X_1 \sim \mathcal{N}(\mu_1, \Sigma_{11}) , \quad (4)$$

such that the marginals (\rightarrow I/1.5.3) of the bivariate normal distribution (\rightarrow II/4.2.1) are univariate normal distributions (\rightarrow II/3.2.1):

$$\begin{bmatrix} X \\ Y \end{bmatrix} \sim \mathcal{N} \left(\begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}, \begin{bmatrix} \sigma_1^2 & \sigma_{12} \\ \sigma_{12} & \sigma_2^2 \end{bmatrix} \right) \Rightarrow X \sim \mathcal{N}(\mu_1, \sigma_1^2) \quad \text{and} \quad Y \sim \mathcal{N}(\mu_2, \sigma_2^2) . \quad (5)$$

The differential entropy of the univariate normal distribution (\rightarrow II/3.2.23) is

$$h(X) = \frac{1}{2} \ln(2\pi\sigma^2 e) \quad (6)$$

and the differential entropy of the multivariate normal distribution (\rightarrow II/4.1.10) is

$$h(x) = \frac{n}{2} \ln(2\pi) + \frac{1}{2} \ln|\Sigma| + \frac{1}{2}n \quad (7)$$

where $|\Sigma|$ is the determinant of the covariance matrix (\rightarrow I/1.16.1) Σ . A two-dimensional covariance matrix can be rewritten in terms of correlations (\rightarrow I/1.16.8) as follows:

$$\begin{aligned} \Sigma &= \begin{bmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{bmatrix} \begin{bmatrix} 1 & \rho \\ \rho & 1 \end{bmatrix} \begin{bmatrix} \sigma_1 & 0 \\ 0 & \sigma_2 \end{bmatrix} \\ &= \begin{bmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 \end{bmatrix} . \end{aligned} \quad (8)$$

Combining (3) with (6) and (7), applying $n = 2$, we get:

$$\begin{aligned}
I(X, Y) &\stackrel{(3)}{=} h(X) + h(Y) - h(X, Y) \\
&\stackrel{(5)}{=} h[\mathcal{N}(\mu_1, \sigma_1^2)] + h[\mathcal{N}(\mu_2, \sigma_2^2)] - h[\mathcal{N}(\mu, \Sigma)] \\
&\stackrel{(8)}{=} \left[\frac{1}{2} \ln(2\pi\sigma_1^2 e) \right] + \left[\frac{1}{2} \ln(2\pi\sigma_2^2 e) \right] - \left[\frac{2}{2} \ln(2\pi) + \frac{1}{2} \ln \left| \begin{bmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 \end{bmatrix} \right| + \frac{1}{2} \cdot 2 \right] \\
&= \left(\frac{2}{2} \ln(2\pi) + \frac{2}{2} \ln(e) - \ln(2\pi) - 1 \right) + \left(\frac{1}{2} \ln(\sigma_1^2) + \frac{1}{2} \ln(\sigma_2^2) - \frac{1}{2} \ln \left| \begin{bmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 \end{bmatrix} \right| \right) \\
&= \frac{1}{2} [\ln(\sigma_1^2) + \ln(\sigma_2^2) - \ln(\sigma_1^2\sigma_2^2 - (\rho\sigma_1\sigma_2)^2)] \\
&= \frac{1}{2} \ln \left[\frac{\sigma_1^2\sigma_2^2}{\sigma_1^2\sigma_2^2 - (\rho\sigma_1\sigma_2)^2} \right] \\
&= \frac{1}{2} \ln \left[\frac{\sigma_1^2\sigma_2^2}{\sigma_1^2\sigma_2^2(1 - \rho^2)} \right] \\
&= \frac{1}{2} \ln \left[\frac{1}{1 - \rho^2} \right] \\
&= -\frac{1}{2} \ln(1 - \rho^2) .
\end{aligned} \tag{9}$$

Sources:

- Krafft, Peter (2013): “Correlation and Mutual Information”; in: *Princeton University Department of Computer Science: Laboratory for Intelligent Probabilistic Systems*, February 13, 2013; URL: <https://lips.cs.princeton.edu/correlation-and-mutual-information/>.

4.2.6 Linear combination

Theorem: Let X and Y follow a bivariate normal distribution (\rightarrow II/4.2.1):

$$\begin{bmatrix} X \\ Y \end{bmatrix} \sim \mathcal{N} \left(\begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}, \begin{bmatrix} \sigma_1^2 & \sigma_{12} \\ \sigma_{12} & \sigma_2^2 \end{bmatrix} \right) . \tag{1}$$

Then, any linear combination of X and Y follows a univariate normal distribution (\rightarrow II/3.2.1):

$$Z = aX + bY \sim \mathcal{N}(a\mu_1 + b\mu_2, a^2\sigma_1^2 + 2ab\sigma_{12} + b^2\sigma_2^2) . \tag{2}$$

Proof: The linear transformation theorem for the multivariate normal distribution (\rightarrow II/4.1.14) states that

$$X \sim \mathcal{N}(\mu, \Sigma) \quad \Rightarrow \quad Y = AX + c \sim \mathcal{N}(A\mu + c, A\Sigma A^T) \tag{3}$$

where $X \in \mathbb{R}^n$, $A \in \mathbb{R}^{n \times n}$ and $c \in \mathbb{R}^n$. In the present case, we have

$$X \in \mathbb{R}^2 \quad \text{and} \quad A = \begin{bmatrix} a & b \end{bmatrix} \in \mathbb{R}^{1 \times 2} \quad \text{and} \quad c = 0 \in \mathbb{R} , \tag{4}$$

such that

$$Z = A \begin{bmatrix} X \\ Y \end{bmatrix} + c = \begin{bmatrix} a & b \end{bmatrix} \begin{bmatrix} X \\ Y \end{bmatrix} + 0 = aX + bY . \quad (5)$$

Combining (3), (1) and (5), it follows that

$$\begin{aligned} Z &\sim \mathcal{N} \left(\begin{bmatrix} a & b \end{bmatrix} \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}, \begin{bmatrix} a & b \end{bmatrix} \begin{bmatrix} \sigma_1^2 & \sigma_{12} \\ \sigma_{12} & \sigma_2^2 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} \right) \\ &\sim \mathcal{N} \left(a\mu_1 + b\mu_2, \begin{bmatrix} a\sigma_1^2 + b\sigma_{12} & a\sigma_{12} + b\sigma_2^2 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} \right) \\ &\sim \mathcal{N} (a\mu_1 + b\mu_2, (a^2\sigma_1^2 + ab\sigma_{12}) + (ab\sigma_{12} + b^2\sigma_2^2)) \\ &\sim \mathcal{N} (a\mu_1 + b\mu_2, a^2\sigma_1^2 + 2ab\sigma_{12} + b^2\sigma_2^2) . \end{aligned} \quad (6)$$

■

Sources:

- Wikipedia (2024): “Misconceptions about the normal distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2024-10-25; URL: https://en.wikipedia.org/wiki/Misconceptions_about_the_normal_distribution.

4.3 Multivariate t-distribution

4.3.1 Definition

Definition: Let X be an n -dimensional random vector (\rightarrow I/1.2.3). Then, X is said to follow a multivariate t -distribution with mean μ , scale matrix Σ and degrees of freedom ν

$$X \sim t(\mu, \Sigma, \nu) , \quad (1)$$

if and only if its probability density function (\rightarrow I/1.7.1) is given by

$$t(x; \mu, \Sigma, \nu) = \sqrt{\frac{1}{(\nu\pi)^n |\Sigma|}} \frac{\Gamma([\nu + n]/2)}{\Gamma(\nu/2)} \left[1 + \frac{1}{\nu} (x - \mu)^T \Sigma^{-1} (x - \mu) \right]^{-(\nu+n)/2} \quad (2)$$

where μ is an n -dimensional real vector, Σ is an $n \times n$ positive-definite matrix and $\nu > 0$.

Sources:

- Koch KR (2007): “Multivariate t-Distribution”; in: *Introduction to Bayesian Statistics*, ch. 2.5.2, pp. 53-55; URL: <https://www.springer.com/gp/book/9783540727231>; DOI: 10.1007/978-3-540-72726-2.

4.3.2 Probability density function

Theorem: Let X be a random vector (\rightarrow I/1.2.3) following a multivariate t-distribution (\rightarrow II/4.3.1):

$$X \sim t(\mu, \Sigma, \nu) . \quad (1)$$

Then, the probability density function (\rightarrow I/1.7.1) of X is

$$f_X(x) = \sqrt{\frac{1}{(\nu\pi)^n |\Sigma|}} \frac{\Gamma([\nu+n]/2)}{\Gamma(\nu/2)} \left[1 + \frac{1}{\nu} (x - \mu)^T \Sigma^{-1} (x - \mu) \right]^{-(\nu+n)/2} . \quad (2)$$

Proof: This follows directly from the definition of the multivariate t-distribution (\rightarrow II/4.3.1). ■

4.3.3 Relationship to F-distribution

Theorem: Let X be a n -dimensional random vector (\rightarrow I/1.2.3) following a multivariate t-distribution (\rightarrow II/4.3.1) with mean μ , scale matrix Σ and degrees of freedom ν :

$$X \sim t(\mu, \Sigma, \nu) . \quad (1)$$

Then, the centered, weighted and standardized quadratic form of X follows an F-distribution (\rightarrow II/3.8.1) with degrees of freedom n and ν :

$$(X - \mu)^T \Sigma^{-1} (X - \mu) / n \sim F(n, \nu) . \quad (2)$$

Proof: The linear transformation theorem for the multivariate t-distribution states

$$x \sim t(\mu, \Sigma, \nu) \quad \Rightarrow \quad y = Ax + b \sim t(A\mu + b, A\Sigma A^T, \nu) \quad (3)$$

where x is an n -dimensional random vector (\rightarrow I/1.2.3) following a multivariate t-distribution (\rightarrow II/4.3.1), A is an $m \times n$ matrix and b is an $m \times 1$ vector. Define the following quantities

$$\begin{aligned} Y &= \Sigma^{-1/2} (X - \mu) = \Sigma^{-1/2} X - \Sigma^{-1/2} \mu \\ Z &= Y^T Y / n = (X - \mu)^T \Sigma^{-1} (X - \mu) / n \end{aligned} \quad (4)$$

where $\Sigma^{-1/2}$ is a matrix square root of the inverse of Σ . Then, applying (3) to (4) with (1), one obtains the distribution of Y as

$$\begin{aligned} Y &\sim t(\Sigma^{-1/2} \mu - \Sigma^{-1/2} \mu, \Sigma^{-1/2} \Sigma \Sigma^{-1/2}, \nu) \\ &= t(0_n, \Sigma^{-1/2} \Sigma^{1/2} \Sigma^{1/2} \Sigma^{-1/2}, \nu) \\ &= t(0_n, I_n, \nu) , \end{aligned} \quad (5)$$

i.e. the marginal distributions (\rightarrow I/1.5.3) of the individual entries of Y are univariate t-distributions (\rightarrow II/3.3.1) with ν degrees of freedom:

$$Y_i \sim t(\nu), \quad i = 1, \dots, n . \quad (6)$$

Note that, when X follows a t-distribution with n degrees of freedom, this is equivalent to (\rightarrow II/3.3.1) an expression of X in terms of a standard normal (\rightarrow II/3.2.3) random variable Z and a chi-squared (\rightarrow II/3.7.1) random variable V :

$$X \sim t(n) \quad \Leftrightarrow \quad X = \frac{Z}{\sqrt{V/n}} \quad \text{with independent} \quad Z \sim \mathcal{N}(0, 1) \quad \text{and} \quad V \sim \chi^2(n). \quad (7)$$

With that, Z from (4) can be rewritten as follows:

$$\begin{aligned} Z &\stackrel{(4)}{=} Y^T Y / n \\ &= \frac{1}{n} \sum_{i=1}^n Y_i^2 \\ &\stackrel{(7)}{=} \frac{1}{n} \sum_{i=1}^n \left(\frac{Z_i}{\sqrt{V/\nu}} \right)^2 \\ &= \frac{(\sum_{i=1}^n Z_i^2) / n}{V/\nu}. \end{aligned} \quad (8)$$

Because by definition, the sum of squared standard normal random variables follows a chi-squared distribution (\rightarrow II/3.7.1)

$$X_i \sim \mathcal{N}(0, 1), \quad i = 1, \dots, n \quad \Rightarrow \quad \sum_{i=1}^n X_i^2 \sim \chi^2(n), \quad (9)$$

the quantity Z becomes a ratio of the following form

$$Z = \frac{W/n}{V/\nu} \quad \text{with} \quad W \sim \chi^2(n) \quad \text{and} \quad V \sim \chi^2(\nu), \quad (10)$$

such that Z , by definition, follows an F-distribution (\rightarrow II/3.8.1):

$$Z = \frac{W/n}{V/\nu} \sim F(n, \nu). \quad (11)$$

■

Sources:

- Lin, Pi-Erh (1972): “Some Characterizations of the Multivariate t Distribution”; in: *Journal of Multivariate Analysis*, vol. 2, pp. 339-344, Lemma 2; URL: <https://core.ac.uk/download/pdf/81139018.pdf>; DOI: 10.1016/0047-259X(72)90021-8.
- Nadarajah, Saralees; Kotz, Samuel (2005): “Mathematical Properties of the Multivariate t Distribution”; in: *Acta Applicandae Mathematicae*, vol. 89, pp. 53-84, page 56; URL: <https://link.springer.com/content/pdf/10.1007/s10440-005-9003-4.pdf>; DOI: 10.1007/s10440-005-9003-4.

4.4 Normal-gamma distribution

4.4.1 Definition

Definition: Let X be an n -dimensional random vector (\rightarrow I/1.2.3) and let Y be a positive random variable (\rightarrow I/1.2.2). Then, X and Y are said to follow a normal-gamma distribution

$$X, Y \sim \text{NG}(\mu, \Lambda, a, b) , \quad (1)$$

if the distribution of X conditional on Y is a multivariate normal distribution (\rightarrow II/4.1.1) with mean vector μ and covariance matrix $(y\Lambda)^{-1}$ and Y follows a gamma distribution (\rightarrow II/3.4.1) with shape parameter a and rate parameter b :

$$\begin{aligned} X|Y &\sim \mathcal{N}(\mu, (Y\Lambda)^{-1}) \\ Y &\sim \text{Gam}(a, b) . \end{aligned} \quad (2)$$

The $n \times n$ matrix Λ is referred to as the precision matrix (\rightarrow I/1.16.12) of the normal-gamma distribution.

Sources:

- Koch KR (2007): “Normal-Gamma Distribution”; in: *Introduction to Bayesian Statistics*, ch. 2.5.3, pp. 55-56, eq. 2.212; URL: <https://www.springer.com/gp/book/9783540727231>; DOI: 10.1007/978-3-540-72726-2.

4.4.2 Special case of normal-Wishart distribution

Theorem: The normal-gamma distribution (\rightarrow II/4.4.1) is a special case of the normal-Wishart distribution (\rightarrow II/5.3.1) where the number of columns of the random matrices (\rightarrow I/1.2.4) is $p = 1$.

Proof: Let X be an $n \times p$ real matrix and let Y be a $p \times p$ positive-definite symmetric matrix, such that X and Y jointly follow a normal-Wishart distribution (\rightarrow II/5.3.1):

$$X, Y \sim \text{NW}(M, U, V, \nu) . \quad (1)$$

Then, X and Y are described by the probability density function (\rightarrow II/5.3.2)

$$\begin{aligned} p(X, Y) = & \frac{1}{\sqrt{(2\pi)^{np}|U|^p|V|^\nu}} \cdot \frac{\sqrt{2^{-\nu p}}}{\Gamma_p\left(\frac{\nu}{2}\right)} \cdot |Y|^{(\nu+n-p-1)/2} \\ & \exp \left[-\frac{1}{2} \text{tr} \left(Y \left[(X - M)^T U^{-1} (X - M) + V^{-1} \right] \right) \right] \end{aligned} \quad (2)$$

where $|A|$ is a matrix determinant, A^{-1} is a matrix inverse and $\Gamma_p(x)$ is the multivariate gamma function of order p . If $p = 1$, then $\Gamma_p(x) = \Gamma(x)$ is the ordinary gamma function, $x = X$ is a column vector and $y = Y$ is a real number. Thus, the probability density function (\rightarrow I/1.7.1) of x and y can be developed as

$$\begin{aligned}
p(x, y) &= \frac{1}{\sqrt{(2\pi)^n |U| |V|^\nu}} \cdot \frac{\sqrt{2^{-\nu}}}{\Gamma\left(\frac{\nu}{2}\right)} \cdot y^{(\nu+n-2)/2} \cdot \\
&\quad \exp \left[-\frac{1}{2} \text{tr} \left(y \left[(x - M)^T U^{-1} (x - M) + V^{-1} \right] \right) \right] \\
&= \sqrt{\frac{|U^{-1}|}{(2\pi)^n}} \cdot \frac{\sqrt{(2|V|)^{-\nu}}}{\Gamma\left(\frac{\nu}{2}\right)} \cdot y^{\frac{\nu}{2} + \frac{n}{2} - 1} \cdot \\
&\quad \exp \left[-\frac{1}{2} \left(y \left[(x - M)^T U^{-1} (x - M) + 2(2V)^{-1} \right] \right) \right] \\
&= \sqrt{\frac{|U^{-1}|}{(2\pi)^n}} \cdot \frac{\left(\frac{1}{2|V|}\right)^{\frac{\nu}{2}}}{\Gamma\left(\frac{\nu}{2}\right)} \cdot y^{\frac{\nu}{2} + \frac{n}{2} - 1} \cdot \\
&\quad \exp \left[-\frac{y}{2} \left((x - M)^T U^{-1} (x - M) + 2 \left(\frac{1}{2V} \right) \right) \right]
\end{aligned} \tag{3}$$

In the matrix-normal distribution (\rightarrow II/5.1.1), we have $M \in \mathbb{R}^{n \times p}$, $U \in \mathbb{R}^{n \times n}$, $V \in \mathbb{R}^{p \times p}$ and $\nu \in \mathbb{R}$. Thus, with $p = 1$, M becomes a column vector and V becomes a real number, such that $V = |V| = 1/V^{-1}$. Finally, substituting $\mu = M$, $\Lambda = U^{-1}$, $a = \frac{\nu}{2}$ and $b = \frac{1}{2V}$, we get

$$p(x, y) = \sqrt{\frac{|\Lambda|}{(2\pi)^n}} \frac{b^a}{\Gamma(a)} \cdot y^{a + \frac{n}{2} - 1} \exp \left[-\frac{y}{2} \left((x - \mu)^T \Lambda (x - \mu) + 2b \right) \right] \tag{4}$$

which is the probability density function of the normal-gamma distribution (\rightarrow II/4.4.3). ■

4.4.3 Probability density function

Theorem: Let x and y follow a normal-gamma distribution (\rightarrow II/4.4.1):

$$x, y \sim \text{NG}(\mu, \Lambda, a, b). \tag{1}$$

Then, the joint probability (\rightarrow I/1.3.2) density function (\rightarrow I/1.7.1) of x and y is

$$p(x, y) = \sqrt{\frac{|\Lambda|}{(2\pi)^n}} \frac{b^a}{\Gamma(a)} \cdot y^{a + \frac{n}{2} - 1} \exp \left[-\frac{y}{2} \left((x - \mu)^T \Lambda (x - \mu) + 2b \right) \right]. \tag{2}$$

Proof: The normal-gamma distribution (\rightarrow II/4.4.1) is defined as X conditional on Y following a multivariate distribution (\rightarrow II/4.1.1) and Y following a gamma distribution (\rightarrow II/3.4.1):

$$\begin{aligned}
X|Y &\sim \mathcal{N}(\mu, (Y\Lambda)^{-1}) \\
Y &\sim \text{Gam}(a, b).
\end{aligned} \tag{3}$$

Thus, using the probability density function of the multivariate normal distribution (\rightarrow II/4.1.4) and the probability density function of the gamma distribution (\rightarrow II/3.4.7), we have the following probabilities:

$$\begin{aligned}
p(x|y) &= \mathcal{N}(x; \mu, (y\Lambda)^{-1}) \\
&= \sqrt{\frac{|y\Lambda|}{(2\pi)^n}} \exp \left[-\frac{1}{2}(x - \mu)^T (y\Lambda)(x - \mu) \right] \\
p(y) &= \text{Gam}(y; a, b) \\
&= \frac{b^a}{\Gamma(a)} y^{a-1} \exp[-by] .
\end{aligned} \tag{4}$$

The law of conditional probability (\rightarrow I/1.3.4) implies that

$$p(x, y) = p(x|y) p(y) , \tag{5}$$

such that the normal-gamma density function becomes:

$$p(x, y) = \sqrt{\frac{|y\Lambda|}{(2\pi)^n}} \exp \left[-\frac{1}{2}(x - \mu)^T (y\Lambda)(x - \mu) \right] \cdot \frac{b^a}{\Gamma(a)} y^{a-1} \exp[-by] . \tag{6}$$

Using the relation $|yA| = y^n|A|$ for an $n \times n$ matrix A and rearranging the terms, we have:

$$p(x, y) = \sqrt{\frac{|\Lambda|}{(2\pi)^n}} \frac{b^a}{\Gamma(a)} \cdot y^{a+\frac{n}{2}-1} \exp \left[-\frac{y}{2} ((x - \mu)^T \Lambda (x - \mu) + 2b) \right] . \tag{7}$$

■

Sources:

- Koch KR (2007): “Normal-Gamma Distribution”; in: *Introduction to Bayesian Statistics*, ch. 2.5.3, pp. 55-56, eq. 2.212; URL: <https://www.springer.com/gp/book/9783540727231>; DOI: 10.1007/978-3-540-72726-2.

4.4.4 Mean

Theorem: Let $x \in \mathbb{R}^n$ and $y > 0$ follow a normal-gamma distribution (\rightarrow II/4.4.1):

$$x, y \sim \text{NG}(\mu, \Lambda, a, b) . \tag{1}$$

Then, the expected value (\rightarrow I/1.12.1) of x and y is

$$\mathbb{E}[(x, y)] = \left(\mu, \frac{a}{b} \right) . \tag{2}$$

Proof: Consider the random vector (\rightarrow I/1.2.3)

$$\begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} x_1 \\ \vdots \\ x_n \\ y \end{bmatrix} . \tag{3}$$

According to the expected value of a random vector (\rightarrow I/1.12.16), its expected value is

$$\mathbb{E} \left(\begin{bmatrix} x \\ y \end{bmatrix} \right) = \begin{bmatrix} \mathbb{E}(x_1) \\ \vdots \\ \mathbb{E}(x_n) \\ \mathbb{E}(y) \end{bmatrix} = \begin{bmatrix} \mathbb{E}(x) \\ \mathbb{E}(y) \end{bmatrix} . \quad (4)$$

When x and y are jointly normal-gamma distributed, then (\rightarrow II/4.4.1) by definition x follows a multivariate normal distribution (\rightarrow II/4.1.1) conditional on y and y follows a univariate gamma distribution (\rightarrow II/3.4.1):

$$x, y \sim \text{NG}(\mu, \Lambda, a, b) \quad \Leftrightarrow \quad x|y \sim \mathcal{N}(\mu, (y\Lambda)^{-1}) \quad \wedge \quad y \sim \text{Gam}(a, b) . \quad (5)$$

Thus, with the expected value of the multivariate normal distribution (\rightarrow II/4.1.6) and the law of conditional probability (\rightarrow I/1.3.4), $\mathbb{E}(x)$ becomes

$$\begin{aligned} \mathbb{E}(x) &= \iint x \cdot p(x, y) \, dx \, dy \\ &= \iint x \cdot p(x|y) \cdot p(y) \, dx \, dy \\ &= \int p(y) \int x \cdot p(x|y) \, dx \, dy \\ &= \int p(y) \langle x \rangle_{\mathcal{N}(\mu, (y\Lambda)^{-1})} \, dy \\ &= \int p(y) \cdot \mu \, dy \\ &= \mu \int p(y) \, dy \\ &= \mu , \end{aligned} \quad (6)$$

and with the expected value of the gamma distribution (\rightarrow II/3.4.11), $\mathbb{E}(y)$ becomes

$$\begin{aligned} \mathbb{E}(y) &= \int y \cdot p(y) \, dy \\ &= \langle y \rangle_{\text{Gam}(a, b)} \\ &= \frac{a}{b} . \end{aligned} \quad (7)$$

Thus, the expectation of the random vector in equations (3) and (4) is

$$\mathbb{E} \left(\begin{bmatrix} x \\ y \end{bmatrix} \right) = \begin{bmatrix} \mu \\ a/b \end{bmatrix} , \quad (8)$$

as indicated by equation (2).

■

4.4.5 Covariance

Theorem: Let $x \in \mathbb{R}^n$ and $y > 0$ follow a normal-gamma distribution (\rightarrow II/4.4.1):

$$x, y \sim \text{NG}(\mu, \Lambda, a, b) . \quad (1)$$

Then,

1) the covariance (\rightarrow I/1.15.1) of x , conditional (\rightarrow I/1.5.4) on y is

$$\text{Cov}(x|y) = \frac{1}{y} \Lambda^{-1} ; \quad (2)$$

2) the covariance (\rightarrow I/1.15.1) of x , unconditional (\rightarrow I/1.5.3) on y is

$$\text{Cov}(x) = \frac{b}{a-1} \Lambda^{-1} ; \quad (3)$$

3) the variance (\rightarrow I/1.13.1) of y is

$$\text{Var}(y) = \frac{a}{b^2} . \quad (4)$$

Proof:

1) According to the definition of the normal-gamma distribution (\rightarrow II/4.4.1), the distribution of x given y is a multivariate normal distribution (\rightarrow II/4.1.1):

$$x|y \sim \mathcal{N}(\mu, (y\Lambda)^{-1}) . \quad (5)$$

The covariance of the multivariate normal distribution (\rightarrow II/4.1.8) is

$$x \sim \mathcal{N}(\mu, \Sigma) \quad \Rightarrow \quad \text{Cov}(x) = \Sigma , \quad (6)$$

such that we have:

$$\text{Cov}(x|y) = (y\Lambda)^{-1} = \frac{1}{y} \Lambda^{-1} . \quad (7)$$

2) The marginal distribution of the normal-gamma distribution (\rightarrow II/4.4.8) with respect to x is a multivariate t-distribution (\rightarrow II/4.3.1):

$$x \sim t\left(\mu, \left(\frac{a}{b}\Lambda\right)^{-1}, 2a\right) . \quad (8)$$

The covariance of the multivariate t-distribution is

$$x \sim t(\mu, \Sigma, \nu) \quad \Rightarrow \quad \text{Cov}(x) = \frac{\nu}{\nu-2} \Sigma , \quad (9)$$

such that we have:

$$\text{Cov}(x) = \frac{2a}{2a-2} \left(\frac{a}{b}\Lambda\right)^{-1} = \frac{a}{a-1} \frac{b}{a} \Lambda^{-1} = \frac{b}{a-1} \Lambda^{-1} . \quad (10)$$

3) The marginal distribution of the normal-gamma distribution (\rightarrow II/4.4.8) with respect to y is a univariate gamma distribution (\rightarrow II/3.4.1):

$$y \sim \text{Gam}(a, b) . \quad (11)$$

The variance of the gamma distribution (\rightarrow II/3.4.14) is

$$x \sim \text{Gam}(a, b) \quad \Rightarrow \quad \text{Var}(x) = \frac{a}{b^2}, \quad (12)$$

such that we have:

$$\text{Var}(y) = \frac{a}{b^2}. \quad (13)$$

■

4.4.6 Differential entropy

Theorem: Let x be an n -dimensional random vector (\rightarrow I/1.2.3) and let y be a positive random variable (\rightarrow I/1.2.2). Assume that x and y are jointly normal-gamma distributed:

$$(x, y) \sim \text{NG}(\mu, \Lambda^{-1}, a, b) \quad (1)$$

Then, the differential entropy (\rightarrow I/2.2.1) of x in nats is

$$\begin{aligned} h(x, y) = & \frac{n}{2} \ln(2\pi) - \frac{1}{2} \ln |\Lambda| + \frac{1}{2}n \\ & + a + \ln \Gamma(a) - \frac{n-2+2a}{2} \psi(a) + \frac{n-2}{2} \ln b. \end{aligned} \quad (2)$$

Proof: The probability density function of the normal-gamma distribution (\rightarrow II/4.4.3) is

$$p(x, y) = p(x|y) \cdot p(y) = \mathcal{N}(x; \mu, (y\Lambda)^{-1}) \cdot \text{Gam}(y; a, b). \quad (3)$$

The differential entropy of the multivariate normal distribution (\rightarrow II/4.1.10) is

$$h(x) = \frac{n}{2} \ln(2\pi) + \frac{1}{2} \ln |\Sigma| + \frac{1}{2}n \quad (4)$$

and the differential entropy of the univariate gamma distribution (\rightarrow II/3.4.17) is

$$h(y) = a + \ln \Gamma(a) + (1-a) \cdot \psi(a) - \ln b \quad (5)$$

where $\Gamma(x)$ is the gamma function and $\psi(x)$ is the digamma function.

The differential entropy of a continuous random variable (\rightarrow I/2.2.1) in nats is given by

$$h(Z) = - \int_{\mathcal{Z}} p(z) \ln p(z) dz \quad (6)$$

which, applied to the normal-gamma distribution (\rightarrow II/4.4.1) over x and y , yields

$$h(x, y) = - \int_0^\infty \int_{\mathbb{R}^n} p(x, y) \ln p(x, y) dx dy. \quad (7)$$

Using the law of conditional probability (\rightarrow I/1.3.4), this can be evaluated as follows:

$$\begin{aligned}
h(x, y) &= - \int_0^\infty \int_{\mathbb{R}^n} p(x|y) p(y) \ln p(x|y) p(y) dx dy \\
&= - \int_0^\infty \int_{\mathbb{R}^n} p(x|y) p(y) \ln p(x|y) dx dy - \int_0^\infty \int_{\mathbb{R}^n} p(x|y) p(y) \ln p(y) dx dy \\
&= \int_0^\infty p(y) \int_{\mathbb{R}^n} p(x|y) \ln p(x|y) dx dy + \int_0^\infty p(y) \ln p(y) \int_{\mathbb{R}^n} p(x|y) dx dy \\
&= \langle h(x|y) \rangle_{p(y)} + h(y) .
\end{aligned} \tag{8}$$

In other words, the differential entropy of the normal-gamma distribution over x and y is equal to the sum of a multivariate normal entropy regarding x conditional on y , expected over y , and a univariate gamma entropy regarding y .

From equations (3) and (4), the first term becomes

$$\begin{aligned}
\langle h(x|y) \rangle_{p(y)} &= \left\langle \frac{n}{2} \ln(2\pi) + \frac{1}{2} \ln |(y\Lambda)^{-1}| + \frac{1}{2}n \right\rangle_{p(y)} \\
&= \left\langle \frac{n}{2} \ln(2\pi) - \frac{1}{2} \ln |(y\Lambda)| + \frac{1}{2}n \right\rangle_{p(y)} \\
&= \left\langle \frac{n}{2} \ln(2\pi) - \frac{1}{2} \ln(y^n |\Lambda|) + \frac{1}{2}n \right\rangle_{p(y)} \\
&= \frac{n}{2} \ln(2\pi) - \frac{1}{2} \ln |\Lambda| + \frac{1}{2}n - \left\langle \frac{n}{2} \ln y \right\rangle_{p(y)}
\end{aligned} \tag{9}$$

and using the relation (\rightarrow II/3.4.15) $y \sim \text{Gam}(a, b) \Rightarrow \langle \ln y \rangle = \psi(a) - \ln(b)$, we have

$$\langle h(x|y) \rangle_{p(y)} = \frac{n}{2} \ln(2\pi) - \frac{1}{2} \ln |\Lambda| + \frac{1}{2}n - \frac{n}{2} \psi(a) + \frac{n}{2} \ln b . \tag{10}$$

By plugging (10) and (5) into (8), one arrives at the differential entropy given by (2). ■

4.4.7 Kullback-Leibler divergence

Theorem: Let x be an n -dimensional random vector (\rightarrow I/1.2.3) and let y be a positive random variable (\rightarrow I/1.2.2). Assume two normal-gamma distributions (\rightarrow II/4.4.1) P and Q specifying the joint distribution of x and y as

$$\begin{aligned}
P : (x, y) &\sim \text{NG}(\mu_1, \Lambda_1^{-1}, a_1, b_1) \\
Q : (x, y) &\sim \text{NG}(\mu_2, \Lambda_2^{-1}, a_2, b_2) .
\end{aligned} \tag{1}$$

Then, the Kullback-Leibler divergence (\rightarrow I/2.5.1) of P from Q is given by

$$\begin{aligned}
\text{KL}[P || Q] &= \frac{1}{2} \frac{a_1}{b_1} [(\mu_2 - \mu_1)^T \Lambda_2 (\mu_2 - \mu_1)] + \frac{1}{2} \text{tr}(\Lambda_2 \Lambda_1^{-1}) - \frac{1}{2} \ln \frac{|\Lambda_2|}{|\Lambda_1|} - \frac{n}{2} \\
&\quad + a_2 \ln \frac{b_1}{b_2} - \ln \frac{\Gamma(a_1)}{\Gamma(a_2)} + (a_1 - a_2) \psi(a_1) - (b_1 - b_2) \frac{a_1}{b_1} .
\end{aligned} \tag{2}$$

Proof: The probability density function of the normal-gamma distribution (\rightarrow II/4.4.3) is

$$p(x, y) = p(x|y) \cdot p(y) = \mathcal{N}(x; \mu, (y\Lambda)^{-1}) \cdot \text{Gam}(y; a, b) . \quad (3)$$

The Kullback-Leibler divergence of the multivariate normal distribution (\rightarrow II/4.1.12) is

$$\text{KL}[P || Q] = \frac{1}{2} \left[(\mu_2 - \mu_1)^T \Sigma_2^{-1} (\mu_2 - \mu_1) + \text{tr}(\Sigma_2^{-1} \Sigma_1) - \ln \frac{|\Sigma_1|}{|\Sigma_2|} - n \right] \quad (4)$$

and the Kullback-Leibler divergence of the univariate gamma distribution (\rightarrow II/3.4.18) is

$$\text{KL}[P || Q] = a_2 \ln \frac{b_1}{b_2} - \ln \frac{\Gamma(a_1)}{\Gamma(a_2)} + (a_1 - a_2) \psi(a_1) - (b_1 - b_2) \frac{a_1}{b_1} \quad (5)$$

where $\Gamma(x)$ is the gamma function and $\psi(x)$ is the digamma function.

The KL divergence for a continuous random variable (\rightarrow I/2.5.1) is given by

$$\text{KL}[P || Q] = \int_{\mathcal{Z}} p(z) \ln \frac{p(z)}{q(z)} dz \quad (6)$$

which, applied to the normal-gamma distribution (\rightarrow II/4.4.1) over x and y , yields

$$\text{KL}[P || Q] = \int_0^\infty \int_{\mathbb{R}^n} p(x, y) \ln \frac{p(x, y)}{q(x, y)} dx dy . \quad (7)$$

Using the law of conditional probability (\rightarrow I/1.3.4), this can be evaluated as follows:

$$\begin{aligned} \text{KL}[P || Q] &= \int_0^\infty \int_{\mathbb{R}^n} p(x|y) p(y) \ln \frac{p(x|y) p(y)}{q(x|y) q(y)} dx dy \\ &= \int_0^\infty \int_{\mathbb{R}^n} p(x|y) p(y) \ln \frac{p(x|y)}{q(x|y)} dx dy + \int_0^\infty \int_{\mathbb{R}^n} p(x|y) p(y) \ln \frac{p(y)}{q(y)} dx dy \\ &= \int_0^\infty p(y) \int_{\mathbb{R}^n} p(x|y) \ln \frac{p(x|y)}{q(x|y)} dx dy + \int_0^\infty p(y) \ln \frac{p(y)}{q(y)} \int_{\mathbb{R}^n} p(x|y) dx dy \\ &= \langle \text{KL}[p(x|y) || q(x|y)] \rangle_{p(y)} + \text{KL}[p(y) || q(y)] . \end{aligned} \quad (8)$$

In other words, the KL divergence between two normal-gamma distributions over x and y is equal to the sum of a multivariate normal KL divergence regarding x conditional on y , expected over y , and a univariate gamma KL divergence regarding y .

From equations (3) and (4), the first term becomes

$$\begin{aligned} &\langle \text{KL}[p(x|y) || q(x|y)] \rangle_{p(y)} \\ &= \left\langle \frac{1}{2} \left[(\mu_2 - \mu_1)^T (y\Lambda_2) (\mu_2 - \mu_1) + \text{tr}((y\Lambda_2)(y\Lambda_1)^{-1}) - \ln \frac{|(y\Lambda_1)^{-1}|}{|(y\Lambda_2)^{-1}|} - n \right] \right\rangle_{p(y)} \\ &= \left\langle \frac{y}{2} (\mu_2 - \mu_1)^T \Lambda_2 (\mu_2 - \mu_1) + \frac{1}{2} \text{tr}(\Lambda_2 \Lambda_1^{-1}) - \frac{1}{2} \ln \frac{|\Lambda_2|}{|\Lambda_1|} - \frac{n}{2} \right\rangle_{p(y)} \end{aligned} \quad (9)$$

and using the relation (\rightarrow II/3.4.11) $y \sim \text{Gam}(a, b) \Rightarrow \langle y \rangle = a/b$, we have

$$\langle \text{KL}[p(x|y) || q(x|y)] \rangle_{p(y)} = \frac{1}{2} \frac{a_1}{b_1} (\mu_2 - \mu_1)^T \Lambda_2 (\mu_2 - \mu_1) + \frac{1}{2} \text{tr}(\Lambda_2 \Lambda_1^{-1}) - \frac{1}{2} \ln \frac{|\Lambda_2|}{|\Lambda_1|} - \frac{n}{2} . \quad (10)$$

By plugging (10) and (5) into (8), one arrives at the KL divergence given by (2). ■

Sources:

- Soch J, Allefeld A (2016): “Kullback-Leibler Divergence for the Normal-Gamma Distribution”; in: *arXiv math.ST*, 1611.01437; URL: <https://arxiv.org/abs/1611.01437>.

4.4.8 Marginal distributions

Theorem: Let x and y follow a normal-gamma distribution (\rightarrow II/4.4.1):

$$x, y \sim \text{NG}(\mu, \Lambda, a, b) . \quad (1)$$

Then, the marginal distribution (\rightarrow I/1.5.3) of y is a gamma distribution (\rightarrow II/3.4.1)

$$y \sim \text{Gam}(a, b) \quad (2)$$

and the marginal distribution (\rightarrow I/1.5.3) of x is a multivariate t-distribution (\rightarrow II/4.3.1)

$$x \sim t \left(\mu, \left(\frac{a}{b} \Lambda \right)^{-1}, 2a \right) . \quad (3)$$

Proof: The probability density function of the normal-gamma distribution (\rightarrow II/4.4.3) is given by

$$\begin{aligned} p(x, y) &= p(x|y) \cdot p(y) \\ p(x|y) &= \mathcal{N}(x; \mu, (y\Lambda)^{-1}) \\ p(y) &= \text{Gam}(y; a, b) . \end{aligned} \quad (4)$$

Using the law of marginal probability (\rightarrow I/1.3.3), the marginal distribution of y can be derived as

$$\begin{aligned} p(y) &= \int p(x, y) \, dx \\ &= \int \mathcal{N}(x; \mu, (y\Lambda)^{-1}) \text{Gam}(y; a, b) \, dx \\ &= \text{Gam}(y; a, b) \int \mathcal{N}(x; \mu, (y\Lambda)^{-1}) \, dx \\ &= \text{Gam}(y; a, b) \end{aligned} \quad (5)$$

which is the probability density function of the gamma distribution (\rightarrow II/3.4.7) with shape parameter a and rate parameter b .

Using the law of marginal probability (\rightarrow I/1.3.3), the marginal distribution of x can be derived as

$$\begin{aligned}
p(x) &= \int p(x, y) \, dy \\
&= \int \mathcal{N}(x; \mu, (y\Lambda)^{-1}) \text{Gam}(y; a, b) \, dy \\
&= \int \sqrt{\frac{|y\Lambda|}{(2\pi)^n}} \exp\left[-\frac{1}{2}(x - \mu)^T(y\Lambda)(x - \mu)\right] \cdot \frac{b^a}{\Gamma(a)} y^{a-1} \exp[-by] \, dy \\
&= \int \sqrt{\frac{y^n|\Lambda|}{(2\pi)^n}} \exp\left[-\frac{1}{2}(x - \mu)^T(y\Lambda)(x - \mu)\right] \cdot \frac{b^a}{\Gamma(a)} y^{a-1} \exp[-by] \, dy \\
&= \int \sqrt{\frac{|\Lambda|}{(2\pi)^n}} \cdot \frac{b^a}{\Gamma(a)} \cdot y^{a+\frac{n}{2}-1} \cdot \exp\left[-\left(b + \frac{1}{2}(x - \mu)^T\Lambda(x - \mu)\right)y\right] \, dy \\
&= \int \sqrt{\frac{|\Lambda|}{(2\pi)^n}} \cdot \frac{b^a}{\Gamma(a)} \cdot \frac{\Gamma(a + \frac{n}{2})}{(b + \frac{1}{2}(x - \mu)^T\Lambda(x - \mu))^{a+\frac{n}{2}}} \cdot \text{Gam}\left(y; a + \frac{n}{2}, b + \frac{1}{2}(x - \mu)^T\Lambda(x - \mu)\right) \, dy \\
&= \sqrt{\frac{|\Lambda|}{(2\pi)^n}} \cdot \frac{b^a}{\Gamma(a)} \cdot \frac{\Gamma(a + \frac{n}{2})}{(b + \frac{1}{2}(x - \mu)^T\Lambda(x - \mu))^{a+\frac{n}{2}}} \int \text{Gam}\left(y; a + \frac{n}{2}, b + \frac{1}{2}(x - \mu)^T\Lambda(x - \mu)\right) \, dy \\
&= \sqrt{\frac{|\Lambda|}{(2\pi)^n}} \cdot \frac{b^a}{\Gamma(a)} \cdot \frac{\Gamma(a + \frac{n}{2})}{(b + \frac{1}{2}(x - \mu)^T\Lambda(x - \mu))^{a+\frac{n}{2}}} \\
&= \frac{\sqrt{|\Lambda|}}{(2\pi)^{\frac{n}{2}}} \cdot \frac{\Gamma(\frac{2a+n}{2})}{\Gamma(\frac{2a}{2})} \cdot b^a \cdot \left(b + \frac{1}{2}(x - \mu)^T\Lambda(x - \mu)\right)^{-(a+\frac{n}{2})} \\
&= \frac{\sqrt{|\Lambda|}}{\pi^{\frac{n}{2}}} \cdot \frac{\Gamma(\frac{2a+n}{2})}{\Gamma(\frac{2a}{2})} \cdot \left(\frac{1}{b}\right)^{-a} \cdot \left(b + \frac{1}{2}(x - \mu)^T\Lambda(x - \mu)\right)^{-a} \cdot 2^{-\frac{n}{2}} \cdot \left(b + \frac{1}{2}(x - \mu)^T\Lambda(x - \mu)\right)^{-\frac{n}{2}} \\
&= \frac{\sqrt{|\Lambda|}}{\pi^{\frac{n}{2}}} \cdot \frac{\Gamma(\frac{2a+n}{2})}{\Gamma(\frac{2a}{2})} \cdot \left(1 + \frac{1}{2b}(x - \mu)^T\Lambda(x - \mu)\right)^{-a} \cdot (2b + (x - \mu)^T\Lambda(x - \mu))^{-\frac{n}{2}} \\
&= \frac{\sqrt{|\Lambda|}}{\pi^{\frac{n}{2}}} \cdot \frac{\Gamma(\frac{2a+n}{2})}{\Gamma(\frac{2a}{2})} \cdot \left(\frac{1}{2a}\right)^{-a} \cdot \left(2a + (x - \mu)^T\left(\frac{a}{b}\Lambda\right)(x - \mu)\right)^{-a} \cdot \left(\frac{b}{a}\right)^{-\frac{n}{2}} \cdot \left(2a + (x - \mu)^T\left(\frac{a}{b}\Lambda\right)(x - \mu)\right)^{-\frac{n}{2}} \\
&= \frac{\sqrt{\left(\frac{a}{b}\right)^n |\Lambda|}}{(2a)^{-a} \pi^{\frac{n}{2}}} \cdot \frac{\Gamma(\frac{2a+n}{2})}{\Gamma(\frac{2a}{2})} \cdot \left(2a + (x - \mu)^T\left(\frac{a}{b}\Lambda\right)(x - \mu)\right)^{-a} \cdot \left(2a + (x - \mu)^T\left(\frac{a}{b}\Lambda\right)(x - \mu)\right)^{-\frac{n}{2}} \\
&= \frac{\sqrt{\left(\frac{a}{b}\right)^n |\Lambda|}}{(2a)^{-a} \pi^{\frac{n}{2}}} \cdot \frac{\Gamma(\frac{2a+n}{2})}{\Gamma(\frac{2a}{2})} \cdot (2a)^{-a} \cdot \left(1 + \frac{1}{2a}(x - \mu)^T\left(\frac{a}{b}\Lambda\right)(x - \mu)\right)^{-a} \cdot (2a)^{-\frac{n}{2}} \cdot \left(1 + \frac{1}{2a}(x - \mu)^T\left(\frac{a}{b}\Lambda\right)(x - \mu)\right)^{-\frac{n}{2}} \\
&= \frac{\sqrt{\left(\frac{a}{b}\right)^n |\Lambda|}}{(2a)^{\frac{n}{2}} \pi^{\frac{n}{2}}} \cdot \frac{\Gamma(\frac{2a+n}{2})}{\Gamma(\frac{2a}{2})} \cdot \left(1 + \frac{1}{2a}(x - \mu)^T\left(\frac{a}{b}\Lambda\right)(x - \mu)\right)^{-\frac{2a+n}{2}} \\
&= \sqrt{\frac{\left|\frac{a}{b}\Lambda\right|}{(2a\pi)^n}} \cdot \frac{\Gamma(\frac{2a+n}{2})}{\Gamma(\frac{2a}{2})} \cdot \left(1 + \frac{1}{2a}(x - \mu)^T\left(\frac{a}{b}\Lambda\right)(x - \mu)\right)^{-\frac{2a+n}{2}}
\end{aligned}$$

(6)

which is the probability density function of a multivariate t-distribution (\rightarrow II/4.3.2) with mean vector μ , shape matrix $\left(\frac{a}{b}\Lambda\right)^{-1}$ and $2a$ degrees of freedom.



4.4.9 Conditional distributions

Theorem: Let x and y follow a normal-gamma distribution (\rightarrow II/4.4.1):

$$x, y \sim \text{NG}(\mu, \Lambda, a, b) . \quad (1)$$

Then,

1) the conditional distribution (\rightarrow I/1.5.4) of x given y is a multivariate normal distribution (\rightarrow II/4.1.1)

$$x|y \sim \mathcal{N}(\mu, (y\Lambda)^{-1}) ; \quad (2)$$

2) the conditional distribution (\rightarrow I/1.5.4) of a subset vector x_1 , given the complement vector x_2 and y , is also a multivariate normal distribution (\rightarrow II/4.1.1)

$$x_1|x_2, y \sim \mathcal{N}(\mu_{1|2}(y), \Sigma_{1|2}(y)) \quad (3)$$

with the conditional mean (\rightarrow I/1.12.1) and covariance (\rightarrow I/1.15.1)

$$\begin{aligned} \mu_{1|2}(y) &= \mu_1 + \Sigma_{12}\Sigma_{22}^{-1}(x_2 - \mu_2) \\ \Sigma_{1|2}(y) &= \Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21} \end{aligned} \quad (4)$$

where μ_1, μ_2 and $\Sigma_{11}, \Sigma_{12}, \Sigma_{22}, \Sigma_{21}$ are block-wise components (\rightarrow II/4.1.16) of μ and $\Sigma(y) = (y\Lambda)^{-1}$;

3) the conditional distribution (\rightarrow I/1.5.4) of y given x is a gamma distribution (\rightarrow II/3.4.1)

$$y|x \sim \text{Gam}\left(a + \frac{n}{2}, b + \frac{1}{2}(x - \mu)^T \Lambda (x - \mu)\right) \quad (5)$$

where n is the dimensionality of x .

Proof:

1) This follows from the definition of the normal-gamma distribution (\rightarrow II/4.4.1):

$$\begin{aligned} p(x, y) &= p(x|y) \cdot p(y) \\ &= \mathcal{N}(x; \mu, (y\Lambda)^{-1}) \cdot \text{Gam}(y; a, b) . \end{aligned} \quad (6)$$

2) This follows from (2) and the conditional distributions of the multivariate normal distribution (\rightarrow II/4.1.16):

$$\begin{aligned} x &\sim \mathcal{N}(\mu, \Sigma) \\ \Rightarrow x_1|x_2 &\sim \mathcal{N}(\mu_{1|2}, \Sigma_{1|2}) \\ \mu_{1|2} &= \mu_1 + \Sigma_{12}\Sigma_{22}^{-1}(x_2 - \mu_2) \\ \Sigma_{1|2} &= \Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21} . \end{aligned} \quad (7)$$

3) The conditional density of y given x follows from Bayes' theorem (\rightarrow I/5.3.2) as

$$p(y|x) = \frac{p(x|y) \cdot p(y)}{p(x)} . \quad (8)$$

The conditional distribution (\rightarrow I/1.5.4) of x given y is a multivariate normal distribution (\rightarrow II/4.4.3)

$$p(x|y) = \mathcal{N}(x; \mu, (y\Lambda)^{-1}) = \sqrt{\frac{|y\Lambda|}{(2\pi)^n}} \exp \left[-\frac{1}{2}(x - \mu)^T (y\Lambda)(x - \mu) \right], \quad (9)$$

the marginal distribution (\rightarrow I/1.5.3) of y is a gamma distribution (\rightarrow II/4.4.8)

$$p(y) = \text{Gam}(y; a, b) = \frac{b^a}{\Gamma(a)} y^{a-1} \exp[-by] \quad (10)$$

and the marginal distribution (\rightarrow I/1.5.3) of x is a multivariate t-distribution (\rightarrow II/4.4.8)

$$\begin{aligned} p(x) &= t \left(x; \mu, \left(\frac{a}{b} \Lambda \right)^{-1}, 2a \right) \\ &= \sqrt{\frac{\left| \frac{a}{b} \Lambda \right|}{(2a\pi)^n}} \cdot \frac{\Gamma\left(\frac{2a+n}{2}\right)}{\Gamma\left(\frac{2a}{2}\right)} \cdot \left(1 + \frac{1}{2a}(x - \mu)^T \left(\frac{a}{b} \Lambda \right) (x - \mu) \right)^{-\frac{2a+n}{2}} \\ &= \sqrt{\frac{|\Lambda|}{(2\pi)^n}} \cdot \frac{\Gamma\left(a + \frac{n}{2}\right)}{\Gamma(a)} \cdot b^a \cdot \left(b + \frac{1}{2}(x - \mu)^T \Lambda (x - \mu) \right)^{-(a + \frac{n}{2})}. \end{aligned} \quad (11)$$

Plugging (9), (10) and (11) into (8), we obtain

$$\begin{aligned} p(y|x) &= \frac{\sqrt{\frac{|y\Lambda|}{(2\pi)^n}} \exp \left[-\frac{1}{2}(x - \mu)^T (y\Lambda)(x - \mu) \right] \cdot \frac{b^a}{\Gamma(a)} y^{a-1} \exp[-by]}{\sqrt{\frac{|\Lambda|}{(2\pi)^n}} \cdot \frac{\Gamma\left(a + \frac{n}{2}\right)}{\Gamma(a)} \cdot b^a \cdot \left(b + \frac{1}{2}(x - \mu)^T \Lambda (x - \mu) \right)^{-(a + \frac{n}{2})}} \\ &= y^{\frac{n}{2}} \cdot \exp \left[-\frac{1}{2}(x - \mu)^T (y\Lambda)(x - \mu) \right] \cdot y^{a-1} \cdot \exp[-by] \cdot \frac{1}{\Gamma\left(a + \frac{n}{2}\right)} \cdot \left(b + \frac{1}{2}(x - \mu)^T \Lambda (x - \mu) \right)^{a + \frac{n}{2}} \\ &= \frac{\left(b + \frac{1}{2}(x - \mu)^T \Lambda (x - \mu) \right)^{a + \frac{n}{2}}}{\Gamma\left(a + \frac{n}{2}\right)} \cdot y^{a + \frac{n}{2} - 1} \cdot \exp \left[- \left(b + \frac{1}{2}(x - \mu)^T \Lambda (x - \mu) \right) y \right] \end{aligned} \quad (12)$$

which is the probability density function of a gamma distribution (\rightarrow II/3.4.7) with shape and rate parameters

$$a + \frac{n}{2} \quad \text{and} \quad b + \frac{1}{2}(x - \mu)^T \Lambda (x - \mu), \quad (13)$$

such that

$$p(y|x) = \text{Gam} \left(y; a + \frac{n}{2}, b + \frac{1}{2}(x - \mu)^T \Lambda (x - \mu) \right). \quad (14)$$

■

4.4.10 Drawing samples

Theorem: Let $Z_1 \in \mathbb{R}^n$ be a random vector (\rightarrow I/1.2.3) with all entries independently following a standard normal distribution (\rightarrow II/3.2.3) and let $Z_2 \in \mathbb{R}$ be a random variable (\rightarrow I/1.2.2) following a standard gamma distribution (\rightarrow II/3.4.3) with shape a . Moreover, let $A \in \mathbb{R}^{n \times n}$ be a matrix, such that $AA^T = \Lambda^{-1}$.

Then, $X = \mu + AZ_1/\sqrt{Z_2/b}$ and $Y = Z_2/b$ jointly follow a normal-gamma distribution (\rightarrow II/4.4.1) with mean vector (\rightarrow I/1.12.16) μ , precision matrix (\rightarrow I/1.16.12) Λ , shape parameter a and rate parameter b :

$$\left(X = \mu + AZ_1/\sqrt{Z_2/b}, Y = Z_2/b \right) \sim \text{NG}(\mu, \Lambda, a, b) . \quad (1)$$

Proof: If all entries of Z_1 are independent and standard normally distributed (\rightarrow II/3.2.3)

$$z_{1i} \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, 1) \quad \text{for all } i = 1, \dots, n , \quad (2)$$

this implies a multivariate normal distribution with diagonal covariance matrix (\rightarrow II/4.1.17):

$$Z_1 \sim \mathcal{N}(0_n, I_n) \quad (3)$$

where 0_n is an $n \times 1$ matrix of zeros and I_n is the $n \times n$ identity matrix.

If the distribution of Z_2 is a standard gamma distribution (\rightarrow II/3.4.3)

$$Z_2 \sim \text{Gam}(a, 1) , \quad (4)$$

then due to the relationship between gamma and standard gamma distribution (\rightarrow II/3.4.4), we have:

$$Y = \frac{Z_2}{b} \sim \text{Gam}(a, b) . \quad (5)$$

Moreover, using the linear transformation theorem for the multivariate normal distribution (\rightarrow II/4.1.14), it follows that:

$$\begin{aligned} Z_1 &\sim \mathcal{N}(0_n, I_n) \\ X = \mu + \frac{1}{\sqrt{Z_2/b}} AZ_1 &\sim \mathcal{N} \left(\mu + \frac{1}{\sqrt{Z_2/b}} A 0_n, \left(\frac{1}{\sqrt{Z_2/b}} A \right) I_n \left(\frac{1}{\sqrt{Z_2/b}} A \right)^T \right) \\ X &\sim \mathcal{N} \left(\mu + 0_n, \left(\frac{1}{\sqrt{Y}} \right)^2 AA^T \right) \\ X &\sim \mathcal{N}(\mu, (Y\Lambda)^{-1}) . \end{aligned} \quad (6)$$

Thus, Y follows a gamma distribution (\rightarrow II/3.4.1) and the distribution of X conditional on Y is a multivariate normal distribution (\rightarrow II/4.1.1):

$$\begin{aligned} X|Y &\sim \mathcal{N}(\mu, (Y\Lambda)^{-1}) \\ Y &\sim \text{Gam}(a, b) . \end{aligned} \quad (7)$$

This means that, by definition (\rightarrow II/4.4.1), X and Y jointly follow a normal-gamma distribution (\rightarrow II/4.4.1):

$$X, Y \sim \text{NG}(\mu, \Lambda, a, b) , \quad (8)$$

Thus, given Z_1 defined by (2) and Z_2 defined by (4), X and Y defined by (1) are a sample (\rightarrow I/1.1.6) from $\text{NG}(\mu, \Lambda, a, b)$. ■

Sources:

- Wikipedia (2022): “Normal-gamma distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-09-22; URL: https://en.wikipedia.org/wiki/Normal-gamma_distribution#Generating_normal-gamma_random_variates.

4.5 Dirichlet distribution

4.5.1 Definition

Definition: Let X be a $1 \times k$ random vector (\rightarrow I/1.2.3). Then, X is said to follow a Dirichlet distribution with concentration parameters $\alpha = [\alpha_1, \dots, \alpha_k]$

$$X \sim \text{Dir}(\alpha) , \quad (1)$$

if and only if its probability density function (\rightarrow I/1.7.1) is given by

$$\text{Dir}(x; \alpha) = \frac{\Gamma\left(\sum_{i=1}^k \alpha_i\right)}{\prod_{i=1}^k \Gamma(\alpha_i)} \prod_{i=1}^k x_i^{\alpha_i-1} \quad (2)$$

where $\alpha_i > 0$ for all $i = 1, \dots, k$, and the density is zero, if $x_i \notin [0, 1]$ for any $i = 1, \dots, k$ or $\sum_{i=1}^k x_i \neq 1$.

Sources:

- Wikipedia (2020): “Dirichlet distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-05-10; URL: https://en.wikipedia.org/wiki/Dirichlet_distribution#Probability_density_function.

4.5.2 Probability density function

Theorem: Let X be a random vector (\rightarrow I/1.2.3) following a Dirichlet distribution (\rightarrow II/4.5.1):

$$X \sim \text{Dir}(\alpha) . \quad (1)$$

Then, the probability density function (\rightarrow I/1.7.1) of X is

$$f_X(x) = \frac{\Gamma\left(\sum_{i=1}^k \alpha_i\right)}{\prod_{i=1}^k \Gamma(\alpha_i)} \prod_{i=1}^k x_i^{\alpha_i-1} . \quad (2)$$

Proof: This follows directly from the definition of the Dirichlet distribution (\rightarrow II/4.5.1). ■

4.5.3 Kullback-Leibler divergence

Theorem: Let X be an $1 \times k$ random vector (\rightarrow I/1.2.3). Assume two Dirichlet distributions (\rightarrow II/4.5.1) P and Q specifying the probability distribution of X as

$$\begin{aligned} P : X &\sim \text{Dir}(\alpha_1) \\ Q : X &\sim \text{Dir}(\alpha_2) . \end{aligned} \quad (1)$$

Then, the Kullback-Leibler divergence (\rightarrow I/2.5.1) of P from Q is given by

$$\text{KL}[P \parallel Q] = \ln \frac{\Gamma\left(\sum_{i=1}^k \alpha_{1i}\right)}{\Gamma\left(\sum_{i=1}^k \alpha_{2i}\right)} + \sum_{i=1}^k \ln \frac{\Gamma(\alpha_{2i})}{\Gamma(\alpha_{1i})} + \sum_{i=1}^k (\alpha_{1i} - \alpha_{2i}) \left[\psi(\alpha_{1i}) - \psi\left(\sum_{i=1}^k \alpha_{1i}\right) \right] . \quad (2)$$

Proof: The KL divergence for a continuous random variable (\rightarrow I/2.5.1) is given by

$$\text{KL}[P \parallel Q] = \int_{\mathcal{X}} p(x) \ln \frac{p(x)}{q(x)} dx \quad (3)$$

which, applied to the Dirichlet distributions (\rightarrow II/4.1.1) in (1), yields

$$\begin{aligned} \text{KL}[P \parallel Q] &= \int_{\mathcal{X}^k} \text{Dir}(x; \alpha_1) \ln \frac{\text{Dir}(x; \alpha_1)}{\text{Dir}(x; \alpha_2)} dx \\ &= \left\langle \ln \frac{\text{Dir}(x; \alpha_1)}{\text{Dir}(x; \alpha_2)} \right\rangle_{p(x)} \end{aligned} \quad (4)$$

where \mathcal{X}^k is the set $\left\{x \in \mathbb{R}^k \mid \sum_{i=1}^k x_i = 1, 0 \leq x_i \leq 1, i = 1, \dots, k\right\}$.

Using the probability density function of the Dirichlet distribution (\rightarrow II/4.5.2), this becomes:

$$\begin{aligned} \text{KL}[P \parallel Q] &= \left\langle \ln \frac{\frac{\Gamma\left(\sum_{i=1}^k \alpha_{1i}\right)}{\prod_{i=1}^k \Gamma(\alpha_{1i})} \prod_{i=1}^k x_i^{\alpha_{1i}-1}}{\frac{\Gamma\left(\sum_{i=1}^k \alpha_{2i}\right)}{\prod_{i=1}^k \Gamma(\alpha_{2i})} \prod_{i=1}^k x_i^{\alpha_{2i}-1}} \right\rangle_{p(x)} \\ &= \left\langle \ln \left(\frac{\Gamma\left(\sum_{i=1}^k \alpha_{1i}\right)}{\Gamma\left(\sum_{i=1}^k \alpha_{2i}\right)} \cdot \frac{\prod_{i=1}^k \Gamma(\alpha_{2i})}{\prod_{i=1}^k \Gamma(\alpha_{1i})} \cdot \prod_{i=1}^k x_i^{\alpha_{1i}-\alpha_{2i}} \right) \right\rangle_{p(x)} \\ &= \left\langle \ln \frac{\Gamma\left(\sum_{i=1}^k \alpha_{1i}\right)}{\Gamma\left(\sum_{i=1}^k \alpha_{2i}\right)} + \sum_{i=1}^k \ln \frac{\Gamma(\alpha_{2i})}{\Gamma(\alpha_{1i})} + \sum_{i=1}^k (\alpha_{1i} - \alpha_{2i}) \cdot \ln(x_i) \right\rangle_{p(x)} \\ &= \ln \frac{\Gamma\left(\sum_{i=1}^k \alpha_{1i}\right)}{\Gamma\left(\sum_{i=1}^k \alpha_{2i}\right)} + \sum_{i=1}^k \ln \frac{\Gamma(\alpha_{2i})}{\Gamma(\alpha_{1i})} + \sum_{i=1}^k (\alpha_{1i} - \alpha_{2i}) \cdot \langle \ln x_i \rangle_{p(x)} . \end{aligned} \quad (5)$$

Using the expected value of a logarithmized Dirichlet variate

$$X \sim \text{Dir}(\alpha) \Rightarrow \langle \ln x_i \rangle = \psi(\alpha_i) - \psi\left(\sum_{i=1}^k \alpha_i\right), \quad (6)$$

the Kullback-Leibler divergence from (5) becomes:

$$\text{KL}[P \parallel Q] = \ln \frac{\Gamma\left(\sum_{i=1}^k \alpha_{1i}\right)}{\Gamma\left(\sum_{i=1}^k \alpha_{2i}\right)} + \sum_{i=1}^k \ln \frac{\Gamma(\alpha_{2i})}{\Gamma(\alpha_{1i})} + \sum_{i=1}^k (\alpha_{1i} - \alpha_{2i}) \cdot \left[\psi(\alpha_{1i}) - \psi\left(\sum_{i=1}^k \alpha_{1i}\right) \right] \quad (7)$$

■

Sources:

- Penny, William D. (2001): “KL-Divergences of Normal, Gamma, Dirichlet and Wishart densities”; in: *University College, London*, p. 2, eqs. 8-9; URL: <https://www.fil.ion.ucl.ac.uk/~wpenny/publications/densities.ps>.

4.5.4 Exceedance probabilities

Theorem: Let $r = [r_1, \dots, r_k]$ be a random vector (\rightarrow I/1.2.3) following a Dirichlet distribution (\rightarrow II/4.5.1) with concentration parameters $\alpha = [\alpha_1, \dots, \alpha_k]$:

$$r \sim \text{Dir}(\alpha). \quad (1)$$

1) If $k = 2$, then the exceedance probability (\rightarrow I/1.3.11) for r_1 is

$$\varphi_1 = 1 - \frac{B\left(\frac{1}{2}; \alpha_1, \alpha_2\right)}{B(\alpha_1, \alpha_2)} \quad (2)$$

where $B(x, y)$ is the beta function and $B(x; a, b)$ is the incomplete beta function.

2) If $k > 2$, then the exceedance probability (\rightarrow I/1.3.11) for r_i is

$$\varphi_i = \int_0^\infty \prod_{j \neq i} \left(\frac{\gamma(\alpha_j, q_j)}{\Gamma(\alpha_j)} \right) \frac{q_i^{\alpha_i-1} \exp[-q_i]}{\Gamma(\alpha_i)} dq_i. \quad (3)$$

where $\Gamma(x)$ is the gamma function and $\gamma(s, x)$ is the lower incomplete gamma function.

Proof: In the context of the Dirichlet distribution (\rightarrow II/4.5.1), the exceedance probability (\rightarrow I/1.3.11) for a particular r_i is defined as:

$$\begin{aligned} \varphi_i &= p\left(\forall j \in \{1, \dots, k \mid j \neq i\} : r_i > r_j \mid \alpha\right) \\ &= p\left(\bigwedge_{j \neq i} r_i > r_j \mid \alpha\right). \end{aligned} \quad (4)$$

The probability density function of the Dirichlet distribution (\rightarrow II/4.5.2) is given by:

$$\text{Dir}(r; \alpha) = \frac{\Gamma\left(\sum_{i=1}^k \alpha_i\right)}{\prod_{i=1}^k \Gamma(\alpha_i)} \prod_{i=1}^k r_i^{\alpha_i-1}. \quad (5)$$

Note that the probability density function is only calculated, if

$$r_i \in [0, 1] \quad \text{for } i = 1, \dots, k \quad \text{and} \quad \sum_{i=1}^k r_i = 1, \quad (6)$$

and defined to be zero otherwise (\rightarrow II/4.5.1).

1) If $k = 2$, the probability density function of the Dirichlet distribution (\rightarrow II/4.5.2) reduces to

$$p(r) = \frac{\Gamma(\alpha_1 + \alpha_2)}{\Gamma(\alpha_1) \Gamma(\alpha_2)} r_1^{\alpha_1-1} r_2^{\alpha_2-1} \quad (7)$$

which is equivalent to the probability density function of the beta distribution (\rightarrow II/3.9.5)

$$p(r_1) = \frac{r_1^{\alpha_1-1} (1 - r_1)^{\alpha_2-1}}{B(\alpha_1, \alpha_2)} \quad (8)$$

with the beta function given by

$$B(x, y) = \frac{\Gamma(x) \Gamma(y)}{\Gamma(x + y)}. \quad (9)$$

With (6), the exceedance probability for this bivariate case simplifies to

$$\varphi_1 = p(r_1 > r_2) = p(r_1 > 1 - r_1) = p(r_1 > 1/2) = \int_{\frac{1}{2}}^1 p(r_1) dr_1. \quad (10)$$

Using the cumulative distribution function of the beta distribution (\rightarrow II/3.9.7), it evaluates to

$$\varphi_1 = 1 - \int_0^{\frac{1}{2}} p(r_1) dr_1 = 1 - \frac{B(\frac{1}{2}; \alpha_1, \alpha_2)}{B(\alpha_1, \alpha_2)} \quad (11)$$

with the incomplete beta function

$$B(x; a, b) = \int_0^x x^{a-1} (1 - x)^{b-1} dx. \quad (12)$$

2) If $k > 2$, there is no similarly simple expression, because in general

$$\varphi_i = p(r_i = \max(r)) > p(r_i > 1/2) \quad \text{for } i = 1, \dots, k, \quad (13)$$

i.e. exceedance probabilities cannot be evaluated using a simple threshold on r_i , because r_i might be the maximal element in r without being larger than 1/2. Instead, we make use of the relationship between the Dirichlet and the gamma distribution which states that

$$\begin{aligned} Y_1 &\sim \text{Gam}(\alpha_1, \beta), \dots, Y_k \sim \text{Gam}(\alpha_k, \beta), Y_s = \sum_{i=1}^k Y_i \\ \Rightarrow X &= (X_1, \dots, X_k) = \left(\frac{Y_1}{Y_s}, \dots, \frac{Y_k}{Y_s} \right) \sim \text{Dir}(\alpha_1, \dots, \alpha_k). \end{aligned} \quad (14)$$

The probability density function of the gamma distribution (\rightarrow II/3.4.7) is given by

$$\text{Gam}(x; a, b) = \frac{b^a}{\Gamma(a)} x^{a-1} \exp[-bx] \quad \text{for } x > 0. \quad (15)$$

Consider the gamma random variables (\rightarrow II/3.4.1)

$$q_1 \sim \text{Gam}(\alpha_1, 1), \dots, q_k \sim \text{Gam}(\alpha_k, 1), q_s = \sum_{j=1}^k q_j \quad (16)$$

and the Dirichlet random vector (\rightarrow II/4.5.1)

$$r = (r_1, \dots, r_k) = \left(\frac{q_1}{q_s}, \dots, \frac{q_k}{q_s} \right) \sim \text{Dir}(\alpha_1, \dots, \alpha_k). \quad (17)$$

Obviously, it holds that

$$r_i > r_j \Leftrightarrow q_i > q_j \quad \text{for } i, j = 1, \dots, k \quad \text{with } j \neq i. \quad (18)$$

Therefore, consider the probability that q_i is larger than q_j , given q_i is known. This probability is equal to the probability that q_j is smaller than q_i , given q_i is known

$$p(q_i > q_j | q_i) = p(q_j < q_i | q_i) \quad (19)$$

which can be expressed in terms of the cumulative distribution function of the gamma distribution (\rightarrow II/3.4.9) as

$$p(q_j < q_i | q_i) = \int_0^{q_i} \text{Gam}(q_j; \alpha_j, 1) dq_j = \frac{\gamma(\alpha_j, q_i)}{\Gamma(\alpha_j)} \quad (20)$$

where $\Gamma(x)$ is the gamma function and $\gamma(s, x)$ is the lower incomplete gamma function. Since the gamma variates are independent of each other, these probabilities factorize:

$$p(\forall_{j \neq i} [q_i > q_j] | q_i) = \prod_{j \neq i} p(q_i > q_j | q_i) = \prod_{j \neq i} \frac{\gamma(\alpha_j, q_i)}{\Gamma(\alpha_j)}. \quad (21)$$

In order to obtain the exceedance probability φ_i , the dependency on q_i in this probability still has to be removed. From equations (4) and (18), it follows that

$$\varphi_i = p(\forall_{j \neq i} [r_i > r_j]) = p(\forall_{j \neq i} [q_i > q_j]). \quad (22)$$

Using the law of marginal probability (\rightarrow I/1.3.3), we have

$$\varphi_i = \int_0^\infty p(\forall_{j \neq i} [q_i > q_j] | q_i) p(q_i) dq_i. \quad (23)$$

With (21) and (16), this becomes

$$\varphi_i = \int_0^\infty \prod_{j \neq i} (p(q_i > q_j | q_i)) \cdot \text{Gam}(q_i; \alpha_i, 1) dq_i. \quad (24)$$

And with (20) and (15), it becomes

$$\varphi_i = \int_0^\infty \prod_{j \neq i} \left(\frac{\gamma(\alpha_j, q_i)}{\Gamma(\alpha_j)} \right) \cdot \frac{q_i^{\alpha_i-1} \exp[-q_i]}{\Gamma(\alpha_i)} dq_i. \quad (25)$$

In other words, the exceedance probability (\rightarrow I/1.3.11) for one element from a Dirichlet-distributed (\rightarrow II/4.5.1) random vector (\rightarrow I/1.2.3) is an integral from zero to infinity where the first term in the integrand conforms to a product of gamma (\rightarrow II/3.4.1) cumulative distribution functions (\rightarrow I/1.8.1) and the second term is a gamma (\rightarrow II/3.4.1) probability density function (\rightarrow I/1.7.1).

■

Sources:

- Soch J, Allefeld C (2016): “Exceedance Probabilities for the Dirichlet Distribution”; in: *arXiv stat.AP*, 1611.01439; URL: <https://arxiv.org/abs/1611.01439>.

5 Matrix-variate continuous distributions

5.1 Matrix-normal distribution

5.1.1 Definition

Definition: Let X be an $n \times p$ random matrix (\rightarrow I/1.2.4). Then, X is said to be matrix-normally distributed with mean M , covariance (\rightarrow I/1.16.1) across rows U and covariance (\rightarrow I/1.16.1) across columns V

$$X \sim \mathcal{MN}(M, U, V), \quad (1)$$

if and only if its probability density function (\rightarrow I/1.7.1) is given by

$$\mathcal{MN}(X; M, U, V) = \frac{1}{\sqrt{(2\pi)^{np}|V|^n|U|^p}} \cdot \exp \left[-\frac{1}{2} \text{tr} (V^{-1}(X - M)^T U^{-1}(X - M)) \right] \quad (2)$$

where M is an $n \times p$ real matrix, U is an $n \times n$ positive-definite matrix and V is a $p \times p$ positive-definite matrix.

Sources:

- Wikipedia (2020): “Matrix normal distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-01-27; URL: https://en.wikipedia.org/wiki/Matrix_normal_distribution#Definition.

5.1.2 Equivalence to multivariate normal distribution

Theorem: The matrix X is matrix-normally distributed (\rightarrow II/5.1.1)

$$X \sim \mathcal{MN}(M, U, V), \quad (1)$$

if and only if $\text{vec}(X)$ is multivariate normally distributed (\rightarrow II/4.1.1)

$$\text{vec}(X) \sim \mathcal{N}(\text{vec}(M), V \otimes U) \quad (2)$$

where $\text{vec}(X)$ is the vectorization operator and \otimes is the Kronecker product.

Proof: The probability density function of the matrix-normal distribution (\rightarrow II/5.1.3) with $n \times p$ mean M , $n \times n$ covariance across rows U and $p \times p$ covariance across columns V is

$$\mathcal{MN}(X; M, U, V) = \frac{1}{\sqrt{(2\pi)^{np}|V|^n|U|^p}} \cdot \exp \left[-\frac{1}{2} \text{tr} (V^{-1}(X - M)^T U^{-1}(X - M)) \right]. \quad (3)$$

Using the trace property $\text{tr}(ABC) = \text{tr}(BCA)$, we have:

$$\mathcal{MN}(X; M, U, V) = \frac{1}{\sqrt{(2\pi)^{np}|V|^n|U|^p}} \cdot \exp \left[-\frac{1}{2} \text{tr} ((X - M)^T U^{-1}(X - M) V^{-1}) \right]. \quad (4)$$

Using the trace-vectorization relation $\text{tr}(A^T B) = \text{vec}(A)^T \text{vec}(B)$, we have:

$$\mathcal{MN}(X; M, U, V) = \frac{1}{\sqrt{(2\pi)^{np}|V|^n|U|^p}} \cdot \exp \left[-\frac{1}{2} \text{vec}(X - M)^T \text{vec} (U^{-1}(X - M) V^{-1}) \right]. \quad (5)$$

Using the vectorization-Kronecker relation $\text{vec}(ABC) = (C^T \otimes A) \text{vec}(B)$, we have:

$$\mathcal{MN}(X; M, U, V) = \frac{1}{\sqrt{(2\pi)^{np}|V|^n|U|^p}} \cdot \exp \left[-\frac{1}{2} \text{vec}(X - M)^T (V^{-1} \otimes U^{-1}) \text{vec}(X - M) \right]. \quad (6)$$

Using the Kronecker product property $(A^{-1} \otimes B^{-1}) = (A \otimes B)^{-1}$, we have:

$$\mathcal{MN}(X; M, U, V) = \frac{1}{\sqrt{(2\pi)^{np}|V|^n|U|^p}} \cdot \exp \left[-\frac{1}{2} \text{vec}(X - M)^T (V \otimes U)^{-1} \text{vec}(X - M) \right]. \quad (7)$$

Using the vectorization property $\text{vec}(A + B) = \text{vec}(A) + \text{vec}(B)$, we have:

$$\mathcal{MN}(X; M, U, V) = \frac{1}{\sqrt{(2\pi)^{np}|V|^n|U|^p}} \cdot \exp \left[-\frac{1}{2} [\text{vec}(X) - \text{vec}(M)]^T (V \otimes U)^{-1} [\text{vec}(X) - \text{vec}(M)] \right]. \quad (8)$$

Using the Kronecker-determinant relation $|A \otimes B| = |A|^m |B|^n$, we have:

$$\mathcal{MN}(X; M, U, V) = \frac{1}{\sqrt{(2\pi)^{np}|V \otimes U|}} \cdot \exp \left[-\frac{1}{2} [\text{vec}(X) - \text{vec}(M)]^T (V \otimes U)^{-1} [\text{vec}(X) - \text{vec}(M)] \right]. \quad (9)$$

This is the probability density function of the multivariate normal distribution (\rightarrow II/4.1.4) with the $np \times 1$ mean vector $\text{vec}(M)$ and the $np \times np$ covariance matrix $V \otimes U$:

$$\mathcal{MN}(X; M, U, V) = \mathcal{N}(\text{vec}(X); \text{vec}(M), V \otimes U). \quad (10)$$

By showing that the probability density functions (\rightarrow I/1.7.1) are identical, it is proven that the associated probability distributions (\rightarrow I/1.5.1) are equivalent. ■

Sources:

- Wikipedia (2020): “Matrix normal distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-01-20; URL: https://en.wikipedia.org/wiki/Matrix_normal_distribution#Proof.

5.1.3 Probability density function

Theorem: Let X be a random matrix (\rightarrow I/1.2.4) following a matrix-normal distribution (\rightarrow II/5.1.1):

$$X \sim \mathcal{MN}(M, U, V). \quad (1)$$

Then, the probability density function (\rightarrow I/1.7.1) of X is

$$f(X) = \frac{1}{\sqrt{(2\pi)^{np}|V|^n|U|^p}} \cdot \exp \left[-\frac{1}{2} \text{tr} (V^{-1} (X - M)^T U^{-1} (X - M)) \right]. \quad (2)$$

Proof: This follows directly from the definition of the matrix-normal distribution (\rightarrow II/5.1.1). ■

5.1.4 Mean

Theorem: Let X be a random matrix (\rightarrow I/1.2.4) following a matrix-normal distribution (\rightarrow II/5.1.1):

$$X \sim \mathcal{MN}(M, U, V) . \quad (1)$$

Then, the mean or expected value (\rightarrow I/1.12.1) of X is

$$E(X) = M . \quad (2)$$

Proof: When X follows a matrix-normal distribution (\rightarrow II/5.1.1), its vectorized version follows a multivariate normal distribution (\rightarrow II/5.1.2)

$$\text{vec}(X) \sim \mathcal{N}(\text{vec}(M), V \otimes U) \quad (3)$$

and the expected value of this multivariate normal distribution is (\rightarrow II/4.1.6)

$$E[\text{vec}(X)] = \text{vec}(M) . \quad (4)$$

Since the expected value of a random matrix is calculated element-wise (\rightarrow I/1.12.19), we can invert the vectorization operator to get:

$$E[X] = M . \quad (5)$$

■

Sources:

- Wikipedia (2022): “Matrix normal distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-09-15; URL: https://en.wikipedia.org/wiki/Matrix_normal_distribution#Expected_values.

5.1.5 Covariance

Theorem: Let X be an $n \times p$ random matrix (\rightarrow I/1.2.4) following a matrix-normal distribution (\rightarrow II/5.1.1):

$$X \sim \mathcal{MN}(M, U, V) . \quad (1)$$

Then,

1) the covariance matrix (\rightarrow I/1.16.1) of each row of X is a scalar multiple of V

$$\text{Cov}(x_{i,\bullet}^T) \propto V \quad \text{for all } i = 1, \dots, n ; \quad (2)$$

2) the covariance matrix (\rightarrow I/1.16.1) of each column of X is a scalar multiple of U

$$\text{Cov}(x_{\bullet,j}) \propto U \quad \text{for all } j = 1, \dots, p . \quad (3)$$

Proof:

1) The marginal distribution (\rightarrow I/1.5.3) of a given row of X is a multivariate normal distribution (\rightarrow II/5.1.10)

$$x_{i,\bullet}^T \sim \mathcal{N}(m_{i,\bullet}^T, u_{ii}V) , \quad (4)$$

and the covariance of this multivariate normal distribution (\rightarrow II/4.1.8) is

$$\text{Cov}(x_{i,\bullet}^T) = u_{ii}V \propto V . \quad (5)$$

2) The marginal distribution (\rightarrow I/1.5.3) of a given column of X is a multivariate normal distribution (\rightarrow II/5.1.10)

$$x_{\bullet,j} \sim \mathcal{N}(m_{\bullet,j}, v_{jj}U) , \quad (6)$$

and the covariance of this multivariate normal distribution (\rightarrow II/4.1.8) is

$$\text{Cov}(x_{\bullet,j}) = v_{jj}U \propto U . \quad (7)$$

Sources:

- Wikipedia (2022): “Matrix normal distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-09-15; URL: https://en.wikipedia.org/wiki/Matrix_normal_distribution#Expected_values.

5.1.6 Differential entropy

Theorem: Let X be an $n \times p$ random matrix (\rightarrow I/1.2.4) following a matrix-normal distribution (\rightarrow II/5.1.1)

$$X \sim \mathcal{MN}(M, U, V) . \quad (1)$$

Then, the differential entropy (\rightarrow I/2.2.1) of X in nats is

$$h(X) = \frac{np}{2} \ln(2\pi) + \frac{n}{2} \ln |V| + \frac{p}{2} \ln |U| + \frac{np}{2} . \quad (2)$$

Proof: The matrix-normal distribution is equivalent to the multivariate normal distribution (\rightarrow II/5.1.2),

$$X \sim \mathcal{MN}(M, U, V) \Leftrightarrow \text{vec}(X) \sim \mathcal{N}(\text{vec}(M), V \otimes U) , \quad (3)$$

and the differential entropy for the multivariate normal distribution (\rightarrow II/4.1.10) in nats is

$$X \sim \mathcal{N}(\mu, \Sigma) \Rightarrow h(X) = \frac{n}{2} \ln(2\pi) + \frac{1}{2} \ln |\Sigma| + \frac{1}{2}n \quad (4)$$

where X is an n -dimensional random vector (\rightarrow I/1.2.3). Thus, we can plug the distribution parameters from (1) into the differential entropy in (4) using the relationship given by (3):

$$h(X) = \frac{np}{2} \ln(2\pi) + \frac{1}{2} \ln |V \otimes U| + \frac{1}{2}np . \quad (5)$$

Using the Kronecker product property

$$|A \otimes B| = |A|^m |B|^n \quad \text{where} \quad A \in \mathbb{R}^{n \times n} \quad \text{and} \quad B \in \mathbb{R}^{m \times m} , \quad (6)$$

the differential entropy from (5) becomes:

$$\begin{aligned} h(X) &= \frac{np}{2} \ln(2\pi) + \frac{1}{2} \ln (|V|^n |U|^p) + \frac{1}{2}np \\ &= \frac{np}{2} \ln(2\pi) + \frac{n}{2} \ln |V| + \frac{p}{2} \ln |U| + \frac{np}{2} . \end{aligned} \quad (7)$$



5.1.7 Kullback-Leibler divergence

Theorem: Let X be an $n \times p$ random matrix (\rightarrow I/1.2.4). Assume two matrix-normal distributions (\rightarrow II/5.1.1) P and Q specifying the probability distribution of X as

$$\begin{aligned} P : X &\sim \mathcal{MN}(M_1, U_1, V_1) \\ Q : X &\sim \mathcal{MN}(M_2, U_2, V_2) . \end{aligned} \quad (1)$$

Then, the Kullback-Leibler divergence (\rightarrow I/2.5.1) of P from Q is given by

$$\begin{aligned} \text{KL}[P \parallel Q] &= \frac{1}{2} \left[\text{vec}(M_2 - M_1)^T \text{vec}(U_2^{-1}(M_2 - M_1)V_2^{-1}) \right. \\ &\quad \left. + \text{tr}((V_2^{-1}V_1) \otimes (U_2^{-1}U_1)) - n \ln \frac{|V_1|}{|V_2|} - p \ln \frac{|U_1|}{|U_2|} - np \right] . \end{aligned} \quad (2)$$

Proof: The matrix-normal distribution is equivalent to the multivariate normal distribution (\rightarrow II/5.1.2),

$$X \sim \mathcal{MN}(M, U, V) \quad \Leftrightarrow \quad \text{vec}(X) \sim \mathcal{N}(\text{vec}(M), V \otimes U) , \quad (3)$$

and the Kullback-Leibler divergence for the multivariate normal distribution (\rightarrow II/4.1.12) is

$$\text{KL}[P \parallel Q] = \frac{1}{2} \left[(\mu_2 - \mu_1)^T \Sigma_2^{-1} (\mu_2 - \mu_1) + \text{tr}(\Sigma_2^{-1} \Sigma_1) - \ln \frac{|\Sigma_1|}{|\Sigma_2|} - n \right] \quad (4)$$

where X is an n -dimensional random vector (\rightarrow I/1.2.3).

Thus, we can plug the distribution parameters from (1) into the KL divergence in (4) using the relationship given by (3)

$$\begin{aligned} \text{KL}[P \parallel Q] &= \frac{1}{2} \left[(\text{vec}(M_2) - \text{vec}(M_1))^T (V_2 \otimes U_2)^{-1} (\text{vec}(M_2) - \text{vec}(M_1)) \right. \\ &\quad \left. + \text{tr}((V_2 \otimes U_2)^{-1} (V_1 \otimes U_1)) - \ln \frac{|V_1 \otimes U_1|}{|V_2 \otimes U_2|} - np \right] . \end{aligned} \quad (5)$$

Using the vectorization operator and Kronecker product properties

$$\text{vec}(A) + \text{vec}(B) = \text{vec}(A + B) \quad (6)$$

$$(A \otimes B)^{-1} = A^{-1} \otimes B^{-1} \quad (7)$$

$$(A \otimes B)(C \otimes D) = (AC) \otimes (BD) \quad (8)$$

$$|A \otimes B| = |A|^m |B|^n \quad \text{where} \quad A \in \mathbb{R}^{n \times n} \quad \text{and} \quad B \in \mathbb{R}^{m \times m} , \quad (9)$$

the Kullback-Leibler divergence from (5) becomes:

$$\begin{aligned} \text{KL}[P || Q] = & \frac{1}{2} [\text{vec}(M_2 - M_1)^T (V_2^{-1} \otimes U_2^{-1}) \text{vec}(M_2 - M_1) \\ & + \text{tr}((V_2^{-1}V_1) \otimes (U_2^{-1}U_1)) - n \ln \frac{|V_1|}{|V_2|} - p \ln \frac{|U_1|}{|U_2|} - np] . \end{aligned} \quad (10)$$

Using the relationship between Kronecker product and vectorization operator

$$(C^T \otimes A) \text{vec}(B) = \text{vec}(ABC) , \quad (11)$$

we finally have:

$$\begin{aligned} \text{KL}[P || Q] = & \frac{1}{2} [\text{vec}(M_2 - M_1)^T \text{vec}(U_2^{-1}(M_2 - M_1)V_2^{-1}) \\ & + \text{tr}((V_2^{-1}V_1) \otimes (U_2^{-1}U_1)) - n \ln \frac{|V_1|}{|V_2|} - p \ln \frac{|U_1|}{|U_2|} - np] . \end{aligned} \quad (12)$$

■

5.1.8 Transposition

Theorem: Let X be an $n \times p$ random matrix (\rightarrow I/1.2.4) following a matrix-normal distribution (\rightarrow II/5.1.1):

$$X \sim \mathcal{MN}(M, U, V) . \quad (1)$$

Then, the transpose of X also has a matrix-normal distribution:

$$X^T \sim \mathcal{MN}(M^T, V, U) . \quad (2)$$

Proof: For a random vector (\rightarrow I/1.2.3) $X \in \mathbb{R}^n$ with probability density function (\rightarrow I/1.7.1) $f_X(x)$, the probability density function of the invertible function (\rightarrow I/1.7.5) $Y = g(X)$ is

$$f_Y(y) = \begin{cases} f_X(g^{-1}(y)) |J_{g^{-1}}(y)| , & \text{if } y \in \mathcal{Y} \\ 0 , & \text{if } y \notin \mathcal{Y} \end{cases} \quad (3)$$

where $|J_{g^{-1}}(y)|$ is the determinant of the Jacobian matrix

$$J_{g^{-1}}(y) = \begin{bmatrix} \frac{dx_1}{dy_1} & \cdots & \frac{dx_1}{dy_n} \\ \vdots & \ddots & \vdots \\ \frac{dx_n}{dy_1} & \cdots & \frac{dx_n}{dy_n} \end{bmatrix} \quad (4)$$

and \mathcal{Y} is the set of possible outcomes of Y :

$$\mathcal{Y} = \{y = g(x) : x \in \mathcal{X}\} . \quad (5)$$

In the present case, we have $Y = g(X) = X^T$ and $X = g^{-1}(Y) = Y^T$ and all $Y \in \mathcal{Y} = \mathbb{R}^{p \times n}$. For the vectorized matrices X and Y , the Jacobian matrix is

$$J_{g^{-1}}(Y) = \begin{bmatrix} \frac{dx_{11}}{dy_{11}} & \frac{dx_{11}}{dy_{21}} & \cdots & \frac{dx_{11}}{dy_{pn}} \\ \frac{dx_{21}}{dy_{11}} & \frac{dx_{21}}{dy_{21}} & \cdots & \frac{dx_{21}}{dy_{pn}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{dx_{np}}{dy_{11}} & \frac{dx_{np}}{dy_{21}} & \cdots & \frac{dx_{np}}{dy_{pn}} \end{bmatrix} \in \mathbb{R}^{np}. \quad (6)$$

Because by transposition, $y_{ji} = x_{ij}$, we have

$$\frac{dx_{ij}}{dy_{kl}} = \begin{cases} 1, & \text{if } k = j \text{ and } l = i \\ 0, & \text{otherwise.} \end{cases} \quad (7)$$

Thus, $J_{g^{-1}}(Y)$ is row-equivalent to I_{np} and $|J_{g^{-1}}(Y)| = |I_{np}| = 1$. Therefore, we have:

$$\begin{aligned} f_Y(Y) &= f_X(g^{-1}(Y)) |J_{g^{-1}}(Y)| \\ &= \mathcal{MN}(Y^T; M, U, V) |I_{np}| \\ &= \mathcal{MN}(Y^T; M, U, V). \end{aligned} \quad (8)$$

The probability density function of the matrix-normal distribution (\rightarrow II/5.1.3) is:

$$f(X) = \mathcal{MN}(X; M, U, V) = \frac{1}{\sqrt{(2\pi)^{np} |V|^n |U|^p}} \cdot \exp \left[-\frac{1}{2} \text{tr} (V^{-1} (X - M)^T U^{-1} (X - M)) \right]. \quad (9)$$

Thus, substituting $X = Y^T$, we get:

$$f(Y) = \frac{1}{\sqrt{(2\pi)^{np} |U|^p |V|^n}} \cdot \exp \left[-\frac{1}{2} \text{tr} (V^{-1} (Y^T - M)^T U^{-1} (Y^T - M)) \right]. \quad (10)$$

Using $(A + B)^T = (A^T + B^T)$, we have:

$$f(Y) = \frac{1}{\sqrt{(2\pi)^{np} |U|^p |V|^n}} \cdot \exp \left[-\frac{1}{2} \text{tr} (V^{-1} (Y - M^T) U^{-1} (Y - M^T)^T) \right]. \quad (11)$$

Using $\text{tr}(ABC) = \text{tr}(CAB)$, we obtain

$$f(Y) = \frac{1}{\sqrt{(2\pi)^{np} |U|^p |V|^n}} \cdot \exp \left[-\frac{1}{2} \text{tr} (U^{-1} (Y - M^T)^T V^{-1} (Y - M^T)) \right] \quad (12)$$

which is the probability density function of a matrix-normal distribution (\rightarrow II/5.1.3) with mean M^T , covariance across rows V and covariance across columns U :

$$f(Y) = \mathcal{MN}(Y; M^T, V, U). \quad (13)$$

■

5.1.9 Linear transformation

Theorem: Let X be an $n \times p$ random matrix (\rightarrow I/1.2.4) following a matrix-normal distribution (\rightarrow II/5.1.1):

$$X \sim \mathcal{MN}(M, U, V) . \quad (1)$$

Then, a linear transformation of X is also matrix-normally distributed

$$Y = AXB + C \sim \mathcal{MN}(AMB + C, AUA^T, B^TVB) \quad (2)$$

where A is an $r \times n$ matrix of full rank $r \leq n$ and B is a $p \times s$ matrix of full rank $s \leq p$ and C is an $r \times s$ matrix.

Proof: The matrix-normal distribution is equivalent to the multivariate normal distribution (\rightarrow II/5.1.2),

$$X \sim \mathcal{MN}(M, U, V) \Leftrightarrow \text{vec}(X) \sim \mathcal{N}(\text{vec}(M), V \otimes U) , \quad (3)$$

and the linear transformation theorem for the multivariate normal distribution (\rightarrow II/4.1.14) states:

$$x \sim \mathcal{N}(\mu, \Sigma) \Rightarrow y = Ax + b \sim \mathcal{N}(A\mu + b, A\Sigma A^T) . \quad (4)$$

The vectorization of $Y = AXB + C$ is

$$\begin{aligned} \text{vec}(Y) &= \text{vec}(AXB + C) \\ &= \text{vec}(AXB) + \text{vec}(C) \\ &= (B^T \otimes A)\text{vec}(X) + \text{vec}(C) \end{aligned} \quad (5)$$

and the Kronecker product obeys

$$(A \otimes B)(C \otimes D) = (AC) \otimes (BD) . \quad (6)$$

Using (3) and (4), we have

$$\begin{aligned} \text{vec}(Y) &\sim \mathcal{N}((B^T \otimes A)\text{vec}(M) + \text{vec}(C), (B^T \otimes A)(V \otimes U)(B^T \otimes A)^T) \\ &= \mathcal{N}(\text{vec}(AMB) + \text{vec}(C), (B^TV \otimes AU)(B^T \otimes A)^T) \\ &= \mathcal{N}(\text{vec}(AMB + C), B^TVB \otimes AUA^T) . \end{aligned} \quad (7)$$

Using (3), we finally have:

$$Y \sim \mathcal{MN}(AMB + C, AUA^T, B^TVB) . \quad (8)$$

■

5.1.10 Marginal distributions

Theorem: Let X be an $n \times p$ random matrix (\rightarrow I/1.2.4) following a matrix-normal distribution (\rightarrow II/5.1.1):

$$X \sim \mathcal{MN}(M, U, V) . \quad (1)$$

Then,

1) the marginal distribution (\rightarrow I/1.5.3) of any subset matrix $X_{I,J}$, obtained by dropping some rows and/or columns from X , is also a matrix-normal distribution (\rightarrow II/5.1.1)

$$X_{I,J} \sim \mathcal{MN}(M_{I,J}, U_{I,I}, V_{J,J}) \quad (2)$$

where $I \subseteq \{1, \dots, n\}$ is an (ordered) subset of all row indices and $J \subseteq \{1, \dots, p\}$ is an (ordered) subset of all column indices, such that $M_{I,J}$ is the matrix dropping the irrelevant rows and columns (the ones not in the subset, i.e. marginalized out) from the mean matrix M ; $U_{I,I}$ is the matrix dropping rows not in I from U ; and $V_{J,J}$ is the matrix dropping columns not in J from V ;

2) the marginal distribution (\rightarrow I/1.5.3) of each row vector is a multivariate normal distribution (\rightarrow II/4.1.1)

$$x_{i,\bullet}^T \sim \mathcal{N}(m_{i,\bullet}^T, u_{ii}V) \quad (3)$$

where $m_{i,\bullet}$ is the i -th row of M and u_{ii} is the i -th diagonal entry of U ;

3) the marginal distribution (\rightarrow I/1.5.3) of each column vector is a multivariate normal distribution (\rightarrow II/4.1.1)

$$x_{\bullet,j} \sim \mathcal{N}(m_{\bullet,j}, v_{jj}U) \quad (4)$$

where $m_{\bullet,j}$ is the j -th column of M and v_{jj} is the j -th diagonal entry of V ; and

4) the marginal distribution (\rightarrow I/1.5.3) of one element of X is a univariate normal distribution (\rightarrow II/3.2.1)

$$x_{ij} \sim \mathcal{N}(m_{ij}, u_{ii}v_{jj}) \quad (5)$$

where m_{ij} is the (i, j) -th entry of M .

Proof:

1) Define a selector matrix A , such that $a_{ij} = 1$, if the i -th row in the subset matrix should be the j -th row from the original matrix (and $a_{ij} = 0$ otherwise)

$$A \in \mathbb{R}^{|I| \times n}, \quad \text{s.t.} \quad a_{ij} = \begin{cases} 1, & \text{if } I_i = j \\ 0, & \text{otherwise} \end{cases} \quad (6)$$

and define a selector matrix B , such that $b_{ij} = 1$, if the j -th column in the subset matrix should be the i -th column from the original matrix (and $b_{ij} = 0$ otherwise)

$$B \in \mathbb{R}^{p \times |J|}, \quad \text{s.t.} \quad b_{ij} = \begin{cases} 1, & \text{if } J_j = i \\ 0, & \text{otherwise} . \end{cases} \quad (7)$$

Then, $X_{I,J}$ can be expressed as

$$X_{I,J} = AXB \quad (8)$$

and we can apply the linear transformation theorem (\rightarrow II/5.1.9) to give

$$X_{I,J} \sim \mathcal{MN}(AMB, AUA^T, B^TVB) . \quad (9)$$

Finally, we see that $AMB = M_{I,J}$, $AUA^T = U_{I,I}$ and $B^TVB = V_{J,J}$.

2) This is a special case of 1). Setting A to the i -th elementary row vector in n dimensions and B to the $p \times p$ identity matrix

$$A = e_i, \quad B = I_p , \quad (10)$$

the i -th row of X can be expressed as

$$\begin{aligned} x_{i,\bullet} &= AXB = e_i X I_p = e_i X \\ &\stackrel{(9)}{\sim} \mathcal{MN}(m_{i,\bullet}, u_{ii}, V) . \end{aligned} \quad (11)$$

Thus, the transpose of the row vector is distributed as (\rightarrow II/5.1.8)

$$x_{i,\bullet}^T \sim \mathcal{MN}(m_{i,\bullet}^T, V, u_{ii}) \quad (12)$$

which is equivalent to a multivariate normal distribution (\rightarrow II/5.1.2):

$$x_{i,\bullet}^T \sim \mathcal{N}(m_{i,\bullet}^T, u_{ii}V) . \quad (13)$$

3) This is a special case of 1). Setting A to the $n \times n$ identity matrix and B to the j -th elementary row vector in p dimensions

$$A = I_n, \quad B = e_j^T , \quad (14)$$

the j -th column of X can be expressed as

$$\begin{aligned} x_{\bullet,j} &= AXB = I_n X e_j^T = X e_j^T \\ &\stackrel{(9)}{\sim} \mathcal{MN}(m_{\bullet,j}, U, v_{jj}) \end{aligned} \quad (15)$$

which is equivalent to a multivariate normal distribution (\rightarrow II/5.1.2):

$$x_{\bullet,j} \sim \mathcal{N}(m_{\bullet,j}, v_{jj}U) . \quad (16)$$

4) This is a special case of 2) and 3). Setting A to the i -th elementary row vector in n dimensions and B to the j -th elementary row vector in p dimensions

$$A = e_i, \quad B = e_j^T , \quad (17)$$

the (i, j) -th entry of X can be expressed as

$$\begin{aligned} x_{ij} &= AXB = e_i X e_j^T \\ &\stackrel{(9)}{\sim} \mathcal{MN}(m_{ij}, u_{ii}, v_{jj}) . \end{aligned} \quad (18)$$

As x_{ij} is a scalar, this is equivalent to a univariate normal distribution (\rightarrow II/3.2.1) as a special case (\rightarrow II/3.2.2) of the matrix-normal distribution (\rightarrow II/4.1.2):

$$x_{ij} \sim \mathcal{N}(m_{ij}, u_{ii}v_{jj}) . \quad (19)$$

■

5.1.11 Redundancy of parameters

Theorem: The covariance parameters of the matrix-normal distribution (\rightarrow II/5.1.1) are redundant up to a scalar factor, i.e. the two probability distributions (\rightarrow I/1.5.1)

$$\begin{aligned} X &\sim \mathcal{MN}(M, U, V) \\ X &\sim \mathcal{MN}\left(M, a \cdot U, \frac{1}{a} \cdot V\right) \end{aligned} \quad (1)$$

are equivalent for any $a \in \mathbb{R}$ with $a > 0$ where $X \in \mathbb{R}^{n \times p}$ is a random matrix (\rightarrow I/1.2.4) and $U \in \mathbb{R}^{n \times n}$ and $V \in \mathbb{R}^{p \times p}$ are positive-definite matrices.

Proof: Since U and V must be positive-definite in the matrix-normal distribution (\rightarrow II/5.1.1), the scalar a must be larger than zero. A random matrix follows a matrix-normal distribution, if and only if its vectorization is multivariate normally distributed (\rightarrow II/5.1.2)

$$X \sim \mathcal{MN}(M, U, V) \quad \Leftrightarrow \quad \text{vec}(X) \sim \mathcal{N}(\text{vec}(M), V \otimes U) \quad (2)$$

where $\text{vec}(X)$ is the vectorization operator and \otimes is the Kronecker product. Thus, the second distribution in (1) is equivalent to

$$\begin{aligned} X \sim \mathcal{MN}\left(M, a \cdot U, \frac{1}{a} \cdot V\right) &\Leftrightarrow \text{vec}(X) \sim \mathcal{N}\left(\text{vec}(M), \frac{1}{a} V \otimes aU\right) \\ &\sim \mathcal{N}\left(\text{vec}(M), \frac{1}{a} (V \otimes aU)\right) \\ &\sim \mathcal{N}\left(\text{vec}(M), \frac{a}{a} (V \otimes U)\right) \\ &\sim \mathcal{N}(\text{vec}(M), V \otimes U) \end{aligned} \quad (3)$$

which proves the equivalence of the two distributions in (1).

■

Sources:

- Glanz, Hunter; Carvalho, Luis (2013): “An Expectation-Maximization Algorithm for the Matrix Normal Distribution”; in: *arXiv stat.ME*, sect. 2.1, p. 3; URL: <https://arxiv.org/abs/1309.6609>; DOI: 10.48550/arXiv.1309.6609.

5.1.12 Redundancy of parameters

Theorem: The covariance parameters of the matrix-normal distribution (\rightarrow II/5.1.1) are redundant up to a scalar factor, i.e. the two probability distributions (\rightarrow I/1.5.1)

$$\begin{aligned} X &\sim \mathcal{MN}(M, U, V) \\ X &\sim \mathcal{MN}\left(M, a \cdot U, \frac{1}{a} \cdot V\right) \end{aligned} \quad (1)$$

are equivalent for any $a \in \mathbb{R}$ with $a > 0$ where $X \in \mathbb{R}^{n \times p}$ is a random matrix (\rightarrow I/1.2.4) and $U \in \mathbb{R}^{n \times n}$ and $V \in \mathbb{R}^{p \times p}$ are positive-definite matrices.

Proof: The probability density function of the matrix-normal distribution (\rightarrow II/5.1.3) is

$$\begin{aligned} X &\sim \mathcal{MN}(M, U, V) \\ \Rightarrow f(X) &= \frac{1}{\sqrt{(2\pi)^{np} |V|^n |U|^p}} \cdot \exp \left[-\frac{1}{2} \text{tr} (V^{-1} (X - M)^T U^{-1} (X - M)) \right]. \end{aligned} \quad (2)$$

Using the inverse matrix property $(cA)^{-1} = (1/c)A^{-1}$ and the matrix determinant property $|cA| = c^n |A|$, the probability density function (\rightarrow I/1.7.1) of the second distribution in (1) becomes

$$\begin{aligned} p(X) &= \frac{1}{\sqrt{(2\pi)^{np} \left|\frac{1}{a}V\right|^n |aU|^p}} \cdot \exp \left[-\frac{1}{2} \text{tr} \left(\left(\frac{1}{a}V\right)^{-1} (X - M)^T (aU)^{-1} (X - M) \right) \right] \\ &= \frac{1}{\sqrt{(2\pi)^{np} \left(\left(\frac{1}{a}\right)^p |V|\right)^n (a^n |U|)^p}} \cdot \exp \left[-\frac{1}{2} \text{tr} \left(\frac{a}{a} V^{-1} (X - M)^T U^{-1} (X - M) \right) \right] \\ &= \frac{1}{\sqrt{(2\pi)^{np} \left(\frac{1}{a}\right)^{np} a^{np} |V|^n |U|^p}} \cdot \exp \left[-\frac{1}{2} \text{tr} (V^{-1} (X - M)^T U^{-1} (X - M)) \right] \\ &= \frac{1}{\sqrt{(2\pi)^{np} |V|^n |U|^p}} \cdot \exp \left[-\frac{1}{2} \text{tr} (V^{-1} (X - M)^T U^{-1} (X - M)) \right] \end{aligned} \quad (3)$$

which is equal to the probability density function (\rightarrow I/1.7.1) of the first distribution in (1). ■

Sources:

- Glanz, Hunter; Carvalho, Luis (2013): “An Expectation-Maximization Algorithm for the Matrix Normal Distribution”; in: *arXiv stat.ME*, sect. 2.1, p. 3; URL: <https://arxiv.org/abs/1309.6609>; DOI: 10.48550/arXiv.1309.6609.

5.1.13 Drawing samples

Theorem: Let $X \in \mathbb{R}^{n \times p}$ be a random matrix (\rightarrow I/1.2.4) with all entries independently following a standard normal distribution (\rightarrow II/3.2.3). Moreover, let $A \in \mathbb{R}^{n \times n}$ and $B \in \mathbb{R}^{p \times p}$, such that $AA^T = U$ and $B^T B = V$.

Then, $Y = M + AXB$ follows a matrix-normal distribution (\rightarrow II/5.1.1) with mean (\rightarrow I/1.12.19) M , covariance (\rightarrow I/1.16.1) across rows U and covariance (\rightarrow I/1.16.1) across columns V :

$$Y = M + AXB \sim \mathcal{MN}(M, U, V) . \quad (1)$$

Proof: If all entries of X are independent and standard normally distributed (\rightarrow II/3.2.3)

$$x_{ij} \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, 1) \quad \text{for all } i = 1, \dots, n \quad \text{and } j = 1, \dots, p , \quad (2)$$

this implies a multivariate normal distribution with diagonal covariance matrix (\rightarrow II/4.1.17)

$$\begin{aligned} \text{vec}(X) &\sim \mathcal{N}(\text{vec}(0_{np}), I_{np}) \\ &\sim \mathcal{N}(\text{vec}(0_{np}), I_p \otimes I_n) \end{aligned} \quad (3)$$

where 0_{np} is an $n \times p$ matrix of zeros and I_n is the $n \times n$ identity matrix.

Due to the relationship between multivariate and matrix-normal distribution (\rightarrow II/5.1.2), we have:

$$X \sim \mathcal{MN}(0_{np}, I_n, I_p) . \quad (4)$$

Thus, with the linear transformation theorem for the matrix-normal distribution (\rightarrow II/5.1.9), it follows that

$$\begin{aligned} Y = M + AXB &\sim \mathcal{MN}(M + A0_{np}B, AI_nA^T, B^T I_p B) \\ &\sim \mathcal{MN}(M, AA^T, B^T B) \\ &\sim \mathcal{MN}(M, U, V) . \end{aligned} \quad (5)$$

Thus, given X defined by (2), Y defined by (1) is a sample (\rightarrow I/1.1.6) from $\mathcal{MN}(M, U, V)$. ■

Sources:

- Wikipedia (2021): “Matrix normal distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-12-07; URL: https://en.wikipedia.org/wiki/Matrix_normal_distribution#Drawing_values_from_the_distribution.

5.2 Wishart distribution

5.2.1 Definition

Definition: Let X be an $n \times p$ matrix following a matrix-normal distribution (\rightarrow II/5.1.1) with mean zero, independence across rows and covariance across columns V :

$$X \sim \mathcal{MN}(0, I_n, V) . \quad (1)$$

Define the scatter matrix S as the product of the transpose of X with itself:

$$S = X^T X = \sum_{i=1}^n x_i^T x_i . \quad (2)$$

Then, the matrix S is said to follow a Wishart distribution with scale matrix V and degrees of freedom n

$$S \sim \mathcal{W}(V, n) \quad (3)$$

where $n > p - 1$ and V is a positive definite symmetric covariance matrix.

Sources:

- Wikipedia (2020): “Wishart distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-03-22; URL: https://en.wikipedia.org/wiki/Wishart_distribution#Definition.

5.2.2 Kullback-Leibler divergence

Theorem: Let S be a $p \times p$ random matrix (\rightarrow I/1.2.4). Assume two Wishart distributions (\rightarrow II/5.2.1) P and Q specifying the probability distribution of S as

$$\begin{aligned} P : S &\sim \mathcal{W}(V_1, n_1) \\ Q : S &\sim \mathcal{W}(V_2, n_2) . \end{aligned} \quad (1)$$

Then, the Kullback-Leibler divergence (\rightarrow I/2.5.1) of P from Q is given by

$$\text{KL}[P \parallel Q] = \frac{1}{2} \left[n_2 (\ln |V_2| - \ln |V_1|) + n_1 \text{tr}(V_2^{-1} V_1) + 2 \ln \frac{\Gamma_p(\frac{n_2}{2})}{\Gamma_p(\frac{n_1}{2})} + (n_1 - n_2) \psi_p\left(\frac{n_1}{2}\right) - n_1 p \right] \quad (2)$$

where $\Gamma_p(x)$ is the multivariate gamma function

$$\Gamma_p(x) = \pi^{p(p-1)/4} \prod_{j=1}^k \Gamma\left(x - \frac{j-1}{2}\right) \quad (3)$$

and $\psi_p(x)$ is the multivariate digamma function

$$\psi_p(x) = \frac{d \ln \Gamma_p(x)}{dx} = \sum_{j=1}^k \psi\left(x - \frac{j-1}{2}\right) . \quad (4)$$

Proof: The KL divergence for a continuous random variable (\rightarrow I/2.5.1) is given by

$$\text{KL}[P \parallel Q] = \int_{\mathcal{X}} p(x) \ln \frac{p(x)}{q(x)} dx \quad (5)$$

which, applied to the Wishart distributions (\rightarrow II/5.2.1) in (1), yields

$$\begin{aligned} \text{KL}[P \parallel Q] &= \int_{\mathcal{S}^p} \mathcal{W}(S; V_1, n_1) \ln \frac{\mathcal{W}(S; V_1, n_1)}{\mathcal{W}(S; V_2, n_2)} dS \\ &= \left\langle \ln \frac{\mathcal{W}(S; \alpha_1)}{\mathcal{W}(S; \alpha_2)} \right\rangle_{p(S)} \end{aligned} \quad (6)$$

where \mathcal{S}^p is the set of all positive-definite symmetric $p \times p$ matrices.

Using the probability density function of the Wishart distribution, this becomes:

$$\begin{aligned}
 \text{KL}[P || Q] &= \left\langle \ln \frac{\frac{1}{\sqrt{2^{n_1 p} |V_1|^{n_1} \Gamma_p(\frac{n_1}{2})}} \cdot |S|^{(n_1 - p - 1)/2} \cdot \exp \left[-\frac{1}{2} \text{tr}(V_1^{-1} S) \right]}{\frac{1}{\sqrt{2^{n_2 p} |V_2|^{n_2} \Gamma_p(\frac{n_2}{2})}} \cdot |S|^{(n_2 - p - 1)/2} \cdot \exp \left[-\frac{1}{2} \text{tr}(V_2^{-1} S) \right]} \right\rangle_{p(S)} \\
 &= \left\langle \ln \left(\sqrt{2^{(n_2 - n_1)p}} \cdot \frac{|V_2|^{n_2}}{|V_1|^{n_1}} \cdot \frac{\Gamma_p(\frac{n_2}{2})}{\Gamma_p(\frac{n_1}{2})} \cdot |S|^{(n_1 - n_2)/2} \cdot \exp \left[-\frac{1}{2} \text{tr}(V_1^{-1} S) + \frac{1}{2} \text{tr}(V_2^{-1} S) \right] \right) \right\rangle_{p(S)} \\
 &= \left\langle \frac{(n_2 - n_1)p}{2} \ln 2 + \frac{n_2}{2} \ln |V_2| - \frac{n_1}{2} \ln |V_1| + \ln \frac{\Gamma_p(\frac{n_2}{2})}{\Gamma_p(\frac{n_1}{2})} \right. \\
 &\quad \left. + \frac{n_1 - n_2}{2} \ln |S| - \frac{1}{2} \text{tr}(V_1^{-1} S) + \frac{1}{2} \text{tr}(V_2^{-1} S) \right\rangle_{p(S)} \\
 &= \frac{(n_2 - n_1)p}{2} \ln 2 + \frac{n_2}{2} \ln |V_2| - \frac{n_1}{2} \ln |V_1| + \ln \frac{\Gamma_p(\frac{n_2}{2})}{\Gamma_p(\frac{n_1}{2})} \\
 &\quad + \frac{n_1 - n_2}{2} \langle \ln |S| \rangle_{p(S)} - \frac{1}{2} \langle \text{tr}(V_1^{-1} S) \rangle_{p(S)} + \frac{1}{2} \langle \text{tr}(V_2^{-1} S) \rangle_{p(S)} .
 \end{aligned} \tag{7}$$

Using the expected value of a Wishart random matrix

$$S \sim \mathcal{W}(V, n) \quad \Rightarrow \quad \langle S \rangle = nV , \tag{8}$$

such that the expected value of the matrix trace (\rightarrow I/1.12.20) becomes

$$\langle \text{tr}(AS) \rangle = \text{tr}(\langle AS \rangle) = \text{tr}(A \langle S \rangle) = \text{tr}(A \cdot (nV)) = n \cdot \text{tr}(AV) , \tag{9}$$

and the expected value of a Wishart log-determinant

$$S \sim \mathcal{W}(V, n) \quad \Rightarrow \quad \langle \ln |S| \rangle = \psi_p \left(\frac{n}{2} \right) + p \cdot \ln 2 + \ln |V| , \tag{10}$$

the Kullback-Leibler divergence from (7) becomes:

$$\begin{aligned}
 \text{KL}[P || Q] &= \frac{(n_2 - n_1)p}{2} \ln 2 + \frac{n_2}{2} \ln |V_2| - \frac{n_1}{2} \ln |V_1| + \ln \frac{\Gamma_p(\frac{n_2}{2})}{\Gamma_p(\frac{n_1}{2})} \\
 &\quad + \frac{n_1 - n_2}{2} \left[\psi_p \left(\frac{n_1}{2} \right) + p \cdot \ln 2 + \ln |V_1| \right] - \frac{n_1}{2} \text{tr}(V_1^{-1} V_1) + \frac{n_1}{2} \text{tr}(V_2^{-1} V_1) \\
 &= \frac{n_2}{2} (\ln |V_2| - \ln |V_1|) + \ln \frac{\Gamma_p(\frac{n_2}{2})}{\Gamma_p(\frac{n_1}{2})} + \frac{n_1 - n_2}{2} \psi_p \left(\frac{n_1}{2} \right) - \frac{n_1}{2} \text{tr}(I_p) + \frac{n_1}{2} \text{tr}(V_2^{-1} V_1) \\
 &= \frac{1}{2} \left[n_2 (\ln |V_2| - \ln |V_1|) + n_1 \text{tr}(V_2^{-1} V_1) + 2 \ln \frac{\Gamma_p(\frac{n_2}{2})}{\Gamma_p(\frac{n_1}{2})} + (n_1 - n_2) \psi_p \left(\frac{n_1}{2} \right) - n_1 p \right] .
 \end{aligned} \tag{11}$$

■

Sources:

- Penny, William D. (2001): “KL-Divergences of Normal, Gamma, Dirichlet and Wishart densities”; in: *University College, London*, pp. 2-3, eqs. 13/15; URL: <https://www.fil.ion.ucl.ac.uk/~wpenny/publications/densities.ps>.
- Wikipedia (2021): “Wishart distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-12-02; URL: https://en.wikipedia.org/wiki/Wishart_distribution#KL-divergence.

5.3 Normal-Wishart distribution

5.3.1 Definition

Definition: Let X be an $n \times p$ random matrix (\rightarrow I/1.2.4) and let Y be a $p \times p$ positive-definite symmetric matrix. Then, X and Y are said to follow a normal-Wishart distribution

$$X, Y \sim \text{NW}(M, U, V, \nu), \quad (1)$$

if the distribution of X conditional on Y is a matrix-normal distribution (\rightarrow II/5.1.1) with mean M , covariance across rows U , covariance across columns Y^{-1} and Y follows a Wishart distribution (\rightarrow II/5.2.1) with scale matrix V and degrees of freedom ν :

$$\begin{aligned} X|Y &\sim \mathcal{MN}(M, U, Y^{-1}) \\ Y &\sim \mathcal{W}(V, \nu). \end{aligned} \quad (2)$$

The $p \times p$ matrix Y can be seen as the precision matrix (\rightarrow I/1.16.12) across the columns of the $n \times p$ matrix X .

Sources:

- Bishop, Christopher M. (2006): “Appendix B. Probability Distributions”; in: *Pattern Recognition for Machine Learning*, p. 690, eq. B.53; URL: <http://users.isr.ist.utl.pt/~wurmd/Livros/school/Bishop%20-%20Pattern%20Recognition%20And%20Machine%20Learning%20-%20Springer%20%202006.pdf>.

5.3.2 Probability density function

Theorem: Let X and Y follow a normal-Wishart distribution (\rightarrow II/5.3.1):

$$X, Y \sim \text{NW}(M, U, V, \nu). \quad (1)$$

Then, the joint probability (\rightarrow I/1.3.2) density function (\rightarrow I/1.7.1) of X and Y is

$$\begin{aligned} p(X, Y) &= \frac{1}{\sqrt{(2\pi)^{np} |U|^p |V|^\nu}} \cdot \frac{\sqrt{2^{-\nu p}}}{\Gamma_p\left(\frac{\nu}{2}\right)} \cdot |Y|^{(\nu+n-p-1)/2} \\ &\quad \exp \left[-\frac{1}{2} \text{tr} \left(Y \left[(X - M)^T U^{-1} (X - M) + V^{-1} \right] \right) \right]. \end{aligned} \quad (2)$$

Proof: The normal-Wishart distribution (\rightarrow II/5.3.1) is defined as X conditional on Y following a matrix-normal distribution (\rightarrow II/5.1.1) and Y following a Wishart distribution (\rightarrow II/5.2.1):

$$\begin{aligned} X|Y &\sim \mathcal{MN}(M, U, Y^{-1}) \\ Y &\sim \mathcal{W}(V, \nu) . \end{aligned} \quad (3)$$

Thus, using the probability density function of the matrix-normal distribution (\rightarrow II/5.1.3) and the probability density function of the Wishart distribution, we have the following probabilities:

$$\begin{aligned} p(X|Y) &= \mathcal{MN}(X; M, U, Y^{-1}) \\ &= \sqrt{\frac{|Y|^n}{(2\pi)^{np}|U|^p}} \cdot \exp \left[-\frac{1}{2} \text{tr} (Y(X - M)^T U^{-1}(X - M)) \right] \\ p(Y) &= \mathcal{W}(Y; V, \nu) \\ &= \frac{1}{\Gamma_p\left(\frac{\nu}{2}\right)} \cdot \frac{1}{\sqrt{2^{\nu p}|V|^\nu}} \cdot |Y|^{(\nu-p-1)/2} \cdot \exp \left[-\frac{1}{2} \text{tr} (V^{-1}Y) \right] . \end{aligned} \quad (4)$$

The law of conditional probability (\rightarrow I/1.3.4) implies that

$$p(X, Y) = p(X|Y) p(Y) , \quad (5)$$

such that the normal-Wishart density function becomes:

$$\begin{aligned} p(X, Y) &= \mathcal{MN}(X; M, U, Y^{-1}) \cdot \mathcal{W}(Y; V, \nu) \\ &= \sqrt{\frac{|Y|^n}{(2\pi)^{np}|U|^p}} \cdot \exp \left[-\frac{1}{2} \text{tr} (Y(X - M)^T U^{-1}(X - M)) \right] \cdot \\ &\quad \frac{1}{\Gamma_p\left(\frac{\nu}{2}\right)} \cdot \frac{1}{\sqrt{2^{\nu p}|V|^\nu}} \cdot |Y|^{(\nu-p-1)/2} \cdot \exp \left[-\frac{1}{2} \text{tr} (V^{-1}Y) \right] \\ &= \frac{1}{\sqrt{(2\pi)^{np}|U|^p|V|^\nu}} \cdot \frac{\sqrt{2^{-\nu p}}}{\Gamma_p\left(\frac{\nu}{2}\right)} \cdot |Y|^{(\nu+n-p-1)/2} \cdot \\ &\quad \exp \left[-\frac{1}{2} \text{tr} (Y [(X - M)^T U^{-1}(X - M) + V^{-1}]) \right] . \end{aligned} \quad (6)$$

■

Sources:

- Bishop, Christopher M. (2006): “Appendix B. Probability Distributions”; in: *Pattern Recognition for Machine Learning*, p. 690, eq. B.53; URL: <http://users.isr.ist.utl.pt/~wurmd/Livros/school/Bishop%20-%20Pattern%20Recognition%20And%20Machine%20Learning%20-%20Springer%20%202006.pdf>.

5.3.3 Mean

Theorem: Let $X \in \mathbb{R}^{n \times p}$ and $Y \in \mathbb{R}^{p \times p}$ follow a normal-Wishart distribution (\rightarrow II/5.3.1):

$$X, Y \sim \text{NW}(M, U, V, \nu) . \quad (1)$$

Then, the expected value (\rightarrow I/1.12.1) of X and Y is

$$E[(X, Y)] = (M, \nu V) . \quad (2)$$

Proof: Consider the random matrix (\rightarrow I/1.2.4)

$$\begin{bmatrix} X \\ Y \end{bmatrix} = \begin{bmatrix} x_{11} & \dots & x_{1p} \\ \vdots & \ddots & \vdots \\ x_{n1} & \dots & x_{np} \\ y_{11} & \dots & y_{1p} \\ \vdots & \ddots & \vdots \\ y_{p1} & \dots & y_{pp} \end{bmatrix} . \quad (3)$$

According to the expected value of a random matrix (\rightarrow I/1.12.19), its expected value is

$$E\left(\begin{bmatrix} X \\ Y \end{bmatrix}\right) = \begin{bmatrix} E(x_{11}) & \dots & E(x_{1p}) \\ \vdots & \ddots & \vdots \\ E(x_{n1}) & \dots & E(x_{np}) \\ E(y_{11}) & \dots & E(y_{1p}) \\ \vdots & \ddots & \vdots \\ E(y_{p1}) & \dots & E(y_{pp}) \end{bmatrix} = \begin{bmatrix} E(X) \\ E(Y) \end{bmatrix} . \quad (4)$$

When X and Y are jointly normal-Wishart distributed, then (\rightarrow II/5.3.1) by definition X follows a matrix-normal distribution (\rightarrow II/5.1.1) conditional on Y and Y follows a Wishart distribution (\rightarrow II/5.2.1):

$$X, Y \sim \text{NW}(M, U, V, \nu) \Leftrightarrow X|Y \sim \mathcal{MN}(M, U, Y^{-1}) \quad \wedge \quad Y \sim \mathcal{W}(V, \nu) . \quad (5)$$

Thus, with the expected value of the matrix-variate normal distribution (\rightarrow II/5.1.4) and the law of conditional probability (\rightarrow I/1.3.4), $E(X)$ becomes

$$\begin{aligned} E(X) &= \iint X \cdot p(X, Y) \, dX \, dY \\ &= \iint X \cdot p(X|Y) \cdot p(Y) \, dX \, dY \\ &= \int p(Y) \int X \cdot p(X|Y) \, dX \, dY \\ &= \int p(Y) \langle X \rangle_{\mathcal{MN}(M, U, Y^{-1})} \, dY \\ &= \int p(Y) \cdot M \, dY \\ &= M \int p(Y) \, dY \\ &= M , \end{aligned} \quad (6)$$

and with the expected value of the Wishart distribution, $E(Y)$ becomes

$$\begin{aligned} E(Y) &= \int Y \cdot p(Y) \, dY \\ &= \langle Y \rangle_{\mathcal{W}(V, \nu)} \\ &= \nu V . \end{aligned} \tag{7}$$

Thus, the expectation of the random matrix in equations (3) and (4) is

$$E \left(\begin{bmatrix} X \\ Y \end{bmatrix} \right) = \begin{bmatrix} M \\ \nu V \end{bmatrix} , \tag{8}$$

as indicated by equation (2).

■

Chapter III

Statistical Models

1 Univariate normal data

1.1 Univariate Gaussian

1.1.1 Definition

Definition: A univariate Gaussian data set is given by a set of real numbers $y = \{y_1, \dots, y_n\}$, independent and identically distributed (\rightarrow I/1.2.8) according to a normal distribution (\rightarrow II/3.2.1) with unknown mean μ and unknown variance σ^2 :

$$y_i \sim \mathcal{N}(\mu, \sigma^2), \quad i = 1, \dots, n. \quad (1)$$

Sources:

- Bishop, Christopher M. (2006): “Example: The univariate Gaussian”; in: *Pattern Recognition for Machine Learning*, ch. 10.1.3, p. 470, eq. 10.21; URL: <http://users.isr.ist.utl.pt/~wurmd/Livros/school/Bishop%20-%20Pattern%20Recognition%20And%20Machine%20Learning%20-%20Springer%20%202006.pdf>.

1.1.2 Maximum likelihood estimation

Theorem: Let there be a univariate Gaussian data set (\rightarrow III/1.1.1) $y = \{y_1, \dots, y_n\}$:

$$y_i \sim \mathcal{N}(\mu, \sigma^2), \quad i = 1, \dots, n. \quad (1)$$

Then, the maximum likelihood estimates (\rightarrow I/4.1.3) for mean μ and variance σ^2 are given by

$$\begin{aligned} \hat{\mu} &= \frac{1}{n} \sum_{i=1}^n y_i \\ \hat{\sigma}^2 &= \frac{1}{n} \sum_{i=1}^n (y_i - \bar{y})^2. \end{aligned} \quad (2)$$

Proof: The likelihood function (\rightarrow I/5.1.2) for each observation is given by the probability density function of the normal distribution (\rightarrow II/3.2.10)

$$p(y_i | \mu, \sigma^2) = \mathcal{N}(y_i; \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \cdot \exp \left[-\frac{1}{2} \left(\frac{y_i - \mu}{\sigma} \right)^2 \right] \quad (3)$$

and because observations are independent (\rightarrow I/1.3.6), the likelihood function for all observations is the product of the individual ones:

$$p(y | \mu, \sigma^2) = \prod_{i=1}^n p(y_i | \mu) = \sqrt{\frac{1}{(2\pi\sigma^2)^n}} \cdot \exp \left[-\frac{1}{2} \sum_{i=1}^n \left(\frac{y_i - \mu}{\sigma} \right)^2 \right]. \quad (4)$$

This can be developed into

$$\begin{aligned}
p(y|\mu, \sigma^2) &= \left(\frac{1}{2\pi\sigma^2} \right)^{n/2} \cdot \exp \left[-\frac{1}{2} \sum_{i=1}^n \left(\frac{y_i^2 - 2y_i\mu + \mu^2}{\sigma^2} \right) \right] \\
&= \left(\frac{1}{2\pi\sigma^2} \right)^{n/2} \cdot \exp \left[-\frac{1}{2\sigma^2} (y^T y - 2n\bar{y}\mu + n\mu^2) \right]
\end{aligned} \tag{5}$$

where $\bar{y} = \frac{1}{n} \sum_{i=1}^n y_i$ is the mean of data points and $y^T y = \sum_{i=1}^n y_i^2$ is the sum of squared data points. Thus, the log-likelihood function (\rightarrow I/4.1.2) is

$$\text{LL}(\mu, \sigma^2) = \log p(y|\mu, \sigma^2) = -\frac{n}{2} \log(2\pi\sigma^2) - \frac{1}{2\sigma^2} (y^T y - 2n\bar{y}\mu + n\mu^2) . \tag{6}$$

The derivative of the log-likelihood function (6) with respect to μ is

$$\frac{d\text{LL}(\mu, \sigma^2)}{d\mu} = \frac{n\bar{y}}{\sigma^2} - \frac{n\mu}{\sigma^2} = \frac{n}{\sigma^2} (\bar{y} - \mu) \tag{7}$$

and setting this derivative to zero gives the MLE for μ :

$$\begin{aligned}
\frac{d\text{LL}(\hat{\mu}, \sigma^2)}{d\mu} &= 0 \\
0 &= \frac{n}{\sigma^2} (\bar{y} - \hat{\mu}) \\
0 &= \bar{y} - \hat{\mu} \\
\hat{\mu} &= \bar{y} \\
\hat{\mu} &= \frac{1}{n} \sum_{i=1}^n y_i .
\end{aligned} \tag{8}$$

The derivative of the log-likelihood function (6) at $\hat{\mu}$ with respect to σ^2 is

$$\begin{aligned}
\frac{d\text{LL}(\hat{\mu}, \sigma^2)}{d\sigma^2} &= -\frac{n}{2} \frac{1}{\sigma^2} + \frac{1}{2(\sigma^2)^2} (y^T y - 2n\bar{y}\hat{\mu} + n\hat{\mu}^2) \\
&= -\frac{n}{2\sigma^2} + \frac{1}{2(\sigma^2)^2} \sum_{i=1}^n (y_i^2 - 2y_i\hat{\mu} + \hat{\mu}^2) \\
&= -\frac{n}{2\sigma^2} + \frac{1}{2(\sigma^2)^2} \sum_{i=1}^n (y_i - \hat{\mu})^2
\end{aligned} \tag{9}$$

and setting this derivative to zero gives the MLE for σ^2 :

$$\begin{aligned}
\frac{dLL(\hat{\mu}, \hat{\sigma}^2)}{d\sigma^2} &= 0 \\
0 &= \frac{1}{2(\hat{\sigma}^2)^2} \sum_{i=1}^n (y_i - \hat{\mu})^2 \\
\frac{n}{2\hat{\sigma}^2} &= \frac{1}{2(\hat{\sigma}^2)^2} \sum_{i=1}^n (y_i - \hat{\mu})^2 \\
\frac{2(\hat{\sigma}^2)^2}{n} \cdot \frac{n}{2\hat{\sigma}^2} &= \frac{2(\hat{\sigma}^2)^2}{n} \cdot \frac{1}{2(\hat{\sigma}^2)^2} \sum_{i=1}^n (y_i - \hat{\mu})^2 \\
\hat{\sigma}^2 &= \frac{1}{n} \sum_{i=1}^n (y_i - \hat{\mu})^2 \\
\hat{\sigma}^2 &= \frac{1}{n} \sum_{i=1}^n (y_i - \bar{y})^2
\end{aligned} \tag{10}$$

Together, (8) and (10) constitute the MLE for the univariate Gaussian. ■

Sources:

- Bishop CM (2006): “Bayesian inference for the Gaussian”; in: *Pattern Recognition for Machine Learning*, pp. 93-94, eqs. 2.121, 2.122; URL: <http://users.isr.ist.utl.pt/~wurmd/Livros/school/Bishop%20-%20Pattern%20Recognition%20And%20Machine%20Learning%20-%20Springer%20%202006.pdf>.

1.1.3 One-sample t-test

Theorem: Let

$$y_i \sim \mathcal{N}(\mu, \sigma^2), \quad i = 1, \dots, n \tag{1}$$

be a univariate Gaussian data set (\rightarrow III/1.1.1) with unknown mean μ and unknown variance σ^2 . Then, the test statistic (\rightarrow I/4.3.5)

$$t = \frac{\bar{y} - \mu_0}{s/\sqrt{n}} \tag{2}$$

with sample mean (\rightarrow I/1.12.2) \bar{y} and sample variance (\rightarrow I/1.13.2) s^2 follows a Student's t-distribution (\rightarrow II/3.3.1) with $n - 1$ degrees of freedom (\rightarrow I/1.5.12)

$$t \sim t(n - 1) \tag{3}$$

under the null hypothesis (\rightarrow I/4.3.2)

$$H_0 : \mu = \mu_0 . \tag{4}$$

Proof: The sample mean (\rightarrow I/1.12.2) is given by

$$\bar{y} = \frac{1}{n} \sum_{i=1}^n y_i \quad (5)$$

and the sample variance (\rightarrow I/1.13.2) is given by

$$s^2 = \frac{1}{n-1} \sum_{i=1}^n (y_i - \bar{y})^2 . \quad (6)$$

Using the linear combination formula for normal random variables (\rightarrow II/3.2.26), the sample mean follows a normal distribution (\rightarrow II/3.2.1) with the following parameters:

$$\bar{y} = \frac{1}{n} \sum_{i=1}^n y_i \sim \mathcal{N} \left(\frac{1}{n} n\mu, \left(\frac{1}{n} \right)^2 n\sigma^2 \right) = \mathcal{N} (\mu, \sigma^2/n) . \quad (7)$$

Again employing the linear combination theorem and applying the null hypothesis from (4), the distribution of $Z = \sqrt{n}(\bar{y} - \mu_0)/\sigma$ becomes standard normal (\rightarrow II/3.2.3)

$$Z = \frac{\sqrt{n}(\bar{y} - \mu_0)}{\sigma} \sim \mathcal{N} \left(\frac{\sqrt{n}}{\sigma}(\mu - \mu_0), \left(\frac{\sqrt{n}}{\sigma} \right)^2 \frac{\sigma^2}{n} \right) \stackrel{(4)}{=} \mathcal{N} (0, 1) . \quad (8)$$

Because sample variances calculated from independent normal random variables follow a chi-squared distribution (\rightarrow II/3.2.7), the distribution of $V = (n-1)s^2/\sigma^2$ is

$$V = \frac{(n-1)s^2}{\sigma^2} \sim \chi^2(n-1) . \quad (9)$$

Finally, since the ratio of a standard normal random variable and the square root of a chi-squared random variable follows a t-distribution (\rightarrow II/3.3.1), the distribution of the test statistic (\rightarrow I/4.3.5) is given by

$$t = \frac{\bar{y} - \mu_0}{s/\sqrt{n}} = \frac{Z}{\sqrt{V/(n-1)}} \sim t(n-1) . \quad (10)$$

This means that the null hypothesis (\rightarrow I/4.3.2) can be rejected when t is as extreme or more extreme than the critical value (\rightarrow I/4.3.9) obtained from the Student's t-distribution (\rightarrow II/3.3.1) with $n-1$ degrees of freedom (\rightarrow I/1.5.12) using a significance level (\rightarrow I/4.3.8) α .

■

Sources:

- Wikipedia (2021): “Student’s t-distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-03-12; URL: https://en.wikipedia.org/wiki/Student%27s_t-distribution#Derivation.

1.1.4 Two-sample t-test

Theorem: Let

$$\begin{aligned} y_{1i} &\sim \mathcal{N}(\mu_1, \sigma^2), & i &= 1, \dots, n_1 \\ y_{2i} &\sim \mathcal{N}(\mu_2, \sigma^2), & i &= 1, \dots, n_2 \end{aligned} \quad (1)$$

be two univariate Gaussian data sets (\rightarrow III/1.1.1) representing two groups of unequal size n_1 and n_2 with unknown means μ_1 and μ_2 and equal unknown variance σ^2 . Then, the test statistic (\rightarrow I/4.3.5)

$$t = \frac{(\bar{y}_1 - \bar{y}_2) - \mu_\Delta}{s_p \cdot \sqrt{\frac{1}{n_1} + \frac{1}{n_2}}} \quad (2)$$

with sample means (\rightarrow I/1.12.2) \bar{y}_1 and \bar{y}_2 and pooled standard deviation (\rightarrow I/1.19.3) s_p follows a Student's t-distribution (\rightarrow II/3.3.1) with $n_1 + n_2 - 2$ degrees of freedom (\rightarrow I/1.5.12)

$$t \sim t(n_1 + n_2 - 2) \quad (3)$$

under the null hypothesis (\rightarrow I/4.3.2)

$$H_0 : \mu_1 - \mu_2 = \mu_\Delta . \quad (4)$$

Proof: The sample means (\rightarrow I/1.12.2) are given by

$$\begin{aligned} \bar{y}_1 &= \frac{1}{n_1} \sum_{i=1}^{n_1} y_{1i} \\ \bar{y}_2 &= \frac{1}{n_2} \sum_{i=1}^{n_2} y_{2i} \end{aligned} \quad (5)$$

and the pooled standard deviation (\rightarrow I/1.19.3) is given by

$$s_p = \sqrt{\frac{(n_1 - 1)s_1^2 + (n_2 - 1)s_2^2}{n_1 + n_2 - 2}} \quad (6)$$

with the sample variances (\rightarrow I/1.13.2)

$$\begin{aligned} s_1^2 &= \frac{1}{n_1 - 1} \sum_{i=1}^{n_1} (y_{1i} - \bar{y}_1)^2 \\ s_2^2 &= \frac{1}{n_2 - 1} \sum_{i=1}^{n_2} (y_{2i} - \bar{y}_2)^2 . \end{aligned} \quad (7)$$

Using the linear combination formula for normal random variables (\rightarrow II/3.2.26), the sample means follows normal distributions (\rightarrow II/3.2.1) with the following parameters:

$$\begin{aligned} \bar{y}_1 &= \frac{1}{n_1} \sum_{i=1}^{n_1} y_{1i} \sim \mathcal{N} \left(\frac{1}{n_1} n_1 \mu_1, \left(\frac{1}{n_1} \right)^2 n_1 \sigma^2 \right) = \mathcal{N} (\mu_1, \sigma^2/n_1) \\ \bar{y}_2 &= \frac{1}{n_2} \sum_{i=1}^{n_2} y_{2i} \sim \mathcal{N} \left(\frac{1}{n_2} n_2 \mu_2, \left(\frac{1}{n_2} \right)^2 n_2 \sigma^2 \right) = \mathcal{N} (\mu_2, \sigma^2/n_2) . \end{aligned} \quad (8)$$

Again employing the linear combination theorem and applying the null hypothesis from (4), the distribution of $Z = ((\bar{y}_1 - \bar{y}_2) - \mu_\Delta) / (\sigma \sqrt{1/n_1 + 1/n_2})$ becomes standard normal (\rightarrow II/3.2.3)

$$Z = \frac{(\bar{y}_1 - \bar{y}_2) - \mu_\Delta}{\sigma \cdot \sqrt{\frac{1}{n_1} + \frac{1}{n_2}}} \sim \mathcal{N} \left(\frac{(\mu_1 - \mu_2) - \mu_\Delta}{\sigma \cdot \sqrt{\frac{1}{n_1} + \frac{1}{n_2}}}, \left(\frac{1}{\sigma \cdot \sqrt{\frac{1}{n_1} + \frac{1}{n_2}}} \right)^2 \left(\frac{\sigma^2}{n_1} + \frac{\sigma^2}{n_2} \right) \right) \stackrel{(4)}{=} \mathcal{N}(0, 1) . \quad (9)$$

Because sample variances calculated from independent normal random variables follow a chi-squared distribution (\rightarrow II/3.2.7), the distribution of $V = (n_1 + n_2 - 2) s_p^2 / \sigma^2$ is

$$V = \frac{(n_1 + n_2 - 2) s_p^2}{\sigma^2} \sim \chi^2(n_1 + n_2 - 2) . \quad (10)$$

Finally, since the ratio of a standard normal random variable and the square root of a chi-squared random variable follows a t-distribution (\rightarrow II/3.3.1), the distribution of the test statistic (\rightarrow I/4.3.5) is given by

$$t = \frac{(\bar{y}_1 - \bar{y}_2) - \mu_\Delta}{s_p \cdot \sqrt{\frac{1}{n_1} + \frac{1}{n_2}}} = \frac{Z}{\sqrt{V/(n_1 + n_2 - 2)}} \sim t(n_1 + n_2 - 2) . \quad (11)$$

This means that the null hypothesis (\rightarrow I/4.3.2) can be rejected when t is as extreme or more extreme than the critical value (\rightarrow I/4.3.9) obtained from the Student's t-distribution (\rightarrow II/3.3.1) with $n_1 + n_2 - 2$ degrees of freedom (\rightarrow I/1.5.12) using a significance level (\rightarrow I/4.3.8) α .

■

Sources:

- Wikipedia (2021): “Student’s t-distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-03-12; URL: https://en.wikipedia.org/wiki/Student%27s_t-distribution#Derivation.
- Wikipedia (2021): “Student’s t-test”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-03-12; URL: [https://en.wikipedia.org/wiki/Student%27s_t-test#Equal_or_unequal_sample_sizes,_similar_variances_\(1/2_%3C_sX1/sX2_%3C_2\)](https://en.wikipedia.org/wiki/Student%27s_t-test#Equal_or_unequal_sample_sizes,_similar_variances_(1/2_%3C_sX1/sX2_%3C_2)).

1.1.5 Paired t-test

Theorem: Let y_{i1} and y_{i2} with $i = 1, \dots, n$ be paired observations, such that

$$y_{i1} \sim \mathcal{N}(y_{i2} + \mu, \sigma^2), \quad i = 1, \dots, n \quad (1)$$

is a univariate Gaussian data set (\rightarrow III/1.1.1) with unknown shift μ and unknown variance σ^2 . Then, the test statistic (\rightarrow I/4.3.5)

$$t = \frac{\bar{d} - \mu_0}{s_d / \sqrt{n}} \quad \text{where} \quad d_i = y_{i1} - y_{i2} \quad (2)$$

with sample mean (\rightarrow I/1.12.2) \bar{d} and sample variance (\rightarrow I/1.13.2) s_d^2 follows a Student’s t-distribution (\rightarrow II/3.3.1) with $n - 1$ degrees of freedom (\rightarrow I/1.5.12)

$$t \sim t(n - 1) \quad (3)$$

under the null hypothesis (\rightarrow I/4.3.2)

$$H_0 : \mu = \mu_0 . \quad (4)$$

Proof: Define the pair-wise difference $d_i = y_{i1} - y_{i2}$ which, as a linear transformation of a normal random variable (\rightarrow II/4.1.14), is distributed as

$$d_i = y_{i1} - y_{i2} \sim \mathcal{N}(\mu, \sigma^2), \quad i = 1, \dots, n. \quad (5)$$

Therefore, d_1, \dots, d_n satisfy the conditions of the one-sample t-test (\rightarrow III/1.1.3) which results in the test statistic given by (2). ■

Sources:

- Wikipedia (2021): “Student’s t-test”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-03-12; URL: https://en.wikipedia.org/wiki/Student%27s_t-test#Dependent_t-test_for_paired_samples.

1.1.6 F-test for equality of variances

Theorem: Let

$$\begin{aligned} y_{1i} &\sim \mathcal{N}(\mu_1, \sigma_1^2), & i = 1, \dots, n_1 \\ y_{2i} &\sim \mathcal{N}(\mu_2, \sigma_2^2), & i = 1, \dots, n_2 \end{aligned} \quad (1)$$

be two univariate Gaussian data sets (\rightarrow III/1.1.1) representing two groups of unequal size n_1 and n_2 with unknown means μ_1 and μ_2 and unknown variances σ_1^2 and σ_2^2 . Then, the test statistic (\rightarrow I/4.3.5)

$$F = \frac{s_1^2}{s_2^2} = \frac{\frac{1}{n_1-1} \sum_{i=1}^{n_1} (y_{1i} - \bar{y}_1)^2}{\frac{1}{n_2-1} \sum_{i=1}^{n_2} (y_{2i} - \bar{y}_2)^2} \quad (2)$$

with sample means (\rightarrow I/1.12.2) \bar{y}_1 and \bar{y}_2 and sample variances (\rightarrow I/1.13.2) s_1^2 and s_2^2 follows an F-distribution (\rightarrow II/3.8.1) with numerator degrees of freedom $n_1 - 1$ and denominator degrees of freedom $n_2 - 1$

$$F \sim F(n_1 - 1, n_2 - 1) \quad (3)$$

under the null hypothesis (\rightarrow I/4.3.2) that the two variances (\rightarrow II/3.2.1) are equal:

$$H_0 : \sigma_1^2 = \sigma_2^2. \quad (4)$$

Proof: We know that, for a sample of normal random variables, the sample variance is following a chi-squared distribution (\rightarrow II/3.2.7):

$$X_i \sim \mathcal{N}(\mu, \sigma^2), \quad i = 1, \dots, n \quad \Rightarrow \quad V = (n-1) \frac{s^2}{\sigma^2} \sim \chi^2(n-1). \quad (5)$$

Thus, we have:

$$\begin{aligned} V_1 &= (n_1 - 1) \frac{s_1^2}{\sigma_1^2} \sim \chi^2(n_1 - 1) \quad \text{and} \\ V_2 &= (n_2 - 1) \frac{s_2^2}{\sigma_2^2} \sim \chi^2(n_2 - 1). \end{aligned} \quad (6)$$

Moreover, by definition, the ratio of two chi-squared random variables, divided by their degrees of freedom, is following an F-distribution (\rightarrow II/3.8.1):

$$X_1 \sim \chi^2(d_1), X_2 \sim \chi^2(d_2) \Rightarrow Y = \frac{X_1/d_1}{X_2/d_2} \sim F(d_1, d_2). \quad (7)$$

Thus, we have:

$$\begin{aligned} F &= \frac{V_1/(n_1 - 1)}{V_2/(n_2 - 1)} \\ &= \frac{(n_1 - 1) \frac{s_1^2}{\sigma_1^2} / (n_1 - 1)}{(n_2 - 1) \frac{s_2^2}{\sigma_2^2} / (n_2 - 1)} \\ &= \frac{s_1^2/\sigma_1^2}{s_2^2/\sigma_2^2} \\ &\stackrel{(4)}{=} \frac{s_1^2}{s_2^2}. \end{aligned} \quad (8)$$

This means that the null hypothesis (\rightarrow I/4.3.2) of equal variances can be rejected when F is as extreme or more extreme than the critical value (\rightarrow I/4.3.9) obtained from the F-distribution (\rightarrow II/3.8.1) with degrees of freedom (\rightarrow I/1.5.12) $n_1 - 1$ and $n_2 - 1$ using a significance level (\rightarrow I/4.3.8) α . ■

Sources:

- Wikipedia (2024): “F-test of equality of variances”; in: *Wikipedia, the free encyclopedia*, retrieved on 2024-07-05; URL: https://en.wikipedia.org/wiki/F-test_of_equality_of_variances#The_test.

1.1.7 Power analysis for one-sample t-test

Theorem: Let there be n i.i.d. (\rightarrow I/1.2.8) observations $Y_1, \dots, Y_n \sim N(\mu, \sigma^2)$ with both μ and σ^2 unknown. Further, let $z_x = \Phi^{-1}(1 - x)$, where Φ is the cumulative distribution function (\rightarrow I/1.8.1) of a standard normal distribution (\rightarrow II/3.2.3). Equivalently, with $Z \sim \mathcal{N}(0, 1)$, let

$$z_x = \Phi^{-1}(1 - x) \Leftrightarrow \Phi(z_x) = 1 - x \Leftrightarrow \Pr(Z \leq z_x) = 1 - x \Leftrightarrow \Pr(z_x \leq Z) = x. \quad (1)$$

1) One-sided one-sample t-test:

We perform a one-sided (\rightarrow I/4.3.4) one-sample t-test (\rightarrow III/1.1.3) of the null hypothesis (\rightarrow I/4.3.2) $H_0 : \mu \leq \mu_0$ vs. $H_1 : \mu > \mu_0$. The test has significance level (\rightarrow I/4.3.8) α . If H_1 is true and $\mu = \mu_0 + \delta$, then the power (\rightarrow I/4.3.7) of the test is

$$\Phi\left(\frac{\delta\sqrt{n}}{\sigma} - z_\alpha\right). \quad (2)$$

If we keep α, n, σ^2 the same as before and require that the power is at least $1 - \beta$, then the minimum detectable effect (\rightarrow I/4.3.12) is

$$\frac{(z_\alpha + z_\beta)\sigma}{\sqrt{n}}. \quad (3)$$

If we keep α , σ^2 , δ , β the same as before, then the minimum required sample size (\rightarrow I/4.3.13) is

$$\frac{\sigma^2(z_\alpha + z_\beta)^2}{\delta^2}. \quad (4)$$

2) Two-sided one-sample t-test:

We perform a two-sided (\rightarrow I/4.3.4) one-sample t-test (\rightarrow III/1.1.3) of hypothesis $H_0 : \mu = \mu_0$ vs. $H_1 : \mu \neq \mu_0$. The test has size α . If H_1 is true and $\mu = \mu_0 + \delta$ (assuming $\delta > 0$ without loss of generality), then the power (\rightarrow I/4.3.7) of the test is

$$\Phi\left(\frac{\delta\sqrt{n}}{\sigma} - z_{\alpha/2}\right) + \Phi\left(-z_{\alpha/2} - \frac{\delta\sqrt{n}}{\sigma}\right) \approx \Phi\left(\frac{\delta\sqrt{n}}{\sigma} - z_{\alpha/2}\right). \quad (5)$$

If we keep α , n , σ^2 the same as before, and require that the power is at least $1 - \beta$, then the minimum detectable effect (\rightarrow I/4.3.12) is

$$\frac{(z_{\alpha/2} + z_\beta)\sigma}{\sqrt{n}}. \quad (6)$$

If we keep α , σ^2 , δ , β the same as before then the minimum required sample size (\rightarrow I/4.3.12) is

$$\frac{\sigma^2(z_{\alpha/2} + z_\beta)^2}{\delta^2}. \quad (7)$$

Proof: The t -statistic is

$$T = \frac{\bar{Y} - \mu_0}{s/\sqrt{n}}. \quad (8)$$

which has a t -distribution (\rightarrow III/1.1.3) with $n - 1$ degrees of freedom (\rightarrow I/1.5.12). Unless n is very small, the $t(n - 1)$ distribution is very close to a $\mathcal{N}(0, 1)$ distribution and for this proof, we will assume that this is a good approximation.

1) One-sided one-sample t-test:

The test has size (\rightarrow I/4.3.6) α , we reject the null, if

$$T > z_\alpha. \quad (9)$$

So the power (\rightarrow I/4.3.7) of the test is

$$\Pr\left(\frac{\bar{Y} - \mu_0}{s/\sqrt{n}} > z_\alpha\right). \quad (10)$$

If the true mean is $\mu = \mu_0 + \delta$, where $\delta > 0$, then the power is

$$\Pr\left(\frac{\bar{Y} - \mu_0 - \delta}{s/\sqrt{n}} + \frac{\delta\sqrt{n}}{s} > z_\alpha\right). \quad (11)$$

Now that we're subtracting the true mean, the first term in the sum has a t -distribution (\rightarrow II/3.3.1), which we approximate with a $\mathcal{N}(0, 1)$ distribution, denoted as Z . We also approximate s with σ , since it should be a good approximation, and the error here doesn't make much difference to the calculation. The power is therefore approximately

$$\Pr\left(Z > z_\alpha - \frac{\delta\sqrt{n}}{\sigma}\right) = \Pr\left(Z < \frac{\delta\sqrt{n}}{\sigma} - z_\alpha\right) = \Phi\left(\frac{\delta\sqrt{n}}{\sigma} - z_\alpha\right). \quad (12)$$

To calculate the minimum detectable effect (\rightarrow I/4.3.12), we want the smallest δ , such that the power is at least $1 - \beta$. If the power is at least $1 - \beta$, then

$$1 - \beta \leq \Phi \left(\frac{\delta\sqrt{n}}{\sigma} - z_{\alpha} \right) . \quad (13)$$

Using $z_{\beta} = \Phi^{-1}(1 - \beta)$ and rearranging, we get

$$z_{\beta} + z_{\alpha} \leq \frac{\delta\sqrt{n}}{\sigma} . \quad (14)$$

Therefore,

$$\frac{(z_{\beta} + z_{\alpha})\sigma}{\sqrt{n}} \leq \delta , \quad (15)$$

and taking the minimum value for δ gives the minimum detectable effect.

To calculate the minimum required sample size (\rightarrow I/4.3.13), we want the smallest n , such that the power is at least $1 - \beta$. Rearranging (13), we have

$$\frac{\sigma^2(z_{\alpha} + z_{\beta})^2}{\delta^2} \leq n . \quad (16)$$

2) Two-sided one-sample t-test:

The test has size (\rightarrow I/4.3.6) α , we reject the null, if

$$|T| > z_{\alpha/2} . \quad (17)$$

So the power (\rightarrow I/4.3.7) of the test is

$$\Pr \left(\left(\frac{\bar{Y} - \mu_0}{s/\sqrt{n}} > z_{\alpha/2} \right) \wedge \left(\frac{\bar{Y} - \mu_0}{s/\sqrt{n}} < -z_{\alpha/2} \right) \right) . \quad (18)$$

If the true mean is $\mu = \mu_0 + \delta$ (where $\delta > 0$ without loss of generality), then the power is

$$\Pr \left(\left(\frac{\bar{Y} - \mu_0 - \delta}{s/\sqrt{n}} + \frac{\delta\sqrt{n}}{\sigma} > z_{\alpha/2} \right) \wedge \left(\frac{\bar{Y} - \mu_0 - \delta}{s/\sqrt{n}} + \frac{\delta\sqrt{n}}{\sigma} < -z_{\alpha/2} \right) \right) . \quad (19)$$

As before, we use a $\mathcal{N}(0, 1)$ distribution and we approximate s with σ . The power is therefore approximately

$$\Phi \left(\frac{\delta\sqrt{n}}{\sigma} - z_{\alpha/2} \right) + \Phi \left(-z_{\alpha/2} - \frac{\delta\sqrt{n}}{\sigma} \right) . \quad (20)$$

If we have a large enough δ , then the second term, which is the probability of rejecting the null hypothesis, but with a sign error on δ , will be small. For the later calculations, we will set it to 0 and use the approximation

$$\Phi \left(\frac{\delta\sqrt{n}}{\sigma} - z_{\alpha/2} \right) \quad (21)$$

for the power. To calculate the minimum detectable effect (\rightarrow I/4.3.12), we want the smallest δ , such that the power is at least $1 - \beta$. If the power is at least $1 - \beta$, then

$$1 - \beta \leq \Phi \left(\frac{\delta\sqrt{n}}{\sigma} - z_{\alpha/2} \right) . \quad (22)$$

Using $z_\beta = \Phi^{-1}(1 - \beta)$ and rearranging, we get

$$z_\beta + z_{\alpha/2} \leq \frac{\delta\sqrt{n}}{\sigma}. \quad (23)$$

Therefore,

$$\frac{(z_\beta + z_{\alpha/2})\sigma}{\sqrt{n}} \leq \delta, \quad (24)$$

and taking the minimum value for δ gives the minimum detectable effect.

To calculate the minimum required sample size (\rightarrow I/4.3.13), we want the smallest n , such that the power is at least $1 - \beta$. Rearranging (22), we have

$$\frac{\sigma^2(z_{\alpha/2} + z_\beta)^2}{\delta^2} \leq n. \quad (25)$$

■

Sources:

- Sylvain Chabé-Ferret (2025): “Power Analysis”; in: *Statistical Tools for Causal Inference*, retrieved on 2025-07-05; URL: <https://chabefer.github.io/STCI/Power.html>.

1.1.8 Conjugate prior distribution

Theorem: Let

$$y = \{y_1, \dots, y_n\}, \quad y_i \sim \mathcal{N}(\mu, \sigma^2), \quad i = 1, \dots, n \quad (1)$$

be a univariate Gaussian data set (\rightarrow III/1.1.1) with unknown mean μ and unknown variance σ^2 . Then, the conjugate prior (\rightarrow I/5.2.5) for this model is a normal-gamma distribution (\rightarrow II/4.4.1)

$$p(\mu, \tau) = \mathcal{N}(\mu; \mu_0, (\tau\lambda_0)^{-1}) \cdot \text{Gam}(\tau; a_0, b_0) \quad (2)$$

where $\tau = 1/\sigma^2$ is the inverse variance or precision.

Proof: By definition, a conjugate prior (\rightarrow I/5.2.5) is a prior distribution (\rightarrow I/5.1.3) that, when combined with the likelihood function (\rightarrow I/5.1.2), leads to a posterior distribution (\rightarrow I/5.1.9) that belongs to the same family of probability distributions (\rightarrow I/1.5.1). This is fulfilled when the prior density and the likelihood function are proportional to the model parameters in the same way, i.e. the model parameters appear in the same functional form in both.

Equation (1) implies the following likelihood function (\rightarrow I/5.1.2)

$$\begin{aligned} p(y|\mu, \sigma^2) &= \prod_{i=1}^n \mathcal{N}(y_i; \mu, \sigma^2) \\ &= \prod_{i=1}^n \frac{1}{\sqrt{2\pi\sigma^2}} \cdot \exp \left[-\frac{1}{2} \left(\frac{y_i - \mu}{\sigma} \right)^2 \right] \\ &= \frac{1}{(\sqrt{2\pi\sigma^2})^n} \cdot \exp \left[-\frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \mu)^2 \right] \end{aligned} \quad (3)$$

which, for mathematical convenience, can also be parametrized as

$$\begin{aligned}
p(y|\mu, \tau) &= \prod_{i=1}^n \mathcal{N}(y_i; \mu, \tau^{-1}) \\
&= \prod_{i=1}^n \sqrt{\frac{\tau}{2\pi}} \cdot \exp \left[-\frac{\tau}{2} (y_i - \mu)^2 \right] \\
&= \left(\sqrt{\frac{\tau}{2\pi}} \right)^n \cdot \exp \left[-\frac{\tau}{2} \sum_{i=1}^n (y_i - \mu)^2 \right]
\end{aligned} \tag{4}$$

using the inverse variance or precision $\tau = 1/\sigma^2$.

Separating constant and variable terms, we have:

$$p(y|\mu, \tau) = \sqrt{\frac{1}{(2\pi)^n}} \cdot \tau^{n/2} \cdot \exp \left[-\frac{\tau}{2} \sum_{i=1}^n (y_i - \mu)^2 \right]. \tag{5}$$

Expanding the product in the exponent, we have

$$\begin{aligned}
p(y|\mu, \tau) &= \sqrt{\frac{1}{(2\pi)^n}} \cdot \tau^{n/2} \cdot \exp \left[-\frac{\tau}{2} \sum_{i=1}^n (y_i^2 - 2\mu y_i + \mu^2) \right] \\
&= \sqrt{\frac{1}{(2\pi)^n}} \cdot \tau^{n/2} \cdot \exp \left[-\frac{\tau}{2} \left(\sum_{i=1}^n y_i^2 - 2\mu \sum_{i=1}^n y_i + n\mu^2 \right) \right] \\
&= \sqrt{\frac{1}{(2\pi)^n}} \cdot \tau^{n/2} \cdot \exp \left[-\frac{\tau}{2} (y^T y - 2\mu n\bar{y} + n\mu^2) \right] \\
&= \sqrt{\frac{1}{(2\pi)^n}} \cdot \tau^{n/2} \cdot \exp \left[-\frac{\tau n}{2} \left(\frac{1}{n} y^T y - 2\mu\bar{y} + \mu^2 \right) \right]
\end{aligned} \tag{6}$$

where $\bar{y} = \frac{1}{n} \sum_{i=1}^n y_i$ is the mean of data points and $y^T y = \sum_{i=1}^n y_i^2$ is the sum of squared data points. Completing the square over μ , finally gives

$$p(y|\mu, \tau) = \sqrt{\frac{1}{(2\pi)^n}} \cdot \tau^{n/2} \cdot \exp \left[-\frac{\tau n}{2} \left((\mu - \bar{y})^2 - \bar{y}^2 + \frac{1}{n} y^T y \right) \right] \tag{7}$$

In other words, the likelihood function (\rightarrow I/5.1.2) is proportional to a power of τ times an exponential of τ and an exponential of a squared form of μ , weighted by τ :

$$p(y|\mu, \tau) \propto \tau^{n/2} \cdot \exp \left[-\frac{\tau}{2} (y^T y - n\bar{y}^2) \right] \cdot \exp \left[-\frac{\tau n}{2} (\mu - \bar{y})^2 \right]. \tag{8}$$

The same is true for a normal-gamma distribution (\rightarrow II/4.4.1) over μ and τ

$$p(\mu, \tau) = \mathcal{N}(\mu; \mu_0, (\tau\lambda_0)^{-1}) \cdot \text{Gam}(\tau; a_0, b_0) \tag{9}$$

the probability density function of which (\rightarrow II/4.4.3)

$$p(\mu, \tau) = \sqrt{\frac{\tau \lambda_0}{2\pi}} \cdot \exp \left[-\frac{\tau \lambda_0}{2} (\mu - \mu_0)^2 \right] \cdot \frac{b_0^{a_0}}{\Gamma(a_0)} \tau^{a_0-1} \exp[-b_0 \tau] \quad (10)$$

exhibits the same proportionality

$$p(\mu, \tau) \propto \tau^{a_0+1/2-1} \cdot \exp[-\tau b_0] \cdot \exp \left[-\frac{\tau \lambda_0}{2} (\mu - \mu_0)^2 \right] \quad (11)$$

and is therefore conjugate relative to the likelihood. ■

Sources:

- Bishop CM (2006): “Bayesian inference for the Gaussian”; in: *Pattern Recognition for Machine Learning*, pp. 97-102, eq. 2.154; URL: <http://users.isr.ist.utl.pt/~wurmd/Livros/school/Bishop%20-%20Pattern%20Recognition%20And%20Machine%20Learning%20-%20Springer%20%202006.pdf>.

1.1.9 Posterior distribution

Theorem: Let

$$y = \{y_1, \dots, y_n\}, \quad y_i \sim \mathcal{N}(\mu, \sigma^2), \quad i = 1, \dots, n \quad (1)$$

be a univariate Gaussian data set (\rightarrow III/1.1.1) with unknown mean μ and unknown variance σ^2 . Moreover, assume a normal-gamma prior distribution (\rightarrow III/1.1.8) over the model parameters μ and $\tau = 1/\sigma^2$:

$$p(\mu, \tau) = \mathcal{N}(\mu; \mu_0, (\tau \lambda_0)^{-1}) \cdot \text{Gam}(\tau; a_0, b_0) . \quad (2)$$

Then, the posterior distribution (\rightarrow I/5.1.9) is also a normal-gamma distribution (\rightarrow II/4.4.1)

$$p(\mu, \tau | y) = \mathcal{N}(\mu; \mu_n, (\tau \lambda_n)^{-1}) \cdot \text{Gam}(\tau; a_n, b_n) \quad (3)$$

and the posterior hyperparameters (\rightarrow I/5.1.9) are given by

$$\begin{aligned} \mu_n &= \frac{\lambda_0 \mu_0 + n \bar{y}}{\lambda_0 + n} \\ \lambda_n &= \lambda_0 + n \\ a_n &= a_0 + \frac{n}{2} \\ b_n &= b_0 + \frac{1}{2} (y^T y + \lambda_0 \mu_0^2 - \lambda_n \mu_n^2) . \end{aligned} \quad (4)$$

Proof: According to Bayes’ theorem (\rightarrow I/5.3.2), the posterior distribution (\rightarrow I/5.1.9) is given by

$$p(\mu, \tau | y) = \frac{p(y | \mu, \tau) p(\mu, \tau)}{p(y)} . \quad (5)$$

Since $p(y)$ is just a normalization factor, the posterior is proportional (\rightarrow I/5.1.10) to the numerator:

$$p(\mu, \tau | y) \propto p(y | \mu, \tau) p(\mu, \tau) = p(y, \mu, \tau) . \quad (6)$$

Equation (1) implies the following likelihood function (\rightarrow I/5.1.2)

$$\begin{aligned}
 p(y|\mu, \sigma^2) &= \prod_{i=1}^n \mathcal{N}(y_i; \mu, \sigma^2) \\
 &= \prod_{i=1}^n \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp \left[-\frac{1}{2} \left(\frac{y_i - \mu}{\sigma} \right)^2 \right] \\
 &= \frac{1}{(\sqrt{2\pi}\sigma^2)^n} \cdot \exp \left[-\frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \mu)^2 \right]
 \end{aligned} \tag{7}$$

which, for mathematical convenience, can also be parametrized as

$$\begin{aligned}
 p(y|\mu, \tau) &= \prod_{i=1}^n \mathcal{N}(y_i; \mu, \tau^{-1}) \\
 &= \prod_{i=1}^n \sqrt{\frac{\tau}{2\pi}} \cdot \exp \left[-\frac{\tau}{2} (y_i - \mu)^2 \right] \\
 &= \left(\sqrt{\frac{\tau}{2\pi}} \right)^n \cdot \exp \left[-\frac{\tau}{2} \sum_{i=1}^n (y_i - \mu)^2 \right]
 \end{aligned} \tag{8}$$

using the inverse variance or precision $\tau = 1/\sigma^2$.

Combining the likelihood function (\rightarrow I/5.1.2) (8) with the prior distribution (\rightarrow I/5.1.3) (2), the joint likelihood (\rightarrow I/5.1.7) of the model is given by

$$\begin{aligned}
 p(y, \mu, \tau) &= p(y|\mu, \tau) p(\mu, \tau) \\
 &= \left(\sqrt{\frac{\tau}{2\pi}} \right)^n \cdot \exp \left[-\frac{\tau}{2} \sum_{i=1}^n (y_i - \mu)^2 \right] \cdot \\
 &\quad \sqrt{\frac{\tau\lambda_0}{2\pi}} \cdot \exp \left[-\frac{\tau\lambda_0}{2} (\mu - \mu_0)^2 \right] \cdot \\
 &\quad \frac{b_0^{a_0}}{\Gamma(a_0)} \tau^{a_0-1} \exp[-b_0\tau] .
 \end{aligned} \tag{9}$$

Collecting identical variables gives:

$$\begin{aligned}
 p(y, \mu, \tau) &= \sqrt{\frac{\tau^{n+1}\lambda_0}{(2\pi)^{n+1}}} \frac{b_0^{a_0}}{\Gamma(a_0)} \tau^{a_0-1} \exp[-b_0\tau] \cdot \\
 &\quad \exp \left[-\frac{\tau}{2} \left(\sum_{i=1}^n (y_i - \mu)^2 + \lambda_0 (\mu - \mu_0)^2 \right) \right] .
 \end{aligned} \tag{10}$$

Expanding the products in the exponent (\rightarrow III/1.1.8) gives

$$p(y, \mu, \tau) = \sqrt{\frac{\tau^{n+1} \lambda_0}{(2\pi)^{n+1}}} \frac{b_0^{a_0}}{\Gamma(a_0)} \tau^{a_0-1} \exp[-b_0 \tau] \cdot \exp \left[-\frac{\tau}{2} ((y^T y - 2\mu n \bar{y} + n\mu^2) + \lambda_0(\mu^2 - 2\mu\mu_0 + \mu_0^2)) \right] \quad (11)$$

where $\bar{y} = \frac{1}{n} \sum_{i=1}^n y_i$ and $y^T y = \sum_{i=1}^n y_i^2$, such that

$$p(y, \mu, \tau) = \sqrt{\frac{\tau^{n+1} \lambda_0}{(2\pi)^{n+1}}} \frac{b_0^{a_0}}{\Gamma(a_0)} \tau^{a_0-1} \exp[-b_0 \tau] \cdot \exp \left[-\frac{\tau}{2} (\mu^2(\lambda_0 + n) - 2\mu(\lambda_0\mu_0 + n\bar{y}) + (y^T y + \lambda_0\mu_0^2)) \right] \quad (12)$$

Completing the square over μ , we finally have

$$p(y, \mu, \tau) = \sqrt{\frac{\tau^{n+1} \lambda_0}{(2\pi)^{n+1}}} \frac{b_0^{a_0}}{\Gamma(a_0)} \tau^{a_0-1} \exp[-b_0 \tau] \cdot \exp \left[-\frac{\tau \lambda_n}{2} (\mu - \mu_n)^2 - \frac{\tau}{2} (y^T y + \lambda_0\mu_0^2 - \lambda_n\mu_n^2) \right] \quad (13)$$

with the posterior hyperparameters (\rightarrow I/5.1.9)

$$\begin{aligned} \mu_n &= \frac{\lambda_0\mu_0 + n\bar{y}}{\lambda_0 + n} \\ \lambda_n &= \lambda_0 + n . \end{aligned} \quad (14)$$

Ergo, the joint likelihood is proportional to

$$p(y, \mu, \tau) \propto \tau^{1/2} \cdot \exp \left[-\frac{\tau \lambda_n}{2} (\mu - \mu_n)^2 \right] \cdot \tau^{a_n-1} \cdot \exp [-b_n \tau] \quad (15)$$

with the posterior hyperparameters (\rightarrow I/5.1.9)

$$\begin{aligned} a_n &= a_0 + \frac{n}{2} \\ b_n &= b_0 + \frac{1}{2} (y^T y + \lambda_0\mu_0^2 - \lambda_n\mu_n^2) . \end{aligned} \quad (16)$$

From the term in (13), we can isolate the posterior distribution over μ given τ :

$$p(\mu|\tau, y) = \mathcal{N}(\mu; \mu_n, (\tau \lambda_n)^{-1}) . \quad (17)$$

From the remaining term, we can isolate the posterior distribution over τ :

$$p(\tau|y) = \text{Gam}(\tau; a_n, b_n) . \quad (18)$$

Together, (17) and (18) constitute the joint (\rightarrow I/1.3.2) posterior distribution (\rightarrow I/5.1.9) of μ and τ .

**Sources:**

- Bishop CM (2006): “Bayesian inference for the Gaussian”; in: *Pattern Recognition for Machine Learning*, pp. 97-102, eq. 2.154; URL: <http://users.isr.ist.utl.pt/~wurmd/Livros/school/Bishop%20-%20Pattern%20Recognition%20And%20Machine%20Learning%20-%20Springer%20%202006.pdf>.

1.1.10 Log model evidence**Theorem:** Let

$$m : y = \{y_1, \dots, y_n\}, \quad y_i \sim \mathcal{N}(\mu, \sigma^2), \quad i = 1, \dots, n \quad (1)$$

be a univariate Gaussian data set (\rightarrow III/1.1.1) with unknown mean μ and unknown variance σ^2 . Moreover, assume a normal-gamma prior distribution (\rightarrow III/1.1.8) over the model parameters μ and $\tau = 1/\sigma^2$:

$$p(\mu, \tau) = \mathcal{N}(\mu; \mu_0, (\tau \lambda_0)^{-1}) \cdot \text{Gam}(\tau; a_0, b_0) . \quad (2)$$

Then, the log model evidence (\rightarrow IV/3.1.3) for this model is

$$\log p(y|m) = -\frac{n}{2} \log(2\pi) + \frac{1}{2} \log \frac{\lambda_0}{\lambda_n} + \log \Gamma(a_n) - \log \Gamma(a_0) + a_0 \log b_0 - a_n \log b_n \quad (3)$$

where the posterior hyperparameters (\rightarrow I/5.1.9) are given by

$$\begin{aligned} \mu_n &= \frac{\lambda_0 \mu_0 + n \bar{y}}{\lambda_0 + n} \\ \lambda_n &= \lambda_0 + n \\ a_n &= a_0 + \frac{n}{2} \\ b_n &= b_0 + \frac{1}{2} (y^T y + \lambda_0 \mu_0^2 - \lambda_n \mu_n^2) . \end{aligned} \quad (4)$$

Proof: According to the law of marginal probability (\rightarrow I/1.3.3), the model evidence (\rightarrow I/5.1.15) for this model is:

$$p(y|m) = \iint p(y|\mu, \tau) p(\mu, \tau) d\mu d\tau . \quad (5)$$

According to the law of conditional probability (\rightarrow I/1.3.4), the integrand is equivalent to the joint likelihood (\rightarrow I/5.1.7):

$$p(y|m) = \iint p(y, \mu, \tau) d\mu d\tau . \quad (6)$$

Equation (1) implies the following likelihood function (\rightarrow I/5.1.2)

$$\begin{aligned}
p(y|\mu, \sigma^2) &= \prod_{i=1}^n \mathcal{N}(y_i; \mu, \sigma^2) \\
&= \prod_{i=1}^n \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp \left[-\frac{1}{2} \left(\frac{y_i - \mu}{\sigma} \right)^2 \right] \\
&= \frac{1}{(\sqrt{2\pi}\sigma^2)^n} \cdot \exp \left[-\frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \mu)^2 \right]
\end{aligned} \tag{7}$$

which, for mathematical convenience, can also be parametrized as

$$\begin{aligned}
p(y|\mu, \tau) &= \prod_{i=1}^n \mathcal{N}(y_i; \mu, \tau^{-1}) \\
&= \prod_{i=1}^n \sqrt{\frac{\tau}{2\pi}} \cdot \exp \left[-\frac{\tau}{2} (y_i - \mu)^2 \right] \\
&= \left(\sqrt{\frac{\tau}{2\pi}} \right)^n \cdot \exp \left[-\frac{\tau}{2} \sum_{i=1}^n (y_i - \mu)^2 \right]
\end{aligned} \tag{8}$$

using the inverse variance or precision $\tau = 1/\sigma^2$.

When deriving the posterior distribution (\rightarrow III/1.1.9) $p(\mu, \tau|y)$, the joint likelihood $p(y, \mu, \tau)$ is obtained as

$$\begin{aligned}
p(y, \mu, \tau) &= \sqrt{\frac{\tau^{n+1} \lambda_0}{(2\pi)^{n+1}}} \frac{b_0^{a_0}}{\Gamma(a_0)} \tau^{a_0-1} \exp[-b_0 \tau] \cdot \\
&\quad \exp \left[-\frac{\tau \lambda_n}{2} (\mu - \mu_n)^2 - \frac{\tau}{2} (y^T y + \lambda_0 \mu_0^2 - \lambda_n \mu_n^2) \right] .
\end{aligned} \tag{9}$$

Using the probability density function of the normal distribution (\rightarrow II/3.2.10), we can rewrite this as

$$\begin{aligned}
p(y, \mu, \tau) &= \sqrt{\frac{\tau^n}{(2\pi)^n}} \sqrt{\frac{\tau \lambda_0}{2\pi}} \sqrt{\frac{2\pi}{\tau \lambda_n}} \frac{b_0^{a_0}}{\Gamma(a_0)} \tau^{a_0-1} \exp[-b_0 \tau] \cdot \\
&\quad \mathcal{N}(\mu; \mu_n, (\tau \lambda_n)^{-1}) \exp \left[-\frac{\tau}{2} (y^T y + \lambda_0 \mu_0^2 - \lambda_n \mu_n^2) \right] .
\end{aligned} \tag{10}$$

Now, μ can be integrated out easily:

$$\begin{aligned}
\int p(y, \mu, \tau) d\mu &= \sqrt{\frac{1}{(2\pi)^n}} \sqrt{\frac{\lambda_0}{\lambda_n}} \frac{b_0^{a_0}}{\Gamma(a_0)} \tau^{a_0+n/2-1} \exp[-b_0 \tau] \cdot \\
&\quad \exp \left[-\frac{\tau}{2} (y^T y + \lambda_0 \mu_0^2 - \lambda_n \mu_n^2) \right] .
\end{aligned} \tag{11}$$

Using the probability density function of the gamma distribution (\rightarrow II/3.4.7), we can rewrite this as

$$\int p(y, \mu, \tau) d\mu = \sqrt{\frac{1}{(2\pi)^n}} \sqrt{\frac{\lambda_0}{\lambda_n}} \frac{b_0^{a_0}}{\Gamma(a_0)} \frac{\Gamma(a_n)}{b_n^{a_n}} \text{Gam}(\tau; a_n, b_n) . \quad (12)$$

Finally, τ can also be integrated out:

$$\iint p(y, \mu, \tau) d\mu d\tau = \sqrt{\frac{1}{(2\pi)^n}} \sqrt{\frac{\lambda_0}{\lambda_n}} \frac{\Gamma(a_n)}{\Gamma(a_0)} \frac{b_0^{a_0}}{b_n^{a_n}} . \quad (13)$$

Thus, the log model evidence (\rightarrow IV/3.1.3) of this model is given by

$$\log p(y|m) = -\frac{n}{2} \log(2\pi) + \frac{1}{2} \log \frac{\lambda_0}{\lambda_n} + \log \Gamma(a_n) - \log \Gamma(a_0) + a_0 \log b_0 - a_n \log b_n . \quad (14)$$

Sources:

- Bishop CM (2006): “Bayesian Linear Regression”; in: *Pattern Recognition for Machine Learning*, pp. 152-161, ex. 3.23, eq. 3.118; URL: <http://users.isr.ist.utl.pt/~wurmd/Livros/school/Bishop%20-%20Pattern%20Recognition%20And%20Machine%20Learning%20-%20Springer%20%202006.pdf>.

1.1.11 Accuracy and complexity

Theorem: Let

$$m : y = \{y_1, \dots, y_n\}, \quad y_i \sim \mathcal{N}(\mu, \sigma^2), \quad i = 1, \dots, n \quad (1)$$

be a univariate Gaussian data set (\rightarrow III/1.1.1) with unknown mean μ and unknown variance σ^2 . Moreover, assume a normal-gamma prior distribution (\rightarrow III/1.1.8) over the model parameters μ and $\tau = 1/\sigma^2$:

$$p(\mu, \tau) = \mathcal{N}(\mu; \mu_0, (\tau \lambda_0)^{-1}) \cdot \text{Gam}(\tau; a_0, b_0) . \quad (2)$$

Then, accuracy and complexity (\rightarrow IV/3.1.6) of this model are

$$\begin{aligned} \text{Acc}(m) &= -\frac{1}{2} \frac{a_n}{b_n} (y^T y - 2n\bar{y}\mu_n + n\mu_n^2) - \frac{1}{2} n \lambda_n^{-1} + \frac{n}{2} (\psi(a_n) - \log(b_n)) - \frac{n}{2} \log(2\pi) \\ \text{Com}(m) &= \frac{1}{2} \frac{a_n}{b_n} [\lambda_0(\mu_0 - \mu_n)^2 - 2(b_n - b_0)] + \frac{1}{2} \frac{\lambda_0}{\lambda_n} - \frac{1}{2} \log \frac{\lambda_0}{\lambda_n} - \frac{1}{2} \\ &\quad + a_0 \cdot \log \frac{b_n}{b_0} - \log \frac{\Gamma(a_n)}{\Gamma(a_0)} + (a_n - a_0) \cdot \psi(a_n) \end{aligned} \quad (3)$$

where μ_n and λ_n as well as a_n and b_n are the posterior hyperparameters for the univariate Gaussian (\rightarrow III/1.1.9) and \bar{y} is the sample mean (\rightarrow I/1.12.2).

Proof: Model accuracy and complexity are defined as (\rightarrow IV/3.1.6)

$$\begin{aligned} \text{LME}(m) &= \text{Acc}(m) - \text{Com}(m) \\ \text{Acc}(m) &= \langle \log p(y|\mu, \tau, m) \rangle_{p(\mu, \tau|y, m)} \\ \text{Com}(m) &= \text{KL} [p(\mu, \tau|y, m) || p(\mu, \tau|m)] . \end{aligned} \quad (4)$$

The accuracy term is the expectation (\rightarrow I/1.12.1) of the log-likelihood function (\rightarrow I/4.1.2) $\log p(y|\mu, \tau)$ with respect to the posterior distribution (\rightarrow I/5.1.9) $p(\mu, \tau|y)$. With the log-likelihood function for the univariate Gaussian (\rightarrow III/1.1.2) and the posterior distribution for the univariate Gaussian (\rightarrow III/1.1.9), the model accuracy of m evaluates to:

$$\begin{aligned}
\text{Acc}(m) &= \langle \log p(y|\mu, \tau) \rangle_{p(\mu, \tau|y)} \\
&= \left\langle \left\langle \log p(y|\mu, \tau) \right\rangle_{p(\mu|\tau, y)} \right\rangle_{p(\tau|y)} \\
&= \left\langle \left\langle \frac{n}{2} \log(\tau) - \frac{n}{2} \log(2\pi) - \frac{\tau}{2} (y^T y - 2n\bar{y}\mu + n\mu^2) \right\rangle_{\mathcal{N}(\mu_n, (\tau\lambda_n)^{-1})} \right\rangle_{\text{Gam}(a_n, b_n)} \\
&= \left\langle \frac{n}{2} \log(\tau) - \frac{n}{2} \log(2\pi) - \frac{\tau}{2} (y^T y - 2n\bar{y}\mu_n + n\mu_n^2) - \frac{1}{2} n\lambda_n^{-1} \right\rangle_{\text{Gam}(a_n, b_n)} \quad (5) \\
&= \frac{n}{2} (\psi(a_n) - \log(b_n)) - \frac{n}{2} \log(2\pi) - \frac{1}{2} \frac{a_n}{b_n} (y^T y - 2n\bar{y}\mu_n + n\mu_n^2) - \frac{1}{2} n\lambda_n^{-1} \\
&= -\frac{1}{2} \frac{a_n}{b_n} (y^T y - 2n\bar{y}\mu_n + n\mu_n^2) - \frac{1}{2} n\lambda_n^{-1} + \frac{n}{2} (\psi(a_n) - \log(b_n)) - \frac{n}{2} \log(2\pi)
\end{aligned}$$

The complexity penalty is the Kullback-Leibler divergence (\rightarrow I/2.5.1) of the posterior distribution (\rightarrow I/5.1.9) $p(\mu, \tau|y)$ from the prior distribution (\rightarrow I/5.1.3) $p(\mu, \tau)$. With the prior distribution (\rightarrow III/1.1.8) given by (2), the posterior distribution for the univariate Gaussian (\rightarrow III/1.1.9) and the Kullback-Leibler divergence of the normal-gamma distribution (\rightarrow II/4.4.7), the model complexity of m evaluates to:

$$\begin{aligned}
\text{Com}(m) &= \text{KL} [p(\mu, \tau|y) || p(\mu, \tau)] \\
&= \text{KL} [\text{NG}(\mu_n, \lambda_n^{-1}, a_n, b_n) || \text{NG}(\mu_0, \lambda_0^{-1}, a_0, b_0)] \\
&= \frac{1}{2} \frac{a_n}{b_n} [\lambda_0(\mu_0 - \mu_n)^2] + \frac{1}{2} \frac{\lambda_0}{\lambda_n} - \frac{1}{2} \log \frac{\lambda_0}{\lambda_n} - \frac{1}{2} \\
&\quad + a_0 \cdot \log \frac{b_n}{b_0} - \log \frac{\Gamma(a_n)}{\Gamma(a_0)} + (a_n - a_0) \cdot \psi(a_n) - (b_n - b_0) \cdot \frac{a_n}{b_n} \quad (6) \\
&= \frac{1}{2} \frac{a_n}{b_n} [\lambda_0(\mu_0 - \mu_n)^2 - 2(b_n - b_0)] + \frac{1}{2} \frac{\lambda_0}{\lambda_n} - \frac{1}{2} \log \frac{\lambda_0}{\lambda_n} - \frac{1}{2} \\
&\quad + a_0 \cdot \log \frac{b_n}{b_0} - \log \frac{\Gamma(a_n)}{\Gamma(a_0)} + (a_n - a_0) \cdot \psi(a_n) .
\end{aligned}$$

A control calculation confirms that

$$\text{Acc}(m) - \text{Com}(m) = \text{LME}(m) \quad (7)$$

where $\text{LME}(m)$ is the log model evidence for the univariate Gaussian (\rightarrow III/1.1.10).

■

1.1.12 Cross-validated log model evidence

Theorem: Let

$$y = \{y_1, \dots, y_n\}, \quad y_i \sim \mathcal{N}(\mu, \sigma^2), \quad i = 1, \dots, n \quad (1)$$

be a univariate Gaussian data set (\rightarrow III/1.1.1) with unknown mean μ and unknown variance σ^2 . Moreover, assume two statistical models (\rightarrow I/5.1.6), one assuming that μ is zero (null model (\rightarrow I/4.3.2)), the other imposing a normal distribution (\rightarrow III/1.1.8) as the prior distribution (\rightarrow I/5.1.3) on the mean parameter (\rightarrow I/1.12.1) μ (alternative (\rightarrow I/4.3.3)) and both imposing a gamma distribution (\rightarrow III/1.1.8) on the precision parameter (\rightarrow I/1.13.13) $\tau = 1/\sigma^2$:

$$\begin{aligned} m_0 : y_i &\sim \mathcal{N}(\mu, \tau^{-1}), \quad \mu = 0, \quad \tau \sim \text{Gam}(a_0, b_0) \\ m_1 : y_i &\sim \mathcal{N}(\mu, \tau^{-1}), \quad \mu|\tau \sim \mathcal{N}(\mu_0, (\tau\lambda_0)^{-1}), \quad \tau \sim \text{Gam}(a_0, b_0) \end{aligned} \quad (2)$$

Then, the cross-validated log model evidences (\rightarrow IV/3.1.9) of m_0 and m_1 are

$$\begin{aligned} \text{cvLME}(m_0) &= -\frac{n}{2} \log(2\pi) + S \cdot \log \Gamma\left(\frac{n}{2}\right) - S \cdot \log \Gamma\left(\frac{1}{2} \frac{S-1}{S} n\right) \\ &\quad - \frac{S \cdot n}{2} \log \left[\frac{1}{2} (y^T y) \right] + \frac{n_1}{2} \sum_{i=1}^S \log \left[\frac{1}{2} (y_1^{(i)T} y_1^{(i)}) \right] \\ \text{cvLME}(m_1) &= -\frac{n}{2} \log(2\pi) + \frac{S}{2} \log \left(\frac{S-1}{S} \right) + S \cdot \log \Gamma\left(\frac{n}{2}\right) - S \cdot \log \Gamma\left(\frac{1}{2} \frac{S-1}{S} n\right) \\ &\quad - \frac{S \cdot n}{2} \log \left[\frac{1}{2} (y^T y - n\bar{y}^2) \right] + \frac{n_1}{2} \sum_{i=1}^S \log \left[\frac{1}{2} (y_1^{(i)T} y_1^{(i)} - n_1 \bar{y}_1^{(i)}) \right] \end{aligned} \quad (3)$$

where \bar{y} is the sample mean (\rightarrow I/1.12.2), $y_1^{(i)}$ are the training data in the i -th cross-validation fold with n_1 data points and S is the number of data subsets (\rightarrow IV/3.1.9).

Proof: For evaluation of the cross-validated log model evidences (\rightarrow IV/3.1.9) (cvLME), we assume that n data points are divided into $S \mid n$ data subsets without remainder. Then, the number of training data points n_1 and test data points n_2 are given by

$$\begin{aligned} n &= n_1 + n_2 \\ n_1 &= \frac{S-1}{S} n \\ n_2 &= \frac{1}{S} n, \end{aligned} \quad (4)$$

such that training data y_1 and test data y_2 in the i -th cross-validation fold are

$$\begin{aligned} y &= \{y_1, \dots, y_n\} \\ y_1^{(i)} &= \left\{ x \in y \mid x \notin y_2^{(i)} \right\} = y \setminus y_2^{(i)} \\ y_2^{(i)} &= \{y_{(i-1) \cdot n_2 + 1}, \dots, y_{i \cdot n_2}\} . \end{aligned} \quad (5)$$

First, we have a look at the alternative m_1 assuming $\mu \neq 0$. To begin, the training data $y_1^{(i)}$ are analyzed using a non-informative prior distribution (\rightarrow I/5.2.3) and applying the posterior distribution for the univariate Gaussian (\rightarrow III/1.1.9):

$$\begin{aligned}
\mu_0^{(1)} = 0 &\Rightarrow \mu_n^{(1)} = \frac{\lambda_0^{(1)} \mu_0^{(1)} + n_1 \bar{y}_1^{(i)}}{\lambda_0^{(1)} + n_1} = \bar{y}_1^{(i)} \\
\lambda_0^{(1)} = 0 &\Rightarrow \lambda_n^{(1)} = \lambda_0^{(1)} + n_1 = n_1 \\
a_0^{(1)} = 0 &\Rightarrow a_n^{(1)} = a_0^{(1)} + \frac{n_1}{2} = \frac{n_1}{2} \\
b_0^{(1)} = 0 &\Rightarrow b_n^{(1)} = b_0^{(1)} + \frac{1}{2} \left(y_1^{(i)T} y_1^{(i)} + \lambda_0^{(1)} \mu_0^{(1)2} - \lambda_n^{(1)} \mu_n^{(1)2} \right) = \frac{1}{2} \left(y_1^{(i)T} y_1^{(i)} - n_1 \left(\bar{y}_1^{(i)} \right)^2 \right).
\end{aligned} \tag{6}$$

This results in a posterior characterized by $\mu_n^{(1)}$, $\lambda_n^{(1)}$, $a_n^{(1)}$ and $b_n^{(1)}$. Then, the test data $y_2^{(i)}$ are analyzed using this posterior as an informative prior distribution (\rightarrow I/5.2.3), again applying the posterior distribution for the univariate Gaussian (\rightarrow III/1.1.9):

$$\begin{aligned}
\mu_0^{(2)} &= \mu_n^{(1)} = \bar{y}_1^{(i)} \\
\Rightarrow \mu_n^{(2)} &= \frac{\lambda_0^{(2)} \mu_0^{(2)} + n_2 \bar{y}_2^{(i)}}{\lambda_0^{(2)} + n_2} \\
&= \frac{n_1 \bar{y}_1^{(i)} + n_2 \bar{y}_2^{(i)}}{n_1 + n_2} \\
&= \frac{n \bar{y}}{n} = \bar{y} \\
\lambda_0^{(2)} &= \lambda_n^{(1)} = n_1 \\
\Rightarrow \lambda_n^{(2)} &= \lambda_0^{(2)} + n_2 = n_1 + n_2 = n \\
a_0^{(2)} &= a_n^{(1)} = \frac{n_1}{2} \\
\Rightarrow a_n^{(2)} &= a_0^{(2)} + \frac{n_2}{2} = \frac{n_1}{2} + \frac{n_2}{2} = \frac{n}{2} \\
b_0^{(2)} &= b_n^{(1)} = \frac{1}{2} \left(y_1^{(i)T} y_1^{(i)} - n_1 \bar{y}_1^{(i)2} \right) \\
\Rightarrow b_n^{(2)} &= b_0^{(2)} + \frac{1}{2} \left(y_2^{(i)T} y_2^{(i)} + \lambda_0^{(2)} \mu_0^{(2)2} - \lambda_n^{(2)} \mu_n^{(2)2} \right) \\
&= \frac{1}{2} \left(y_1^{(i)T} y_1^{(i)} - n_1 \left(\bar{y}_1^{(i)} \right)^2 \right) + \frac{1}{2} \left(y_2^{(i)T} y_2^{(i)} + n_1 \left(\bar{y}_1^{(i)} \right)^2 - n \bar{y}^2 \right) \\
&= \frac{1}{2} \left(y^T y - n \bar{y}^2 \right).
\end{aligned} \tag{7}$$

In the test data, we now have a prior characterized by $\mu_0^{(2)}$, $\lambda_0^{(2)}$, $a_0^{(2)}$ and $b_0^{(2)}$ and a posterior characterized by $\mu_n^{(2)}$, $\lambda_n^{(2)}$, $a_n^{(2)}$ and $b_n^{(2)}$. Applying the log model evidence for the univariate Gaussian (\rightarrow III/1.1.10), the out-of-sample log model evidence (\rightarrow IV/3.1.9) (oosLME) therefore follows as

$$\begin{aligned}
\text{oosLME}_i(m_1) &= -\frac{n_2}{2} \log(2\pi) + \frac{1}{2} \log \frac{\lambda_0^{(2)}}{\lambda_n^{(2)}} + \log \Gamma(a_n^{(2)}) - \log \Gamma(a_0^{(2)}) \\
&\quad + a_0^{(2)} \log b_0^{(2)} - a_n^{(2)} \log b_n^{(2)} \\
&= -\frac{n_2}{2} \log(2\pi) + \frac{1}{2} \log \left(\frac{n_1}{n} \right) + \log \Gamma \left(\frac{n}{2} \right) - \log \Gamma \left(\frac{n_1}{2} \right) \\
&\quad + \frac{n_1}{2} \log \left[\frac{1}{2} \left(y_1^{(i)\text{T}} y_1^{(i)} - n_1 \bar{y}_1^{(i)} \right) \right] - \frac{n}{2} \log \left[\frac{1}{2} (y^{\text{T}} y - n \bar{y}^2) \right] \\
&= -\frac{n}{2S} \log(2\pi) + \frac{1}{2} \log \left(\frac{S-1}{S} \right) + \log \Gamma \left(\frac{n}{2} \right) - \log \Gamma \left(\frac{(S-1)n}{2S} \right) \\
&\quad + \frac{(S-1)n}{2S} \log \left[\frac{1}{2} \left(y_1^{(i)\text{T}} y_1^{(i)} - n_1 \bar{y}_1^{(i)} \right) \right] - \frac{n}{2} \log \left[\frac{1}{2} (y^{\text{T}} y - n \bar{y}^2) \right].
\end{aligned} \tag{8}$$

By definition, the cross-validated log model evidence is the sum of out-of-sample log model evidences (\rightarrow IV/3.1.9) over cross-validation folds, such that the cvLME of m_1 is:

$$\begin{aligned}
\text{cvLME}(m_1) &= \sum_{i=1}^S \text{oosLME}_i(m_1) \\
&= \sum_{i=1}^S \left(-\frac{n}{2S} \log(2\pi) + \frac{1}{2} \log \left(\frac{S-1}{S} \right) + \log \Gamma \left(\frac{n}{2} \right) - \log \Gamma \left(\frac{(S-1)n}{2S} \right) \right. \\
&\quad \left. + \frac{(S-1)n}{2S} \log \left[\frac{1}{2} \left(y_1^{(i)\text{T}} y_1^{(i)} - n_1 \bar{y}_1^{(i)} \right) \right] - \frac{n}{2} \log \left[\frac{1}{2} (y^{\text{T}} y - n \bar{y}^2) \right] \right) \\
&= -\frac{n}{2} \log(2\pi) + \frac{S}{2} \log \left(\frac{S-1}{S} \right) + S \cdot \log \Gamma \left(\frac{n}{2} \right) - S \cdot \log \Gamma \left(\frac{1}{2} \frac{S-1}{S} n \right) \\
&\quad - \frac{S \cdot n}{2} \log \left[\frac{1}{2} (y^{\text{T}} y - n \bar{y}^2) \right] + \frac{n_1}{2} \sum_{i=1}^S \log \left[\frac{1}{2} \left(y_1^{(i)\text{T}} y_1^{(i)} - n_1 \bar{y}_1^{(i)} \right) \right].
\end{aligned} \tag{9}$$

Next, we consider the null model m_0 assuming $\mu = 0$. Because this model has no parameter for μ , there are no hyperparameters μ_0 and λ_0 , but only hyperparameters a_0 and b_0 for the parameter τ . In the first step, the training data $y_1^{(i)}$ are analyzed using a non-informative prior distribution (\rightarrow I/5.2.3) and applying the posterior distribution for the univariate Gaussian (\rightarrow III/1.1.9):

$$\begin{aligned}
a_0^{(1)} = 0 &\Rightarrow a_n^{(1)} = a_0^{(1)} + \frac{n_1}{2} = \frac{n_1}{2} \\
b_0^{(1)} = 0 &\Rightarrow b_n^{(1)} = b_0^{(1)} + \frac{1}{2} \left(y_1^{(i)\text{T}} y_1^{(i)} \right) = \frac{1}{2} \left(y_1^{(i)\text{T}} y_1^{(i)} \right).
\end{aligned} \tag{10}$$

In the second step, the test data $y_2^{(i)}$ are analyzed using this posterior as an informative prior distribution (\rightarrow I/5.2.3), again applying the posterior distribution for the univariate Gaussian (\rightarrow III/1.1.9):

$$\begin{aligned}
a_0^{(2)} &= a_n^{(1)} = \frac{n_1}{2} \\
\Rightarrow a_n^{(2)} &= a_0^{(2)} + \frac{n_2}{2} = \frac{n_1}{2} + \frac{n_2}{2} = \frac{n}{2} \\
b_0^{(2)} &= b_n^{(1)} = \frac{1}{2} \left(y_1^{(i)\top} y_1^{(i)} \right) \\
\Rightarrow b_n^{(2)} &= b_0^{(2)} + \frac{1}{2} \left(y_2^{(i)\top} y_2^{(i)} \right) = \frac{1}{2} \left(y_1^{(i)\top} y_1^{(i)} \right) + \frac{1}{2} \left(y_2^{(i)\top} y_2^{(i)} \right) = \frac{1}{2} (y^\top y) .
\end{aligned} \tag{11}$$

In the test data, we now have a prior characterized by $a_0^{(2)}$ and $b_0^{(2)}$ and a posterior characterized $a_n^{(2)}$ and $b_n^{(2)}$. Applying the log model evidence for the univariate Gaussian (\rightarrow III/1.1.10), the out-of-sample log model evidence (\rightarrow IV/3.1.9) (oosLME) therefore follows as

$$\begin{aligned}
\text{oosLME}_i(m_1) &= -\frac{n_2}{2} \log(2\pi) + \log \Gamma(a_n^{(2)}) - \log \Gamma(a_0^{(2)}) \\
&\quad + a_0^{(2)} \log b_0^{(2)} - a_n^{(2)} \log b_n^{(2)} \\
&= -\frac{n_2}{2} \log(2\pi) + \log \Gamma\left(\frac{n}{2}\right) - \log \Gamma\left(\frac{n_1}{2}\right) \\
&\quad + \frac{n_1}{2} \log \left[\frac{1}{2} \left(y_1^{(i)\top} y_1^{(i)} \right) \right] - \frac{n}{2} \log \left[\frac{1}{2} (y^\top y) \right] \\
&= -\frac{n}{2S} \log(2\pi) + \log \Gamma\left(\frac{n}{2}\right) - \log \Gamma\left(\frac{(S-1)n}{2S}\right) \\
&\quad + \frac{(S-1)n}{2S} \log \left[\frac{1}{2} \left(y_1^{(i)\top} y_1^{(i)} \right) \right] - \frac{n}{2} \log \left[\frac{1}{2} (y^\top y) \right] .
\end{aligned} \tag{12}$$

Again, because the cross-validated log model evidence is the sum of out-of-sample log model evidences (\rightarrow IV/3.1.9) over cross-validation folds, the cvLME of m_0 becomes:

$$\begin{aligned}
\text{cvLME}(m_0) &= \sum_{i=1}^S \text{oosLME}_i(m_0) \\
&= \sum_{i=1}^S \left(-\frac{n}{2S} \log(2\pi) + \log \Gamma\left(\frac{n}{2}\right) - \log \Gamma\left(\frac{(S-1)n}{2S}\right) \right. \\
&\quad \left. + \frac{(S-1)n}{2S} \log \left[\frac{1}{2} \left(y_1^{(i)\top} y_1^{(i)} \right) \right] - \frac{n}{2} \log \left[\frac{1}{2} (y^\top y) \right] \right) \\
&= -\frac{n}{2} \log(2\pi) + S \cdot \log \Gamma\left(\frac{n}{2}\right) - S \cdot \log \Gamma\left(\frac{1}{2} \frac{S-1}{S} n\right) \\
&\quad - \frac{S \cdot n}{2} \log \left[\frac{1}{2} (y^\top y) \right] + \frac{n_1}{2} \sum_{i=1}^S \log \left[\frac{1}{2} \left(y_1^{(i)\top} y_1^{(i)} \right) \right] .
\end{aligned} \tag{13}$$

Together, (13) and (9) conform to the results given in (3). ■

1.1.13 Cross-validated log Bayes factor

Theorem: Let

$$y = \{y_1, \dots, y_n\}, \quad y_i \sim \mathcal{N}(\mu, \sigma^2), \quad i = 1, \dots, n \quad (1)$$

be a univariate Gaussian data set (\rightarrow III/1.1.1) with unknown mean μ and unknown variance σ^2 . Moreover, assume two statistical models (\rightarrow I/5.1.6), one assuming that μ is zero (null model (\rightarrow I/4.3.2)), the other imposing a normal distribution (\rightarrow III/1.1.8) as the prior distribution (\rightarrow I/5.1.3) on the mean parameter (\rightarrow I/1.12.1) μ (alternative (\rightarrow I/4.3.3)) and both imposing a gamma distribution (\rightarrow III/1.1.8) on the precision parameter (\rightarrow I/1.13.13) $\tau = 1/\sigma^2$:

$$\begin{aligned} m_0 : y_i &\sim \mathcal{N}(\mu, \tau^{-1}), \quad \mu = 0, \quad \tau \sim \text{Gam}(a_0, b_0) \\ m_1 : y_i &\sim \mathcal{N}(\mu, \tau^{-1}), \quad \mu|\tau \sim \mathcal{N}(\mu_0, (\tau\lambda_0)^{-1}), \quad \tau \sim \text{Gam}(a_0, b_0) \end{aligned} \quad (2)$$

Then, the cross-validated (\rightarrow IV/3.1.9) log Bayes factor (\rightarrow IV/3.3.6) in favor of m_1 against m_0 is

$$\text{cvLBF}_{10} = \frac{S}{2} \log \left(\frac{S-1}{S} \right) - \frac{S \cdot n}{2} \left[\log \left(1 - \frac{n\bar{y}^2}{y^T y} \right) \right] + \frac{n_1}{2} \sum_{i=1}^S \left[\log \left(1 - \frac{n_1 \bar{y}_1^{(i)}}{y_1^{(i)T} y_1^{(i)}} \right) \right] \quad (3)$$

where \bar{y} is the sample mean (\rightarrow I/1.12.2), $y_1^{(i)}$ are the training data in the i -th cross-validation fold with n_1 data points and S is the number of data subsets (\rightarrow IV/3.1.9).

Proof: The relationship between log Bayes factor and log model evidences (\rightarrow IV/3.3.8) also holds for cross-validated log bayes factor (\rightarrow IV/3.3.6) (cvLBF) and cross-validated log model evidences (\rightarrow IV/3.1.9) (cvLME):

$$\text{cvLBF}_{12} = \text{cvLME}(m_1) - \text{cvLME}(m_2). \quad (4)$$

The cross-validated log model evidences (\rightarrow IV/3.1.9) of m_0 and m_1 are given by (\rightarrow III/1.1.12)

$$\begin{aligned} \text{cvLME}(m_0) &= -\frac{n}{2} \log(2\pi) + S \cdot \log \Gamma \left(\frac{n}{2} \right) - S \cdot \log \Gamma \left(\frac{1}{2} \frac{S-1}{S} n \right) \\ &\quad - \frac{S \cdot n}{2} \log \left[\frac{1}{2} (y^T y) \right] + \frac{n_1}{2} \sum_{i=1}^S \log \left[\frac{1}{2} (y_1^{(i)T} y_1^{(i)}) \right] \\ \text{cvLME}(m_1) &= -\frac{n}{2} \log(2\pi) + \frac{S}{2} \log \left(\frac{S-1}{S} \right) + S \cdot \log \Gamma \left(\frac{n}{2} \right) - S \cdot \log \Gamma \left(\frac{1}{2} \frac{S-1}{S} n \right) \\ &\quad - \frac{S \cdot n}{2} \log \left[\frac{1}{2} (y^T y - n\bar{y}^2) \right] + \frac{n_1}{2} \sum_{i=1}^S \log \left[\frac{1}{2} (y_1^{(i)T} y_1^{(i)} - n_1 \bar{y}_1^{(i)}) \right]. \end{aligned} \quad (5)$$

Subtracting the two cvLMEs from each other, the cvLBF emerges as

$$\begin{aligned}
\text{cvLBF}_{10} &= \text{cvLME}(m_1) - \text{LME}(m_0) \\
&= + \frac{S}{2} \log \left(\frac{S-1}{S} \right) - \frac{S \cdot n}{2} \left[\log \left(\frac{1}{2} (y^T y - n \bar{y}^2) \right) - \log \left(\frac{1}{2} (y^T y) \right) \right] \\
&\quad + \frac{n_1}{2} \sum_{i=1}^S \left[\log \left(\frac{1}{2} (y_1^{(i)T} y_1^{(i)} - n_1 \bar{y}_1^{(i)}) \right) - \log \left(\frac{1}{2} (y_1^{(i)T} y_1^{(i)}) \right) \right] \\
&= \frac{S}{2} \log \left(\frac{S-1}{S} \right) - \frac{S \cdot n}{2} \left[\log \left(\frac{y^T y - n \bar{y}^2}{y^T y} \right) \right] + \frac{n_1}{2} \sum_{i=1}^S \left[\log \left(\frac{y_1^{(i)T} y_1^{(i)} - n_1 \bar{y}_1^{(i)}}{y_1^{(i)T} y_1^{(i)}} \right) \right] \\
&= \frac{S}{2} \log \left(\frac{S-1}{S} \right) - \frac{S \cdot n}{2} \left[\log \left(1 - \frac{n \bar{y}^2}{y^T y} \right) \right] + \frac{n_1}{2} \sum_{i=1}^S \left[\log \left(1 - \frac{n_1 \bar{y}_1^{(i)}}{y_1^{(i)T} y_1^{(i)}} \right) \right] .
\end{aligned} \tag{6}$$

■

1.2 Univariate Gaussian with known variance

1.2.1 Definition

Definition: A univariate Gaussian data set with known variance is given by a set of real numbers $y = \{y_1, \dots, y_n\}$, independent and identically distributed (\rightarrow I/1.2.8) according to a normal distribution (\rightarrow II/3.2.1) with unknown mean μ and known variance σ^2 :

$$y_i \sim \mathcal{N}(\mu, \sigma^2), \quad i = 1, \dots, n . \tag{1}$$

Sources:

- Bishop, Christopher M. (2006): “Bayesian inference for the Gaussian”; in: *Pattern Recognition for Machine Learning*, ch. 2.3.6, p. 97, eq. 2.137; URL: <http://users.isr.ist.utl.pt/~wurmd/Livros/school/Bishop%20-%20Pattern%20Recognition%20And%20Machine%20Learning%20-%20Springer%20%202006.pdf>.

1.2.2 Maximum likelihood estimation

Theorem: Let there be univariate Gaussian data with known variance (\rightarrow III/1.2.1) $y = \{y_1, \dots, y_n\}$:

$$y_i \sim \mathcal{N}(\mu, \sigma^2), \quad i = 1, \dots, n . \tag{1}$$

Then, the maximum likelihood estimate (\rightarrow I/4.1.3) for the mean μ is given by

$$\hat{\mu} = \bar{y} \tag{2}$$

where \bar{y} is the sample mean (\rightarrow I/1.12.2)

$$\bar{y} = \frac{1}{n} \sum_{i=1}^n y_i . \tag{3}$$

Proof: The likelihood function (\rightarrow I/5.1.2) for each observation is given by the probability density function of the normal distribution (\rightarrow II/3.2.10)

$$p(y_i|\mu) = \mathcal{N}(y_i; \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \cdot \exp \left[-\frac{1}{2} \left(\frac{y_i - \mu}{\sigma} \right)^2 \right] \quad (4)$$

and because observations are independent (\rightarrow I/1.3.6), the likelihood function for all observations is the product of the individual ones:

$$p(y|\mu) = \prod_{i=1}^n p(y_i|\mu) = \sqrt{\frac{1}{(2\pi\sigma^2)^n}} \cdot \exp \left[-\frac{1}{2} \sum_{i=1}^n \left(\frac{y_i - \mu}{\sigma} \right)^2 \right] . \quad (5)$$

This can be developed into

$$\begin{aligned} p(y|\mu) &= \left(\frac{1}{2\pi\sigma^2} \right)^{n/2} \cdot \exp \left[-\frac{1}{2} \sum_{i=1}^n \left(\frac{y_i^2 - 2y_i\mu + \mu^2}{\sigma^2} \right) \right] \\ &= \left(\frac{1}{2\pi\sigma^2} \right)^{n/2} \cdot \exp \left[-\frac{1}{2\sigma^2} (y^T y - 2n\bar{y}\mu + n\mu^2) \right] \end{aligned} \quad (6)$$

where $\bar{y} = \frac{1}{n} \sum_{i=1}^n y_i$ is the mean (\rightarrow I/1.12.2) of data points (\rightarrow I/1.1.5) and $y^T y = \sum_{i=1}^n y_i^2$ is the sum of squared data points (\rightarrow I/1.1.5). Thus, the log-likelihood function (\rightarrow I/4.1.2) is

$$\text{LL}(\mu) = \log p(y|\mu) = -\frac{n}{2} \log(2\pi\sigma^2) - \frac{1}{2\sigma^2} (y^T y - 2n\bar{y}\mu + n\mu^2) . \quad (7)$$

The derivatives of the log-likelihood with respect to μ are

$$\begin{aligned} \frac{d\text{LL}(\mu)}{d\mu} &= \frac{n\bar{y}}{\sigma^2} - \frac{n\mu}{\sigma^2} = \frac{n}{\sigma^2} (\bar{y} - \mu) \\ \frac{d^2\text{LL}(\mu)}{d\mu^2} &= -\frac{n}{\sigma^2} . \end{aligned} \quad (8)$$

Setting the first derivative to zero, we obtain:

$$\begin{aligned} \frac{d\text{LL}(\hat{\mu})}{d\mu} &= 0 \\ 0 &= \frac{n}{\sigma^2} (\bar{y} - \hat{\mu}) \\ 0 &= \bar{y} - \hat{\mu} \\ \hat{\mu} &= \bar{y} \end{aligned} \quad (9)$$

Plugging this value into the second derivative, we confirm:

$$\frac{d^2\text{LL}(\hat{\mu})}{d\mu^2} = -\frac{n}{\sigma^2} < 0 . \quad (10)$$

This demonstrates that the estimate (\rightarrow I/3.1.1) $\hat{\mu} = \bar{y}$ maximizes the likelihood (\rightarrow I/5.1.2) $p(y|\mu)$. ■

Sources:

- Bishop, Christopher M. (2006): “Bayesian inference for the Gaussian”; in: *Pattern Recognition for Machine Learning*, ch. 2.3.6, p. 98, eq. 2.143; URL: <http://users.isr.ist.utl.pt/~wurmd/Livros/school/Bishop%20-%20Pattern%20Recognition%20And%20Machine%20Learning%20-%20Springer%20%202006.pdf>.

1.2.3 One-sample z-test

Theorem: Let

$$y_i \sim \mathcal{N}(\mu, \sigma^2), \quad i = 1, \dots, n \quad (1)$$

be a univariate Gaussian data set (\rightarrow III/1.2.1) with unknown mean μ and known variance σ^2 . Then, the test statistic (\rightarrow I/4.3.5)

$$z = \sqrt{n} \frac{\bar{y} - \mu_0}{\sigma} \quad (2)$$

with sample mean (\rightarrow I/1.12.2) \bar{y} follows a standard normal distribution (\rightarrow II/3.2.3)

$$z \sim \mathcal{N}(0, 1) \quad (3)$$

under the null hypothesis (\rightarrow I/4.3.2)

$$H_0 : \mu = \mu_0 . \quad (4)$$

Proof: The sample mean (\rightarrow I/1.12.2) is given by

$$\bar{y} = \frac{1}{n} \sum_{i=1}^n y_i . \quad (5)$$

Using the linear combination formula for normal random variables (\rightarrow II/3.2.26), the sample mean follows a normal distribution (\rightarrow II/3.2.1) with the following parameters:

$$\bar{y} = \frac{1}{n} \sum_{i=1}^n y_i \sim \mathcal{N} \left(\frac{1}{n} n \mu, \left(\frac{1}{n} \right)^2 n \sigma^2 \right) = \mathcal{N}(\mu, \sigma^2/n) . \quad (6)$$

Again employing the linear combination theorem, the distribution of $z = \sqrt{n/\sigma^2}(\bar{y} - \mu_0)$ becomes

$$z = \sqrt{\frac{n}{\sigma^2}}(\bar{y} - \mu_0) \sim \mathcal{N} \left(\sqrt{\frac{n}{\sigma^2}}(\mu - \mu_0), \left(\sqrt{\frac{n}{\sigma^2}} \right)^2 \frac{\sigma^2}{n} \right) = \mathcal{N} \left(\sqrt{n} \frac{\mu - \mu_0}{\sigma}, 1 \right) , \quad (7)$$

such that, under the null hypothesis in (4), we have:

$$z \sim \mathcal{N}(0, 1), \quad \text{if } \mu = \mu_0 . \quad (8)$$

This means that the null hypothesis (\rightarrow I/4.3.2) can be rejected when z is as extreme or more extreme than the critical value (\rightarrow I/4.3.9) obtained from the standard normal distribution (\rightarrow II/3.2.3) using a significance level (\rightarrow I/4.3.8) α . ■

Sources:

- Wikipedia (2021): “Z-test”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-03-24; URL: https://en.wikipedia.org/wiki/Z-test#Use_in_location_testing.
- Wikipedia (2021): “Gauß-Test”; in: *Wikipedia – Die freie Enzyklopädie*, retrieved on 2021-03-24; URL: <https://de.wikipedia.org/wiki/Gau%C3%9F-Test#Einstichproben-Gau%C3%9F-Test>.

1.2.4 Two-sample z-test

Theorem: Let

$$\begin{aligned} y_{1i} &\sim \mathcal{N}(\mu_1, \sigma_1^2), & i = 1, \dots, n_1 \\ y_{2i} &\sim \mathcal{N}(\mu_2, \sigma_2^2), & i = 1, \dots, n_2 \end{aligned} \quad (1)$$

be two univariate Gaussian data sets (\rightarrow III/1.1.1) representing two groups of unequal size n_1 and n_2 with unknown means μ_1 and μ_2 and unknown variances σ_1^2 and σ_2^2 . Then, the test statistic (\rightarrow I/4.3.5)

$$z = \frac{(\bar{y}_1 - \bar{y}_2) - \mu_\Delta}{\sqrt{\frac{\sigma_1^2}{n_1} + \frac{\sigma_2^2}{n_2}}} \quad (2)$$

with sample means (\rightarrow I/1.12.2) \bar{y}_1 and \bar{y}_2 follows a standard normal distribution (\rightarrow II/3.2.3)

$$z \sim \mathcal{N}(0, 1) \quad (3)$$

under the null hypothesis (\rightarrow I/4.3.2)

$$H_0 : \mu_1 - \mu_2 = \mu_\Delta . \quad (4)$$

Proof: The sample means (\rightarrow I/1.12.2) are given by

$$\begin{aligned} \bar{y}_1 &= \frac{1}{n_1} \sum_{i=1}^{n_1} y_{1i} \\ \bar{y}_2 &= \frac{1}{n_2} \sum_{i=1}^{n_2} y_{2i} . \end{aligned} \quad (5)$$

Using the linear combination formula for normal random variables (\rightarrow II/3.2.26), the sample means follows normal distributions (\rightarrow II/3.2.1) with the following parameters:

$$\begin{aligned} \bar{y}_1 &= \frac{1}{n_1} \sum_{i=1}^{n_1} y_{1i} \sim \mathcal{N} \left(\frac{1}{n_1} n_1 \mu_1, \left(\frac{1}{n_1} \right)^2 n_1 \sigma_1^2 \right) = \mathcal{N}(\mu_1, \sigma_1^2/n_1) \\ \bar{y}_2 &= \frac{1}{n_2} \sum_{i=1}^{n_2} y_{2i} \sim \mathcal{N} \left(\frac{1}{n_2} n_2 \mu_2, \left(\frac{1}{n_2} \right)^2 n_2 \sigma_2^2 \right) = \mathcal{N}(\mu_2, \sigma_2^2/n_2) . \end{aligned} \quad (6)$$

Again employing the linear combination theorem, the distribution of $z = [(\bar{y}_1 - \bar{y}_2) - \mu_\Delta] / \sigma_\Delta$ becomes

$$z = \frac{(\bar{y}_1 - \bar{y}_2) - \mu_\Delta}{\sigma_\Delta} \sim \mathcal{N} \left(\frac{(\mu_1 - \mu_2) - \mu_\Delta}{\sigma_\Delta}, \left(\frac{1}{\sigma_\Delta} \right)^2 \sigma_\Delta^2 \right) = \mathcal{N} \left(\frac{(\mu_1 - \mu_2) - \mu_\Delta}{\sigma_\Delta}, 1 \right) \quad (7)$$

where σ_Δ is the pooled standard deviation (\rightarrow I/1.19.3)

$$\sigma_\Delta = \sqrt{\frac{\sigma_1^2}{n_1} + \frac{\sigma_2^2}{n_2}} , \quad (8)$$

such that, under the null hypothesis in (4), we have:

$$z \sim \mathcal{N}(0, 1), \quad \text{if } \mu_\Delta = \mu_1 - \mu_2. \quad (9)$$

This means that the null hypothesis (\rightarrow I/4.3.2) can be rejected when z is as extreme or more extreme than the critical value (\rightarrow I/4.3.9) obtained from the standard normal distribution (\rightarrow II/3.2.3) using a significance level (\rightarrow I/4.3.8) α . ■

Sources:

- Wikipedia (2021): “Z-test”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-03-24; URL: https://en.wikipedia.org/wiki/Z-test#Use_in_location_testing.
- Wikipedia (2021): “Gauß-Test”; in: *Wikipedia – Die freie Enzyklopädie*, retrieved on 2021-03-24; URL: https://de.wikipedia.org/wiki/Gau%C3%9F-Test#Zweistichproben-Gau%C3%9F-Test_f%C3%BCr_unabh%C3%A4ngige_Stichproben.

1.2.5 Paired z-test

Theorem: Let y_{i1} and y_{i2} with $i = 1, \dots, n$ be paired observations, such that

$$y_{i1} \sim \mathcal{N}(y_{i2} + \mu, \sigma^2), \quad i = 1, \dots, n \quad (1)$$

is a univariate Gaussian data set (\rightarrow III/1.2.1) with unknown shift μ and known variance σ^2 . Then, the test statistic (\rightarrow I/4.3.5)

$$z = \sqrt{n} \frac{\bar{d} - \mu_0}{\sigma} \quad \text{where} \quad d_i = y_{i1} - y_{i2} \quad (2)$$

with sample mean (\rightarrow I/1.12.2) \bar{d} follows a standard normal distribution (\rightarrow II/3.2.3)

$$z \sim \mathcal{N}(0, 1) \quad (3)$$

under the null hypothesis (\rightarrow I/4.3.2)

$$H_0 : \mu = \mu_0. \quad (4)$$

Proof: Define the pair-wise difference $d_i = y_{i1} - y_{i2}$ which, as a linear transformation of a normal random variable (\rightarrow II/4.1.14), is distributed as

$$d_i = y_{i1} - y_{i2} \sim \mathcal{N}(\mu, \sigma^2), \quad i = 1, \dots, n. \quad (5)$$

Therefore, d_1, \dots, d_n satisfy the conditions of the one-sample z-test (\rightarrow III/1.2.3) which results in the test statistic given by (2). ■

Sources:

- Wikipedia (2021): “Z-test”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-03-24; URL: https://en.wikipedia.org/wiki/Z-test#Use_in_location_testing.
- Wikipedia (2021): “Gauß-Test”; in: *Wikipedia – Die freie Enzyklopädie*, retrieved on 2021-03-24; URL: [https://de.wikipedia.org/wiki/Gau%C3%9F-Test#Zweistichproben-Gau%C3%9F-Test_f%C3%BCr_abh%C3%A4ngige_\(verbundene\)_Stichproben](https://de.wikipedia.org/wiki/Gau%C3%9F-Test#Zweistichproben-Gau%C3%9F-Test_f%C3%BCr_abh%C3%A4ngige_(verbundene)_Stichproben).

1.2.6 Conjugate prior distribution

Theorem: Let

$$y = \{y_1, \dots, y_n\}, \quad y_i \sim \mathcal{N}(\mu, \sigma^2), \quad i = 1, \dots, n \quad (1)$$

be a univariate Gaussian data set (\rightarrow III/1.2.1) with unknown mean μ and known variance σ^2 . Then, the conjugate prior (\rightarrow I/5.2.5) for this model is a normal distribution (\rightarrow II/3.2.1)

$$p(\mu) = \mathcal{N}(\mu; \mu_0, \lambda_0^{-1}) \quad (2)$$

with prior (\rightarrow I/5.1.3) mean (\rightarrow I/1.12.1) μ_0 and prior (\rightarrow I/5.1.3) precision (\rightarrow I/1.13.13) λ_0 .

Proof: By definition, a conjugate prior (\rightarrow I/5.2.5) is a prior distribution (\rightarrow I/5.1.3) that, when combined with the likelihood function (\rightarrow I/5.1.2), leads to a posterior distribution (\rightarrow I/5.1.9) that belongs to the same family of probability distributions (\rightarrow I/1.5.1). This is fulfilled when the prior density and the likelihood function are proportional to the model parameters in the same way, i.e. the model parameters appear in the same functional form in both.

Equation (1) implies the following likelihood function (\rightarrow I/5.1.2)

$$\begin{aligned} p(y|\mu) &= \prod_{i=1}^n \mathcal{N}(y_i; \mu, \sigma^2) \\ &= \prod_{i=1}^n \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp \left[-\frac{1}{2} \left(\frac{y_i - \mu}{\sigma} \right)^2 \right] \\ &= \left(\sqrt{\frac{1}{2\pi\sigma^2}} \right)^n \cdot \exp \left[-\frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \mu)^2 \right] \end{aligned} \quad (3)$$

which, for mathematical convenience, can also be parametrized as

$$\begin{aligned} p(y|\mu) &= \prod_{i=1}^n \mathcal{N}(y_i; \mu, \tau^{-1}) \\ &= \prod_{i=1}^n \sqrt{\frac{\tau}{2\pi}} \cdot \exp \left[-\frac{\tau}{2} (y_i - \mu)^2 \right] \\ &= \left(\sqrt{\frac{\tau}{2\pi}} \right)^n \cdot \exp \left[-\frac{\tau}{2} \sum_{i=1}^n (y_i - \mu)^2 \right] \end{aligned} \quad (4)$$

using the inverse variance or precision $\tau = 1/\sigma^2$.

Expanding the product in the exponent, we have

$$\begin{aligned}
p(y|\mu) &= \left(\frac{\tau}{2\pi}\right)^{n/2} \cdot \exp \left[-\frac{\tau}{2} \sum_{i=1}^n (y_i^2 - 2\mu y_i + \mu^2) \right] \\
&= \left(\frac{\tau}{2\pi}\right)^{n/2} \cdot \exp \left[-\frac{\tau}{2} \left(\sum_{i=1}^n y_i^2 - 2\mu \sum_{i=1}^n y_i + n\mu^2 \right) \right] \\
&= \left(\frac{\tau}{2\pi}\right)^{n/2} \cdot \exp \left[-\frac{\tau}{2} (y^T y - 2\mu n\bar{y} + n\mu^2) \right] \\
&= \left(\frac{\tau}{2\pi}\right)^{n/2} \cdot \exp \left[-\frac{\tau n}{2} \left(\frac{1}{n} y^T y - 2\mu\bar{y} + \mu^2 \right) \right]
\end{aligned} \tag{5}$$

where $\bar{y} = \frac{1}{n} \sum_{i=1}^n y_i$ is the mean of data points and $y^T y = \sum_{i=1}^n y_i^2$ is the sum of squared data points. Completing the square over μ , finally gives

$$p(y|\mu) = \left(\frac{\tau}{2\pi}\right)^{n/2} \cdot \exp \left[-\frac{\tau n}{2} \left((\mu - \bar{y})^2 - \bar{y}^2 + \frac{1}{n} y^T y \right) \right] \tag{6}$$

In other words, the likelihood function (\rightarrow I/5.1.2) is proportional to an exponential of a squared form of μ , weighted by some constant:

$$p(y|\mu) \propto \exp \left[-\frac{\tau n}{2} (\mu - \bar{y})^2 \right]. \tag{7}$$

The same is true for a normal distribution (\rightarrow II/3.2.1) over μ

$$p(\mu) = \mathcal{N}(\mu; \mu_0, \lambda_0^{-1}) \tag{8}$$

the probability density function of which (\rightarrow II/3.2.10)

$$p(\mu) = \sqrt{\frac{\lambda_0}{2\pi}} \cdot \exp \left[-\frac{\lambda_0}{2} (\mu - \mu_0)^2 \right] \tag{9}$$

exhibits the same proportionality

$$p(\mu) \propto \exp \left[-\frac{\lambda_0}{2} (\mu - \mu_0)^2 \right] \tag{10}$$

and is therefore conjugate relative to the likelihood. ■

Sources:

- Bishop, Christopher M. (2006): “Bayesian inference for the Gaussian”; in: *Pattern Recognition for Machine Learning*, ch. 2.3.6, pp. 97-98, eq. 2.138; URL: <http://users.isr.ist.utl.pt/~wurmd/Livros/school/Bishop%20-%20Pattern%20Recognition%20And%20Machine%20Learning%20-%20Springer%20%202006.pdf>.

1.2.7 Posterior distribution

Theorem: Let

$$y = \{y_1, \dots, y_n\}, \quad y_i \sim \mathcal{N}(\mu, \sigma^2), \quad i = 1, \dots, n \quad (1)$$

be a univariate Gaussian data set (\rightarrow III/1.2.1) with unknown mean μ and known variance σ^2 . Moreover, assume a normal distribution (\rightarrow III/1.2.6) over the model parameter μ :

$$p(\mu) = \mathcal{N}(\mu; \mu_0, \lambda_0^{-1}) . \quad (2)$$

Then, the posterior distribution (\rightarrow I/5.1.9) is also a normal distribution (\rightarrow II/3.2.1)

$$p(\mu|y) = \mathcal{N}(\mu; \mu_n, \lambda_n^{-1}) \quad (3)$$

and the posterior hyperparameters (\rightarrow I/5.1.9) are given by

$$\begin{aligned} \mu_n &= \frac{\lambda_0 \mu_0 + \tau n \bar{y}}{\lambda_0 + \tau n} \\ \lambda_n &= \lambda_0 + \tau n \end{aligned} \quad (4)$$

with the sample mean (\rightarrow I/1.12.2) \bar{y} and the inverse variance or precision (\rightarrow I/1.13.13) $\tau = 1/\sigma^2$.

Proof: According to Bayes' theorem (\rightarrow I/5.3.2), the posterior distribution (\rightarrow I/5.1.9) is given by

$$p(\mu|y) = \frac{p(y|\mu) p(\mu)}{p(y)} . \quad (5)$$

Since $p(y)$ is just a normalization factor, the posterior is proportional (\rightarrow I/5.1.10) to the numerator:

$$p(\mu|y) \propto p(y|\mu) p(\mu) = p(y, \mu) . \quad (6)$$

Equation (1) implies the following likelihood function (\rightarrow I/5.1.2)

$$\begin{aligned} p(y|\mu) &= \prod_{i=1}^n \mathcal{N}(y_i; \mu, \sigma^2) \\ &= \prod_{i=1}^n \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp \left[-\frac{1}{2} \left(\frac{y_i - \mu}{\sigma} \right)^2 \right] \\ &= \left(\sqrt{\frac{1}{2\pi\sigma^2}} \right)^n \cdot \exp \left[-\frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \mu)^2 \right] \end{aligned} \quad (7)$$

which, for mathematical convenience, can also be parametrized as

$$\begin{aligned} p(y|\mu) &= \prod_{i=1}^n \mathcal{N}(y_i; \mu, \tau^{-1}) \\ &= \prod_{i=1}^n \sqrt{\frac{\tau}{2\pi}} \cdot \exp \left[-\frac{\tau}{2} (y_i - \mu)^2 \right] \\ &= \left(\sqrt{\frac{\tau}{2\pi}} \right)^n \cdot \exp \left[-\frac{\tau}{2} \sum_{i=1}^n (y_i - \mu)^2 \right] \end{aligned} \quad (8)$$

using the inverse variance or precision $\tau = 1/\sigma^2$.

Combining the likelihood function (\rightarrow I/5.1.2) (8) with the prior distribution (\rightarrow I/5.1.3) (2), the joint likelihood (\rightarrow I/5.1.7) of the model is given by

$$\begin{aligned} p(y, \mu) &= p(y|\mu) p(\mu) \\ &= \left(\sqrt{\frac{\tau}{2\pi}} \right)^n \cdot \exp \left[-\frac{\tau}{2} \sum_{i=1}^n (y_i - \mu)^2 \right] \cdot \sqrt{\frac{\lambda_0}{2\pi}} \cdot \exp \left[-\frac{\lambda_0}{2} (\mu - \mu_0)^2 \right] . \end{aligned} \quad (9)$$

Rearranging the terms, we then have:

$$p(y, \mu) = \left(\frac{\tau}{2\pi} \right)^{n/2} \cdot \sqrt{\frac{\lambda_0}{2\pi}} \cdot \exp \left[-\frac{\tau}{2} \sum_{i=1}^n (y_i - \mu)^2 - \frac{\lambda_0}{2} (\mu - \mu_0)^2 \right] . \quad (10)$$

Expanding the products in the exponent (\rightarrow III/1.2.6) gives

$$\begin{aligned} p(y, \mu) &= \left(\frac{\tau}{2\pi} \right)^{\frac{n}{2}} \cdot \left(\frac{\lambda_0}{2\pi} \right)^{\frac{1}{2}} \cdot \exp \left[-\frac{1}{2} \left(\sum_{i=1}^n \tau (y_i - \mu)^2 + \lambda_0 (\mu - \mu_0)^2 \right) \right] \\ &= \left(\frac{\tau}{2\pi} \right)^{\frac{n}{2}} \cdot \left(\frac{\lambda_0}{2\pi} \right)^{\frac{1}{2}} \cdot \exp \left[-\frac{1}{2} \left(\sum_{i=1}^n \tau (y_i^2 - 2y_i\mu + \mu^2) + \lambda_0 (\mu^2 - 2\mu\mu_0 + \mu_0^2) \right) \right] \\ &= \left(\frac{\tau}{2\pi} \right)^{\frac{n}{2}} \cdot \left(\frac{\lambda_0}{2\pi} \right)^{\frac{1}{2}} \cdot \exp \left[-\frac{1}{2} (\tau (y^T y - 2n\bar{y}\mu + n\mu^2) + \lambda_0 (\mu^2 - 2\mu\mu_0 + \mu_0^2)) \right] \\ &= \left(\frac{\tau}{2\pi} \right)^{\frac{n}{2}} \cdot \left(\frac{\lambda_0}{2\pi} \right)^{\frac{1}{2}} \cdot \exp \left[-\frac{1}{2} (\mu^2 (\tau n + \lambda_0) - 2\mu (\tau n\bar{y} + \lambda_0\mu_0) + (\tau y^T y + \lambda_0\mu_0^2)) \right] \end{aligned} \quad (11)$$

where $\bar{y} = \frac{1}{n} \sum_{i=1}^n y_i$ and $y^T y = \sum_{i=1}^n y_i^2$. Completing the square in μ then yields

$$p(y, \mu) = \left(\frac{\tau}{2\pi} \right)^{\frac{n}{2}} \cdot \left(\frac{\lambda_0}{2\pi} \right)^{\frac{1}{2}} \cdot \exp \left[-\frac{\lambda_n}{2} (\mu - \mu_n)^2 + f_n \right] \quad (12)$$

with the posterior hyperparameters (\rightarrow I/5.1.9)

$$\begin{aligned} \mu_n &= \frac{\lambda_0\mu_0 + \tau n\bar{y}}{\lambda_0 + \tau n} \\ \lambda_n &= \lambda_0 + \tau n \end{aligned} \quad (13)$$

and the remaining independent term

$$f_n = -\frac{1}{2} (\tau y^T y + \lambda_0\mu_0^2 - \lambda_n\mu_n^2) . \quad (14)$$

Ergo, the joint likelihood in (12) is proportional to

$$p(y, \mu) \propto \exp \left[-\frac{\lambda_n}{2} (\mu - \mu_n)^2 \right] , \quad (15)$$

such that the posterior distribution over μ is given by

$$p(\mu|y) = \mathcal{N}(\mu; \mu_n, \lambda_n^{-1}) . \quad (16)$$

with the posterior hyperparameters given in (13). ■

Sources:

- Bishop, Christopher M. (2006): “Bayesian inference for the Gaussian”; in: *Pattern Recognition for Machine Learning*, ch. 2.3.6, p. 98, eqs. 2.139-2.142; URL: <http://users.isr.ist.utl.pt/~wurmd/Livros/school/Bishop%20-%20Pattern%20Recognition%20And%20Machine%20Learning%20-%20Springer%202006.pdf>.

1.2.8 Log model evidence

Theorem: Let

$$m : y = \{y_1, \dots, y_n\}, \quad y_i \sim \mathcal{N}(\mu, \sigma^2), \quad i = 1, \dots, n \quad (1)$$

be a univariate Gaussian data set (\rightarrow III/1.2.1) with unknown mean μ and known variance σ^2 . Moreover, assume a normal distribution (\rightarrow III/1.2.6) over the model parameter μ :

$$p(\mu) = \mathcal{N}(\mu; \mu_0, \lambda_0^{-1}) . \quad (2)$$

Then, the log model evidence (\rightarrow IV/3.1.3) for this model is

$$\log p(y|m) = \frac{n}{2} \log \left(\frac{\tau}{2\pi} \right) + \frac{1}{2} \log \left(\frac{\lambda_0}{\lambda_n} \right) - \frac{1}{2} (\tau y^T y + \lambda_0 \mu_0^2 - \lambda_n \mu_n^2) . \quad (3)$$

where the posterior hyperparameters (\rightarrow I/5.1.9) are given by

$$\begin{aligned} \mu_n &= \frac{\lambda_0 \mu_0 + \tau n \bar{y}}{\lambda_0 + \tau n} \\ \lambda_n &= \lambda_0 + \tau n \end{aligned} \quad (4)$$

with the sample mean (\rightarrow I/1.12.2) \bar{y} and the inverse variance or precision (\rightarrow I/1.13.13) $\tau = 1/\sigma^2$.

Proof: According to the law of marginal probability (\rightarrow I/1.3.3), the model evidence (\rightarrow I/5.1.15) for this model is:

$$p(y|m) = \int p(y|\mu) p(\mu) d\mu . \quad (5)$$

According to the law of conditional probability (\rightarrow I/1.3.4), the integrand is equivalent to the joint likelihood (\rightarrow I/5.1.7):

$$p(y|m) = \int p(y, \mu) d\mu . \quad (6)$$

Equation (1) implies the following likelihood function (\rightarrow I/5.1.2)

$$\begin{aligned}
p(y|\mu, \sigma^2) &= \prod_{i=1}^n \mathcal{N}(y_i; \mu, \sigma^2) \\
&= \prod_{i=1}^n \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp \left[-\frac{1}{2} \left(\frac{y_i - \mu}{\sigma} \right)^2 \right] \\
&= \left(\sqrt{\frac{1}{2\pi\sigma^2}} \right)^n \cdot \exp \left[-\frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \mu)^2 \right]
\end{aligned} \tag{7}$$

which, for mathematical convenience, can also be parametrized as

$$\begin{aligned}
p(y|\mu, \tau) &= \prod_{i=1}^n \mathcal{N}(y_i; \mu, \tau^{-1}) \\
&= \prod_{i=1}^n \sqrt{\frac{\tau}{2\pi}} \cdot \exp \left[-\frac{\tau}{2} (y_i - \mu)^2 \right] \\
&= \left(\sqrt{\frac{\tau}{2\pi}} \right)^n \cdot \exp \left[-\frac{\tau}{2} \sum_{i=1}^n (y_i - \mu)^2 \right]
\end{aligned} \tag{8}$$

using the inverse variance or precision $\tau = 1/\sigma^2$.

When deriving the posterior distribution (\rightarrow III/1.2.7) $p(\mu|y)$, the joint likelihood $p(y, \mu)$ is obtained as

$$\begin{aligned}
p(y, \mu) &= p(y|\mu) p(\mu) \\
&= \left(\frac{\tau}{2\pi} \right)^{\frac{n}{2}} \cdot \exp \left[-\frac{\tau}{2} \sum_{i=1}^n (y_i - \mu)^2 \right] \cdot \sqrt{\frac{\lambda_0}{2\pi}} \cdot \exp \left[-\frac{\lambda_0}{2} (\mu - \mu_0)^2 \right] \\
&= \left(\frac{\tau}{2\pi} \right)^{\frac{n}{2}} \cdot \sqrt{\frac{\lambda_0}{2\pi}} \cdot \exp \left[-\frac{\lambda_0}{2} (\mu^2 - 2\mu\mu_0 + \mu_0^2) - \frac{\tau}{2} (y^T y - 2\mu n\bar{y} + n\mu^2) \right] \\
&= \left(\frac{\tau}{2\pi} \right)^{\frac{n}{2}} \cdot \sqrt{\frac{\lambda_0}{2\pi}} \cdot \exp \left[-\frac{1}{2} (\mu^2(\lambda_0 + \tau n) - 2\mu(\lambda_0\mu_0 + \tau n\bar{y}) + \lambda_0\mu_0^2 + \tau y^T y) \right] \\
&= \left(\frac{\tau}{2\pi} \right)^{\frac{n}{2}} \cdot \sqrt{\frac{\lambda_0}{2\pi}} \cdot \exp \left[-\frac{\lambda_0 + \tau n}{2} (\mu^2 - 2\mu\mu_n + \mu_n^2) - \frac{1}{2} (\tau y^T y + \lambda_0\mu_0^2 - (\lambda_0 + \tau n)\mu_n^2) \right] \\
&= \left(\frac{\tau}{2\pi} \right)^{\frac{n}{2}} \cdot \sqrt{\frac{\lambda_0}{2\pi}} \cdot \exp \left[-\frac{\lambda_n}{2} (\mu - \mu_n)^2 - \frac{1}{2} (\tau y^T y + \lambda_0\mu_0^2 - \lambda_n\mu_n^2) \right].
\end{aligned} \tag{9}$$

Using the probability density function of the normal distribution (\rightarrow II/3.2.10), we can rewrite this as

$$p(y, \mu) = \left(\frac{\tau}{2\pi} \right)^{\frac{n}{2}} \cdot \sqrt{\frac{\lambda_0}{2\pi}} \cdot \sqrt{\frac{2\pi}{\lambda_n}} \cdot \mathcal{N}(\mu; \mu_n, \lambda_n^{-1}) \cdot \exp \left[-\frac{1}{2} (\tau y^T y + \lambda_0\mu_0^2 - \lambda_n\mu_n^2) \right]. \tag{10}$$

Now, μ can be integrated out using the properties of the probability density function (\rightarrow I/1.7.1):

$$p(y|m) = \int p(y, \mu) d\mu = \left(\frac{\tau}{2\pi}\right)^{\frac{n}{2}} \cdot \sqrt{\frac{\lambda_0}{\lambda_n}} \cdot \exp \left[-\frac{1}{2} (\tau y^T y + \lambda_0 \mu_0^2 - \lambda_n \mu_n^2) \right] . \quad (11)$$

Thus, the log model evidence (\rightarrow IV/3.1.3) of this model is given by

$$\log p(y|m) = \frac{n}{2} \log \left(\frac{\tau}{2\pi} \right) + \frac{1}{2} \log \left(\frac{\lambda_0}{\lambda_n} \right) - \frac{1}{2} (\tau y^T y + \lambda_0 \mu_0^2 - \lambda_n \mu_n^2) . \quad (12)$$

■

1.2.9 Accuracy and complexity

Theorem: Let

$$y = \{y_1, \dots, y_n\}, \quad y_i \sim \mathcal{N}(\mu, \sigma^2), \quad i = 1, \dots, n \quad (1)$$

be a univariate Gaussian data set (\rightarrow III/1.2.1) with unknown mean μ and known variance σ^2 . Moreover, assume a statistical model (\rightarrow I/5.1.6) imposing a normal distribution (\rightarrow III/1.2.6) as the prior distribution (\rightarrow I/5.1.3) on the model parameter μ :

$$m : y_i \sim \mathcal{N}(\mu, \sigma^2), \quad \mu \sim \mathcal{N}(\mu_0, \lambda_0^{-1}) . \quad (2)$$

Then, accuracy and complexity (\rightarrow IV/3.1.6) of this model are

$$\begin{aligned} \text{Acc}(m) &= \frac{n}{2} \log \left(\frac{\tau}{2\pi} \right) - \frac{1}{2} \left[\tau y^T y - 2\tau n \bar{y} \mu_n + \tau n \mu_n^2 + \frac{\tau n}{\lambda_n} \right] \\ \text{Com}(m) &= \frac{1}{2} \left[\frac{\lambda_0}{\lambda_n} + \lambda_0 (\mu_0 - \mu_n)^2 - 1 + \log \left(\frac{\lambda_0}{\lambda_n} \right) \right] \end{aligned} \quad (3)$$

where μ_n and λ_n are the posterior hyperparameters for the univariate Gaussian with known variance (\rightarrow III/1.2.7), $\tau = 1/\sigma^2$ is the inverse variance or precision (\rightarrow I/1.13.13) and \bar{y} is the sample mean (\rightarrow I/1.12.2).

Proof: Model accuracy and complexity are defined as (\rightarrow IV/3.1.6)

$$\begin{aligned} \text{LME}(m) &= \text{Acc}(m) - \text{Com}(m) \\ \text{Acc}(m) &= \langle \log p(y|\mu, m) \rangle_{p(\mu|y, m)} \\ \text{Com}(m) &= \text{KL} [p(\mu|y, m) || p(\mu|m)] . \end{aligned} \quad (4)$$

The accuracy term is the expectation (\rightarrow I/1.12.1) of the log-likelihood function (\rightarrow I/4.1.2) $\log p(y|\mu)$ with respect to the posterior distribution (\rightarrow I/5.1.9) $p(\mu|y)$. With the log-likelihood function for the univariate Gaussian with known variance (\rightarrow III/1.2.2) and the posterior distribution for the univariate Gaussian with known variance (\rightarrow III/1.2.7), the model accuracy of m evaluates to:

$$\begin{aligned} \text{Acc}(m) &= \langle \log p(y|\mu) \rangle_{p(\mu|y)} \\ &= \left\langle \frac{n}{2} \log \left(\frac{\tau}{2\pi} \right) - \frac{\tau}{2} (y^T y - 2n \bar{y} \mu + n \mu^2) \right\rangle_{\mathcal{N}(\mu_n, \lambda_n^{-1})} \\ &= \frac{n}{2} \log \left(\frac{\tau}{2\pi} \right) - \frac{1}{2} \left[\tau y^T y - 2\tau n \bar{y} \mu_n + \tau n \mu_n^2 + \frac{\tau n}{\lambda_n} \right] . \end{aligned} \quad (5)$$

The complexity penalty is the Kullback-Leibler divergence (\rightarrow I/2.5.1) of the posterior distribution (\rightarrow I/5.1.9) $p(\mu|y)$ from the prior distribution (\rightarrow I/5.1.3) $p(\mu)$. With the prior distribution (\rightarrow III/1.2.6) given by (2), the posterior distribution for the univariate Gaussian with known variance (\rightarrow III/1.2.7) and the Kullback-Leibler divergence of the normal distribution (\rightarrow II/3.2.24), the model complexity of m evaluates to:

$$\begin{aligned} \text{Com}(m) &= \text{KL} [p(\mu|y) || p(\mu)] \\ &= \text{KL} [\mathcal{N}(\mu_n, \lambda_n^{-1}) || \mathcal{N}(\mu_0, \lambda_0^{-1})] \\ &= \frac{1}{2} \left[\frac{\lambda_0}{\lambda_n} + \lambda_0(\mu_0 - \mu_n)^2 - 1 + \log \left(\frac{\lambda_0}{\lambda_n} \right) \right] . \end{aligned} \quad (6)$$

A control calculation confirms that

$$\text{Acc}(m) - \text{Com}(m) = \text{LME}(m) \quad (7)$$

where $\text{LME}(m)$ is the log model evidence for the univariate Gaussian with known variance (\rightarrow III/1.2.8). ■

1.2.10 Log Bayes factor

Theorem: Let

$$y = \{y_1, \dots, y_n\}, \quad y_i \sim \mathcal{N}(\mu, \sigma^2), \quad i = 1, \dots, n \quad (1)$$

be a univariate Gaussian data set (\rightarrow III/1.2.1) with unknown mean μ and known variance σ^2 . Moreover, assume two statistical models (\rightarrow I/5.1.6), one assuming that μ is zero (null model (\rightarrow I/4.3.2)), the other imposing a normal distribution (\rightarrow III/1.2.6) as the prior distribution (\rightarrow I/5.1.3) on the model parameter μ (alternative (\rightarrow I/4.3.3)):

$$\begin{aligned} m_0 : y_i &\sim \mathcal{N}(\mu, \sigma^2), \quad \mu = 0 \\ m_1 : y_i &\sim \mathcal{N}(\mu, \sigma^2), \quad \mu \sim \mathcal{N}(\mu_0, \lambda_0^{-1}) . \end{aligned} \quad (2)$$

Then, the log Bayes factor (\rightarrow IV/3.3.6) in favor of m_1 against m_0 is

$$\text{LBF}_{10} = \frac{1}{2} \log \left(\frac{\lambda_0}{\lambda_n} \right) - \frac{1}{2} (\lambda_0 \mu_0^2 - \lambda_n \mu_n^2) \quad (3)$$

where μ_n and λ_n are the posterior hyperparameters for the univariate Gaussian with known variance (\rightarrow III/1.2.7) which are functions of the inverse variance or precision (\rightarrow I/1.13.13) $\tau = 1/\sigma^2$ and the sample mean (\rightarrow I/1.12.2) \bar{y} .

Proof: The log Bayes factor is equal to the difference of two log model evidences (\rightarrow IV/3.3.8):

$$\text{LBF}_{12} = \text{LME}(m_1) - \text{LME}(m_2) . \quad (4)$$

The LME of the alternative m_1 is equal to the log model evidence for the univariate Gaussian with known variance (\rightarrow III/1.2.8):

$$\text{LME}(m_1) = \log p(y|m_1) = \frac{n}{2} \log \left(\frac{\tau}{2\pi} \right) + \frac{1}{2} \log \left(\frac{\lambda_0}{\lambda_n} \right) - \frac{1}{2} (\tau y^T y + \lambda_0 \mu_0^2 - \lambda_n \mu_n^2) . \quad (5)$$

Because the null model m_0 has no free parameter, its log model evidence (\rightarrow IV/3.1.3) (logarithmized marginal likelihood (\rightarrow I/5.1.15)) is equal to the log-likelihood function for the univariate Gaussian with known variance (\rightarrow III/1.2.2) at the value $\mu = 0$:

$$\text{LME}(m_0) = \log p(y|\mu = 0) = \frac{n}{2} \log \left(\frac{\tau}{2\pi} \right) - \frac{1}{2} (\tau y^T y) . \quad (6)$$

Subtracting the two LMEs from each other, the LBF emerges as

$$\text{LBF}_{10} = \text{LME}(m_1) - \text{LME}(m_0) = \frac{1}{2} \log \left(\frac{\lambda_0}{\lambda_n} \right) - \frac{1}{2} (\lambda_0 \mu_0^2 - \lambda_n \mu_n^2) \quad (7)$$

where the posterior hyperparameters (\rightarrow I/5.1.9) are given by (\rightarrow III/1.2.7)

$$\begin{aligned} \mu_n &= \frac{\lambda_0 \mu_0 + \tau n \bar{y}}{\lambda_0 + \tau n} \\ \lambda_n &= \lambda_0 + \tau n \end{aligned} \quad (8)$$

with the sample mean (\rightarrow I/1.12.2) \bar{y} and the inverse variance or precision (\rightarrow I/1.13.13) $\tau = 1/\sigma^2$. ■

1.2.11 Expectation of log Bayes factor

Theorem: Let

$$y = \{y_1, \dots, y_n\}, \quad y_i \sim \mathcal{N}(\mu, \sigma^2), \quad i = 1, \dots, n \quad (1)$$

be a univariate Gaussian data set (\rightarrow III/1.2.1) with unknown mean μ and known variance σ^2 . Moreover, assume two statistical models (\rightarrow I/5.1.6), one assuming that μ is zero (null model (\rightarrow I/4.3.2)), the other imposing a normal distribution (\rightarrow III/1.2.6) as the prior distribution (\rightarrow I/5.1.3) on the model parameter μ (alternative (\rightarrow I/4.3.3)):

$$\begin{aligned} m_0 : y_i &\sim \mathcal{N}(\mu, \sigma^2), \quad \mu = 0 \\ m_1 : y_i &\sim \mathcal{N}(\mu, \sigma^2), \quad \mu \sim \mathcal{N}(\mu_0, \lambda_0^{-1}) . \end{aligned} \quad (2)$$

Then, under the null hypothesis (\rightarrow I/4.3.2) that m_0 generated the data, the expectation (\rightarrow I/1.12.1) of the log Bayes factor (\rightarrow IV/3.3.6) in favor of m_1 with $\mu_0 = 0$ against m_0 is

$$\langle \text{LBF}_{10} \rangle = \frac{1}{2} \log \left(\frac{\lambda_0}{\lambda_n} \right) + \frac{1}{2} \left(\frac{\lambda_n - \lambda_0}{\lambda_n} \right) \quad (3)$$

where λ_n is the posterior precision for the univariate Gaussian with known variance (\rightarrow III/1.2.7).

Proof: The log Bayes factor for the univariate Gaussian with known variance (\rightarrow III/1.2.10) is

$$\text{LBF}_{10} = \frac{1}{2} \log \left(\frac{\lambda_0}{\lambda_n} \right) - \frac{1}{2} (\lambda_0 \mu_0^2 - \lambda_n \mu_n^2) \quad (4)$$

where the posterior hyperparameters (\rightarrow I/5.1.9) are given by (\rightarrow III/1.2.7)

$$\begin{aligned}\mu_n &= \frac{\lambda_0 \mu_0 + \tau n \bar{y}}{\lambda_0 + \tau n} \\ \lambda_n &= \lambda_0 + \tau n\end{aligned}\tag{5}$$

with the sample mean (\rightarrow I/1.12.2) \bar{y} and the inverse variance or precision (\rightarrow I/1.13.13) $\tau = 1/\sigma^2$. Plugging μ_n from (5) into (4), we obtain:

$$\begin{aligned}\text{LBF}_{10} &= \frac{1}{2} \log \left(\frac{\lambda_0}{\lambda_n} \right) - \frac{1}{2} \left(\lambda_0 \mu_0^2 - \lambda_n \frac{(\lambda_0 \mu_0 + \tau n \bar{y})^2}{\lambda_n^2} \right) \\ &= \frac{1}{2} \log \left(\frac{\lambda_0}{\lambda_n} \right) - \frac{1}{2} \left(\lambda_0 \mu_0^2 - \frac{1}{\lambda_n} (\lambda_0^2 \mu_0^2 - 2\tau n \lambda_0 \mu_0 \bar{y} + \tau^2 (n \bar{y})^2) \right)\end{aligned}\tag{6}$$

Because m_1 uses a zero-mean prior distribution (\rightarrow I/5.1.3) with prior mean (\rightarrow I/1.12.1) $\mu_0 = 0$ per construction, the log Bayes factor simplifies to:

$$\text{LBF}_{10} = \frac{1}{2} \log \left(\frac{\lambda_0}{\lambda_n} \right) + \frac{1}{2} \left(\frac{\tau^2 (n \bar{y})^2}{\lambda_n} \right).\tag{7}$$

From (1), we know that the data are distributed as $y_i \sim \mathcal{N}(\mu, \sigma^2)$, such that we can derive the expectation (\rightarrow I/1.12.1) of $(n \bar{y})^2$ as follows:

$$\begin{aligned}\langle (n \bar{y})^2 \rangle &= \left\langle \sum_{i=1}^n \sum_{j=1}^n y_i y_j \right\rangle = \langle n y_i^2 + (n^2 - n) [y_i y_j]_{i \neq j} \rangle \\ &= n(\mu^2 + \sigma^2) + (n^2 - n) \mu^2 \\ &= n^2 \mu^2 + n \sigma^2.\end{aligned}\tag{8}$$

Applying this expected value (\rightarrow I/1.12.1) to (7), the expected LBF emerges as:

$$\begin{aligned}\langle \text{LBF}_{10} \rangle &= \frac{1}{2} \log \left(\frac{\lambda_0}{\lambda_n} \right) + \frac{1}{2} \left(\frac{\tau^2 (n^2 \mu^2 + n \sigma^2)}{\lambda_n} \right) \\ &= \frac{1}{2} \log \left(\frac{\lambda_0}{\lambda_n} \right) + \frac{1}{2} \left(\frac{(\tau n \mu)^2 + \tau n}{\lambda_n} \right)\end{aligned}\tag{9}$$

Under the null hypothesis (\rightarrow I/4.3.2) that m_0 generated the data, the unknown mean is $\mu = 0$, such that the log Bayes factor further simplifies to:

$$\langle \text{LBF}_{10} \rangle = \frac{1}{2} \log \left(\frac{\lambda_0}{\lambda_n} \right) + \frac{1}{2} \left(\frac{\tau n}{\lambda_n} \right).\tag{10}$$

Finally, plugging λ_n from (5) into (10), we obtain:

$$\langle \text{LBF}_{10} \rangle = \frac{1}{2} \log \left(\frac{\lambda_0}{\lambda_n} \right) + \frac{1}{2} \left(\frac{\lambda_n - \lambda_0}{\lambda_n} \right).\tag{11}$$

■

1.2.12 Cross-validated log model evidence

Theorem: Let

$$y = \{y_1, \dots, y_n\}, \quad y_i \sim \mathcal{N}(\mu, \sigma^2), \quad i = 1, \dots, n \quad (1)$$

be a univariate Gaussian data set (\rightarrow III/1.2.1) with unknown mean μ and known variance σ^2 . Moreover, assume two statistical models (\rightarrow I/5.1.6), one assuming that μ is zero (null model (\rightarrow I/4.3.2)), the other imposing a normal distribution (\rightarrow III/1.2.6) as the prior distribution (\rightarrow I/5.1.3) on the model parameter μ (alternative (\rightarrow I/4.3.3)):

$$\begin{aligned} m_0 : y_i &\sim \mathcal{N}(\mu, \sigma^2), \quad \mu = 0 \\ m_1 : y_i &\sim \mathcal{N}(\mu, \sigma^2), \quad \mu \sim \mathcal{N}(\mu_0, \lambda_0^{-1}) . \end{aligned} \quad (2)$$

Then, the cross-validated log model evidences (\rightarrow IV/3.1.9) of m_0 and m_1 are

$$\begin{aligned} \text{cvLME}(m_0) &= \frac{n}{2} \log \left(\frac{\tau}{2\pi} \right) - \frac{1}{2} (\tau y^T y) \\ \text{cvLME}(m_1) &= \frac{n}{2} \log \left(\frac{\tau}{2\pi} \right) + \frac{S}{2} \log \left(\frac{S-1}{S} \right) - \frac{\tau}{2} \left[y^T y + \sum_{i=1}^S \left(\frac{(n_1 \bar{y}_1^{(i)})^2}{n_1} - \frac{(n\bar{y})^2}{n} \right) \right] \end{aligned} \quad (3)$$

where \bar{y} is the sample mean (\rightarrow I/1.12.2), $\tau = 1/\sigma^2$ is the inverse variance or precision (\rightarrow I/1.13.13), $y_1^{(i)}$ are the training data in the i -th cross-validation fold with n_1 data points and S is the number of data subsets (\rightarrow IV/3.1.9).

Proof: For evaluation of the cross-validated log model evidences (\rightarrow IV/3.1.9) (cvLME), we assume that n data points are divided into $S \mid n$ data subsets without remainder. Then, the number of training data points n_1 and test data points n_2 are given by

$$\begin{aligned} n &= n_1 + n_2 \\ n_1 &= \frac{S-1}{S} n \\ n_2 &= \frac{1}{S} n , \end{aligned} \quad (4)$$

such that training data y_1 and test data y_2 in the i -th cross-validation fold are

$$\begin{aligned} y &= \{y_1, \dots, y_n\} \\ y_1^{(i)} &= \{x \in y \mid x \notin y_2^{(i)}\} = y \setminus y_2^{(i)} \\ y_2^{(i)} &= \{y_{(i-1) \cdot n_2 + 1}, \dots, y_{i \cdot n_2}\} . \end{aligned} \quad (5)$$

First, we consider the null model m_0 assuming $\mu = 0$. Because this model has no free parameter, nothing is estimated from the training data and the assumed parameter value is applied to the test data. Consequently, the out-of-sample log model evidence (\rightarrow IV/3.1.9) (oosLME) is equal to the log-likelihood function (\rightarrow III/1.2.2) of the test data at $\mu = 0$:

$$\text{oosLME}_i(m_0) = \log p\left(y_2^{(i)} \mid \mu = 0\right) = \frac{n_2}{2} \log\left(\frac{\tau}{2\pi}\right) - \frac{1}{2} \left[\tau y_2^{(i)\text{T}} y_2^{(i)} \right] . \quad (6)$$

By definition, the cross-validated log model evidence is the sum of out-of-sample log model evidences (\rightarrow IV/3.1.9) over cross-validation folds, such that the cvLME of m_0 is:

$$\begin{aligned} \text{cvLME}(m_0) &= \sum_{i=1}^S \text{oosLME}_i(m_0) \\ &= \sum_{i=1}^S \left(\frac{n_2}{2} \log\left(\frac{\tau}{2\pi}\right) - \frac{1}{2} \left[\tau y_2^{(i)\text{T}} y_2^{(i)} \right] \right) \\ &= \frac{n}{2} \log\left(\frac{\tau}{2\pi}\right) - \frac{1}{2} [\tau y^{\text{T}} y] . \end{aligned} \quad (7)$$

Next, we have a look at the alternative m_1 assuming $\mu \neq 0$. First, the training data $y_1^{(i)}$ are analyzed using a non-informative prior distribution (\rightarrow I/5.2.3) and applying the posterior distribution for the univariate Gaussian with known variance (\rightarrow III/1.2.7):

$$\begin{aligned} \mu_0^{(1)} &= 0 \\ \lambda_0^{(1)} &= 0 \\ \mu_n^{(1)} &= \frac{\tau n_1 \bar{y}_1^{(i)} + \lambda_0^{(1)} \mu_0^{(1)}}{\tau n_1 + \lambda_0^{(1)}} = \bar{y}_1^{(i)} \\ \lambda_n^{(1)} &= \tau n_1 + \lambda_0^{(1)} = \tau n_1 . \end{aligned} \quad (8)$$

This results in a posterior characterized by $\mu_n^{(1)}$ and $\lambda_n^{(1)}$. Then, the test data $y_2^{(i)}$ are analyzed using this posterior as an informative prior distribution (\rightarrow I/5.2.3), again applying the posterior distribution for the univariate Gaussian with known variance (\rightarrow III/1.2.7):

$$\begin{aligned} \mu_0^{(2)} &= \mu_n^{(1)} = \bar{y}_1^{(i)} \\ \lambda_0^{(2)} &= \lambda_n^{(1)} = \tau n_1 \\ \mu_n^{(2)} &= \frac{\tau n_2 \bar{y}_2^{(i)} + \lambda_0^{(2)} \mu_0^{(2)}}{\tau n_2 + \lambda_0^{(2)}} = \bar{y} \\ \lambda_n^{(2)} &= \tau n_2 + \lambda_0^{(2)} = \tau n . \end{aligned} \quad (9)$$

In the test data, we now have a prior characterized by $\mu_0^{(2)}/\lambda_0^{(2)}$ and a posterior characterized $\mu_n^{(2)}/\lambda_n^{(2)}$. Applying the log model evidence for the univariate Gaussian with known variance (\rightarrow III/1.2.8), the out-of-sample log model evidence (\rightarrow IV/3.1.9) (oosLME) therefore follows as

$$\begin{aligned} \text{oosLME}_i(m_1) &= \frac{n_2}{2} \log\left(\frac{\tau}{2\pi}\right) + \frac{1}{2} \log\left(\frac{\lambda_0^{(2)}}{\lambda_n^{(2)}}\right) - \frac{1}{2} \left[\tau y_2^{(i)\text{T}} y_2^{(i)} + \lambda_0^{(2)} \mu_0^{(2)2} - \lambda_n^{(2)} \mu_n^{(2)2} \right] \\ &= \frac{n_2}{2} \log\left(\frac{\tau}{2\pi}\right) + \frac{1}{2} \log\left(\frac{n_1}{n}\right) - \frac{1}{2} \left[\tau y_2^{(i)\text{T}} y_2^{(i)} + \frac{\tau}{n_1} \left(n_1 \bar{y}_1^{(i)} \right)^2 - \frac{\tau}{n} (n \bar{y})^2 \right] . \end{aligned} \quad (10)$$

Again, because the cross-validated log model evidence is the sum of out-of-sample log model evidences (\rightarrow IV/3.1.9) over cross-validation folds, the cvLME of m_1 becomes:

$$\begin{aligned}
 \text{cvLME}(m_1) &= \sum_{i=1}^S \text{oosLME}_i(m_1) \\
 &= \sum_{i=1}^S \left(\frac{n_2}{2} \log \left(\frac{\tau}{2\pi} \right) + \frac{1}{2} \log \left(\frac{n_1}{n} \right) - \frac{1}{2} \left[\tau y_2^{(i)\text{T}} y_2^{(i)} + \frac{\tau}{n_1} \left(n_1 \bar{y}_1^{(i)} \right)^2 - \frac{\tau}{n} (n\bar{y})^2 \right] \right) \\
 &= \frac{S \cdot n_2}{2} \log \left(\frac{\tau}{2\pi} \right) + \frac{S}{2} \log \left(\frac{n_1}{n} \right) - \frac{\tau}{2} \sum_{i=1}^S \left[y_2^{(i)\text{T}} y_2^{(i)} + \frac{\left(n_1 \bar{y}_1^{(i)} \right)^2}{n_1} - \frac{(n\bar{y})^2}{n} \right] \\
 &= \frac{n}{2} \log \left(\frac{\tau}{2\pi} \right) + \frac{S}{2} \log \left(\frac{S-1}{S} \right) - \frac{\tau}{2} \left[y^{\text{T}} y + \sum_{i=1}^S \left(\frac{\left(n_1 \bar{y}_1^{(i)} \right)^2}{n_1} - \frac{(n\bar{y})^2}{n} \right) \right].
 \end{aligned} \tag{11}$$

Together, (7) and (11) conform to the results given in (3). ■

1.2.13 Cross-validated log Bayes factor

Theorem: Let

$$y = \{y_1, \dots, y_n\}, \quad y_i \sim \mathcal{N}(\mu, \sigma^2), \quad i = 1, \dots, n \tag{1}$$

be a univariate Gaussian data set (\rightarrow III/1.2.1) with unknown mean μ and known variance σ^2 . Moreover, assume two statistical models (\rightarrow I/5.1.6), one assuming that μ is zero (null model (\rightarrow I/4.3.2)), the other imposing a normal distribution (\rightarrow III/1.2.6) as the prior distribution (\rightarrow I/5.1.3) on the model parameter μ (alternative (\rightarrow I/4.3.3)):

$$\begin{aligned}
 m_0 : y_i &\sim \mathcal{N}(\mu, \sigma^2), \quad \mu = 0 \\
 m_1 : y_i &\sim \mathcal{N}(\mu, \sigma^2), \quad \mu \sim \mathcal{N}(\mu_0, \lambda_0^{-1}).
 \end{aligned} \tag{2}$$

Then, the cross-validated (\rightarrow IV/3.1.9) log Bayes factor (\rightarrow IV/3.3.6) in favor of m_1 against m_0 is

$$\text{cvLBF}_{10} = \frac{S}{2} \log \left(\frac{S-1}{S} \right) - \frac{\tau}{2} \sum_{i=1}^S \left(\frac{\left(n_1 \bar{y}_1^{(i)} \right)^2}{n_1} - \frac{(n\bar{y})^2}{n} \right) \tag{3}$$

where \bar{y} is the sample mean (\rightarrow I/1.12.2), $\tau = 1/\sigma^2$ is the inverse variance or precision (\rightarrow I/1.13.13), $y_1^{(i)}$ are the training data in the i -th cross-validation fold with n_1 data points and S is the number of data subsets (\rightarrow IV/3.1.9).

Proof: The relationship between log Bayes factor and log model evidences (\rightarrow IV/3.3.8) also holds for cross-validated log bayes factor (\rightarrow IV/3.3.6) (cvLBF) and cross-validated log model evidences (\rightarrow IV/3.1.9) (cvLME):

$$\text{cvLBF}_{12} = \text{cvLME}(m_1) - \text{cvLME}(m_2) . \quad (4)$$

The cross-validated log model evidences (\rightarrow IV/3.1.9) of m_0 and m_1 are given by (\rightarrow III/1.2.12)

$$\begin{aligned} \text{cvLME}(m_0) &= \frac{n}{2} \log \left(\frac{\tau}{2\pi} \right) - \frac{1}{2} (\tau y^T y) \\ \text{cvLME}(m_1) &= \frac{n}{2} \log \left(\frac{\tau}{2\pi} \right) + \frac{S}{2} \log \left(\frac{S-1}{S} \right) - \frac{\tau}{2} \left[y^T y + \sum_{i=1}^S \left(\frac{(n_1 \bar{y}_1^{(i)})^2}{n_1} - \frac{(n\bar{y})^2}{n} \right) \right] . \end{aligned} \quad (5)$$

Subtracting the two cvLMEs from each other, the cvLBF emerges as

$$\begin{aligned} \text{cvLBF}_{10} &= \text{cvLME}(m_1) - \text{LME}(m_0) \\ &= \left(\frac{n}{2} \log \left(\frac{\tau}{2\pi} \right) + \frac{S}{2} \log \left(\frac{S-1}{S} \right) - \frac{\tau}{2} \left[y^T y + \sum_{i=1}^S \left(\frac{(n_1 \bar{y}_1^{(i)})^2}{n_1} - \frac{(n\bar{y})^2}{n} \right) \right] \right) \\ &\quad - \left(\frac{n}{2} \log \left(\frac{\tau}{2\pi} \right) - \frac{1}{2} (\tau y^T y) \right) \\ &= \frac{S}{2} \log \left(\frac{S-1}{S} \right) - \frac{\tau}{2} \sum_{i=1}^S \left(\frac{(n_1 \bar{y}_1^{(i)})^2}{n_1} - \frac{(n\bar{y})^2}{n} \right) . \end{aligned} \quad (6)$$

■

1.2.14 Expectation of cross-validated log Bayes factor

Theorem: Let

$$y = \{y_1, \dots, y_n\}, \quad y_i \sim \mathcal{N}(\mu, \sigma^2), \quad i = 1, \dots, n \quad (1)$$

be a univariate Gaussian data set (\rightarrow III/1.2.1) with unknown mean μ and known variance σ^2 . Moreover, assume two statistical models (\rightarrow I/5.1.6), one assuming that μ is zero (null model (\rightarrow I/4.3.2)), the other imposing a normal distribution (\rightarrow III/1.2.6) as the prior distribution (\rightarrow I/5.1.3) on the model parameter μ (alternative (\rightarrow I/4.3.3)):

$$\begin{aligned} m_0 : y_i &\sim \mathcal{N}(\mu, \sigma^2), \quad \mu = 0 \\ m_1 : y_i &\sim \mathcal{N}(\mu, \sigma^2), \quad \mu \sim \mathcal{N}(\mu_0, \lambda_0^{-1}) . \end{aligned} \quad (2)$$

Then, the expectation (\rightarrow I/1.12.1) of the cross-validated (\rightarrow IV/3.1.9) log Bayes factor (\rightarrow IV/3.3.6) (cvLBF) in favor of m_1 against m_0 is

$$\langle \text{cvLBF}_{10} \rangle = \frac{S}{2} \log \left(\frac{S-1}{S} \right) + \frac{1}{2} [\tau n \mu^2] \quad (3)$$

where $\tau = 1/\sigma^2$ is the inverse variance or precision (\rightarrow I/1.13.13) and S is the number of data subsets (\rightarrow IV/3.1.9).

Proof: The cross-validated log Bayes factor for the univariate Gaussian with known variance (\rightarrow III/1.2.13) is

$$\text{cvLBF}_{10} = \frac{S}{2} \log \left(\frac{S-1}{S} \right) - \frac{\tau}{2} \sum_{i=1}^S \left(\frac{(n_1 \bar{y}_1^{(i)})^2}{n_1} - \frac{(n\bar{y})^2}{n} \right) \quad (4)$$

From (1), we know that the data are distributed as $y_i \sim \mathcal{N}(\mu, \sigma^2)$, such that we can derive the expectation (\rightarrow I/1.12.1) of $(n\bar{y})^2$ and $(n_1 \bar{y}_1^{(i)})^2$ as follows:

$$\begin{aligned} \langle (n\bar{y})^2 \rangle &= \left\langle \sum_{i=1}^n \sum_{j=1}^n y_i y_j \right\rangle = \langle n y_i^2 + (n^2 - n) [y_i y_j]_{i \neq j} \rangle \\ &= n(\mu^2 + \sigma^2) + (n^2 - n)\mu^2 \\ &= n^2 \mu^2 + n\sigma^2. \end{aligned} \quad (5)$$

Applying this expected value (\rightarrow I/1.12.1) to (4), the expected cvLBF emerges as:

$$\begin{aligned} \langle \text{cvLBF}_{10} \rangle &= \left\langle \frac{S}{2} \log \left(\frac{S-1}{S} \right) - \frac{\tau}{2} \sum_{i=1}^S \left(\frac{(n_1 \bar{y}_1^{(i)})^2}{n_1} - \frac{(n\bar{y})^2}{n} \right) \right\rangle \\ &= \frac{S}{2} \log \left(\frac{S-1}{S} \right) - \frac{\tau}{2} \sum_{i=1}^S \left(\frac{\langle (n_1 \bar{y}_1^{(i)})^2 \rangle}{n_1} - \frac{\langle (n\bar{y})^2 \rangle}{n} \right) \\ &\stackrel{(5)}{=} \frac{S}{2} \log \left(\frac{S-1}{S} \right) - \frac{\tau}{2} \sum_{i=1}^S \left(\frac{n_1^2 \mu^2 + n_1 \sigma^2}{n_1} - \frac{n^2 \mu^2 + n \sigma^2}{n} \right) \\ &= \frac{S}{2} \log \left(\frac{S-1}{S} \right) - \frac{\tau}{2} \sum_{i=1}^S ([n_1 \mu^2 + \sigma^2] - [n \mu^2 + \sigma^2]) \\ &= \frac{S}{2} \log \left(\frac{S-1}{S} \right) - \frac{\tau}{2} \sum_{i=1}^S (n_1 - n) \mu^2 \end{aligned} \quad (6)$$

Because it holds that (\rightarrow III/1.2.12) $n_1 + n_2 = n$ and $n_2 = n/S$, we finally have:

$$\begin{aligned} \langle \text{cvLBF}_{10} \rangle &= \frac{S}{2} \log \left(\frac{S-1}{S} \right) - \frac{\tau}{2} \sum_{i=1}^S (-n_2) \mu^2 \\ &= \frac{S}{2} \log \left(\frac{S-1}{S} \right) + \frac{1}{2} [\tau n \mu^2]. \end{aligned} \quad (7)$$

■

1.3 Analysis of variance

1.3.1 One-way ANOVA

Definition: Consider measurements $y_{ij} \in \mathbb{R}$ from distinct objects $j = 1, \dots, n_i$ in separate groups $i = 1, \dots, k$.

Then, in one-way analysis of variance (ANOVA), these measurements are assumed to come from normal distributions (\rightarrow II/3.2.1)

$$y_{ij} \sim \mathcal{N}(\mu_i, \sigma^2) \quad \text{for all } i = 1, \dots, k \quad \text{and } j = 1, \dots, n_i \quad (1)$$

where

- μ_i is the expected value (\rightarrow I/1.12.1) in group i and
- σ^2 is the common variance (\rightarrow I/1.13.1) across groups.

Alternatively, the model may be written as

$$\begin{aligned} y_{ij} &= \mu_i + \varepsilon_{ij} \\ \varepsilon_{ij} &\stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2) \end{aligned} \quad (2)$$

where ε_{ij} is the error term (\rightarrow III/1.4.1) belonging to observation j in category i and ε_{ij} are the independent and identically distributed (\rightarrow I/1.2.8).

Sources:

- Bortz, Jürgen (1977): “Einfaktorielle Varianzanalyse”; in: *Lehrbuch der Statistik. Für Sozialwissenschaftler*, ch. 12.1, pp. 528ff.; URL: <https://books.google.de/books?id=INCyBgAAQBAJ>.
- Denziloe (2018): “Derive the distribution of the ANOVA F-statistic under the alternative hypothesis”; in: *StackExchange Cross Validated*, retrieved on 2022-11-06; URL: <https://stats.stackexchange.com/questions/355594/derive-the-distribution-of-the-anova-f-statistic-under-the-alternative-hypothesis>.

1.3.2 Treatment sum of squares

Definition: Let there be an analysis of variance (ANOVA) model with one (\rightarrow III/1.3.1), two (\rightarrow III/1.3.8) or multiple factors influencing the measured data y (here, using the reparametrized version (\rightarrow III/1.3.7) of one-way ANOVA (\rightarrow III/1.3.1)):

$$y_{ij} = \mu + \delta_i + \varepsilon_{ij}, \quad \varepsilon_{ij} \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2) . \quad (1)$$

Then, the treatment sum of squares is defined as the explained sum of squares (\rightarrow III/1.5.8) (ESS) for each main effect, i.e. as the sum of squared deviations of the average for each level of the factor, from the average across all observations:

$$\text{SS}_{\text{treat}} = \sum_{i=1}^k \sum_{j=1}^{n_i} (\bar{y}_i - \bar{y})^2 . \quad (2)$$

Here, \bar{y}_i is the mean for the i -th level of the factor (out of k levels), computed from n_i values y_{ij} , and \bar{y} is the mean across all values y_{ij} .

Sources:

- Wikipedia (2022): “Analysis of variance”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-11-15; URL: https://en.wikipedia.org/wiki/Analysis_of_variance#Partitioning_of_the_sum_of_squares.

1.3.3 Ordinary least squares for one-way ANOVA

Theorem: Given the one-way analysis of variance (\rightarrow III/1.3.1) assumption

$$y_{ij} = \mu_i + \varepsilon_{ij}, \quad \varepsilon_{ij} \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2), \quad i = 1, \dots, k, \quad j = 1, \dots, n_i, \quad (1)$$

the parameters minimizing the residual sum of squares (\rightarrow III/1.5.9) are given by

$$\hat{\mu}_i = \bar{y}_i \quad (2)$$

where \bar{y}_i is the sample mean (\rightarrow I/1.12.2) of all observations in group (\rightarrow III/1.3.1) i :

$$\bar{y}_i = \frac{1}{n_i} \sum_{j=1}^{n_i} y_{ij}. \quad (3)$$

Proof: The residual sum of squares (\rightarrow III/1.5.9) for this model is

$$\text{RSS}(\mu) = \sum_{i=1}^k \sum_{j=1}^{n_i} \varepsilon_{ij}^2 = \sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \mu_i)^2 \quad (4)$$

and the derivatives of RSS with respect to μ_i are

$$\begin{aligned} \frac{\text{dRSS}(\mu)}{\text{d}\mu_i} &= \sum_{j=1}^{n_i} \frac{\text{d}}{\text{d}\mu_i} (y_{ij} - \mu_i)^2 \\ &= \sum_{j=1}^{n_i} 2(y_{ij} - \mu_i)(-1) \\ &= 2 \sum_{j=1}^{n_i} (\mu_i - y_{ij}) \\ &= 2n_i\mu_i - 2 \sum_{j=1}^{n_i} y_{ij} \quad \text{for } i = 1, \dots, k. \end{aligned} \quad (5)$$

Setting these derivatives to zero, we obtain the estimates of μ_i :

$$\begin{aligned} 0 &= 2n_i\hat{\mu}_i - 2 \sum_{j=1}^{n_i} y_{ij} \\ \hat{\mu}_i &= \frac{1}{n_i} \sum_{j=1}^{n_i} y_{ij} \quad \text{for } i = 1, \dots, k. \end{aligned} \quad (6)$$

■

1.3.4 Sums of squares in one-way ANOVA

Theorem: Given one-way analysis of variance (\rightarrow III/1.3.1),

$$y_{ij} = \mu_i + \varepsilon_{ij}, \quad \varepsilon_{ij} \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2) \quad (1)$$

sums of squares can be partitioned as follows

$$\text{SS}_{\text{tot}} = \text{SS}_{\text{treat}} + \text{SS}_{\text{res}} \quad (2)$$

where SS_{tot} is the total sum of squares (\rightarrow III/1.5.7), SS_{treat} is the treatment sum of squares (\rightarrow III/1.3.2) (equivalent to explained sum of squares (\rightarrow III/1.5.8)) and SS_{res} is the residual sum of squares (\rightarrow III/1.5.9).

Proof: The total sum of squares (\rightarrow III/1.5.7) for one-way ANOVA (\rightarrow III/1.3.1) is given by

$$\text{SS}_{\text{tot}} = \sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \bar{y})^2 \quad (3)$$

where \bar{y} is the mean across all values y_{ij} . This can be rewritten as

$$\begin{aligned} \sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \bar{y})^2 &= \sum_{i=1}^k \sum_{j=1}^{n_i} [(y_{ij} - \bar{y}_i) + (\bar{y}_i - \bar{y})]^2 \\ &= \sum_{i=1}^k \sum_{j=1}^{n_i} [(y_{ij} - \bar{y}_i)^2 + (\bar{y}_i - \bar{y})^2 + 2(y_{ij} - \bar{y}_i)(\bar{y}_i - \bar{y})] \\ &= \sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_i)^2 + \sum_{i=1}^k \sum_{j=1}^{n_i} (\bar{y}_i - \bar{y})^2 + 2 \sum_{i=1}^k (\bar{y}_i - \bar{y}) \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_i). \end{aligned} \quad (4)$$

Note that the following sum is zero

$$\sum_{j=1}^{n_i} (y_{ij} - \bar{y}_i) = \sum_{j=1}^{n_i} y_{ij} - n_i \cdot \bar{y}_i = \sum_{j=1}^{n_i} y_{ij} - n_i \cdot \frac{1}{n_i} \sum_{j=1}^{n_i} y_{ij}, \quad (5)$$

so that the sum in (4) reduces to

$$\sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \bar{y})^2 = \sum_{i=1}^k \sum_{j=1}^{n_i} (\bar{y}_i - \bar{y})^2 + \sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_i)^2. \quad (6)$$

With the treatment sum of squares (\rightarrow III/1.3.2) for one-way ANOVA (\rightarrow III/1.3.1)

$$\text{SS}_{\text{treat}} = \sum_{i=1}^k \sum_{j=1}^{n_i} (\bar{y}_i - \bar{y})^2 \quad (7)$$

and the residual sum of squares (\rightarrow III/1.5.9) for one-way ANOVA (\rightarrow III/1.3.1)

$$\text{SS}_{\text{res}} = \sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_i)^2, \quad (8)$$

we finally have:

$$SS_{\text{tot}} = SS_{\text{treat}} + SS_{\text{res}} . \quad (9)$$

■

Sources:

- Wikipedia (2022): “Analysis of variance”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-11-15; URL: https://en.wikipedia.org/wiki/Analysis_of_variance#Partitioning_of_the_sum_of_squares.

1.3.5 F-test for main effect in one-way ANOVA

Theorem: Assume the one-way analysis of variance (\rightarrow III/1.3.1) model

$$y_{ij} = \mu_i + \varepsilon_{ij}, \quad \varepsilon_{ij} \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2), \quad i = 1, \dots, k, \quad j = 1, \dots, n_i . \quad (1)$$

Then, the test statistic (\rightarrow I/4.3.5)

$$F = \frac{\frac{1}{k-1} \sum_{i=1}^k n_i (\bar{y}_i - \bar{y})^2}{\frac{1}{n-k} \sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_i)^2} \quad (2)$$

follows an F-distribution (\rightarrow II/3.8.1)

$$F \sim F(k-1, n-k) \quad (3)$$

under the null hypothesis (\rightarrow I/4.3.2)

$$\begin{aligned} H_0 : \mu_1 = \dots = \mu_k \\ H_1 : \mu_i \neq \mu_j \quad \text{for at least one } i, j \in \{1, \dots, k\}, i \neq j . \end{aligned} \quad (4)$$

Proof: Denote sample sizes as

$$\begin{aligned} n_i &= \text{number of samples in category } i \\ n &= \sum_{i=1}^k n_i \end{aligned} \quad (5)$$

and denote sample means as

$$\begin{aligned} \bar{y}_i &= \frac{1}{n_i} \sum_{j=1}^{n_i} y_{ij} \\ \bar{y} &= \frac{1}{n} \sum_{i=1}^k \sum_{j=1}^{n_i} y_{ij} . \end{aligned} \quad (6)$$

Let μ be the common mean (\rightarrow I/1.12.1) according to H_0 given by (4), i.e. $\mu_1 = \dots = \mu_k = \mu$. Under this null hypothesis, we have:

$$y_{ij} \sim \mathcal{N}(\mu, \sigma^2) \quad \text{for all } i = 1, \dots, k, j = 1, \dots, n_i. \quad (7)$$

Thus, the random variable (\rightarrow I/1.2.2) $U_{ij} = (y_{ij} - \mu)/\sigma$ follows a standard normal distribution (\rightarrow II/3.2.4)

$$U_{ij} = \frac{y_{ij} - \mu}{\sigma} \sim \mathcal{N}(0, 1). \quad (8)$$

Now consider the following sum:

$$\begin{aligned} \sum_{i=1}^k \sum_{j=1}^{n_i} U_{ij}^2 &= \sum_{i=1}^k \sum_{j=1}^{n_i} \left(\frac{y_{ij} - \mu}{\sigma} \right)^2 \\ &= \frac{1}{\sigma^2} \sum_{i=1}^k \sum_{j=1}^{n_i} ((y_{ij} - \bar{y}_i) + (\bar{y}_i - \bar{y}) + (\bar{y} - \mu))^2 \\ &= \frac{1}{\sigma^2} \sum_{i=1}^k \sum_{j=1}^{n_i} [(y_{ij} - \bar{y}_i)^2 + (\bar{y}_i - \bar{y})^2 + (\bar{y} - \mu)^2 + 2(y_{ij} - \bar{y}_i)(\bar{y}_i - \bar{y}) + 2(y_{ij} - \bar{y}_i)(\bar{y} - \mu) + 2(\bar{y}_i - \bar{y})(\bar{y} - \mu)] \end{aligned} \quad (9)$$

Because the following sum over j is zero for all i

$$\begin{aligned} \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_i) &= \sum_{j=1}^{n_i} y_{ij} - n_i \bar{y}_i \\ &= \sum_{j=1}^{n_i} y_{ij} - n_i \cdot \frac{1}{n_i} \sum_{j=1}^{n_i} y_{ij} \\ &= 0, \quad i = 1, \dots, k \end{aligned} \quad (10)$$

and the following sum over i and j is also zero

$$\begin{aligned} \sum_{i=1}^k \sum_{j=1}^{n_i} (\bar{y}_i - \bar{y}) &= \sum_{i=1}^k n_i (\bar{y}_i - \bar{y}) \\ &= \sum_{i=1}^k n_i \bar{y}_i - \bar{y} \sum_{i=1}^k n_i \\ &= \sum_{i=1}^k n_i \cdot \frac{1}{n_i} \sum_{j=1}^{n_i} y_{ij} - \bar{y} \cdot \frac{1}{n} \sum_{i=1}^k \sum_{j=1}^{n_i} y_{ij} \\ &= 0, \end{aligned} \quad (11)$$

non-square products in (9) disappear and the sum reduces to

$$\begin{aligned} \sum_{i=1}^k \sum_{j=1}^{n_i} U_{ij}^2 &= \sum_{i=1}^k \sum_{j=1}^{n_i} \left[\left(\frac{y_{ij} - \bar{y}_i}{\sigma} \right)^2 + \left(\frac{\bar{y}_i - \bar{y}}{\sigma} \right)^2 + \left(\frac{\bar{y} - \mu}{\sigma} \right)^2 \right] \\ &= \sum_{i=1}^k \sum_{j=1}^{n_i} \left(\frac{y_{ij} - \bar{y}_i}{\sigma} \right)^2 + \sum_{i=1}^k \sum_{j=1}^{n_i} \left(\frac{\bar{y}_i - \bar{y}}{\sigma} \right)^2 + \sum_{i=1}^k \sum_{j=1}^{n_i} \left(\frac{\bar{y} - \mu}{\sigma} \right)^2. \end{aligned} \quad (12)$$

Cochran's theorem states that, if a sum of squared standard normal (\rightarrow II/3.2.3) random variables (\rightarrow I/1.2.2) can be written as a sum of squared forms

$$\begin{aligned} \sum_{i=1}^n U_i^2 &= \sum_{j=1}^m Q_j \quad \text{where} \quad Q_j = U^T B^{(j)} U \\ &\quad \text{with} \quad \sum_{j=1}^m B^{(j)} = I_n \\ &\quad \text{and} \quad r_j = \text{rank}(B^{(j)}) , \end{aligned} \tag{13}$$

then the terms Q_j are independent (\rightarrow I/1.3.6) and each term Q_j follows a chi-squared distribution (\rightarrow II/3.7.1) with r_j degrees of freedom:

$$Q_j \sim \chi^2(r_j), \quad j = 1, \dots, m . \tag{14}$$

Let U be the n -dimensional column vector of all observations

$$U = \begin{bmatrix} u_1 \\ \vdots \\ u_k \end{bmatrix} \tag{15}$$

where the group-wise $n_i \times 1$ column vectors are

$$u_1 = \begin{bmatrix} (y_{1,1} - \mu)/\sigma \\ \vdots \\ (y_{1,n_1} - \mu)/\sigma \end{bmatrix}, \quad \dots, \quad u_k = \begin{bmatrix} (y_{k,1} - \mu)/\sigma \\ \vdots \\ (y_{k,n_k} - \mu)/\sigma \end{bmatrix} . \tag{16}$$

Then, we observe that the sum in (12) can be represented in the form of (13) using the matrices

$$\begin{aligned} B^{(1)} &= I_n - \text{diag} \left(\frac{1}{n_1} J_{n_1}, \dots, \frac{1}{n_k} J_{n_k} \right) \\ B^{(2)} &= \text{diag} \left(\frac{1}{n_1} J_{n_1}, \dots, \frac{1}{n_k} J_{n_k} \right) - \frac{1}{n} J_n \\ B^{(3)} &= \frac{1}{n} J_n \end{aligned} \tag{17}$$

where J_n is an $n \times n$ matrix of ones and $\text{diag}(A_1, \dots, A_n)$ denotes a block-diagonal matrix composed of A_1, \dots, A_n . We observe that those matrices satisfy

$$\sum_{i=1}^k \sum_{j=1}^{n_i} U_{ij}^2 = Q_1 + Q_2 + Q_3 = U^T B^{(1)} U + U^T B^{(2)} U + U^T B^{(3)} U \tag{18}$$

as well as

$$B^{(1)} + B^{(2)} + B^{(3)} = I_n \tag{19}$$

and their ranks are:

$$\begin{aligned}
\text{rank}(B^{(1)}) &= n - k \\
\text{rank}(B^{(2)}) &= k - 1 \\
\text{rank}(B^{(3)}) &= 1 .
\end{aligned} \tag{20}$$

Let's write down the explained sum of squares (\rightarrow III/1.5.8) and the residual sum of squares (\rightarrow III/1.5.9) for one-way analysis of variance (\rightarrow III/1.3.1) as

$$\begin{aligned}
\text{ESS} &= \sum_{i=1}^k \sum_{j=1}^{n_i} (\bar{y}_i - \bar{y})^2 \\
\text{RSS} &= \sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_i)^2 .
\end{aligned} \tag{21}$$

Then, using (12), (13), (14), (17) and (20), we find that

$$\begin{aligned}
\frac{\text{ESS}}{\sigma^2} &= \sum_{i=1}^k \sum_{j=1}^{n_i} \left(\frac{\bar{y}_i - \bar{y}}{\sigma} \right)^2 = Q_2 = U^T B^{(2)} U \sim \chi^2(k - 1) \\
\frac{\text{RSS}}{\sigma^2} &= \sum_{i=1}^k \sum_{j=1}^{n_i} \left(\frac{y_{ij} - \bar{y}_i}{\sigma} \right)^2 = Q_1 = U^T B^{(1)} U \sim \chi^2(n - k) .
\end{aligned} \tag{22}$$

Because ESS/σ^2 and RSS/σ^2 are also independent by (14), the F-statistic from (2) is equal to the ratio of two independent chi-squared distributed (\rightarrow II/3.7.1) random variables (\rightarrow I/1.2.2) divided by their degrees of freedom

$$\begin{aligned}
F &= \frac{(\text{ESS}/\sigma^2)/(k - 1)}{(\text{RSS}/\sigma^2)/(n - k)} \\
&= \frac{\text{ESS}/(k - 1)}{\text{RSS}/(n - k)} \\
&= \frac{\frac{1}{k-1} \sum_{i=1}^k \sum_{j=1}^{n_i} (\bar{y}_i - \bar{y})^2}{\frac{1}{n-k} \sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_i)^2} \\
&= \frac{\frac{1}{k-1} \sum_{i=1}^k n_i (\bar{y}_i - \bar{y})^2}{\frac{1}{n-k} \sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_i)^2}
\end{aligned} \tag{23}$$

which, by definition of the F-distribution (\rightarrow II/3.8.1), is distributed as

$$F \sim F(k - 1, n - k) \tag{24}$$

under the null hypothesis (\rightarrow I/4.3.2) for the main effect. ■

Sources:

- Denziloe (2018): “Derive the distribution of the ANOVA F-statistic under the alternative hypothesis”; in: *StackExchange Cross Validated*, retrieved on 2022-11-06; URL: <https://stats.stackexchange.com/questions/355594/derive-the-distribution-of-the-anova-f-statistic-under-the-alternative-hypothesis>.

1.3.6 F-statistic in terms of OLS estimates

Theorem: Given the one-way analysis of variance (\rightarrow III/1.3.1) assumption

$$y_{ij} = \mu_i + \varepsilon_{ij}, \quad \varepsilon_{ij} \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2), \quad (1)$$

1) the F-statistic for the main effect (\rightarrow III/1.3.5) can be expressed in terms of ordinary least squares parameter estimates (\rightarrow III/1.3.3) as

$$F = \frac{\frac{1}{k-1} \sum_{i=1}^k n_i (\hat{\mu}_i - \bar{y})^2}{\frac{1}{n-k} \sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \hat{\mu}_i)^2} \quad (2)$$

2) or, when using the reparametrized version of one-way ANOVA (\rightarrow III/1.3.7), the F-statistic can be expressed as

$$F = \frac{\frac{1}{k-1} \sum_{i=1}^k n_i \hat{\delta}_i^2}{\frac{1}{n-k} \sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \hat{\mu} - \hat{\delta}_i)^2} . \quad (3)$$

Proof: The F-statistic for the main effect in one-way ANOVA (\rightarrow III/1.3.5) is given in terms of the sample means (\rightarrow I/1.12.2) as

$$F = \frac{\frac{1}{k-1} \sum_{i=1}^k n_i (\bar{y}_i - \bar{y})^2}{\frac{1}{n-k} \sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_i)^2} \quad (4)$$

where \bar{y}_i is the average of all values y_{ij} from category i and \bar{y} is the grand mean of all values y_{ij} from all categories $i = 1, \dots, k$.

1) The ordinary least squares estimates for one-way ANOVA (\rightarrow III/1.3.3) are

$$\hat{\mu}_i = \bar{y}_i, \quad (5)$$

such that

$$F = \frac{\frac{1}{k-1} \sum_{i=1}^k n_i (\hat{\mu}_i - \bar{y})^2}{\frac{1}{n-k} \sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \hat{\mu}_i)^2} . \quad (6)$$

2) The OLS estimates for reparametrized one-way ANOVA (\rightarrow III/1.3.7) are

$$\begin{aligned} \hat{\mu} &= \bar{y} \\ \hat{\delta}_i &= \bar{y}_i - \bar{y}, \end{aligned} \quad (7)$$

such that

$$F = \frac{\frac{1}{k-1} \sum_{i=1}^k n_i \hat{\delta}_i^2}{\frac{1}{n-k} \sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \hat{\mu} - \hat{\delta}_i)^2} . \quad (8)$$

■

1.3.7 Reparametrization of one-way ANOVA

Theorem: The one-way analysis of variance (\rightarrow III/1.3.1) model

$$y_{ij} = \mu_i + \varepsilon_{ij}, \quad \varepsilon_{ij} \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2) \quad (1)$$

can be rewritten using parameters μ and δ_i instead of μ_i

$$y_{ij} = \mu + \delta_i + \varepsilon_{ij}, \quad \varepsilon_{ij} \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2) \quad (2)$$

with the constraint

$$\sum_{i=1}^k \frac{n_i}{n} \delta_i = 0, \quad (3)$$

in which case

1) the model parameters are related to each other as

$$\delta_i = \mu_i - \mu, \quad i = 1, \dots, k; \quad (4)$$

2) the ordinary least squares estimates (\rightarrow III/1.3.3) are given by

$$\hat{\delta}_i = \bar{y}_i - \bar{y} = \frac{1}{n_i} \sum_{j=1}^{n_i} y_{ij} - \frac{1}{n} \sum_{i=1}^k \sum_{j=1}^{n_i} y_{ij}; \quad (5)$$

3) the following sum of squares (\rightarrow III/1.3.4) is chi-square distributed (\rightarrow II/3.7.1)

$$\frac{1}{\sigma^2} \sum_{i=1}^k \sum_{j=1}^{n_i} (\hat{\delta}_i - \delta_i)^2 \sim \chi^2(k-1); \quad (6)$$

4) and the following test statistic (\rightarrow I/4.3.5) is F-distributed (\rightarrow II/3.8.1)

$$F = \frac{\frac{1}{k-1} \sum_{i=1}^k n_i \hat{\delta}_i^2}{\frac{1}{n-k} \sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_i)^2} \sim F(k-1, n-k) \quad (7)$$

under the null hypothesis for the main effect (\rightarrow III/1.3.5)

$$H_0 : \delta_1 = \dots = \delta_k = 0. \quad (8)$$

Proof:

1) Equating (1) with (2), we get:

$$\begin{aligned} y_{ij} &= \mu + \delta_i + \varepsilon_{ij} = \mu_i + \varepsilon_{ij} = y_{ij} \\ \mu + \delta_i &= \mu_i \\ \delta_i &= \mu_i - \mu. \end{aligned} \quad (9)$$

2) The residual sum of squares (\rightarrow III/1.5.9) for the reparametrized model is

$$\text{RSS}(\mu, \delta) = \sum_{i=1}^k \sum_{j=1}^{n_i} \varepsilon_{ijk}^2 = \sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \mu - \delta_i)^2 \quad (10)$$

and the derivatives of RSS with respect to μ , δ are

$$\begin{aligned}
 \frac{dRSS}{d\mu} &= \sum_{i=1}^k \sum_{j=1}^{n_i} \frac{d}{d\mu} (y_{ij} - \mu - \delta_i)^2 \\
 &= \sum_{i=1}^k \sum_{j=1}^{n_i} -2(y_{ij} - \mu - \delta_i) \\
 &= \sum_{i=1}^k \left(2n_i\mu + 2n_i\delta_i - 2 \sum_{j=1}^{n_i} y_{ij} \right) \\
 &= 2n\mu + 2 \sum_{i=1}^k n_i\delta_i - 2 \sum_{i=1}^k \sum_{j=1}^{n_i} y_{ij}
 \end{aligned} \tag{11}$$

$$\begin{aligned}
 \frac{dRSS}{d\delta_i} &= \sum_{j=1}^{n_i} \frac{d}{d\delta_i} (y_{ij} - \mu - \delta_i)^2 \\
 &= \sum_{j=1}^{n_i} -2(y_{ij} - \mu - \delta_i) \\
 &= 2n_i\mu + 2n_i\delta_i - 2 \sum_{j=1}^{n_i} y_{ij} .
 \end{aligned} \tag{12}$$

Setting these derivatives to zero, we obtain the estimates of μ and δ_i :

$$\begin{aligned}
 0 &= 2n\hat{\mu} + 2 \sum_{i=1}^k n_i\delta_i - 2 \sum_{i=1}^k \sum_{j=1}^{n_i} y_{ij} \\
 \hat{\mu} &= \frac{1}{n} \sum_{i=1}^k \sum_{j=1}^{n_i} y_{ij} - \sum_{i=1}^k \frac{n_i}{n} \delta_i \\
 &\stackrel{(3)}{=} \frac{1}{n} \sum_{i=1}^k \sum_{j=1}^{n_i} y_{ij} \\
 &= \bar{y}
 \end{aligned} \tag{13}$$

$$\begin{aligned}
 0 &= 2n_i\hat{\mu} + 2n_i\hat{\delta}_i - 2 \sum_{j=1}^{n_i} y_{ij} \\
 \hat{\delta}_i &= \frac{1}{n_i} \sum_{j=1}^{n_i} y_{ij} - \hat{\mu} \\
 &\stackrel{(13)}{=} \frac{1}{n_i} \sum_{j=1}^{n_i} y_{ij} - \frac{1}{n} \sum_{i=1}^k \sum_{j=1}^{n_i} y_{ij} \\
 &= \bar{y}_i - \bar{y} .
 \end{aligned} \tag{14}$$

3) Let $U_{ij} = (y_{ij} - \mu - \delta_i)/\sigma$, such that (\rightarrow II/3.2.4) $U_{ij} \sim \mathcal{N}(0, 1)$ and consider the sum of all squared random variables (\rightarrow I/1.2.2) U_{ij} :

$$\begin{aligned} \sum_{i=1}^k \sum_{j=1}^{n_i} U_{ij}^2 &= \sum_{i=1}^k \sum_{j=1}^{n_i} \left(\frac{y_{ij} - \mu - \delta_i}{\sigma} \right)^2 \\ &= \frac{1}{\sigma^2} \sum_{i=1}^k \sum_{j=1}^{n_i} [(y_{ij} - \bar{y}_i) + (\bar{y}_i - \bar{y}) - \delta_i + (\bar{y} - \mu)]^2. \end{aligned} \quad (15)$$

This square of sums, using a number of intermediate steps, can be developed (\rightarrow III/1.3.5) into a sum of squares:

$$\begin{aligned} \sum_{i=1}^k \sum_{j=1}^{n_i} U_{ij}^2 &= \frac{1}{\sigma^2} \sum_{i=1}^k \sum_{j=1}^{n_i} [(y_{ij} - \bar{y}_i)^2 + (\bar{y}_i - \bar{y})^2 + (\bar{y} - \mu)^2] \\ &= \frac{1}{\sigma^2} \left[\sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_i)^2 + \sum_{i=1}^k \sum_{j=1}^{n_i} (\bar{y}_i - \bar{y})^2 + \sum_{i=1}^k \sum_{j=1}^{n_i} (\bar{y} - \mu)^2 \right]. \end{aligned} \quad (16)$$

To this sum, Cochran's theorem for one-way analysis of variance can be applied (\rightarrow III/1.3.5), yielding the distributions:

$$\begin{aligned} \frac{1}{\sigma^2} \sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_i)^2 &\sim \chi^2(n - k) \\ \frac{1}{\sigma^2} \sum_{i=1}^k \sum_{j=1}^{n_i} (\bar{y}_i - \bar{y})^2 &\stackrel{(14)}{=} \frac{1}{\sigma^2} \sum_{i=1}^k \sum_{j=1}^{n_i} (\hat{\delta}_i - \delta_i)^2 \sim \chi^2(k - 1). \end{aligned} \quad (17)$$

4) The ratio of two chi-square distributed (\rightarrow II/3.7.1) random variables (\rightarrow I/1.2.2), divided by their degrees of freedom (\rightarrow I/1.5.12), is defined to be F-distributed (\rightarrow II/3.8.1), so that

$$\begin{aligned} F &= \frac{\left(\frac{1}{\sigma^2} \sum_{i=1}^k \sum_{j=1}^{n_i} (\hat{\delta}_i - \delta_i)^2 \right) / (k - 1)}{\left(\frac{1}{\sigma^2} \sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_i)^2 \right) / (n - k)} \\ &= \frac{\frac{1}{k-1} \sum_{i=1}^k \sum_{j=1}^{n_i} (\hat{\delta}_i - \delta_i)^2}{\frac{1}{n-k} \sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_i)^2} \\ &= \frac{\frac{1}{k-1} \sum_{i=1}^k n_i (\hat{\delta}_i - \delta_i)^2}{\frac{1}{n-k} \sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_i)^2} \\ &\stackrel{(8)}{=} \frac{\frac{1}{k-1} \sum_{i=1}^k n_i \hat{\delta}_i^2}{\frac{1}{n-k} \sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_i)^2} \end{aligned} \quad (18)$$

follows the F-distribution

$$F \sim F(k - 1, n - k) \quad (19)$$

under the null hypothesis.

**Sources:**

- Wikipedia (2022): “Analysis of variance”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-11-15; URL: https://en.wikipedia.org/wiki/Analysis_of_variance#For_a_single_factor.

1.3.8 Two-way ANOVA

Definition: Let there be two factors A and B with levels $i = 1, \dots, a$ and $j = 1, \dots, b$ that are used to group measurements $y_{ijk} \in \mathbb{R}$ from distinct objects $k = 1, \dots, n_{ij}$ into $a \cdot b$ categories $(i, j) \in \{1, \dots, a\} \times \{1, \dots, b\}$.

Then, in two-way analysis of variance (ANOVA), these measurements are assumed to come from normal distributions (\rightarrow II/3.2.1)

$$y_{ijk} \sim \mathcal{N}(\mu_{ij}, \sigma^2) \quad \text{for all } i = 1, \dots, a, \quad j = 1, \dots, b, \quad \text{and } k = 1, \dots, n_{ij} \quad (1)$$

with

$$\mu_{ij} = \mu + \alpha_i + \beta_j + \gamma_{ij} \quad (2)$$

where

- μ is called the “grand mean”;
- α_i is the additive “main effect” of the i -th level of factor A ;
- β_j is the additive “main effect” of the j -th level of factor B ;
- γ_{ij} is the non-additive “interaction effect” of category (i, j) ;
- μ_{ij} is the expected value (\rightarrow I/1.12.1) in category (i, j) ; and
- σ^2 is common variance (\rightarrow I/1.13.1) across all categories.

Alternatively, the model may be written as

$$\begin{aligned} y_{ijk} &= \mu + \alpha_i + \beta_j + \gamma_{ij} + \varepsilon_{ijk} \\ \varepsilon_{ijk} &\sim \mathcal{N}(0, \sigma^2) \end{aligned} \quad (3)$$

where ε_{ijk} is the error term (\rightarrow III/1.4.1) corresponding to observation k belonging to the i -th level of A and the j -th level of B .

As the two-way ANOVA model is underdetermined, the parameters of the model are additionally subject to the constraints

$$\begin{aligned} \sum_{i=1}^a w_{ij} \alpha_i &= 0 \quad \text{for all } j = 1, \dots, b \\ \sum_{j=1}^b w_{ij} \beta_j &= 0 \quad \text{for all } i = 1, \dots, a \\ \sum_{i=1}^a w_{ij} \gamma_{ij} &= 0 \quad \text{for all } j = 1, \dots, b \\ \sum_{j=1}^b w_{ij} \gamma_{ij} &= 0 \quad \text{for all } i = 1, \dots, a \end{aligned} \quad (4)$$

where the weights are $w_{ij} = n_{ij}/n$ and the total sample size (\rightarrow I/1.1.7) is $n = \sum_{i=1}^a \sum_{j=1}^b n_{ij}$.

Sources:

- Bortz, Jürgen (1977): “Zwei- und mehrfaktorielle Varianzanalyse”; in: *Lehrbuch der Statistik. Für Sozialwissenschaftler*, ch. 12.2, pp. 538ff.; URL: <https://books.google.de/books?id=INCyBgAAQBAJ>.
- ttd (2021): “Proof on SSAB/s2 chi2(I-1)(J-1) under the null hypothesis HAB: dij=0 for i=1,...,I and j=1,...,J”; in: *StackExchange CrossValidated*, retrieved on 2022-11-06; URL: <https://stats.stackexchange.com/questions/545807/proof-on-ss-ab-sigma2-sim-chi2-i-1j-1-under-the-null-hypothesis>.

1.3.9 Interaction sum of squares

Definition: Let there be an analysis of variance (ANOVA) model with two (\rightarrow III/1.3.8) or more factors influencing the measured data y (here, using the standard formulation (\rightarrow III/1.3.11) of two-way ANOVA (\rightarrow III/1.3.8)):

$$y_{ijk} = \mu + \alpha_i + \beta_j + \gamma_{ij} + \varepsilon_{ijk}, \quad \varepsilon_{ijk} \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2). \quad (1)$$

Then, the interaction sum of squares is defined as the explained sum of squares (\rightarrow III/1.5.8) (ESS) for each interaction, i.e. as the sum of squared deviations of the average for each cell from the average across all observations, controlling for the treatment sums of squares (\rightarrow III/1.3.2) of the corresponding factors:

$$\begin{aligned} \text{SS}_{A \times B} &= \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} ([\bar{y}_{ij\bullet} - \bar{y}_{\bullet\bullet\bullet}] - [\bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet}] - [\bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet}])^2 \\ &= \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (\bar{y}_{ij\bullet} - \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet j\bullet} + \bar{y}_{\bullet\bullet\bullet})^2. \end{aligned} \quad (2)$$

Here, $\bar{y}_{ij\bullet}$ is the mean for the (i, j) -th cell (out of $a \times b$ cells), computed from n_{ij} values y_{ijk} , $\bar{y}_{i\bullet\bullet}$ and $\bar{y}_{\bullet j\bullet}$ are the level means for the two factors and $\bar{y}_{\bullet\bullet\bullet}$ is the mean across all values y_{ijk} .

Sources:

- Nandy, Siddhartha (2018): “Two-Way Analysis of Variance”; in: *Stat 512: Applied Regression Analysis*, Purdue University, Summer 2018, Ch. 19; URL: <https://www.stat.purdue.edu/~snandy/stat512/topic7.pdf>.

1.3.10 Ordinary least squares for two-way ANOVA

Theorem: Given the two-way analysis of variance (\rightarrow III/1.3.8) assumption

$$\begin{aligned} y_{ijk} &= \mu + \alpha_i + \beta_j + \gamma_{ij} + \varepsilon_{ijk} \\ \varepsilon_{ijk} &\stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2), \quad i = 1, \dots, a, \quad j = 1, \dots, b, \quad k = 1, \dots, n_{ij}, \end{aligned} \quad (1)$$

the parameters minimizing the residual sum of squares (\rightarrow III/1.5.9) and satisfying the constraints for the model parameters (\rightarrow III/1.3.8) are given by

$$\begin{aligned}
\hat{\mu} &= \bar{y}_{\bullet\bullet\bullet} \\
\hat{\alpha}_i &= \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet} \\
\hat{\beta}_j &= \bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet} \\
\hat{\gamma}_{ij} &= \bar{y}_{ij\bullet} - \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet j\bullet} + \bar{y}_{\bullet\bullet\bullet}
\end{aligned} \tag{2}$$

where $\bar{y}_{\bullet\bullet\bullet}$, $\bar{y}_{i\bullet\bullet}$, $\bar{y}_{\bullet j\bullet}$ and $\bar{y}_{ij\bullet}$ are the following sample means (\rightarrow I/1.12.2):

$$\begin{aligned}
\bar{y}_{\bullet\bullet\bullet} &= \frac{1}{n} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} y_{ijk} \\
\bar{y}_{i\bullet\bullet} &= \frac{1}{n_{i\bullet}} \sum_{j=1}^b \sum_{k=1}^{n_{ij}} y_{ijk} \\
\bar{y}_{\bullet j\bullet} &= \frac{1}{n_{\bullet j}} \sum_{i=1}^a \sum_{k=1}^{n_{ij}} y_{ijk} \\
\bar{y}_{ij\bullet} &= \frac{1}{n_{ij}} \sum_{k=1}^{n_{ij}} y_{ijk}
\end{aligned} \tag{3}$$

with the sample size (\rightarrow I/1.1.7) numbers

$$\begin{aligned}
n_{ij} &\text{ -- number of samples in category } (i, j) \\
n_{i\bullet} &= \sum_{j=1}^b n_{ij} \\
n_{\bullet j} &= \sum_{i=1}^a n_{ij} \\
n &= \sum_{i=1}^a \sum_{j=1}^b n_{ij} .
\end{aligned} \tag{4}$$

Proof: In two-way ANOVA, model parameters are subject to the constraints (\rightarrow III/1.3.8)

$$\begin{aligned}
\sum_{i=1}^a w_{ij} \alpha_i &= 0 \quad \text{for all } j = 1, \dots, b \\
\sum_{j=1}^b w_{ij} \beta_j &= 0 \quad \text{for all } i = 1, \dots, a \\
\sum_{i=1}^a w_{ij} \gamma_{ij} &= 0 \quad \text{for all } j = 1, \dots, b \\
\sum_{j=1}^b w_{ij} \gamma_{ij} &= 0 \quad \text{for all } i = 1, \dots, a
\end{aligned} \tag{5}$$

where $w_{ij} = n_{ij}/n$. The residual sum of squares (\rightarrow III/1.5.9) for this model is

$$\text{RSS}(\mu, \alpha, \beta, \gamma) = \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} \varepsilon_{ijk}^2 = \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \mu - \alpha_i - \beta_j - \gamma_{ij})^2 \quad (6)$$

and the derivatives of RSS with respect to μ , α , β and γ are

$$\begin{aligned} \frac{d\text{RSS}}{d\mu} &= \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} \frac{d}{d\mu} (y_{ijk} - \mu - \alpha_i - \beta_j - \gamma_{ij})^2 \\ &= \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} -2(y_{ijk} - \mu - \alpha_i - \beta_j - \gamma_{ij}) \\ &= \sum_{i=1}^a \sum_{j=1}^b \left(2n_{ij}\mu + 2n_{ij}(\alpha_i + \beta_j + \gamma_{ij}) - 2 \sum_{k=1}^{n_{ij}} y_{ijk} \right) \\ &= 2n\mu + 2 \left(\sum_{i=1}^a n_{i\bullet} \alpha_i + \sum_{j=1}^b n_{\bullet j} \beta_j + \sum_{i=1}^a \sum_{j=1}^b n_{ij} \gamma_{ij} \right) - 2 \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} y_{ijk} \end{aligned} \quad (7)$$

$$\begin{aligned} \frac{d\text{RSS}}{d\alpha_i} &= \sum_{j=1}^b \sum_{k=1}^{n_{ij}} \frac{d}{d\alpha_i} (y_{ijk} - \mu - \alpha_i - \beta_j - \gamma_{ij})^2 \\ &= \sum_{j=1}^b \sum_{k=1}^{n_{ij}} -2(y_{ijk} - \mu - \alpha_i - \beta_j - \gamma_{ij}) \\ &= 2n_{i\bullet} \mu + 2n_{i\bullet} \alpha_i + 2 \left(\sum_{j=1}^b n_{ij} \beta_j + \sum_{j=1}^b n_{ij} \gamma_{ij} \right) - 2 \sum_{j=1}^b \sum_{k=1}^{n_{ij}} y_{ijk} \end{aligned} \quad (8)$$

$$\begin{aligned} \frac{d\text{RSS}}{d\beta_j} &= \sum_{i=1}^a \sum_{k=1}^{n_{ij}} \frac{d}{d\beta_j} (y_{ijk} - \mu - \alpha_i - \beta_j - \gamma_{ij})^2 \\ &= \sum_{i=1}^a \sum_{k=1}^{n_{ij}} -2(y_{ijk} - \mu - \alpha_i - \beta_j - \gamma_{ij}) \\ &= 2n_{\bullet j} \mu + 2n_{\bullet j} \beta_j + 2 \left(\sum_{i=1}^a n_{ij} \alpha_i + \sum_{i=1}^a n_{ij} \gamma_{ij} \right) - 2 \sum_{i=1}^a \sum_{k=1}^{n_{ij}} y_{ijk} \end{aligned} \quad (9)$$

$$\begin{aligned} \frac{d\text{RSS}}{d\gamma_{ij}} &= \sum_{k=1}^{n_{ij}} \frac{d}{d\gamma_{ij}} (y_{ijk} - \mu - \alpha_i - \beta_j - \gamma_{ij})^2 \\ &= \sum_{k=1}^{n_{ij}} -2(y_{ijk} - \mu - \alpha_i - \beta_j - \gamma_{ij}) \\ &= 2n_{ij}(\mu + \alpha_i + \beta_j + \gamma_{ij}) - 2 \sum_{k=1}^{n_{ij}} y_{ijk} . \end{aligned} \quad (10)$$

Setting these derivatives to zero, we obtain the estimates of μ , α_i , β_j and γ_{ij} :

$$\begin{aligned}
 0 &= 2n\hat{\mu} + 2 \left(\sum_{i=1}^a n_{i\bullet} \alpha_i + \sum_{j=1}^b n_{\bullet j} \beta_j + \sum_{i=1}^a \sum_{j=1}^b n_{ij} \gamma_{ij} \right) - 2 \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} y_{ijk} \\
 \hat{\mu} &= \frac{1}{n} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} y_{ijk} - \sum_{i=1}^a \frac{n_{i\bullet}}{n} \alpha_i - \sum_{j=1}^b \frac{n_{\bullet j}}{n} \beta_j - \sum_{i=1}^a \sum_{j=1}^b \frac{n_{ij}}{n} \gamma_{ij} \\
 &\stackrel{(4)}{=} \frac{1}{n} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} y_{ijk} - \sum_{j=1}^b \sum_{i=1}^a \frac{n_{ij}}{n} \alpha_i - \sum_{i=1}^a \sum_{j=1}^b \frac{n_{ij}}{n} \beta_j - \sum_{i=1}^a \sum_{j=1}^b \frac{n_{ij}}{n} \gamma_{ij} \\
 &\stackrel{(5)}{=} \frac{1}{n} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} y_{ijk} \\
 &\stackrel{(3)}{=} \bar{y}_{\bullet\bullet\bullet}
 \end{aligned} \tag{11}$$

$$\begin{aligned}
 0 &= 2n_{i\bullet} \hat{\mu} + 2n_{i\bullet} \hat{\alpha}_i + 2 \left(\sum_{j=1}^b n_{ij} \beta_j + \sum_{j=1}^b n_{ij} \gamma_{ij} \right) - 2 \sum_{j=1}^b \sum_{k=1}^{n_{ij}} y_{ijk} \\
 \hat{\alpha}_i &= \frac{1}{n_{i\bullet}} \sum_{j=1}^b \sum_{k=1}^{n_{ij}} y_{ijk} - \hat{\mu} - \sum_{j=1}^b \frac{n_{ij}}{n_{i\bullet}} \beta_j - \sum_{j=1}^b \frac{n_{ij}}{n_{i\bullet}} \gamma_{ij} \\
 &= \frac{1}{n_{i\bullet}} \sum_{j=1}^b \sum_{k=1}^{n_{ij}} y_{ijk} - \hat{\mu} - \frac{n}{n_{i\bullet}} \sum_{j=1}^b \frac{n_{ij}}{n} \beta_j - \frac{n}{n_{i\bullet}} \sum_{j=1}^b \frac{n_{ij}}{n} \gamma_{ij} \\
 &\stackrel{(5)}{=} \frac{1}{n_{i\bullet}} \sum_{j=1}^b \sum_{k=1}^{n_{ij}} y_{ijk} - \frac{1}{n} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} y_{ijk} \\
 &\stackrel{(3)}{=} \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet}
 \end{aligned} \tag{12}$$

$$\begin{aligned}
 0 &= 2n_{\bullet j} \hat{\mu} + 2n_{\bullet j} \hat{\beta}_j + 2 \left(\sum_{i=1}^a n_{ij} \alpha_i + \sum_{i=1}^a n_{ij} \gamma_{ij} \right) - 2 \sum_{i=1}^a \sum_{k=1}^{n_{ij}} y_{ijk} \\
 \hat{\beta}_j &= \frac{1}{n_{\bullet j}} \sum_{i=1}^a \sum_{k=1}^{n_{ij}} y_{ijk} - \hat{\mu} - \sum_{i=1}^a \frac{n_{ij}}{n_{\bullet j}} \alpha_i - \sum_{i=1}^a \frac{n_{ij}}{n_{\bullet j}} \gamma_{ij} \\
 &= \frac{1}{n_{\bullet j}} \sum_{i=1}^a \sum_{k=1}^{n_{ij}} y_{ijk} - \hat{\mu} - \frac{n}{n_{\bullet j}} \sum_{i=1}^a \frac{n_{ij}}{n} \alpha_i - \frac{n}{n_{\bullet j}} \sum_{i=1}^a \frac{n_{ij}}{n} \gamma_{ij} \\
 &\stackrel{(5)}{=} \frac{1}{n_{\bullet j}} \sum_{i=1}^a \sum_{k=1}^{n_{ij}} y_{ijk} - \frac{1}{n} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} y_{ijk} \\
 &\stackrel{(3)}{=} \bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet}
 \end{aligned} \tag{13}$$

$$\begin{aligned}
0 &= 2n_{ij}(\hat{\mu} + \hat{\alpha}_i + \hat{\beta}_j + \hat{\gamma}_{ij}) - 2 \sum_{k=1}^{n_{ij}} y_{ijk} \\
\hat{\gamma}_{ij} &= \frac{1}{n_{ij}} \sum_{k=1}^{n_{ij}} y_{ijk} - \hat{\alpha}_i - \hat{\beta}_j - \hat{\mu} \\
&= \frac{1}{n_{ij}} \sum_{k=1}^{n_{ij}} y_{ijk} - \frac{1}{n_{i\bullet}} \sum_{j=1}^b \sum_{k=1}^{n_{ij}} y_{ijk} - \frac{1}{n_{\bullet j}} \sum_{i=1}^a \sum_{k=1}^{n_{ij}} y_{ijk} + \frac{1}{n} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} y_{ijk} \\
&\stackrel{(3)}{=} \bar{y}_{ij\bullet} - \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet j\bullet} + \bar{y}_{\bullet\bullet\bullet} .
\end{aligned} \tag{14}$$

■

Sources:

- Olbricht, Gayla R. (2011): “Two-Way ANOVA: Interaction”; in: *Stat 512: Applied Regression Analysis*, Purdue University, Spring 2011, Lect. 27; URL: https://www.stat.purdue.edu/~ghobbs/STAT_512/Lecture_Notes/ANOVA/Topic_27.pdf.

1.3.11 Sums of squares in two-way ANOVA

Theorem: Given two-way analysis of variance (\rightarrow III/1.3.8),

$$y_{ijk} = \mu + \alpha_i + \beta_j + \gamma_{ij} + \varepsilon_{ijk}, \quad \varepsilon_{ijk} \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2) \tag{1}$$

sums of squares can be partitioned as follows

$$\text{SS}_{\text{tot}} = \text{SS}_A + \text{SS}_B + \text{SS}_{A \times B} + \text{SS}_{\text{res}} \tag{2}$$

where SS_{tot} is the total sum of squares (\rightarrow III/1.5.7), SS_A , SS_B and $\text{SS}_{A \times B}$ are treatment (\rightarrow III/1.3.2) and interaction sum of squares (\rightarrow III/1.3.9) (summing into the explained sum of squares (\rightarrow III/1.5.8)) and SS_{res} is the residual sum of squares (\rightarrow III/1.5.9).

Proof: The total sum of squares (\rightarrow III/1.5.7) for two-way ANOVA (\rightarrow III/1.3.8) is given by

$$\text{SS}_{\text{tot}} = \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{\bullet\bullet\bullet})^2 \tag{3}$$

where $\bar{y}_{\bullet\bullet\bullet}$ is the mean across all values y_{ijk} . This can be rewritten as

$$\sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{\bullet\bullet\bullet})^2 = \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} [(y_{ijk} - \bar{y}_{ij\bullet}) + (\bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet}) + (\bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet}) +$$

$$(\bar{y}_{ij\bullet} - \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet j\bullet} + \bar{y}_{\bullet\bullet\bullet})]^2$$

It can be shown (\rightarrow III/1.3.12) that the following sums are all zero:

$$\begin{aligned}
\sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet}) &= 0 \\
\sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (\bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet}) &= 0 \\
\sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (\bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet}) &= 0 \\
\sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (\bar{y}_{ij\bullet} - \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet j\bullet} + \bar{y}_{\bullet\bullet\bullet}) &= 0 .
\end{aligned} \tag{5}$$

This means that the sum in (4) reduces to

$$\begin{aligned}
\sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{\bullet\bullet\bullet})^2 &= \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} \left[(y_{ijk} - \bar{y}_{ij\bullet})^2 + (\bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet})^2 + (\bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet})^2 + \right. \\
&\quad \left. (\bar{y}_{ij\bullet} - \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet j\bullet} + \bar{y}_{\bullet\bullet\bullet})^2 \right] \\
&= \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2 + \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (\bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet})^2 + \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (\bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet})^2 + \\
&\quad \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (\bar{y}_{ij\bullet} - \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet j\bullet} + \bar{y}_{\bullet\bullet\bullet})^2 .
\end{aligned} \tag{6}$$

With the treatment sums of squares (\rightarrow III/1.3.2)

$$\begin{aligned}
SS_A &= \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (\bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet})^2 \\
SS_B &= \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (\bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet})^2 ,
\end{aligned} \tag{7}$$

the interaction sum of squares (\rightarrow III/1.3.9)

$$SS_{A \times B} = \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (\bar{y}_{ij\bullet} - \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet j\bullet} + \bar{y}_{\bullet\bullet\bullet})^2 \tag{8}$$

and the residual sum of squares (\rightarrow III/1.5.9) for two-way ANOVA (\rightarrow III/1.3.8)

$$SS_{\text{res}} = \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2 , \tag{9}$$

we finally have:

$$SS_{\text{tot}} = SS_A + SS_B + SS_{A \times B} + SS_{\text{res}} . \quad (10)$$

■

Sources:

- Nandy, Siddhartha (2018): “Two-Way Analysis of Variance”; in: *Stat 512: Applied Regression Analysis*, Purdue University, Summer 2018, Ch. 19; URL: <https://www.stat.purdue.edu/~snandy/stat512/topic7.pdf>.
- Wikipedia (2022): “Analysis of variance”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-11-15; URL: https://en.wikipedia.org/wiki/Analysis_of_variance#Partitioning_of_the_sum_of_squares.

1.3.12 Cochran’s theorem for two-way ANOVA

Theorem: Assume the two-way analysis of variance (\rightarrow III/1.3.8) model

$$y_{ijk} = \mu + \alpha_i + \beta_j + \gamma_{ij} + \varepsilon_{ijk} \quad (1)$$

$$\varepsilon_{ijk} \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2), \quad i = 1, \dots, a, \quad j = 1, \dots, b, \quad k = 1, \dots, n_{ij}$$

under the well-known constraints for the model parameters (\rightarrow III/1.3.8)

$$\begin{aligned} \sum_{i=1}^a \frac{n_{ij}}{n} \alpha_i &= 0 \quad \text{for all } j = 1, \dots, b \\ \sum_{j=1}^b \frac{n_{ij}}{n} \beta_j &= 0 \quad \text{for all } i = 1, \dots, a \\ \sum_{i=1}^a \frac{n_{ij}}{n} \gamma_{ij} &= 0 \quad \text{for all } j = 1, \dots, b \\ \sum_{j=1}^b \frac{n_{ij}}{n} \gamma_{ij} &= 0 \quad \text{for all } i = 1, \dots, a . \end{aligned} \quad (2)$$

Then, the following sums of squares (\rightarrow III/1.3.11) are chi-square distributed (\rightarrow II/3.7.1)

$$\begin{aligned} \frac{1}{\sigma^2} n (\bar{y}_{\bullet\bullet\bullet} - \mu)^2 &= \frac{SS_M}{\sigma^2} \sim \chi^2(1) \\ \frac{1}{\sigma^2} \sum_{i=1}^a n_{i\bullet} ([\bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet}] - \alpha_i)^2 &= \frac{SS_A}{\sigma^2} \sim \chi^2(a-1) \\ \frac{1}{\sigma^2} \sum_{j=1}^b n_{\bullet j} ([\bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet}] - \beta_j)^2 &= \frac{SS_B}{\sigma^2} \sim \chi^2(b-1) \\ \frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b n_{ij} ([\bar{y}_{ij\bullet} - \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet j\bullet} + \bar{y}_{\bullet\bullet\bullet}] - \gamma_{ij})^2 &= \frac{SS_{A \times B}}{\sigma^2} \sim \chi^2((a-1)(b-1)) \\ \frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2 &= \frac{SS_{\text{res}}}{\sigma^2} \sim \chi^2(n - ab) . \end{aligned} \quad (3)$$

Proof: Denote sample sizes as

$$\begin{aligned}
 n_{ij} &= \text{number of samples in category } (i, j) \\
 n_{i\bullet} &= \sum_{j=1}^b n_{ij} \\
 n_{\bullet j} &= \sum_{i=1}^a n_{ij} \\
 n &= \sum_{i=1}^a \sum_{j=1}^b n_{ij}
 \end{aligned} \tag{4}$$

and denote sample means as

$$\begin{aligned}
 \bar{y}_{\bullet\bullet\bullet} &= \frac{1}{n} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} y_{ijk} \\
 \bar{y}_{i\bullet\bullet} &= \frac{1}{n_{i\bullet}} \sum_{j=1}^b \sum_{k=1}^{n_{ij}} y_{ijk} \\
 \bar{y}_{\bullet j\bullet} &= \frac{1}{n_{\bullet j}} \sum_{i=1}^a \sum_{k=1}^{n_{ij}} y_{ijk} \\
 \bar{y}_{ij\bullet} &= \frac{1}{n_{ij}} \sum_{k=1}^{n_{ij}} y_{ijk} .
 \end{aligned} \tag{5}$$

According to the model given by (1), the observations are distributed as:

$$y_{ijk} \sim \mathcal{N}(\mu + \alpha_i + \beta_j + \gamma_{ij}, \sigma^2) \quad \text{for all } i, j, k . \tag{6}$$

Thus, the random variable (\rightarrow I/1.2.2) $U_{ijk} = (y_{ijk} - \mu - \alpha_i - \beta_j - \gamma_{ij})/\sigma$ follows a standard normal distribution (\rightarrow II/3.2.4)

$$U_{ijk} = \frac{y_{ijk} - \mu - \alpha_i - \beta_j - \gamma_{ij}}{\sigma} \sim \mathcal{N}(0, 1) . \tag{7}$$

Now consider the following sum

$$\sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} U_{ijk}^2 = \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} \left(\frac{y_{ijk} - \mu - \alpha_i - \beta_j - \gamma_{ij}}{\sigma} \right)^2 \tag{8}$$

which can be rewritten as follows:

$$\begin{aligned}
\sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} U_{ijk}^2 &= \frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} [(y_{ijk} - \mu - \alpha_i - \beta_j - \gamma_{ij}) - \\
&\quad [\bar{y}_{\bullet\bullet\bullet} + (\bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet}) + (\bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet}) + (\bar{y}_{ij\bullet} - \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet j\bullet} + \bar{y}_{\bullet\bullet\bullet})] + \\
&\quad [\bar{y}_{\bullet\bullet\bullet} + (\bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet}) + (\bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet}) + (\bar{y}_{ij\bullet} - \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet j\bullet} + \bar{y}_{\bullet\bullet\bullet})]]^2 \\
&= \frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} [(y_{ijk} - [\bar{y}_{\bullet\bullet\bullet} + (\bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet}) + (\bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet}) + (\bar{y}_{ij\bullet} - \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet j\bullet} + \bar{y}_{\bullet\bullet\bullet})]) + \\
&\quad (\bar{y}_{\bullet\bullet\bullet} - \mu) + ([\bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet}] - \alpha_i) + ([\bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet}] - \beta_j) + \\
&\quad ([\bar{y}_{ij\bullet} - \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet j\bullet} + \bar{y}_{\bullet\bullet\bullet}] - \gamma_{ij}))^2 \\
&= \frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} [(y_{ijk} - \bar{y}_{ij\bullet}) + (\bar{y}_{\bullet\bullet\bullet} - \mu) + ([\bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet}] - \alpha_i) + \\
&\quad ([\bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet}] - \beta_j) + ([\bar{y}_{ij\bullet} - \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet j\bullet} + \bar{y}_{\bullet\bullet\bullet}] - \gamma_{ij}))^2.
\end{aligned} \tag{9}$$

Note that the following sums are all zero:

$$\begin{aligned}
\sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet}) &= \sum_{i=1}^a \sum_{j=1}^b \left[\sum_{k=1}^{n_{ij}} y_{ijk} - n_{ij} \cdot \bar{y}_{ij\bullet} \right] \\
&\stackrel{(5)}{=} \sum_{i=1}^a \sum_{j=1}^b \left[\sum_{k=1}^{n_{ij}} y_{ijk} - n_{ij} \cdot \frac{1}{n_{ij}} \sum_{k=1}^{n_{ij}} y_{ijk} \right] \\
&= \sum_{i=1}^a \sum_{j=1}^b 0 = 0
\end{aligned} \tag{10}$$

$$\begin{aligned}
\sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} ([\bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet}] - \alpha_i) &= \sum_{i=1}^a n_{i\bullet\bullet} \cdot (\bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet} - \alpha_i) \\
&= \sum_{i=1}^a n_{i\bullet\bullet} \cdot \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet} \sum_{i=1}^a n_{i\bullet\bullet} - \sum_{i=1}^a n_{i\bullet\bullet} \alpha_i \\
&\stackrel{(5)}{=} \sum_{i=1}^a n_{i\bullet\bullet} \cdot \frac{1}{n_{i\bullet\bullet}} \sum_{j=1}^b \sum_{k=1}^{n_{ij}} y_{ijk} - n \cdot \frac{1}{n} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} y_{ijk} - \sum_{i=1}^a n_{i\bullet\bullet} \alpha_i \\
&= - \sum_{i=1}^a n_{i\bullet\bullet} \alpha_i \stackrel{(4)}{=} -n \sum_{i=1}^a \sum_{j=1}^b \frac{n_{ij}}{n} \alpha_i \stackrel{(2)}{=} 0
\end{aligned} \tag{11}$$

$$\begin{aligned}
\sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} ([\bar{y}_{\bullet j \bullet} - \bar{y}_{\bullet \bullet \bullet}] - \beta_j) &= \sum_{j=1}^b n_{\bullet j} \cdot (\bar{y}_{\bullet j \bullet} - \bar{y}_{\bullet \bullet \bullet} - \beta_j) \\
&= \sum_{j=1}^b n_{\bullet j} \cdot \bar{y}_{\bullet j \bullet} - \bar{y}_{\bullet \bullet \bullet} \sum_{j=1}^b n_{\bullet j} - \sum_{j=1}^b n_{\bullet j} \beta_j \\
&\stackrel{(5)}{=} \sum_{j=1}^b n_{\bullet j} \cdot \frac{1}{n_{\bullet j}} \sum_{i=1}^a \sum_{k=1}^{n_{ij}} y_{ijk} - n \cdot \frac{1}{n} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} y_{ijk} - \sum_{j=1}^b n_{\bullet j} \beta_j \\
&= - \sum_{j=1}^b n_{\bullet j} \beta_j \stackrel{(4)}{=} -n \sum_{j=1}^b \sum_{i=1}^a \frac{n_{ij}}{n} \beta_j \stackrel{(2)}{=} 0
\end{aligned} \tag{12}$$

$$\begin{aligned}
&\sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} ([\bar{y}_{ij \bullet} - \bar{y}_{i \bullet \bullet} - \bar{y}_{\bullet j \bullet} + \bar{y}_{\bullet \bullet \bullet}] - \gamma_{ij}) \\
&= \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} [(\bar{y}_{ij \bullet} - \bar{y}_{\bullet \bullet \bullet}) - (\bar{y}_{i \bullet \bullet} - \bar{y}_{\bullet \bullet \bullet}) - (\bar{y}_{\bullet j \bullet} - \bar{y}_{\bullet \bullet \bullet}) - \gamma_{ij}] \\
&= \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (\bar{y}_{ij \bullet} - \bar{y}_{\bullet \bullet \bullet} - \gamma_{ij}) - \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (\bar{y}_{i \bullet \bullet} - \bar{y}_{\bullet \bullet \bullet}) - \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (\bar{y}_{\bullet j \bullet} - \bar{y}_{\bullet \bullet \bullet}) \\
&\stackrel{(12)}{=} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (\bar{y}_{ij \bullet} - \bar{y}_{\bullet \bullet \bullet} - \gamma_{ij}) - \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (\bar{y}_{i \bullet \bullet} - \bar{y}_{\bullet \bullet \bullet}) \\
&\stackrel{(11)}{=} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (\bar{y}_{ij \bullet} - \bar{y}_{\bullet \bullet \bullet} - \gamma_{ij}) \\
&= \sum_{i=1}^a \sum_{j=1}^b n_{ij} \bar{y}_{ij \bullet} - \bar{y}_{\bullet \bullet \bullet} \sum_{i=1}^a \sum_{j=1}^b n_{ij} - \sum_{i=1}^a \sum_{j=1}^b n_{ij} \gamma_{ij} \\
&\stackrel{(5)}{=} \sum_{i=1}^a \sum_{j=1}^b n_{ij} \cdot \frac{1}{n_{ij}} \sum_{k=1}^{n_{ij}} y_{ijk} - n \cdot \frac{1}{n} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} y_{ijk} - \sum_{i=1}^a \sum_{j=1}^b n_{ij} \gamma_{ij} \\
&= - \sum_{i=1}^a \sum_{j=1}^b n_{ij} \gamma_{ij} = - \frac{1}{n} \sum_{i=1}^a \sum_{j=1}^b \frac{n_{ij}}{n} \gamma_{ij} \stackrel{(2)}{=} 0.
\end{aligned} \tag{13}$$

Note further that $\bar{y}_{\bullet \bullet \bullet}$ and μ are not dependent on i, j and k :

$$\bar{y}_{\bullet \bullet \bullet} = \text{const.} \quad \text{and} \quad \mu = \text{const.} \tag{14}$$

Thus, all the non-square products in (9) disappear and the sum reduces to

$$\begin{aligned}
\sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} U_{ijk}^2 &= \frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} [(y_{ijk} - \bar{y}_{ij\bullet})^2 + (\bar{y}_{\bullet\bullet\bullet} - \mu)^2 + ([\bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet}] - \alpha_i)^2 + \\
&\quad ([\bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet}] - \beta_j)^2 + ([\bar{y}_{ij\bullet} - \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet j\bullet} + \bar{y}_{\bullet\bullet\bullet}] - \gamma_{ij})^2] \\
&= \frac{1}{\sigma^2} \left[\sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2 + \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (\bar{y}_{\bullet\bullet\bullet} - \mu)^2 + \right. \\
&\quad \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} ([\bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet}] - \alpha_i)^2 + \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} ([\bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet}] - \beta_j)^2 + \\
&\quad \left. \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} ([\bar{y}_{ij\bullet} - \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet j\bullet} + \bar{y}_{\bullet\bullet\bullet}] - \gamma_{ij})^2 \right] . \tag{15}
\end{aligned}$$

Cochran's theorem states that, if a sum of squared standard normal (\rightarrow II/3.2.3) random variables (\rightarrow I/1.2.2) can be written as a sum of squared forms

$$\begin{aligned}
\sum_{i=1}^n U_i^2 &= \sum_{j=1}^m Q_j \quad \text{where} \quad Q_j = U^T B^{(j)} U \\
&\text{with} \quad \sum_{j=1}^m B^{(j)} = I_n \\
&\text{and} \quad r_j = \text{rank}(B^{(j)}) , \tag{16}
\end{aligned}$$

then the terms Q_j are independent (\rightarrow I/1.3.6) and each term Q_j follows a chi-squared distribution (\rightarrow II/3.7.1) with r_j degrees of freedom:

$$Q_j \sim \chi^2(r_j), \quad j = 1, \dots, m . \tag{17}$$

First, we define the n -dimensional vector U :

$$U = \begin{bmatrix} u_{1\bullet} \\ \vdots \\ u_{a\bullet} \end{bmatrix} \quad \text{where} \quad u_{i\bullet} = \begin{bmatrix} u_{i1} \\ \vdots \\ u_{ib} \end{bmatrix} \quad \text{where} \quad u_{ij} = \begin{bmatrix} (y_{i,j,1} - \mu - \alpha_i - \beta_j - \gamma_{ij})/\sigma \\ \vdots \\ (y_{i,j,n_{ij}} - \mu - \alpha_i - \beta_j - \gamma_{ij})/\sigma \end{bmatrix} . \tag{18}$$

Next, we specify the $n \times n$ matrices B

$$\begin{aligned}
B^{(1)} &= I_n - \text{diag} \left[\text{diag} \left(\frac{1}{n_{11}} J_{n_{11}}, \dots, \frac{1}{n_{1b}} J_{n_{1b}} \right), \dots, \text{diag} \left(\frac{1}{n_{a1}} J_{n_{a1}}, \dots, \frac{1}{n_{ab}} J_{n_{ab}} \right) \right] \\
B^{(2)} &= \frac{1}{n} J_n \\
B^{(3)} &= \text{diag} \left(\frac{1}{n_{1\bullet}} J_{n_{1\bullet}}, \dots, \frac{1}{n_{a\bullet}} J_{n_{a\bullet}} \right) - \frac{1}{n} J_n \\
B^{(4)} &= M_B - \frac{1}{n} J_n \\
B^{(5)} &= \text{diag} \left[\text{diag} \left(\frac{1}{n_{11}} J_{n_{11}}, \dots, \frac{1}{n_{1b}} J_{n_{1b}} \right), \dots, \text{diag} \left(\frac{1}{n_{a1}} J_{n_{a1}}, \dots, \frac{1}{n_{ab}} J_{n_{ab}} \right) \right] \\
&\quad - \text{diag} \left(\frac{1}{n_{1\bullet}} J_{n_{1\bullet}}, \dots, \frac{1}{n_{a\bullet}} J_{n_{a\bullet}} \right) - M_B + \frac{1}{n} J_n
\end{aligned} \tag{19}$$

with the factor B matrix M_B given by

$$M_B = \begin{bmatrix} \text{diag} \left(\frac{1}{n_{\bullet 1}} J_{n_{11}, n_{11}}, \dots, \frac{1}{n_{\bullet b}} J_{n_{1b}, n_{1b}} \right) & \cdots & \text{diag} \left(\frac{1}{n_{\bullet 1}} J_{n_{11}, n_{a1}}, \dots, \frac{1}{n_{\bullet b}} J_{n_{1b}, n_{ab}} \right) \\ \vdots & \ddots & \vdots \\ \text{diag} \left(\frac{1}{n_{\bullet 1}} J_{n_{a1}, n_{11}}, \dots, \frac{1}{n_{\bullet b}} J_{n_{ab}, n_{1b}} \right) & \cdots & \text{diag} \left(\frac{1}{n_{\bullet 1}} J_{n_{a1}, n_{a1}}, \dots, \frac{1}{n_{\bullet b}} J_{n_{ab}, n_{ab}} \right) \end{bmatrix}. \tag{20}$$

where J_n is an $n \times n$ matrix of ones, $J_{n,m}$ is an $n \times m$ matrix of ones and $\text{diag}(A_1, \dots, A_n)$ denotes a block-diagonal matrix composed of A_1, \dots, A_n . We observe that those matrices satisfy

$$\sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} U_{ijk}^2 = \sum_{l=1}^5 Q_l = \sum_{l=1}^5 U^T B^{(l)} U \tag{21}$$

as well as

$$\sum_{l=1}^5 B^{(l)} = I_n \tag{22}$$

and their ranks are

$$\begin{aligned}
\text{rank}(B^{(1)}) &= n - ab \\
\text{rank}(B^{(2)}) &= 1 \\
\text{rank}(B^{(3)}) &= a - 1 \\
\text{rank}(B^{(4)}) &= b - 1 \\
\text{rank}(B^{(5)}) &= (a - 1)(b - 1).
\end{aligned} \tag{23}$$

Thus, the conditions for applying Cochran's theorem given by (16) are fulfilled and we can use (15), (17), (19) and (23) to conclude that

$$\begin{aligned}
\frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (\bar{y}_{\bullet\bullet\bullet} - \mu)^2 &= Q_2 = U^T B^{(2)} U \sim \chi^2(1) \\
\frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} ([\bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet}] - \alpha_i)^2 &= Q_3 = U^T B^{(3)} U \sim \chi^2(a-1) \\
\frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} ([\bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet}] - \beta_j)^2 &= Q_4 = U^T B^{(4)} U \sim \chi^2(b-1) \\
\frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} ([\bar{y}_{ij\bullet} - \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet j\bullet} + \bar{y}_{\bullet\bullet\bullet}] - \gamma_{ij})^2 &= Q_5 = U^T B^{(5)} U \sim \chi^2((a-1)(b-1)) \\
\frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2 &= Q_1 = U^T B^{(1)} U \sim \chi^2(n-ab) .
\end{aligned} \tag{24}$$

Finally, we identify the terms Q with sums of squares in two-way ANOVA (\rightarrow III/1.3.11) and simplify them to reach the expressions given by (3):

$$\begin{aligned}
\frac{SS_M}{\sigma^2} &= \frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (\bar{y}_{\bullet\bullet\bullet} - \mu)^2 = \frac{1}{\sigma^2} n (\bar{y}_{\bullet\bullet\bullet} - \mu)^2 \\
\frac{SS_A}{\sigma^2} &= \frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} ([\bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet}] - \alpha_i)^2 = \frac{1}{\sigma^2} \sum_{i=1}^a n_{i\bullet} ([\bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet}] - \alpha_i)^2 \\
\frac{SS_B}{\sigma^2} &= \frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} ([\bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet}] - \beta_j)^2 = \frac{1}{\sigma^2} \sum_{j=1}^b n_{\bullet j} ([\bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet}] - \beta_j)^2 \\
\frac{SS_{A \times B}}{\sigma^2} &= \frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} ([\bar{y}_{ij\bullet} - \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet j\bullet} + \bar{y}_{\bullet\bullet\bullet}] - \gamma_{ij})^2 = \frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b n_{ij} ([\bar{y}_{ij\bullet} - \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet j\bullet} + \bar{y}_{\bullet\bullet\bullet}] - \gamma_{ij})^2 \\
\frac{SS_{\text{res}}}{\sigma^2} &= \frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2 = \frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2 .
\end{aligned} \tag{25}$$

■

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1.3.13 F-test for main effect in two-way ANOVA

Theorem: Assume the two-way analysis of variance (\rightarrow III/1.3.8) model

$$\begin{aligned}
y_{ijk} &= \mu + \alpha_i + \beta_j + \gamma_{ij} + \varepsilon_{ijk} \\
\varepsilon_{ijk} &\stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2), \quad i = 1, \dots, a, \quad j = 1, \dots, b, \quad k = 1, \dots, n_{ij} .
\end{aligned} \tag{1}$$

Then, the test statistic (\rightarrow I/4.3.5)

$$F_A = \frac{\frac{1}{a-1} \sum_{i=1}^a n_{i\bullet} (\bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet})^2}{\frac{1}{n-ab} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2} \quad (2)$$

follows an F-distribution (\rightarrow II/3.8.1)

$$F_A \sim F(a-1, n-ab) \quad (3)$$

under the null hypothesis (\rightarrow I/4.3.2) for the main effect (\rightarrow III/1.3.8) of factor A

$$\begin{aligned} H_0 : \alpha_1 = \dots = \alpha_a = 0 \\ H_1 : \alpha_i \neq 0 \quad \text{for at least one } i \in \{1, \dots, a\} \end{aligned} \quad (4)$$

and the test statistic (\rightarrow I/4.3.5)

$$F_B = \frac{\frac{1}{b-1} \sum_{j=1}^b n_{\bullet j} (\bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet})^2}{\frac{1}{n-ab} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2} \quad (5)$$

follows an F-distribution (\rightarrow II/3.8.1)

$$F_B \sim F(b-1, n-ab) \quad (6)$$

under the null hypothesis (\rightarrow I/4.3.2) for the main effect (\rightarrow III/1.3.8) of factor B

$$\begin{aligned} H_0 : \beta_1 = \dots = \beta_b = 0 \\ H_1 : \beta_j \neq 0 \quad \text{for at least one } j \in \{1, \dots, b\} . \end{aligned} \quad (7)$$

Proof: Applying Cochran's theorem for two-analysis of variance (\rightarrow III/1.3.12), we find that the following squared sums

$$\begin{aligned} \frac{SS_A}{\sigma^2} &= \frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} ([\bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet}] - \alpha_i)^2 = \frac{1}{\sigma^2} \sum_{i=1}^a n_{i\bullet} ([\bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet}] - \alpha_i)^2 \\ \frac{SS_B}{\sigma^2} &= \frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} ([\bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet}] - \beta_j)^2 = \frac{1}{\sigma^2} \sum_{j=1}^b n_{\bullet j} ([\bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet}] - \beta_j)^2 \\ \frac{SS_{\text{res}}}{\sigma^2} &= \frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2 = \frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2 \end{aligned} \quad (8)$$

are independent (\rightarrow I/1.3.6) and chi-squared distributed (\rightarrow II/3.7.1):

$$\begin{aligned} \frac{SS_A}{\sigma^2} &\sim \chi^2(a-1) \\ \frac{SS_B}{\sigma^2} &\sim \chi^2(b-1) \\ \frac{SS_{\text{res}}}{\sigma^2} &\sim \chi^2(n-ab) . \end{aligned} \quad (9)$$

1) Thus, the F-statistic from (2) is equal to the ratio of two independent (\rightarrow I/1.3.6) chi-squared distributed (\rightarrow II/3.7.1) random variables (\rightarrow I/1.2.2) divided by their degrees of freedom

$$\begin{aligned}
 F_A &= \frac{(\text{SS}_A/\sigma^2)/(a-1)}{(\text{SS}_{\text{res}}/\sigma^2)/(n-ab)} \\
 &= \frac{\text{SS}_A/(a-1)}{\text{SS}_{\text{res}}/(n-ab)} \\
 &\stackrel{(8)}{=} \frac{\frac{1}{a-1} \sum_{i=1}^a n_{i\bullet} ([\bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet}] - \alpha_i)^2}{\frac{1}{n-ab} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2} \\
 &\stackrel{(4)}{=} \frac{\frac{1}{a-1} \sum_{i=1}^a n_{i\bullet} (\bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet})^2}{\frac{1}{n-ab} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2}
 \end{aligned} \tag{10}$$

which, by definition of the F-distribution (\rightarrow II/3.8.1), is distributed as

$$F_A \sim F(a-1, n-ab) \tag{11}$$

under the null hypothesis (\rightarrow I/4.3.2) for main effect of A .

2) Similarly, the F-statistic from (5) is equal to the ratio of two independent chi-squared distributed (\rightarrow II/3.7.1) random variables (\rightarrow I/1.2.2) divided by their degrees of freedom

$$\begin{aligned}
 F_B &= \frac{(\text{SS}_B/\sigma^2)/(b-1)}{(\text{SS}_{\text{res}}/\sigma^2)/(n-ab)} \\
 &= \frac{\text{SS}_B/(b-1)}{\text{SS}_{\text{res}}/(n-ab)} \\
 &\stackrel{(8)}{=} \frac{\frac{1}{b-1} \sum_{j=1}^b n_{\bullet j} ([\bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet}] - \beta_j)^2}{\frac{1}{n-ab} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2} \\
 &\stackrel{(7)}{=} \frac{\frac{1}{b-1} \sum_{j=1}^b n_{\bullet j} (\bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet})^2}{\frac{1}{n-ab} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2}
 \end{aligned} \tag{12}$$

which, by definition of the F-distribution (\rightarrow II/3.8.1), is distributed as

$$F_B \sim F(b-1, n-ab) \tag{13}$$

under the null hypothesis (\rightarrow I/4.3.2) for main effect of B .

■

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1.3.14 F-test for interaction in two-way ANOVA

Theorem: Assume the two-way analysis of variance (\rightarrow III/1.3.8) model

$$\begin{aligned} y_{ijk} &= \mu + \alpha_i + \beta_j + \gamma_{ij} + \varepsilon_{ijk} \\ \varepsilon_{ijk} &\stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2), \quad i = 1, \dots, a, \quad j = 1, \dots, b, \quad k = 1, \dots, n_{ij} . \end{aligned} \quad (1)$$

Then, the test statistic (\rightarrow I/4.3.5)

$$F_{A \times B} = \frac{\frac{1}{(a-1)(b-1)} \sum_{i=1}^a \sum_{j=1}^b n_{ij} (\bar{y}_{ij\bullet} - \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet j\bullet} + \bar{y}_{\bullet\bullet\bullet})^2}{\frac{1}{n-ab} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2} \quad (2)$$

follows an F-distribution (\rightarrow II/3.8.1)

$$F_{A \times B} \sim F((a-1)(b-1), n-ab) \quad (3)$$

under the null hypothesis (\rightarrow I/4.3.2) for the interaction effect (\rightarrow III/1.3.8) of factors A and B

$$\begin{aligned} H_0 &: \gamma_{11} = \dots = \gamma_{ab} = 0 \\ H_1 &: \gamma_{ij} \neq 0 \quad \text{for at least one } (i, j) \in \{1, \dots, a\} \times \{1, \dots, b\} . \end{aligned} \quad (4)$$

Proof: Applying Cochran's theorem for two-analysis of variance (\rightarrow III/1.3.12), we find that the following squared sums

$$\begin{aligned} \frac{SS_{A \times B}}{\sigma^2} &= \frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} ([\bar{y}_{ij\bullet} - \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet j\bullet} + \bar{y}_{\bullet\bullet\bullet}] - \gamma_{ij})^2 \\ &= \frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b n_{ij} ([\bar{y}_{ij\bullet} - \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet j\bullet} + \bar{y}_{\bullet\bullet\bullet}] - \gamma_{ij})^2 \\ \frac{SS_{\text{res}}}{\sigma^2} &= \frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2 \\ &= \frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2 \end{aligned} \quad (5)$$

are independent (\rightarrow I/1.3.6) and chi-squared distributed (\rightarrow II/3.7.1):

$$\begin{aligned} \frac{SS_{A \times B}}{\sigma^2} &\sim \chi^2((a-1)(b-1)) \\ \frac{SS_{\text{res}}}{\sigma^2} &\sim \chi^2(n-ab) . \end{aligned} \quad (6)$$

Thus, the F-statistic from (2) is equal to the ratio of two independent (\rightarrow I/1.3.6) chi-squared distributed (\rightarrow II/3.7.1) random variables (\rightarrow I/1.2.2) divided by their degrees of freedom

$$\begin{aligned}
F_{A \times B} &= \frac{(\text{SS}_{A \times B} / \sigma^2) / ((a-1)(b-1))}{(\text{SS}_{\text{res}} / \sigma^2) / (n-ab)} \\
&= \frac{\text{SS}_{A \times B} / ((a-1)(b-1))}{\text{SS}_{\text{res}} / (n-ab)} \\
&\stackrel{(5)}{=} \frac{\frac{1}{(a-1)(b-1)} \sum_{i=1}^a \sum_{j=1}^b n_{ij} ([\bar{y}_{ij\bullet} - \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet j\bullet} + \bar{y}_{\bullet\bullet\bullet}] - \gamma_{ij})^2}{\frac{1}{n-ab} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2} \\
&\stackrel{(4)}{=} \frac{\frac{1}{(a-1)(b-1)} \sum_{i=1}^a \sum_{j=1}^b n_{ij} (\bar{y}_{ij\bullet} - \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet j\bullet} + \bar{y}_{\bullet\bullet\bullet})^2}{\frac{1}{n-ab} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2}
\end{aligned} \tag{7}$$

which, by definition of the F-distribution (\rightarrow II/3.8.1), is distributed as

$$F_{A \times B} \sim F((a-1)(b-1), n-ab) \tag{8}$$

under the null hypothesis (\rightarrow I/4.3.2) for an interaction of A and B.

■

Sources:

- Nandy, Siddhartha (2018): “Two-Way Analysis of Variance”; in: *Stat 512: Applied Regression Analysis*, Purdue University, Summer 2018, Ch. 19; URL: <https://www.stat.purdue.edu/~snandy/stat512/topic7.pdf>.
- ttd (2021): “Proof on SSAB/s2 chi2(I-1)(J-1) under the null hypothesis HAB: dij=0 for i=1,...,I and j=1,...,J”; in: *StackExchange CrossValidated*, retrieved on 2022-11-10; URL: <https://stats.stackexchange.com/questions/545807/proof-on-ss-ab-sigma2-sim-chi2-i-1-j-1-under-the-null-hypothesis>.

1.3.15 F-test for grand mean in two-way ANOVA

Theorem: Assume the two-way analysis of variance (\rightarrow III/1.3.8) model

$$\begin{aligned}
y_{ijk} &= \mu + \alpha_i + \beta_j + \gamma_{ij} + \varepsilon_{ijk} \\
\varepsilon_{ijk} &\stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2), \quad i = 1, \dots, a, \quad j = 1, \dots, b, \quad k = 1, \dots, n_{ij}.
\end{aligned} \tag{1}$$

Then, the test statistic (\rightarrow I/4.3.5)

$$F_M = \frac{n(\bar{y}_{\bullet\bullet\bullet})^2}{\frac{1}{n-ab} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2} \tag{2}$$

follows an F-distribution (\rightarrow II/3.8.1)

$$F_M \sim F(1, n-ab) \tag{3}$$

under the null hypothesis (\rightarrow I/4.3.2) for the grand mean (\rightarrow III/1.3.8)

$$\begin{aligned}
H_0 : \mu &= 0 \\
H_1 : \mu &\neq 0.
\end{aligned} \tag{4}$$

Proof: Applying Cochran's theorem for two-analysis of variance (\rightarrow III/1.3.12), we find that the following squared sums

$$\begin{aligned}\frac{SS_M}{\sigma^2} &= \frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (\bar{y}_{\bullet\bullet\bullet} - \mu)^2 = \frac{1}{\sigma^2} n(\bar{y}_{\bullet\bullet\bullet} - \mu)^2 \\ \frac{SS_{\text{res}}}{\sigma^2} &= \frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2 = \frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2\end{aligned}\quad (5)$$

are independent (\rightarrow I/1.3.6) and chi-squared distributed (\rightarrow II/3.7.1):

$$\begin{aligned}\frac{SS_M}{\sigma^2} &\sim \chi^2(1) \\ \frac{SS_{\text{res}}}{\sigma^2} &\sim \chi^2(n - ab) .\end{aligned}\quad (6)$$

Thus, the F-statistic from (2) is equal to the ratio of two independent (\rightarrow I/1.3.6) chi-squared distributed (\rightarrow II/3.7.1) random variables (\rightarrow I/1.2.2) divided by their degrees of freedom

$$\begin{aligned}F_M &= \frac{(SS_M/\sigma^2)/(1)}{(SS_{\text{res}}/\sigma^2)/(n - ab)} \\ &= \frac{SS_M/(1)}{SS_{\text{res}}/(n - ab)} \\ &\stackrel{(5)}{=} \frac{n(\bar{y}_{\bullet\bullet\bullet} - \mu)^2}{\frac{1}{n-ab} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2} \\ &\stackrel{(4)}{=} \frac{n(\bar{y}_{\bullet\bullet\bullet})^2}{\frac{1}{n-ab} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2}\end{aligned}\quad (7)$$

which, by definition of the F-distribution (\rightarrow II/3.8.1), is distributed as

$$F_M \sim F(1, n - ab) \quad (8)$$

under the null hypothesis (\rightarrow I/4.3.2) for the grand mean. ■

Sources:

- Nandy, Siddhartha (2018): "Two-Way Analysis of Variance"; in: *Stat 512: Applied Regression Analysis*, Purdue University, Summer 2018, Ch. 19; URL: <https://www.stat.purdue.edu/~snandy/stat512/topic7.pdf>.
- Olbricht, Gayla R. (2011): "Two-Way ANOVA: Interaction"; in: *Stat 512: Applied Regression Analysis*, Purdue University, Spring 2011, Lect. 27; URL: https://www.stat.purdue.edu/~ghobbs/STAT_512/Lecture_Notes/ANOVA/Topic_27.pdf.

1.3.16 F-statistics in terms of OLS estimates

Theorem: Given the two-way analysis of variance (\rightarrow III/1.3.8) assumption

$$y_{ijk} = \mu + \alpha_i + \beta_j + \gamma_{ij} + \varepsilon_{ijk}, \quad \varepsilon_{ijk} \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2), \quad (1)$$

the F-statistics for the grand mean (\rightarrow III/1.3.15), the main effects (\rightarrow III/1.3.13) and the interaction (\rightarrow III/1.3.14) can be expressed in terms of ordinary least squares parameter estimates (\rightarrow III/1.3.10) as

$$\begin{aligned} F_M &= \frac{n\hat{\mu}^2}{\frac{1}{n-ab} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \hat{y}_{ijk})^2} \\ F_A &= \frac{\frac{1}{a-1} \sum_{i=1}^a n_{i\bullet} \hat{\alpha}_i^2}{\frac{1}{n-ab} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \hat{y}_{ijk})^2} \\ F_B &= \frac{\frac{1}{b-1} \sum_{j=1}^b n_{\bullet j} \hat{\beta}_j^2}{\frac{1}{n-ab} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \hat{y}_{ijk})^2} \\ F_{A \times B} &= \frac{\frac{1}{(a-1)(b-1)} \sum_{i=1}^a \sum_{j=1}^b n_{ij} \hat{\gamma}_{ij}^2}{\frac{1}{n-ab} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \hat{y}_{ijk})^2} \end{aligned} \quad (2)$$

where the predicted values \hat{y}_{ijk} are given by

$$\hat{y}_{ijk} = \hat{\mu} + \hat{\alpha}_i + \hat{\beta}_j + \hat{\gamma}_{ij}. \quad (3)$$

Theorem: The F-statistics for the grand mean (\rightarrow III/1.3.15), the main effects (\rightarrow III/1.3.13) and the interaction (\rightarrow III/1.3.14) in two-way ANOVA (\rightarrow III/1.3.8) are calculated as

$$\begin{aligned} F_M &= \frac{n(\bar{y}_{\bullet\bullet\bullet})^2}{\frac{1}{n-ab} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2} \\ F_A &= \frac{\frac{1}{a-1} \sum_{i=1}^a n_{i\bullet} (\bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet})^2}{\frac{1}{n-ab} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2} \\ F_B &= \frac{\frac{1}{b-1} \sum_{j=1}^b n_{\bullet j} (\bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet})^2}{\frac{1}{n-ab} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2} \\ F_{A \times B} &= \frac{\frac{1}{(a-1)(b-1)} \sum_{i=1}^a \sum_{j=1}^b n_{ij} (\bar{y}_{ij\bullet} - \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet j\bullet} + \bar{y}_{\bullet\bullet\bullet})^2}{\frac{1}{n-ab} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2} \end{aligned} \quad (4)$$

and the ordinary least squares estimates for two-way ANOVA (\rightarrow III/1.3.10) are

$$\begin{aligned} \hat{\mu} &= \bar{y}_{\bullet\bullet\bullet} \\ \hat{\alpha}_i &= \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet} \\ \hat{\beta}_j &= \bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet} \\ \hat{\gamma}_{ij} &= \bar{y}_{ij\bullet} - \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet j\bullet} + \bar{y}_{\bullet\bullet\bullet} \end{aligned} \quad (5)$$

where the sample means (\rightarrow I/1.12.2) are given by

$$\begin{aligned}
\bar{y}_{\bullet\bullet\bullet} &= \frac{1}{n} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} y_{ijk} \\
\bar{y}_{i\bullet\bullet} &= \frac{1}{n_{i\bullet}} \sum_{j=1}^b \sum_{k=1}^{n_{ij}} y_{ijk} \\
\bar{y}_{\bullet j\bullet} &= \frac{1}{n_{\bullet j}} \sum_{i=1}^a \sum_{k=1}^{n_{ij}} y_{ijk} \\
\bar{y}_{ij\bullet} &= \frac{1}{n_{ij}} \sum_{k=1}^{n_{ij}} y_{ijk} .
\end{aligned} \tag{6}$$

We first note that the predicted values can be evaluated as

$$\begin{aligned}
\hat{y}_{ijk} &= \hat{\mu} + \hat{\alpha}_i + \hat{\beta}_j + \hat{\gamma}_{ij} \\
&= \bar{y}_{\bullet\bullet\bullet} + (\bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet}) + (\bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet}) + (\bar{y}_{ij\bullet} - \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet j\bullet} + \bar{y}_{\bullet\bullet\bullet}) \\
&= \bar{y}_{i\bullet\bullet} + \bar{y}_{\bullet j\bullet} + \bar{y}_{ij\bullet} - \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet j\bullet} \\
&= \bar{y}_{ij\bullet} .
\end{aligned} \tag{7}$$

Substituting this (7) and the OLS estimates (5) into the F-formulas (4), we obtain:

$$\begin{aligned}
F_M &= \frac{n\hat{\mu}^2}{\frac{1}{n-ab} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \hat{y}_{ijk})^2} \\
F_A &= \frac{\frac{1}{a-1} \sum_{i=1}^a n_{i\bullet} \hat{\alpha}_i^2}{\frac{1}{n-ab} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \hat{y}_{ijk})^2} \\
F_B &= \frac{\frac{1}{b-1} \sum_{j=1}^b n_{\bullet j} \hat{\beta}_j^2}{\frac{1}{n-ab} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \hat{y}_{ijk})^2} \\
F_{A \times B} &= \frac{\frac{1}{(a-1)(b-1)} \sum_{i=1}^a \sum_{j=1}^b n_{ij} \hat{\gamma}_{ij}^2}{\frac{1}{n-ab} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \hat{y}_{ijk})^2} .
\end{aligned} \tag{8}$$

■

1.4 Simple linear regression

1.4.1 Definition

Definition: Let y and x be two $n \times 1$ vectors.

Then, a statement asserting a linear relationship between x and y

$$y = \beta_0 + \beta_1 x + \varepsilon , \tag{1}$$

together with a statement asserting a normal distribution (\rightarrow II/4.1.1) for ε

$$\varepsilon \sim \mathcal{N}(0, \sigma^2 V) \tag{2}$$

is called a univariate simple regression model or simply, “simple linear regression”.

- y is called “dependent variable”, “measured data” or “signal”;
- x is called “independent variable”, “predictor” or “covariate”;
- V is called “covariance matrix” or “covariance structure”;
- β_1 is called “slope of the regression line (\rightarrow III/1.4.10)”;
- β_0 is called “intercept of the regression line (\rightarrow III/1.4.10)”;
- ε is called “noise”, “errors” or “error terms”;
- σ^2 is called “noise variance” or “error variance”;
- n is the number of observations.

When the covariance structure V is equal to the $n \times n$ identity matrix, this is called simple linear regression with independent and identically distributed (\rightarrow I/1.2.8) (i.i.d.) observations:

$$V = I_n \quad \Rightarrow \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 I_n) \quad \Rightarrow \quad \varepsilon_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2) . \quad (3)$$

In this case, the linear regression model can also be written as

$$y_i = \beta_0 + \beta_1 x_i + \varepsilon_i, \quad \varepsilon_i \sim \mathcal{N}(0, \sigma^2) . \quad (4)$$

Otherwise, it is called simple linear regression with correlated observations (\rightarrow I/1.17.1).

Sources:

- Wikipedia (2021): “Simple linear regression”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-10-27; URL: https://en.wikipedia.org/wiki/Simple_linear_regression#Fitting_the_regression_line.

1.4.2 Special case of multiple linear regression

Theorem: Simple linear regression (\rightarrow III/1.4.1) is a special case of multiple linear regression (\rightarrow III/1.5.1) with design matrix X and regression coefficients β

$$X = \begin{bmatrix} 1_n & x \end{bmatrix} \quad \text{and} \quad \beta = \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} \quad (1)$$

where 1_n is an $n \times 1$ vector of ones, x is the $n \times 1$ single predictor variable, β_0 is the intercept and β_1 is the slope of the regression line (\rightarrow III/1.4.10).

Proof: Without loss of generality, consider the simple linear regression case with uncorrelated errors (\rightarrow III/1.4.1):

$$y_i = \beta_0 + \beta_1 x_i + \varepsilon_i, \quad \varepsilon_i \sim \mathcal{N}(0, \sigma^2), \quad i = 1, \dots, n . \quad (2)$$

In matrix notation and using the multivariate normal distribution (\rightarrow II/4.1.1), this can also be written as

$$\begin{aligned} y &= \beta_0 1_n + \beta_1 x + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, I_n) \\ y &= \begin{bmatrix} 1_n & x \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, I_n) . \end{aligned} \quad (3)$$

Comparing with the multiple linear regression equations for uncorrelated errors (\rightarrow III/1.5.1), we finally note:

$$y = X\beta + \varepsilon \quad \text{with} \quad X = \begin{bmatrix} 1_n & x \end{bmatrix} \quad \text{and} \quad \beta = \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}. \quad (4)$$

In the case of correlated observations (\rightarrow III/1.4.1), the error distribution changes to (\rightarrow III/1.5.1):

$$\varepsilon \sim \mathcal{N}(0, \sigma^2 V). \quad (5)$$

■

1.4.3 Ordinary least squares

Theorem: Given a simple linear regression model (\rightarrow III/1.4.1) with independent observations

$$y = \beta_0 + \beta_1 x + \varepsilon, \quad \varepsilon_i \sim \mathcal{N}(0, \sigma^2), \quad i = 1, \dots, n, \quad (1)$$

the parameters minimizing the residual sum of squares (\rightarrow III/1.5.9) are given by

$$\begin{aligned} \hat{\beta}_0 &= \bar{y} - \hat{\beta}_1 \bar{x} \\ \hat{\beta}_1 &= \frac{s_{xy}}{s_x^2} \end{aligned} \quad (2)$$

where \bar{x} and \bar{y} are the sample means (\rightarrow I/1.12.2), s_x^2 is the sample variance (\rightarrow I/1.13.2) of x and s_{xy} is the sample covariance (\rightarrow I/1.15.2) between x and y .

Proof: The residual sum of squares (\rightarrow III/1.5.9) is defined as

$$\text{RSS}(\beta_0, \beta_1) = \sum_{i=1}^n \varepsilon_i^2 = \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)^2. \quad (3)$$

The derivatives of $\text{RSS}(\beta_0, \beta_1)$ with respect to β_0 and β_1 are

$$\begin{aligned} \frac{d\text{RSS}(\beta_0, \beta_1)}{d\beta_0} &= \sum_{i=1}^n 2(y_i - \beta_0 - \beta_1 x_i)(-1) \\ &= -2 \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i) \\ \frac{d\text{RSS}(\beta_0, \beta_1)}{d\beta_1} &= \sum_{i=1}^n 2(y_i - \beta_0 - \beta_1 x_i)(-x_i) \\ &= -2 \sum_{i=1}^n (x_i y_i - \beta_0 x_i - \beta_1 x_i^2) \end{aligned} \quad (4)$$

and setting these derivatives to zero

$$\begin{aligned}
0 &= -2 \sum_{i=1}^n (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i) \\
0 &= -2 \sum_{i=1}^n (x_i y_i - \hat{\beta}_0 x_i - \hat{\beta}_1 x_i^2)
\end{aligned} \tag{5}$$

yields the following equations:

$$\begin{aligned}
\hat{\beta}_1 \sum_{i=1}^n x_i + \hat{\beta}_0 \cdot n &= \sum_{i=1}^n y_i \\
\hat{\beta}_1 \sum_{i=1}^n x_i^2 + \hat{\beta}_0 \sum_{i=1}^n x_i &= \sum_{i=1}^n x_i y_i .
\end{aligned} \tag{6}$$

From the first equation, we can derive the estimate for the intercept:

$$\begin{aligned}
\hat{\beta}_0 &= \frac{1}{n} \sum_{i=1}^n y_i - \hat{\beta}_1 \cdot \frac{1}{n} \sum_{i=1}^n x_i \\
&= \bar{y} - \hat{\beta}_1 \bar{x} .
\end{aligned} \tag{7}$$

From the second equation, we can derive the estimate for the slope:

$$\begin{aligned}
\hat{\beta}_1 \sum_{i=1}^n x_i^2 + \hat{\beta}_0 \sum_{i=1}^n x_i &= \sum_{i=1}^n x_i y_i \\
\hat{\beta}_1 \sum_{i=1}^n x_i^2 + (\bar{y} - \hat{\beta}_1 \bar{x}) \sum_{i=1}^n x_i &\stackrel{(7)}{=} \sum_{i=1}^n x_i y_i \\
\hat{\beta}_1 \left(\sum_{i=1}^n x_i^2 - \bar{x} \sum_{i=1}^n x_i \right) &= \sum_{i=1}^n x_i y_i - \bar{y} \sum_{i=1}^n x_i \\
\hat{\beta}_1 &= \frac{\sum_{i=1}^n x_i y_i - \bar{y} \sum_{i=1}^n x_i}{\sum_{i=1}^n x_i^2 - \bar{x} \sum_{i=1}^n x_i} .
\end{aligned} \tag{8}$$

Note that the numerator can be rewritten as

$$\begin{aligned}
\sum_{i=1}^n x_i y_i - \bar{y} \sum_{i=1}^n x_i &= \sum_{i=1}^n x_i y_i - n \bar{x} \bar{y} \\
&= \sum_{i=1}^n x_i y_i - n \bar{x} \bar{y} - n \bar{x} \bar{y} + n \bar{x} \bar{y} \\
&= \sum_{i=1}^n x_i y_i - \bar{y} \sum_{i=1}^n x_i - \bar{x} \sum_{i=1}^n y_i + \sum_{i=1}^n \bar{x} \bar{y} \\
&= \sum_{i=1}^n (x_i y_i - x_i \bar{y} - \bar{x} y_i + \bar{x} \bar{y}) \\
&= \sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})
\end{aligned} \tag{9}$$

and that the denominator can be rewritten as

$$\begin{aligned}
 \sum_{i=1}^n x_i^2 - \bar{x} \sum_{i=1}^n x_i &= \sum_{i=1}^n x_i^2 - n\bar{x}^2 \\
 &= \sum_{i=1}^n x_i^2 - 2n\bar{x}\bar{x} + n\bar{x}^2 \\
 &= \sum_{i=1}^n x_i^2 - 2\bar{x} \sum_{i=1}^n x_i + \sum_{i=1}^n \bar{x}^2 \\
 &= \sum_{i=1}^n (x_i^2 - 2\bar{x}x_i + \bar{x}^2) \\
 &= \sum_{i=1}^n (x_i - \bar{x})^2 .
 \end{aligned} \tag{10}$$

With (9) and (10), the estimate from (8) can be simplified as follows:

$$\begin{aligned}
 \hat{\beta}_1 &= \frac{\sum_{i=1}^n x_i y_i - \bar{y} \sum_{i=1}^n x_i}{\sum_{i=1}^n x_i^2 - \bar{x} \sum_{i=1}^n x_i} \\
 &= \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2} \\
 &= \frac{\frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x})^2} \\
 &= \frac{s_{xy}}{s_x^2} .
 \end{aligned} \tag{11}$$

Together, (7) and (11) constitute the ordinary least squares parameter estimates for simple linear regression.

■

Sources:

- Penny, William (2006): “Linear regression”; in: *Mathematics for Brain Imaging*, ch. 1.2.2, pp. 14-16, eqs. 1.24/1.25; URL: https://ueapsylabs.co.uk/sites/wpenny/mbi/mbi_course.pdf.
- Wikipedia (2021): “Proofs involving ordinary least squares”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-10-27; URL: https://en.wikipedia.org/wiki/Proofs_involving_ordinary_least_squares#Derivation_of_simple_linear_regression_estimators.

1.4.4 Ordinary least squares

Theorem: Given a simple linear regression model (\rightarrow III/1.4.1) with independent observations

$$y_i = \beta_0 + \beta_1 x_i + \varepsilon_i, \quad \varepsilon_i \sim \mathcal{N}(0, \sigma^2), \quad i = 1, \dots, n, \tag{1}$$

the parameters minimizing the residual sum of squares (\rightarrow III/1.5.9) are given by

$$\begin{aligned}\hat{\beta}_0 &= \bar{y} - \hat{\beta}_1 \bar{x} \\ \hat{\beta}_1 &= \frac{s_{xy}}{s_x^2}\end{aligned}\tag{2}$$

where \bar{x} and \bar{y} are the sample means (\rightarrow I/1.12.2), s_x^2 is the sample variance (\rightarrow I/1.13.2) of x and s_{xy} is the sample covariance (\rightarrow I/1.15.2) between x and y .

Proof: Simple linear regression is a special case of multiple linear regression (\rightarrow III/1.4.2) with

$$X = \begin{bmatrix} 1_n & x \end{bmatrix} \quad \text{and} \quad \beta = \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}\tag{3}$$

and ordinary least squares estimates (\rightarrow III/1.5.3) are given by

$$\hat{\beta} = (X^T X)^{-1} X^T y.\tag{4}$$

Writing out equation (4), we have

$$\begin{aligned}\hat{\beta} &= \left(\begin{bmatrix} 1_n^T \\ x^T \end{bmatrix} \begin{bmatrix} 1_n & x \end{bmatrix} \right)^{-1} \begin{bmatrix} 1_n^T \\ x^T \end{bmatrix} y \\ &= \left(\begin{bmatrix} n & n\bar{x} \\ n\bar{x} & x^T x \end{bmatrix} \right)^{-1} \begin{bmatrix} n\bar{y} \\ x^T y \end{bmatrix} \\ &= \frac{1}{nx^T x - (n\bar{x})^2} \begin{bmatrix} x^T x & -n\bar{x} \\ -n\bar{x} & n \end{bmatrix} \begin{bmatrix} n\bar{y} \\ x^T y \end{bmatrix} \\ &= \frac{1}{nx^T x - (n\bar{x})^2} \begin{bmatrix} n\bar{y} x^T x - n\bar{x} x^T y \\ n x^T y - (n\bar{x})(n\bar{y}) \end{bmatrix}.\end{aligned}\tag{5}$$

Thus, the second entry of $\hat{\beta}$ is equal to (\rightarrow III/1.4.3):

$$\begin{aligned}\hat{\beta}_1 &= \frac{n x^T y - (n\bar{x})(n\bar{y})}{nx^T x - (n\bar{x})^2} \\ &= \frac{x^T y - n\bar{x}\bar{y}}{x^T x - n\bar{x}^2} \\ &= \frac{\sum_{i=1}^n x_i y_i - \sum_{i=1}^n \bar{x} \bar{y}}{\sum_{i=1}^n x_i^2 - \sum_{i=1}^n \bar{x}^2} \\ &= \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2} \\ &= \frac{s_{xy}}{s_x^2}.\end{aligned}\tag{6}$$

Moreover, the first entry of $\hat{\beta}$ is equal to:

$$\begin{aligned}
\hat{\beta}_0 &= \frac{n\bar{y}x^T x - n\bar{x}x^T y}{nx^T x - (n\bar{x})^2} \\
&= \frac{\bar{y}x^T x - \bar{x}x^T y}{x^T x - n\bar{x}^2} \\
&= \frac{\bar{y}x^T x - \bar{x}x^T y + n\bar{x}^2\bar{y} - n\bar{x}^2\bar{y}}{x^T x - n\bar{x}^2} \\
&= \frac{\bar{y}(x^T x - n\bar{x}^2) - \bar{x}(x^T y - n\bar{x}\bar{y})}{x^T x - n\bar{x}^2} \\
&= \frac{\bar{y}(x^T x - n\bar{x}^2)}{x^T x - n\bar{x}^2} - \frac{\bar{x}(x^T y - n\bar{x}\bar{y})}{x^T x - n\bar{x}^2} \\
&= \bar{y} - \bar{x} \frac{\sum_{i=1}^n x_i y_i - \sum_{i=1}^n \bar{x} \bar{y}}{\sum_{i=1}^n x_i^2 - \sum_{i=1}^n \bar{x}^2} \\
&= \bar{y} - \hat{\beta}_1 \bar{x} .
\end{aligned} \tag{7}$$

■

1.4.5 Expectation of estimates

Theorem: Assume a simple linear regression model (\rightarrow III/1.4.1) with independent observations

$$y = \beta_0 + \beta_1 x + \varepsilon, \quad \varepsilon_i \sim \mathcal{N}(0, \sigma^2), \quad i = 1, \dots, n \tag{1}$$

and consider estimation using ordinary least squares (\rightarrow III/1.4.3). Then, the expected values (\rightarrow I/1.12.1) of the estimated parameters are

$$\begin{aligned}
E(\hat{\beta}_0) &= \beta_0 \\
E(\hat{\beta}_1) &= \beta_1
\end{aligned} \tag{2}$$

which means that the ordinary least squares solution (\rightarrow III/1.4.3) produces unbiased estimators (\rightarrow I/3.1.2).

Proof: According to the simple linear regression model in (1), the expectation of a single data point is

$$E(y_i) = \beta_0 + \beta_1 x_i . \tag{3}$$

The ordinary least squares estimates for simple linear regression (\rightarrow III/1.4.3) are given by

$$\begin{aligned}
\hat{\beta}_0 &= \frac{1}{n} \sum_{i=1}^n y_i - \hat{\beta}_1 \cdot \frac{1}{n} \sum_{i=1}^n x_i \\
\hat{\beta}_1 &= \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2} .
\end{aligned} \tag{4}$$

If we define the following quantity

$$c_i = \frac{x_i - \bar{x}}{\sum_{i=1}^n (x_i - \bar{x})^2} , \tag{5}$$

we note that

$$\begin{aligned}\sum_{i=1}^n c_i &= \frac{\sum_{i=1}^n (x_i - \bar{x})}{\sum_{i=1}^n (x_i - \bar{x})^2} = \frac{\sum_{i=1}^n x_i - n\bar{x}}{\sum_{i=1}^n (x_i - \bar{x})^2} \\ &= \frac{n\bar{x} - n\bar{x}}{\sum_{i=1}^n (x_i - \bar{x})^2} = 0 ,\end{aligned}\tag{6}$$

and

$$\begin{aligned}\sum_{i=1}^n c_i x_i &= \frac{\sum_{i=1}^n (x_i - \bar{x})x_i}{\sum_{i=1}^n (x_i - \bar{x})^2} = \frac{\sum_{i=1}^n (x_i^2 - \bar{x}x_i)}{\sum_{i=1}^n (x_i - \bar{x})^2} \\ &= \frac{\sum_{i=1}^n x_i^2 - 2n\bar{x}\bar{x} + n\bar{x}^2}{\sum_{i=1}^n (x_i - \bar{x})^2} = \frac{\sum_{i=1}^n (x_i^2 - 2\bar{x}x_i + \bar{x}^2)}{\sum_{i=1}^n (x_i - \bar{x})^2} \\ &= \frac{\sum_{i=1}^n (x_i - \bar{x})^2}{\sum_{i=1}^n (x_i - \bar{x})^2} = 1 .\end{aligned}\tag{7}$$

With (5), the estimate for the slope from (4) becomes

$$\begin{aligned}\hat{\beta}_1 &= \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2} \\ &= \sum_{i=1}^n c_i (y_i - \bar{y}) \\ &= \sum_{i=1}^n c_i y_i - \bar{y} \sum_{i=1}^n c_i\end{aligned}\tag{8}$$

and with (3), (6) and (7), its expectation becomes:

$$\begin{aligned}\mathbb{E}(\hat{\beta}_1) &= \mathbb{E}\left(\sum_{i=1}^n c_i y_i - \bar{y} \sum_{i=1}^n c_i\right) \\ &= \sum_{i=1}^n c_i \mathbb{E}(y_i) - \bar{y} \sum_{i=1}^n c_i \\ &= \beta_1 \sum_{i=1}^n c_i x_i + \beta_0 \sum_{i=1}^n c_i - \bar{y} \sum_{i=1}^n c_i \\ &= \beta_1 .\end{aligned}\tag{9}$$

Finally, with (3) and (9), the expectation of the intercept estimate from (4) becomes

$$\begin{aligned}
E(\hat{\beta}_0) &= E\left(\frac{1}{n} \sum_{i=1}^n y_i - \hat{\beta}_1 \cdot \frac{1}{n} \sum_{i=1}^n x_i\right) \\
&= \frac{1}{n} \sum_{i=1}^n E(y_i) - E(\hat{\beta}_1) \cdot \bar{x} \\
&= \frac{1}{n} \sum_{i=1}^n (\beta_0 + \beta_1 x_i) - \beta_1 \cdot \bar{x} \\
&= \beta_0 + \beta_1 \bar{x} - \beta_1 \bar{x} \\
&= \beta_0 .
\end{aligned} \tag{10}$$

Sources:

- Penny, William (2006): “Finding the uncertainty in estimating the slope”; in: *Mathematics for Brain Imaging*, ch. 1.2.4, pp. 18-20, eq. 1.37; URL: https://ueapsylabs.co.uk/sites/wpenny/mbi/mbi_course.pdf.
- Wikipedia (2021): “Proofs involving ordinary least squares”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-10-27; URL: https://en.wikipedia.org/wiki/Proofs_involving_ordinary_least_squares#Unbiasedness_and_variance_of_%7F%22%60UNIQ--postMath-00000037-QINU%60%22%7F.

1.4.6 Variance of estimates

Theorem: Assume a simple linear regression model (\rightarrow III/1.4.1) with independent observations

$$y = \beta_0 + \beta_1 x + \varepsilon, \quad \varepsilon_i \sim \mathcal{N}(0, \sigma^2), \quad i = 1, \dots, n \tag{1}$$

and consider estimation using ordinary least squares (\rightarrow III/1.4.3). Then, the variances (\rightarrow I/1.13.1) of the estimated parameters are

$$\begin{aligned}
\text{Var}(\hat{\beta}_0) &= \frac{x^T x}{n} \cdot \frac{\sigma^2}{(n-1)s_x^2} \\
\text{Var}(\hat{\beta}_1) &= \frac{\sigma^2}{(n-1)s_x^2}
\end{aligned} \tag{2}$$

where s_x^2 is the sample variance (\rightarrow I/1.13.2) of x and $x^T x$ is the sum of squared values of the covariate.

Proof: According to the simple linear regression model in (1), the variance of a single data point is

$$\text{Var}(y_i) = \text{Var}(\varepsilon_i) = \sigma^2 . \tag{3}$$

The ordinary least squares estimates for simple linear regression (\rightarrow III/1.4.3) are given by

$$\begin{aligned}
\hat{\beta}_0 &= \frac{1}{n} \sum_{i=1}^n y_i - \hat{\beta}_1 \cdot \frac{1}{n} \sum_{i=1}^n x_i \\
\hat{\beta}_1 &= \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2} .
\end{aligned} \tag{4}$$

If we define the following quantity

$$c_i = \frac{x_i - \bar{x}}{\sum_{i=1}^n (x_i - \bar{x})^2}, \quad (5)$$

we note that

$$\begin{aligned} \sum_{i=1}^n c_i^2 &= \sum_{i=1}^n \left(\frac{x_i - \bar{x}}{\sum_{i=1}^n (x_i - \bar{x})^2} \right)^2 \\ &= \frac{\sum_{i=1}^n (x_i - \bar{x})^2}{[\sum_{i=1}^n (x_i - \bar{x})^2]^2} \\ &= \frac{1}{\sum_{i=1}^n (x_i - \bar{x})^2}. \end{aligned} \quad (6)$$

With (5), the estimate for the slope from (4) becomes

$$\begin{aligned} \hat{\beta}_1 &= \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2} \\ &= \sum_{i=1}^n c_i (y_i - \bar{y}) \\ &= \sum_{i=1}^n c_i y_i - \bar{y} \sum_{i=1}^n c_i \end{aligned} \quad (7)$$

and with (3) and (6) as well as invariance (\rightarrow I/1.13.7), scaling (\rightarrow I/1.13.8) and additivity (\rightarrow I/1.13.11) of the variance, the variance of $\hat{\beta}_1$ is:

$$\begin{aligned} \text{Var}(\hat{\beta}_1) &= \text{Var} \left(\sum_{i=1}^n c_i y_i - \bar{y} \sum_{i=1}^n c_i \right) \\ &= \text{Var} \left(\sum_{i=1}^n c_i y_i \right) \\ &= \sum_{i=1}^n c_i^2 \text{Var}(y_i) \\ &= \sigma^2 \sum_{i=1}^n c_i^2 \\ &= \sigma^2 \frac{1}{\sum_{i=1}^n (x_i - \bar{x})^2} \\ &= \frac{\sigma^2}{(n-1) \frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x})^2} \\ &= \frac{\sigma^2}{(n-1) s_x^2}. \end{aligned} \quad (8)$$

Finally, with (3) and (8), the variance of the intercept estimate from (4) becomes:

$$\begin{aligned}
\text{Var}(\hat{\beta}_0) &= \text{Var}\left(\frac{1}{n} \sum_{i=1}^n y_i - \hat{\beta}_1 \cdot \frac{1}{n} \sum_{i=1}^n x_i\right) \\
&= \text{Var}\left(\frac{1}{n} \sum_{i=1}^n y_i\right) + \text{Var}\left(\hat{\beta}_1 \cdot \bar{x}\right) \\
&= \left(\frac{1}{n}\right)^2 \sum_{i=1}^n \text{Var}(y_i) + \bar{x}^2 \cdot \text{Var}(\hat{\beta}_1) \\
&= \frac{1}{n^2} \sum_{i=1}^n \sigma^2 + \bar{x}^2 \frac{\sigma^2}{(n-1)s_x^2} \\
&= \frac{\sigma^2}{n} + \frac{\sigma^2 \bar{x}^2}{(n-1)s_x^2}.
\end{aligned} \tag{9}$$

Applying the formula for the sample variance (\rightarrow I/1.13.2) s_x^2 , we finally get:

$$\begin{aligned}
\text{Var}(\hat{\beta}_0) &= \sigma^2 \left(\frac{1}{n} + \frac{\bar{x}^2}{\sum_{i=1}^n (x_i - \bar{x})^2} \right) \\
&= \sigma^2 \left(\frac{\frac{1}{n} \sum_{i=1}^n (x_i - \bar{x})^2}{\sum_{i=1}^n (x_i - \bar{x})^2} + \frac{\bar{x}^2}{\sum_{i=1}^n (x_i - \bar{x})^2} \right) \\
&= \sigma^2 \left(\frac{\frac{1}{n} \sum_{i=1}^n (x_i^2 - 2\bar{x}x_i + \bar{x}^2) + \bar{x}^2}{\sum_{i=1}^n (x_i - \bar{x})^2} \right) \\
&= \sigma^2 \left(\frac{\left(\frac{1}{n} \sum_{i=1}^n x_i^2 - 2\bar{x} \frac{1}{n} \sum_{i=1}^n x_i + \bar{x}^2\right) + \bar{x}^2}{\sum_{i=1}^n (x_i - \bar{x})^2} \right) \\
&= \sigma^2 \left(\frac{\frac{1}{n} \sum_{i=1}^n x_i^2 - 2\bar{x}^2 + 2\bar{x}^2}{\sum_{i=1}^n (x_i - \bar{x})^2} \right) \\
&= \sigma^2 \left(\frac{\frac{1}{n} \sum_{i=1}^n x_i^2}{(n-1) \frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x})^2} \right) \\
&= \frac{x^T x}{n} \cdot \frac{\sigma^2}{(n-1)s_x^2}.
\end{aligned} \tag{10}$$

■

Sources:

- Penny, William (2006): “Finding the uncertainty in estimating the slope”; in: *Mathematics for Brain Imaging*, ch. 1.2.4, pp. 18-20, eq. 1.37; URL: https://ueapsylabs.co.uk/sites/wpenny/mbi/mbi_course.pdf.
- Wikipedia (2021): “Proofs involving ordinary least squares”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-10-27; URL: https://en.wikipedia.org/wiki/Proofs_involving_ordinary_least_squares#Unbiasedness_and_variance_of_%7F%22%60UNIQ--postMath-00000037-QINU%60%22%7F.

1.4.7 Distribution of estimates

Theorem: Assume a simple linear regression model (\rightarrow III/1.4.1) with independent observations

$$y = \beta_0 + \beta_1 x + \varepsilon, \quad \varepsilon_i \sim \mathcal{N}(0, \sigma^2), \quad i = 1, \dots, n \quad (1)$$

and consider estimation using ordinary least squares (\rightarrow III/1.4.3). Then, the estimated parameters are normally distributed (\rightarrow II/4.1.1) as

$$\begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \end{bmatrix} \sim \mathcal{N} \left(\begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}, \frac{\sigma^2}{(n-1)s_x^2} \cdot \begin{bmatrix} x^T x/n & -\bar{x} \\ -\bar{x} & 1 \end{bmatrix} \right) \quad (2)$$

where \bar{x} is the sample mean (\rightarrow I/1.12.2) and s_x^2 is the sample variance (\rightarrow I/1.13.2) of x .

Proof: Simple linear regression is a special case of multiple linear regression (\rightarrow III/1.4.2) with

$$X = \begin{bmatrix} 1_n & x \end{bmatrix} \quad \text{and} \quad \beta = \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}, \quad (3)$$

such that (1) can also be written as

$$y = X\beta + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 I_n) \quad (4)$$

and ordinary least squares estimates (\rightarrow III/1.5.3) are given by

$$\hat{\beta} = (X^T X)^{-1} X^T y. \quad (5)$$

From (4) and the linear transformation theorem for the multivariate normal distribution (\rightarrow II/4.1.14), it follows that

$$y \sim \mathcal{N}(X\beta, \sigma^2 I_n). \quad (6)$$

From (5), in combination with (6) and the transformation theorem (\rightarrow II/4.1.14), it follows that

$$\begin{aligned} \hat{\beta} &\sim \mathcal{N}((X^T X)^{-1} X^T X\beta, \sigma^2 (X^T X)^{-1} X^T I_n X (X^T X)^{-1}) \\ &\sim \mathcal{N}(\beta, \sigma^2 (X^T X)^{-1}). \end{aligned} \quad (7)$$

Applying (3), the covariance matrix (\rightarrow II/4.1.1) can be further developed as follows:

$$\begin{aligned}
\sigma^2(X^T X)^{-1} &= \sigma^2 \left(\begin{bmatrix} 1_n^T \\ x^T \end{bmatrix} \begin{bmatrix} 1_n & x \end{bmatrix} \right)^{-1} \\
&= \sigma^2 \left(\begin{bmatrix} 1_n^T 1_n & 1_n^T x \\ x^T 1_n & x^T x \end{bmatrix} \right)^{-1} \\
&= \sigma^2 \left(\begin{bmatrix} n & n\bar{x} \\ n\bar{x} & x^T x \end{bmatrix} \right)^{-1} \\
&= \frac{\sigma^2}{nx^T x - (n\bar{x})^2} \begin{bmatrix} x^T x & -n\bar{x} \\ -n\bar{x} & n \end{bmatrix} \\
&= \frac{\sigma^2}{x^T x - n\bar{x}^2} \begin{bmatrix} x^T x/n & -\bar{x} \\ -\bar{x} & 1 \end{bmatrix}.
\end{aligned} \tag{8}$$

Note that the denominator in the first factor is equal to

$$\begin{aligned}
x^T x - n\bar{x}^2 &= x^T x - 2n\bar{x}^2 + n\bar{x}^2 \\
&= \sum_{i=1}^n x_i^2 - 2n\bar{x} \frac{1}{n} \sum_{i=1}^n x_i + \sum_{i=1}^n \bar{x}^2 \\
&= \sum_{i=1}^n x_i^2 - 2 \sum_{i=1}^n x_i \bar{x} + \sum_{i=1}^n \bar{x}^2 \\
&= \sum_{i=1}^n (x_i^2 - 2x_i \bar{x} + \bar{x}^2) \\
&= \sum_{i=1}^n (x_i^2 - \bar{x})^2 \\
&= (n-1) s_x^2.
\end{aligned} \tag{9}$$

Thus, combining (7), (8) and (9), we have

$$\hat{\beta} \sim \mathcal{N} \left(\beta, \frac{\sigma^2}{(n-1) s_x^2} \cdot \begin{bmatrix} x^T x/n & -\bar{x} \\ -\bar{x} & 1 \end{bmatrix} \right) \tag{10}$$

which is equivalent to equation (2). ■

Sources:

- Wikipedia (2021): “Proofs involving ordinary least squares”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-11-09; URL: https://en.wikipedia.org/wiki/Proofs_involving_ordinary_least_squares#Unbiasedness_and_variance_of_%7F'%22%60UNIQ--postMath-00000037-QINU%60%22'%7F.

1.4.8 Correlation of estimates

Theorem: In simple linear regression (\rightarrow III/1.4.1), when the independent variable x is mean-centered (\rightarrow I/1.12.1), the ordinary least squares (\rightarrow III/1.4.3) estimates for slope and intercept are uncorrelated (\rightarrow I/1.17.1).

Proof: The parameter estimates for simple linear regression are bivariate normally distributed under ordinary least squares (\rightarrow III/1.4.7):

$$\begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \end{bmatrix} \sim \mathcal{N} \left(\begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}, \frac{\sigma^2}{(n-1)s_x^2} \cdot \begin{bmatrix} x^T x/n & -\bar{x} \\ -\bar{x} & 1 \end{bmatrix} \right) \quad (1)$$

Because the covariance matrix (\rightarrow I/1.16.1) of the multivariate normal distribution (\rightarrow II/4.1.1) contains the pairwise covariances of the random variables (\rightarrow I/1.2.2), we can deduce that the covariance (\rightarrow I/1.15.1) of $\hat{\beta}_0$ and $\hat{\beta}_1$ is:

$$\text{Cov}(\hat{\beta}_0, \hat{\beta}_1) = -\frac{\sigma^2 \bar{x}}{(n-1)s_x^2} \quad (2)$$

where σ^2 is the noise variance (\rightarrow III/1.4.1), s_x^2 is the sample variance (\rightarrow I/1.13.2) of x and n is the number of observations. When x is mean-centered, we have $\bar{x} = 0$, such that:

$$\text{Cov}(\hat{\beta}_0, \hat{\beta}_1) = 0. \quad (3)$$

Because correlation is equal to covariance divided by standard deviations (\rightarrow I/1.17.1), we can conclude that the correlation of $\hat{\beta}_0$ and $\hat{\beta}_1$ is also zero:

$$\text{Corr}(\hat{\beta}_0, \hat{\beta}_1) = 0. \quad (4)$$

■

1.4.9 Effects of mean-centering

Theorem: In simple linear regression (\rightarrow III/1.4.1), when the dependent variable y and/or the independent variable x are mean-centered (\rightarrow I/1.12.1), the ordinary least squares (\rightarrow III/1.4.3) estimate for the intercept changes, but that of the slope does not.

Proof:

1) Under unaltered y and x , ordinary least squares estimates for simple linear regression (\rightarrow III/1.4.3) are

$$\begin{aligned} \hat{\beta}_0 &= \bar{y} - \hat{\beta}_1 \bar{x} \\ \hat{\beta}_1 &= \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2} = \frac{s_{xy}}{s_x^2} \end{aligned} \quad (1)$$

with sample means (\rightarrow I/1.12.2) \bar{x} and \bar{y} , sample variance (\rightarrow I/1.13.2) s_x^2 and sample covariance (\rightarrow I/1.15.2) s_{xy} , such that $\hat{\beta}_0$ estimates “the mean y at $x = 0$ ”.

2) Let \tilde{x} be the mean-centered covariate vector (\rightarrow III/1.4.1):

$$\tilde{x}_i = x_i - \bar{x} \quad \Rightarrow \quad \bar{\tilde{x}} = 0 . \quad (2)$$

Under this condition, the parameter estimates become

$$\begin{aligned} \hat{\beta}_0 &= \bar{y} - \hat{\beta}_1 \bar{\tilde{x}} \\ &= \bar{y} \\ \hat{\beta}_1 &= \frac{\sum_{i=1}^n (\tilde{x}_i - \bar{\tilde{x}})(y_i - \bar{y})}{\sum_{i=1}^n (\tilde{x}_i - \bar{\tilde{x}})^2} \\ &= \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2} = \frac{s_{xy}}{s_x^2} \end{aligned} \quad (3)$$

and we can see that $\hat{\beta}_1(\tilde{x}, y) = \hat{\beta}_1(x, y)$, but $\hat{\beta}_0(\tilde{x}, y) \neq \hat{\beta}_0(x, y)$, specifically β_0 now estimates “the mean y at the mean x ”.

3) Let \tilde{y} be the mean-centered data vector (\rightarrow III/1.4.1):

$$\tilde{y}_i = y_i - \bar{y} \quad \Rightarrow \quad \bar{\tilde{y}} = 0 . \quad (4)$$

Under this condition, the parameter estimates become

$$\begin{aligned} \hat{\beta}_0 &= \bar{\tilde{y}} - \hat{\beta}_1 \bar{x} \\ &= -\hat{\beta}_1 \bar{x} \\ \hat{\beta}_1 &= \frac{\sum_{i=1}^n (x_i - \bar{x})(\tilde{y}_i - \bar{\tilde{y}})}{\sum_{i=1}^n (x_i - \bar{x})^2} \\ &= \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2} = \frac{s_{xy}}{s_x^2} \end{aligned} \quad (5)$$

and we can see that $\hat{\beta}_1(x, \tilde{y}) = \hat{\beta}_1(x, y)$, but $\hat{\beta}_0(x, \tilde{y}) \neq \hat{\beta}_0(x, y)$, specifically β_0 now estimates “the mean x , multiplied with the negative slope”.

4) Finally, consider mean-centering both x and y :

$$\begin{aligned} \tilde{x}_i &= x_i - \bar{x} \quad \Rightarrow \quad \bar{\tilde{x}} = 0 \\ \tilde{y}_i &= y_i - \bar{y} \quad \Rightarrow \quad \bar{\tilde{y}} = 0 . \end{aligned} \quad (6)$$

Under this condition, the parameter estimates become

$$\begin{aligned} \hat{\beta}_0 &= \bar{\tilde{y}} - \hat{\beta}_1 \bar{\tilde{x}} \\ &= 0 \\ \hat{\beta}_1 &= \frac{\sum_{i=1}^n (\tilde{x}_i - \bar{\tilde{x}})(\tilde{y}_i - \bar{\tilde{y}})}{\sum_{i=1}^n (\tilde{x}_i - \bar{\tilde{x}})^2} \\ &= \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2} = \frac{s_{xy}}{s_x^2} \end{aligned} \quad (7)$$

and we can see that $\hat{\beta}_1(\tilde{x}, \tilde{y}) = \hat{\beta}_1(x, y)$, but $\hat{\beta}_0(\tilde{x}, \tilde{y}) \neq \hat{\beta}_0(x, y)$, specifically β_0 is now forced to become zero.

■

1.4.10 Regression line

Definition: Let there be a simple linear regression with independent observations (\rightarrow III/1.4.1) using dependent variable y and independent variable x :

$$y_i = \beta_0 + \beta_1 x_i + \varepsilon_i, \quad \varepsilon_i \sim \mathcal{N}(0, \sigma^2) . \quad (1)$$

Then, given some parameters $\beta_0, \beta_1 \in \mathbb{R}$, the set

$$L(\beta_0, \beta_1) = \{(x, y) \in \mathbb{R}^2 \mid y = \beta_0 + \beta_1 x\} \quad (2)$$

is called a “regression line” and the set

$$L(\hat{\beta}_0, \hat{\beta}_1) \quad (3)$$

is called the “fitted regression line”, with estimated regression coefficients $\hat{\beta}_0, \hat{\beta}_1$, e.g. obtained via ordinary least squares (\rightarrow III/1.4.3).

Sources:

- Wikipedia (2021): “Simple linear regression”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-10-27; URL: https://en.wikipedia.org/wiki/Simple_linear_regression#Fitting_the_regression_line.

1.4.11 Regression line includes center of mass

Theorem: In simple linear regression (\rightarrow III/1.4.1), the regression line (\rightarrow III/1.4.10) estimated using ordinary least squares (\rightarrow III/1.4.3) includes the point $M(\bar{x}, \bar{y})$.

Proof: The fitted regression line (\rightarrow III/1.4.10) is described by the equation

$$y = \hat{\beta}_0 + \hat{\beta}_1 x \quad \text{where} \quad x, y \in \mathbb{R} . \quad (1)$$

Plugging in the coordinates of M and the ordinary least squares estimate of the intercept (\rightarrow III/1.4.3), we obtain

$$\begin{aligned} \bar{y} &= \hat{\beta}_0 + \hat{\beta}_1 \bar{x} \\ \bar{y} &= \bar{y} - \hat{\beta}_1 \bar{x} + \hat{\beta}_1 \bar{x} \\ \bar{y} &= \bar{y} . \end{aligned} \quad (2)$$

which is a true statement. Thus, the regression line (\rightarrow III/1.4.10) goes through the center of mass point (\bar{x}, \bar{y}) , if the model (\rightarrow III/1.4.1) includes an intercept term β_0 . ■

Sources:

- Wikipedia (2021): “Simple linear regression”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-10-27; URL: https://en.wikipedia.org/wiki/Simple_linear_regression#Numerical_properties.

1.4.12 Projection of data point to regression line

Theorem: Consider simple linear regression (\rightarrow III/1.4.1) and an estimated regression line (\rightarrow III/1.4.10) specified by

$$y = \hat{\beta}_0 + \hat{\beta}_1 x \quad \text{where} \quad x, y \in \mathbb{R} . \quad (1)$$

For any given data point $O(x_o|y_o)$, the point on the regression line $P(x_p|y_p)$ that is closest to this data point is given by:

$$P(w | \hat{\beta}_0 + \hat{\beta}_1 w) \quad \text{with} \quad w = \frac{x_o + (y_o - \hat{\beta}_0)\hat{\beta}_1}{1 + \hat{\beta}_1^2} . \quad (2)$$

Proof: The intersection point of the regression line (\rightarrow III/1.4.10) with the y-axis is

$$S(0|\hat{\beta}_0) . \quad (3)$$

Let a be a vector describing the direction of the regression line, let b be the vector pointing from S to O and let p be the vector pointing from S to P .

Because $\hat{\beta}_1$ is the slope of the regression line, we have

$$a = \begin{pmatrix} 1 \\ \hat{\beta}_1 \end{pmatrix} . \quad (4)$$

Moreover, with the points O and S , we have

$$b = \begin{pmatrix} x_o \\ y_o \end{pmatrix} - \begin{pmatrix} 0 \\ \hat{\beta}_0 \end{pmatrix} = \begin{pmatrix} x_o \\ y_o - \hat{\beta}_0 \end{pmatrix} . \quad (5)$$

Because P is located on the regression line, p is collinear with a and thus a scalar multiple of this vector:

$$p = w \cdot a . \quad (6)$$

Moreover, as P is the point on the regression line which is closest to O , this means that the vector $b - p$ is orthogonal to a , such that the inner product of these two vectors is equal to zero:

$$a^T(b - p) = 0 . \quad (7)$$

Rearranging this equation gives

$$\begin{aligned} a^T(b - p) &= 0 \\ a^T(b - w \cdot a) &= 0 \\ a^T b - w \cdot a^T a &= 0 \\ w \cdot a^T a &= a^T b \\ w &= \frac{a^T b}{a^T a} . \end{aligned} \quad (8)$$

With (4) and (5), w can be calculated as

$$\begin{aligned}
w &= \frac{a^T b}{a^T a} \\
w &= \frac{\begin{pmatrix} 1 \\ \hat{\beta}_1 \end{pmatrix}^T \begin{pmatrix} x_o \\ y_o - \hat{\beta}_0 \end{pmatrix}}{\begin{pmatrix} 1 \\ \hat{\beta}_1 \end{pmatrix}^T \begin{pmatrix} 1 \\ \hat{\beta}_1 \end{pmatrix}} \\
w &= \frac{x_o + (y_o - \hat{\beta}_0)\hat{\beta}_1}{1 + \hat{\beta}_1^2}
\end{aligned} \tag{9}$$

Finally, with the point S (3) and the vector p (6), the coordinates of P are obtained as

$$\begin{pmatrix} x_p \\ y_p \end{pmatrix} = \begin{pmatrix} 0 \\ \hat{\beta}_0 \end{pmatrix} + w \cdot \begin{pmatrix} 1 \\ \hat{\beta}_1 \end{pmatrix} = \begin{pmatrix} w \\ \hat{\beta}_0 + \hat{\beta}_1 w \end{pmatrix}. \tag{10}$$

Together, (10) and (9) constitute the proof of equation (2). ■

Sources:

- Penny, William (2006): “Projections”; in: *Mathematics for Brain Imaging*, ch. 1.4.10, pp. 34-35, eqs. 1.87/1.88; URL: https://ueapsylabs.co.uk/sites/wpenny/mbi/mbi_course.pdf.

1.4.13 Sums of squares

Theorem: Under ordinary least squares (\rightarrow III/1.4.3) for simple linear regression (\rightarrow III/1.4.1), total (\rightarrow III/1.5.7), explained (\rightarrow III/1.5.8) and residual (\rightarrow III/1.5.9) sums of squares are given by

$$\begin{aligned}
\text{TSS} &= (n-1) s_y^2 \\
\text{ESS} &= (n-1) \frac{s_{xy}^2}{s_x^2} \\
\text{RSS} &= (n-1) \left(s_y^2 - \frac{s_{xy}^2}{s_x^2} \right)
\end{aligned} \tag{1}$$

where s_x^2 and s_y^2 are the sample variances (\rightarrow I/1.13.2) of x and y and s_{xy} is the sample covariance (\rightarrow I/1.15.2) between x and y .

Proof: The ordinary least squares parameter estimates (\rightarrow III/1.4.3) are given by

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x} \quad \text{and} \quad \hat{\beta}_1 = \frac{s_{xy}}{s_x^2}. \tag{2}$$

1) The total sum of squares (\rightarrow III/1.5.7) is defined as

$$\text{TSS} = \sum_{i=1}^n (y_i - \bar{y})^2 \tag{3}$$

which can be reformulated as follows:

$$\begin{aligned}
 \text{TSS} &= \sum_{i=1}^n (y_i - \bar{y})^2 \\
 &= (n-1) \frac{1}{n-1} \sum_{i=1}^n (y_i - \bar{y})^2 \\
 &= (n-1) s_y^2 .
 \end{aligned} \tag{4}$$

2) The explained sum of squares (\rightarrow III/1.5.8) is defined as

$$\text{ESS} = \sum_{i=1}^n (\hat{y}_i - \bar{y})^2 \quad \text{where} \quad \hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i \tag{5}$$

which, with the OLS parameter estimates, becomes:

$$\begin{aligned}
 \text{ESS} &= \sum_{i=1}^n (\hat{y}_i - \bar{y})^2 \\
 &= \sum_{i=1}^n (\hat{\beta}_0 + \hat{\beta}_1 x_i - \bar{y})^2 \\
 &\stackrel{(2)}{=} \sum_{i=1}^n (\bar{y} - \hat{\beta}_1 \bar{x} + \hat{\beta}_1 x_i - \bar{y})^2 \\
 &= \sum_{i=1}^n \left(\hat{\beta}_1 (x_i - \bar{x}) \right)^2 \\
 &\stackrel{(2)}{=} \sum_{i=1}^n \left(\frac{s_{xy}}{s_x^2} (x_i - \bar{x}) \right)^2 \\
 &= \left(\frac{s_{xy}}{s_x^2} \right)^2 \sum_{i=1}^n (x_i - \bar{x})^2 \\
 &= \left(\frac{s_{xy}}{s_x^2} \right)^2 (n-1) s_x^2 \\
 &= (n-1) \frac{s_{xy}^2}{s_x^2} .
 \end{aligned} \tag{6}$$

3) The residual sum of squares (\rightarrow III/1.5.9) is defined as

$$\text{RSS} = \sum_{i=1}^n (y_i - \hat{y}_i)^2 \quad \text{where} \quad \hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i \tag{7}$$

which, with the OLS parameter estimates, becomes:

$$\begin{aligned}
\text{RSS} &= \sum_{i=1}^n (y_i - \hat{y}_i)^2 \\
&= \sum_{i=1}^n (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2 \\
&\stackrel{(2)}{=} \sum_{i=1}^n (y_i - \bar{y} + \hat{\beta}_1 \bar{x} - \hat{\beta}_1 x_i)^2 \\
&= \sum_{i=1}^n \left((y_i - \bar{y}) - \hat{\beta}_1 (x_i - \bar{x}) \right)^2 \\
&= \sum_{i=1}^n \left((y_i - \bar{y})^2 - 2\hat{\beta}_1 (x_i - \bar{x})(y_i - \bar{y}) + \hat{\beta}_1^2 (x_i - \bar{x})^2 \right) \\
&= \sum_{i=1}^n (y_i - \bar{y})^2 - 2\hat{\beta}_1 \sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y}) + \hat{\beta}_1^2 \sum_{i=1}^n (x_i - \bar{x})^2 \\
&= (n-1) s_y^2 - 2(n-1) \hat{\beta}_1 s_{xy} + (n-1) \hat{\beta}_1^2 s_x^2 \\
&\stackrel{(2)}{=} (n-1) s_y^2 - 2(n-1) \left(\frac{s_{xy}}{s_x^2} \right) s_{xy} + (n-1) \left(\frac{s_{xy}}{s_x^2} \right)^2 s_x^2 \\
&= (n-1) s_y^2 - (n-1) \frac{s_{xy}^2}{s_x^2} \\
&= (n-1) \left(s_y^2 - \frac{s_{xy}^2}{s_x^2} \right).
\end{aligned} \tag{8}$$

■

1.4.14 Partition of sums of squares

Theorem: Assume a simple linear regression model (\rightarrow III/1.4.1) with independent observations

$$y = \beta_0 + \beta_1 x + \varepsilon, \quad \varepsilon_i \sim \mathcal{N}(0, \sigma^2), \quad i = 1, \dots, n \tag{1}$$

where β_0 and β_1 are intercept and slope parameter (\rightarrow III/1.4.1), respectively. Then, it holds that

$$\text{TSS} = \text{ESS} + \text{RSS} \tag{2}$$

where TSS is the total sum of squares (\rightarrow III/1.5.7), ESS is the explained sum of squares (\rightarrow III/1.5.8) and RSS is the residual sum of squares (\rightarrow III/1.5.9).

Proof: For simple linear regression, total, explained and residual sum squares are given by (\rightarrow III/1.4.13)

$$\begin{aligned}
\text{TSS} &= \sum_{i=1}^n (y_i - \bar{y})^2 \\
\text{ESS} &= \sum_{i=1}^n (\hat{y}_i - \bar{y})^2 = \sum_{i=1}^n (\hat{\beta}_0 + \hat{\beta}_1 x_i - \bar{y})^2 \\
\text{RSS} &= \sum_{i=1}^n (y_i - \hat{y}_i)^2 = \sum_{i=1}^n (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2
\end{aligned} \tag{3}$$

where $\hat{\beta}_0$ and $\hat{\beta}_1$ are the estimated regression coefficients obtained via ordinary least squares (\rightarrow III/1.4.3)

$$\begin{aligned}
\hat{\beta}_0 &= \bar{y} - \hat{\beta}_1 \bar{x} \\
\hat{\beta}_1 &= \frac{s_{xy}}{s_x^2}
\end{aligned} \tag{4}$$

where \bar{x} and \bar{y} are the sample means (\rightarrow I/1.12.2) of x and y , s_{xy} is the unbiased sample covariance (\rightarrow I/1.15.2) of x and y and s_x^2 is the unbiased sample variance (\rightarrow I/1.15.2) of x :

$$\begin{aligned}
s_{xy} &= \frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y}) \\
s_x^2 &= \frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x})^2.
\end{aligned} \tag{5}$$

With that in mind, we start working out the total sum of squares:

$$\begin{aligned}
\text{TSS} &= \sum_{i=1}^n (y_i - \bar{y})^2 \\
&= \sum_{i=1}^n (y_i - \hat{y}_i + \hat{y}_i - \bar{y})^2 \\
&= \sum_{i=1}^n ((y_i - \hat{y}_i) + (\hat{y}_i - \bar{y}))^2 \\
&= \sum_{i=1}^n ((y_i - \hat{y}_i)^2 + 2(y_i - \hat{y}_i)(\hat{y}_i - \bar{y}) + (\hat{y}_i - \bar{y})^2) \\
&= \sum_{i=1}^n (y_i - \hat{y}_i)^2 + \sum_{i=1}^n 2(y_i - \hat{y}_i)(\hat{y}_i - \bar{y}) + \sum_{i=1}^n (\hat{y}_i - \bar{y})^2 \\
&\stackrel{(3)}{=} \text{ESS} + \text{RSS} + \sum_{i=1}^n 2(y_i - \hat{y}_i)(\hat{y}_i - \bar{y}).
\end{aligned} \tag{6}$$

Thus, what remains to be shown is that the following sum is zero:

$$\sum_{i=1}^n 2(y_i - \hat{y}_i)(\hat{y}_i - \bar{y}) \quad (7)$$

Using the expression $\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$ for the fitted signal values (\rightarrow III/1.4.10), we proceed as follows:

$$\begin{aligned} \sum_{i=1}^n 2(y_i - \hat{y}_i)(\hat{y}_i - \bar{y}) &= \sum_{i=1}^n 2(y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)(\hat{\beta}_0 + \hat{\beta}_1 x_i - \bar{y}) \\ &\stackrel{(4)}{=} \sum_{i=1}^n 2(y_i - \bar{y} + \hat{\beta}_1 \bar{x} - \hat{\beta}_1 x_i)(\bar{y} - \hat{\beta}_1 \bar{x} + \hat{\beta}_1 x_i - \bar{y}) \\ &= \sum_{i=1}^n 2 \left((y_i - \bar{y}) - (\hat{\beta}_1 x_i - \hat{\beta}_1 \bar{x}) \right) (\hat{\beta}_1 x_i - \hat{\beta}_1 \bar{x}) \\ &= 2 \sum_{i=1}^n \left((y_i - \bar{y}) - \hat{\beta}_1 (x_i - \bar{x}) \right) \hat{\beta}_1 (x_i - \bar{x}) \\ &= 2 \sum_{i=1}^n \left((y_i - \hat{y}_i) \hat{\beta}_1 (x_i - \bar{x}) - \hat{\beta}_1 (x_i - \bar{x}) \hat{\beta}_1 (x_i - \bar{x}) \right) \\ &= 2 \left[\hat{\beta}_1 \sum_{i=1}^n (y_i - \hat{y}_i)(x_i - \bar{x}) - \hat{\beta}_1^2 \sum_{i=1}^n (x_i - \bar{x})(x_i - \bar{x}) \right]. \end{aligned} \quad (8)$$

Next, we recognize the sample covariance and sample variance terms from (5):

$$\begin{aligned} \sum_{i=1}^n 2(y_i - \hat{y}_i)(\hat{y}_i - \bar{y}) &= 2 \left[\hat{\beta}_1 (n-1) s_{xy} - \hat{\beta}_1^2 (n-1) s_x^2 \right] \\ &= 2(n-1) \left[\hat{\beta}_1 s_{xy} - \hat{\beta}_1^2 s_x^2 \right]. \end{aligned} \quad (9)$$

Now, we can apply to functional form of the estimate $\hat{\beta}_1$ from (4) to get:

$$\begin{aligned} \sum_{i=1}^n 2(y_i - \hat{y}_i)(\hat{y}_i - \bar{y}) &= 2(n-1) \left[\left(\frac{s_{xy}}{s_x^2} \right) s_{xy} - \left(\frac{s_{xy}}{s_x^2} \right)^2 s_x^2 \right] \\ &= 2(n-1) \left[\frac{s_{xy}^2}{s_x^2} - \frac{s_{xy}^2}{s_x^2} \right] \\ &= 2(n-1) \cdot 0 \\ &= 0. \end{aligned} \quad (10)$$

Plugging the result from (10) into (6), we finally get:

$$\text{TSS} = \text{ESS} + \text{RSS}. \quad (11)$$

Sources:

■

- Ostwald, Dirk (2023): “Korrelation”; in: *Allgemeines Lineares Modell*, Einheit (2), Folien 19-23; URL: https://www.ipsy.ovgu.de/ipsy_media/Methodenlehre+I/Sommersemester+2023/Allgemeines+Lineares+Modell/2_Korrelation.pdf.
- Manabu, Hayashi (2021): “TSS = RSS + ESS | Simple Linear Regression”; in: *You Tube*, retrieved on 2024-07-12; URL: <https://www.youtube.com/watch?v=N7pHym1L9b0>.

1.4.15 Transformation matrices

Theorem: Under ordinary least squares (\rightarrow III/1.4.3) for simple linear regression (\rightarrow III/1.4.1), estimation (\rightarrow III/1.5.11), projection (\rightarrow III/1.5.12) and residual-forming (\rightarrow III/1.5.13) matrices are given by

$$\begin{aligned} E &= \frac{1}{(n-1)s_x^2} \begin{bmatrix} (x^T x/n) 1_n^T - \bar{x} x^T \\ -\bar{x} 1_n^T + x^T \end{bmatrix} \\ P &= \frac{1}{(n-1)s_x^2} \begin{bmatrix} (x^T x/n) - 2\bar{x}x_1 + x_1^2 & \cdots & (x^T x/n) - \bar{x}(x_1 + x_n) + x_1x_n \\ \vdots & \ddots & \vdots \\ (x^T x/n) - \bar{x}(x_1 + x_n) + x_1x_n & \cdots & (x^T x/n) - 2\bar{x}x_n + x_n^2 \end{bmatrix} \\ R &= \frac{1}{(n-1)s_x^2} \begin{bmatrix} (n-1)(x^T x/n) + \bar{x}(2x_1 - n\bar{x}) - x_1^2 & \cdots & -(x^T x/n) + \bar{x}(x_1 + x_n) - x_1x_n \\ \vdots & \ddots & \vdots \\ -(x^T x/n) + \bar{x}(x_1 + x_n) - x_1x_n & \cdots & (n-1)(x^T x/n) + \bar{x}(2x_n - n\bar{x}) - x_n^2 \end{bmatrix} \end{aligned} \quad (1)$$

where 1_n is an $n \times 1$ vector of ones, x is the $n \times 1$ single predictor variable, \bar{x} is the sample mean (\rightarrow I/1.12.2) of x and s_x^2 is the sample variance (\rightarrow I/1.13.2) of x .

Proof: Simple linear regression is a special case of multiple linear regression (\rightarrow III/1.4.2) with

$$X = \begin{bmatrix} 1_n & x \end{bmatrix} \quad \text{and} \quad \beta = \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}, \quad (2)$$

such that the simple linear regression model can also be written as

$$y = X\beta + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 I_n). \quad (3)$$

Moreover, we note the following equality (\rightarrow III/1.4.7):

$$x^T x - n\bar{x}^2 = (n-1)s_x^2. \quad (4)$$

1) The estimation matrix is given by (\rightarrow III/1.5.14)

$$E = (X^T X)^{-1} X^T \quad (5)$$

which is a $2 \times n$ matrix and can be reformulated as follows:

$$\begin{aligned}
E &= (X^T X)^{-1} X^T \\
&= \left(\begin{bmatrix} 1_n^T \\ x^T \end{bmatrix} \begin{bmatrix} 1_n & x \end{bmatrix} \right)^{-1} \begin{bmatrix} 1_n^T \\ x^T \end{bmatrix} \\
&= \left(\begin{bmatrix} n & n\bar{x} \\ n\bar{x} & x^T x \end{bmatrix} \right)^{-1} \begin{bmatrix} 1_n^T \\ x^T \end{bmatrix} \\
&= \frac{1}{nx^T x - (n\bar{x})^2} \begin{bmatrix} x^T x & -n\bar{x} \\ -n\bar{x} & n \end{bmatrix} \begin{bmatrix} 1_n^T \\ x^T \end{bmatrix} \\
&= \frac{1}{x^T x - n\bar{x}^2} \begin{bmatrix} x^T x/n & -\bar{x} \\ -\bar{x} & 1 \end{bmatrix} \begin{bmatrix} 1_n^T \\ x^T \end{bmatrix} \\
&\stackrel{(4)}{=} \frac{1}{(n-1)s_x^2} \begin{bmatrix} (x^T x/n) 1_n^T - \bar{x} x^T \\ -\bar{x} 1_n^T + x^T \end{bmatrix}.
\end{aligned} \tag{6}$$

2) The projection matrix is given by (\rightarrow III/1.5.14)

$$P = X(X^T X)^{-1} X^T = X E \tag{7}$$

which is an $n \times n$ matrix and can be reformulated as follows:

$$\begin{aligned}
P = X E &= \begin{bmatrix} 1_n & x \end{bmatrix} \begin{bmatrix} e_1 \\ e_2 \end{bmatrix} \\
&= \frac{1}{(n-1)s_x^2} \begin{bmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} \begin{bmatrix} (x^T x/n) - \bar{x}x_1 & \cdots & (x^T x/n) - \bar{x}x_n \\ -\bar{x} + x_1 & \cdots & -\bar{x} + x_n \end{bmatrix} \\
&= \frac{1}{(n-1)s_x^2} \begin{bmatrix} (x^T x/n) - 2\bar{x}x_1 + x_1^2 & \cdots & (x^T x/n) - \bar{x}(x_1 + x_n) + x_1x_n \\ \vdots & \ddots & \vdots \\ (x^T x/n) - \bar{x}(x_1 + x_n) + x_1x_n & \cdots & (x^T x/n) - 2\bar{x}x_n + x_n^2 \end{bmatrix}.
\end{aligned} \tag{8}$$

3) The residual-forming matrix is given by (\rightarrow III/1.5.14)

$$R = I_n - X(X^T X)^{-1} X^T = I_n - P \tag{9}$$

which also is an $n \times n$ matrix and can be reformulated as follows:

$$\begin{aligned}
R = I_n - P &= \begin{bmatrix} 1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 1 \end{bmatrix} - \begin{bmatrix} p_{11} & \cdots & p_{1n} \\ \vdots & \ddots & \vdots \\ p_{n1} & \cdots & p_{nn} \end{bmatrix} \\
&\stackrel{(4)}{=} \frac{1}{(n-1)s_x^2} \begin{bmatrix} x^T x - n\bar{x}^2 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & x^T x - n\bar{x}^2 \end{bmatrix} \\
&\quad - \frac{1}{(n-1)s_x^2} \begin{bmatrix} (x^T x/n) - 2\bar{x}x_1 + x_1^2 & \cdots & (x^T x/n) - \bar{x}(x_1 + x_n) + x_1 x_n \\ \vdots & \ddots & \vdots \\ (x^T x/n) - \bar{x}(x_1 + x_n) + x_1 x_n & \cdots & (x^T x/n) - 2\bar{x}x_n + x_n^2 \end{bmatrix} \\
&= \frac{1}{(n-1)s_x^2} \begin{bmatrix} (n-1)(x^T x/n) + \bar{x}(2x_1 - n\bar{x}) - x_1^2 & \cdots & -(x^T x/n) + \bar{x}(x_1 + x_n) - x_1 x_n \\ \vdots & \ddots & \vdots \\ -(x^T x/n) + \bar{x}(x_1 + x_n) - x_1 x_n & \cdots & (n-1)(x^T x/n) + \bar{x}(2x_n - n\bar{x}) - x_n^2 \end{bmatrix}.
\end{aligned} \tag{10}$$

■

1.4.16 Weighted least squares

Theorem: Given a simple linear regression model (\rightarrow III/1.4.1) with correlated observations

$$y = \beta_0 + \beta_1 x + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 V), \tag{1}$$

the parameters minimizing the weighted residual sum of squares (\rightarrow III/1.5.9) are given by

$$\begin{aligned}
\hat{\beta}_0 &= \frac{x^T V^{-1} x \mathbf{1}_n^T V^{-1} y - \mathbf{1}_n^T V^{-1} x x^T V^{-1} y}{x^T V^{-1} x \mathbf{1}_n^T V^{-1} \mathbf{1}_n - \mathbf{1}_n^T V^{-1} x x^T V^{-1} \mathbf{1}_n} \\
\hat{\beta}_1 &= \frac{\mathbf{1}_n^T V^{-1} \mathbf{1}_n x^T V^{-1} y - x^T V^{-1} \mathbf{1}_n \mathbf{1}_n^T V^{-1} y}{\mathbf{1}_n^T V^{-1} \mathbf{1}_n x^T V^{-1} x - x^T V^{-1} \mathbf{1}_n \mathbf{1}_n^T V^{-1} x}
\end{aligned} \tag{2}$$

where $\mathbf{1}_n$ is an $n \times 1$ vector of ones.

Proof: Let there be an $n \times n$ square matrix W , such that

$$W V W^T = I_n. \tag{3}$$

Since V is a covariance matrix and thus symmetric (\rightarrow I/1.15.4), W is also symmetric and can be expressed as the matrix square root of the inverse of V :

$$W V W = I_n \quad \Leftrightarrow \quad V = W^{-1} W^{-1} \quad \Leftrightarrow \quad V^{-1} = W W \quad \Leftrightarrow \quad W = V^{-1/2}. \tag{4}$$

Because β_0 is a scalar, (1) may also be written as

$$y = \beta_0 \mathbf{1}_n + \beta_1 x + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 V), \quad (5)$$

Left-multiplying (5) with W , the linear transformation theorem (\rightarrow II/4.1.14) implies that

$$Wy = \beta_0 W\mathbf{1}_n + \beta_1 Wx + W\varepsilon, \quad W\varepsilon \sim \mathcal{N}(0, \sigma^2 W V W^T). \quad (6)$$

Applying (3), we see that (6) is actually a linear regression model (\rightarrow III/1.5.1) with independent observations

$$\tilde{y} = \begin{bmatrix} \tilde{x}_0 & \tilde{x} \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} + \tilde{\varepsilon}, \quad \tilde{\varepsilon} \sim \mathcal{N}(0, \sigma^2 I_n) \quad (7)$$

where $\tilde{y} = Wy$, $\tilde{x}_0 = W\mathbf{1}_n$, $\tilde{x} = Wx$ and $\tilde{\varepsilon} = W\varepsilon$, such that we can apply the ordinary least squares solution (\rightarrow III/1.5.3) giving:

$$\begin{aligned} \hat{\beta} &= (\tilde{X}^T \tilde{X})^{-1} \tilde{X}^T \tilde{y} \\ &= \left(\begin{bmatrix} \tilde{x}_0^T \\ \tilde{x}^T \end{bmatrix} \begin{bmatrix} \tilde{x}_0 & \tilde{x} \end{bmatrix} \right)^{-1} \begin{bmatrix} \tilde{x}_0^T \\ \tilde{x}^T \end{bmatrix} \tilde{y} \\ &= \begin{bmatrix} \tilde{x}_0^T \tilde{x}_0 & \tilde{x}_0^T \tilde{x} \\ \tilde{x}^T \tilde{x}_0 & \tilde{x}^T \tilde{x} \end{bmatrix}^{-1} \begin{bmatrix} \tilde{x}_0^T \\ \tilde{x}^T \end{bmatrix} \tilde{y}. \end{aligned} \quad (8)$$

Applying the inverse of a 2×2 matrix, this reformulates to:

$$\begin{aligned} \hat{\beta} &= \frac{1}{\tilde{x}_0^T \tilde{x}_0 \tilde{x}^T \tilde{x} - \tilde{x}_0^T \tilde{x} \tilde{x}^T \tilde{x}_0} \begin{bmatrix} \tilde{x}^T \tilde{x} & -\tilde{x}_0^T \tilde{x} \\ -\tilde{x}^T \tilde{x}_0 & \tilde{x}_0^T \tilde{x}_0 \end{bmatrix}^{-1} \begin{bmatrix} \tilde{x}_0^T \\ \tilde{x}^T \end{bmatrix} \tilde{y} \\ &= \frac{1}{\tilde{x}_0^T \tilde{x}_0 \tilde{x}^T \tilde{x} - \tilde{x}_0^T \tilde{x} \tilde{x}^T \tilde{x}_0} \begin{bmatrix} \tilde{x}^T \tilde{x} \tilde{x}_0^T - \tilde{x}_0^T \tilde{x} \tilde{x}^T \\ \tilde{x}_0^T \tilde{x}_0 \tilde{x}^T - \tilde{x}^T \tilde{x}_0 \tilde{x}_0^T \end{bmatrix} \tilde{y} \\ &= \frac{1}{\tilde{x}_0^T \tilde{x}_0 \tilde{x}^T \tilde{x} - \tilde{x}_0^T \tilde{x} \tilde{x}^T \tilde{x}_0} \begin{bmatrix} \tilde{x}^T \tilde{x} \tilde{x}_0^T \tilde{y} - \tilde{x}_0^T \tilde{x} \tilde{x}^T \tilde{y} \\ \tilde{x}_0^T \tilde{x}_0 \tilde{x}^T \tilde{y} - \tilde{x}^T \tilde{x}_0 \tilde{x}_0^T \tilde{y} \end{bmatrix}. \end{aligned} \quad (9)$$

Reinserting $\tilde{x}_0 = W\mathbf{1}_n$, $\tilde{x} = Wx$ and $W^T W = W W^T = V^{-1}$, we finally have

$$\begin{aligned} \hat{\beta} &= \frac{1}{\mathbf{1}_n^T W^T W \mathbf{1}_n x^T W^T W x - \mathbf{1}_n^T W^T W x x^T W^T W \mathbf{1}_n} \begin{bmatrix} x^T W^T W x \mathbf{1}_n^T W^T W y - \mathbf{1}_n^T W^T W x x^T W^T W y \\ \mathbf{1}_n^T W^T W \mathbf{1}_n x^T W^T W y - x^T W^T W \mathbf{1}_n \mathbf{1}_n^T W^T W y \end{bmatrix} \\ &= \frac{1}{x^T V^{-1} x \mathbf{1}_n^T V^{-1} \mathbf{1}_n - \mathbf{1}_n^T V^{-1} x x^T V^{-1} \mathbf{1}_n} \begin{bmatrix} x^T V^{-1} x \mathbf{1}_n^T V^{-1} y - \mathbf{1}_n^T V^{-1} x x^T V^{-1} y \\ \mathbf{1}_n^T V^{-1} \mathbf{1}_n x^T V^{-1} y - x^T V^{-1} \mathbf{1}_n \mathbf{1}_n^T V^{-1} y \end{bmatrix} \\ &= \begin{bmatrix} \frac{x^T V^{-1} x \mathbf{1}_n^T V^{-1} y - \mathbf{1}_n^T V^{-1} x x^T V^{-1} y}{x^T V^{-1} x \mathbf{1}_n^T V^{-1} \mathbf{1}_n - \mathbf{1}_n^T V^{-1} x x^T V^{-1} \mathbf{1}_n} \\ \frac{\mathbf{1}_n^T V^{-1} \mathbf{1}_n x^T V^{-1} y - x^T V^{-1} \mathbf{1}_n \mathbf{1}_n^T V^{-1} y}{\mathbf{1}_n^T V^{-1} \mathbf{1}_n x^T V^{-1} x - x^T V^{-1} \mathbf{1}_n \mathbf{1}_n^T V^{-1} x} \end{bmatrix} \end{aligned} \quad (10)$$

which corresponds to the weighted least squares solution (2).

■

1.4.17 Weighted least squares

Theorem: Given a simple linear regression model (\rightarrow III/1.4.1) with correlated observations

$$y = \beta_0 + \beta_1 x + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 V), \quad (1)$$

the parameters minimizing the weighted residual sum of squares (\rightarrow III/1.5.9) are given by

$$\begin{aligned} \hat{\beta}_0 &= \frac{x^T V^{-1} x \mathbf{1}_n^T V^{-1} y - \mathbf{1}_n^T V^{-1} x x^T V^{-1} y}{x^T V^{-1} x \mathbf{1}_n^T V^{-1} \mathbf{1}_n - \mathbf{1}_n^T V^{-1} x x^T V^{-1} \mathbf{1}_n} \\ \hat{\beta}_1 &= \frac{\mathbf{1}_n^T V^{-1} \mathbf{1}_n x^T V^{-1} y - x^T V^{-1} \mathbf{1}_n \mathbf{1}_n^T V^{-1} y}{\mathbf{1}_n^T V^{-1} \mathbf{1}_n x^T V^{-1} x - x^T V^{-1} \mathbf{1}_n \mathbf{1}_n^T V^{-1} x} \end{aligned} \quad (2)$$

where $\mathbf{1}_n$ is an $n \times 1$ vector of ones.

Proof: Simple linear regression is a special case of multiple linear regression (\rightarrow III/1.4.2) with

$$X = \begin{bmatrix} \mathbf{1}_n & x \end{bmatrix} \quad \text{and} \quad \beta = \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} \quad (3)$$

and weighted least squares estimates (\rightarrow III/1.5.21) are given by

$$\hat{\beta} = (X^T V^{-1} X)^{-1} X^T V^{-1} y. \quad (4)$$

Writing out equation (4), we have

$$\begin{aligned} \hat{\beta} &= \left(\begin{bmatrix} \mathbf{1}_n^T \\ x^T \end{bmatrix} V^{-1} \begin{bmatrix} \mathbf{1}_n & x \end{bmatrix} \right)^{-1} \begin{bmatrix} \mathbf{1}_n^T \\ x^T \end{bmatrix} V^{-1} y \\ &= \begin{bmatrix} \mathbf{1}_n^T V^{-1} \mathbf{1}_n & \mathbf{1}_n^T V^{-1} x \\ x^T V^{-1} \mathbf{1}_n & x^T V^{-1} x \end{bmatrix}^{-1} \begin{bmatrix} \mathbf{1}_n^T V^{-1} y \\ x^T V^{-1} y \end{bmatrix} \\ &= \frac{1}{x^T V^{-1} x \mathbf{1}_n^T V^{-1} \mathbf{1}_n - \mathbf{1}_n^T V^{-1} x x^T V^{-1} \mathbf{1}_n} \begin{bmatrix} x^T V^{-1} x & -\mathbf{1}_n^T V^{-1} x \\ -x^T V^{-1} \mathbf{1}_n & \mathbf{1}_n^T V^{-1} \mathbf{1}_n \end{bmatrix} \begin{bmatrix} \mathbf{1}_n^T V^{-1} y \\ x^T V^{-1} y \end{bmatrix} \\ &= \frac{1}{x^T V^{-1} x \mathbf{1}_n^T V^{-1} \mathbf{1}_n - \mathbf{1}_n^T V^{-1} x x^T V^{-1} \mathbf{1}_n} \begin{bmatrix} x^T V^{-1} x \mathbf{1}_n^T V^{-1} y - \mathbf{1}_n^T V^{-1} x x^T V^{-1} y \\ \mathbf{1}_n^T V^{-1} \mathbf{1}_n x^T V^{-1} y - x^T V^{-1} \mathbf{1}_n \mathbf{1}_n^T V^{-1} y \end{bmatrix}. \end{aligned} \quad (5)$$

Thus, the first entry of $\hat{\beta}$ is equal to (\rightarrow III/1.4.16):

$$\hat{\beta}_0 = \frac{x^T V^{-1} x \mathbf{1}_n^T V^{-1} y - \mathbf{1}_n^T V^{-1} x x^T V^{-1} y}{x^T V^{-1} x \mathbf{1}_n^T V^{-1} \mathbf{1}_n - \mathbf{1}_n^T V^{-1} x x^T V^{-1} \mathbf{1}_n}. \quad (6)$$

Moreover, the second entry of $\hat{\beta}$ is equal to (\rightarrow III/1.4.16):

$$\hat{\beta}_1 = \frac{1_n^T V^{-1} 1_n x^T V^{-1} y - x^T V^{-1} 1_n 1_n^T V^{-1} y}{1_n^T V^{-1} 1_n x^T V^{-1} x - x^T V^{-1} 1_n 1_n^T V^{-1} x} . \quad (7)$$

■

1.4.18 Maximum likelihood estimation

Theorem: Given a simple linear regression model (\rightarrow III/1.5.1) with independent observations

$$y_i = \beta_0 + \beta_1 x_i + \varepsilon_i, \quad \varepsilon_i \sim \mathcal{N}(0, \sigma^2), \quad i = 1, \dots, n, \quad (1)$$

the maximum likelihood estimates (\rightarrow I/4.1.3) of β_0 , β_1 and σ^2 are given by

$$\begin{aligned} \hat{\beta}_0 &= \bar{y} - \hat{\beta}_1 \bar{x} \\ \hat{\beta}_1 &= \frac{s_{xy}}{s_x^2} \\ \hat{\sigma}^2 &= \frac{1}{n} \sum_{i=1}^n (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2 \end{aligned} \quad (2)$$

where \bar{x} and \bar{y} are the sample means (\rightarrow I/1.12.2), s_x^2 is the sample variance (\rightarrow I/1.13.2) of x and s_{xy} is the sample covariance (\rightarrow I/1.15.2) between x and y .

Proof: With the probability density function of the normal distribution (\rightarrow II/3.2.10) and probability under independence (\rightarrow I/1.3.6), the linear regression equation (1) implies the following likelihood function (\rightarrow I/5.1.2)

$$\begin{aligned} p(y|\beta_0, \beta_1, \sigma^2) &= \prod_{i=1}^n p(y_i|\beta_0, \beta_1, \sigma^2) \\ &= \prod_{i=1}^n \mathcal{N}(y_i; \beta_0 + \beta_1 x_i, \sigma^2) \\ &= \prod_{i=1}^n \frac{1}{\sqrt{2\pi\sigma}} \cdot \exp \left[-\frac{(y_i - \beta_0 - \beta_1 x_i)^2}{2\sigma^2} \right] \\ &= \frac{1}{\sqrt{(2\pi\sigma^2)^n}} \cdot \exp \left[-\frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)^2 \right] \end{aligned} \quad (3)$$

and the log-likelihood function (\rightarrow I/4.1.2)

$$\begin{aligned} \text{LL}(\beta_0, \beta_1, \sigma^2) &= \log p(y|\beta_0, \beta_1, \sigma^2) \\ &= -\frac{n}{2} \log(2\pi) - \frac{n}{2} \log(\sigma^2) - \frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)^2 . \end{aligned} \quad (4)$$

The derivative of the log-likelihood function (4) with respect to β_0 is

$$\frac{dLL(\beta_0, \beta_1, \sigma^2)}{d\beta_0} = \frac{1}{\sigma^2} \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i) \quad (5)$$

and setting this derivative to zero gives the MLE for β_0 :

$$\begin{aligned} \frac{dLL(\hat{\beta}_0, \hat{\beta}_1, \hat{\sigma}^2)}{d\beta_0} &= 0 \\ 0 &= \frac{1}{\hat{\sigma}^2} \sum_{i=1}^n (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i) \\ 0 &= \sum_{i=1}^n y_i - n\hat{\beta}_0 - \hat{\beta}_1 \sum_{i=1}^n x_i \\ \hat{\beta}_0 &= \frac{1}{n} \sum_{i=1}^n y_i - \hat{\beta}_1 \frac{1}{n} \sum_{i=1}^n x_i \\ \hat{\beta}_0 &= \bar{y} - \hat{\beta}_1 \bar{x} . \end{aligned} \quad (6)$$

The derivative of the log-likelihood function (4) at $\hat{\beta}_0$ with respect to β_1 is

$$\frac{dLL(\hat{\beta}_0, \beta_1, \sigma^2)}{d\beta_1} = \frac{1}{\sigma^2} \sum_{i=1}^n (x_i y_i - \hat{\beta}_0 x_i - \beta_1 x_i^2) \quad (7)$$

and setting this derivative to zero gives the MLE for β_1 :

$$\begin{aligned} \frac{dLL(\hat{\beta}_0, \hat{\beta}_1, \hat{\sigma}^2)}{d\beta_1} &= 0 \\ 0 &= \frac{1}{\hat{\sigma}^2} \sum_{i=1}^n (x_i y_i - \hat{\beta}_0 x_i - \hat{\beta}_1 x_i^2) \\ 0 &= \sum_{i=1}^n x_i y_i - \hat{\beta}_0 \sum_{i=1}^n x_i - \hat{\beta}_1 \sum_{i=1}^n x_i^2 \\ 0 &\stackrel{(6)}{=} \sum_{i=1}^n x_i y_i - (\bar{y} - \hat{\beta}_1 \bar{x}) \sum_{i=1}^n x_i - \hat{\beta}_1 \sum_{i=1}^n x_i^2 \\ 0 &= \sum_{i=1}^n x_i y_i - \bar{y} \sum_{i=1}^n x_i + \hat{\beta}_1 \bar{x} \sum_{i=1}^n x_i - \hat{\beta}_1 \sum_{i=1}^n x_i^2 \\ 0 &= \sum_{i=1}^n x_i y_i - n\bar{x}\bar{y} + \hat{\beta}_1 n\bar{x}^2 - \hat{\beta}_1 \sum_{i=1}^n x_i^2 \\ \hat{\beta}_1 &= \frac{\sum_{i=1}^n x_i y_i - \sum_{i=1}^n \bar{x}\bar{y}}{\sum_{i=1}^n x_i^2 - \sum_{i=1}^n \bar{x}^2} \\ \hat{\beta}_1 &= \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2} \\ \hat{\beta}_1 &= \frac{s_{xy}}{s_x^2} . \end{aligned} \quad (8)$$

The derivative of the log-likelihood function (4) at $(\hat{\beta}_0, \hat{\beta}_1)$ with respect to σ^2 is

$$\frac{dLL(\hat{\beta}_0, \hat{\beta}_1, \sigma^2)}{d\sigma^2} = -\frac{n}{2\sigma^2} + \frac{1}{2(\sigma^2)^2} \sum_{i=1}^n (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2 \quad (9)$$

and setting this derivative to zero gives the MLE for σ^2 :

$$\begin{aligned} \frac{dLL(\hat{\beta}_0, \hat{\beta}_1, \hat{\sigma}^2)}{d\hat{\sigma}^2} &= 0 \\ 0 &= -\frac{n}{2\hat{\sigma}^2} + \frac{1}{2(\hat{\sigma}^2)^2} \sum_{i=1}^n (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2 \\ \frac{n}{2\hat{\sigma}^2} &= \frac{1}{2(\hat{\sigma}^2)^2} \sum_{i=1}^n (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2 \\ \hat{\sigma}^2 &= \frac{1}{n} \sum_{i=1}^n (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2. \end{aligned} \quad (10)$$

Together, (6), (8) and (10) constitute the MLE for simple linear regression. ■

1.4.19 Maximum likelihood estimation

Theorem: Given a simple linear regression model (\rightarrow III/1.5.1) with independent observations

$$y_i = \beta_0 + \beta_1 x_i + \varepsilon_i, \quad \varepsilon_i \sim \mathcal{N}(0, \sigma^2), \quad i = 1, \dots, n, \quad (1)$$

the maximum likelihood estimates (\rightarrow I/4.1.3) of β_0 , β_1 and σ^2 are given by

$$\begin{aligned} \hat{\beta}_0 &= \bar{y} - \hat{\beta}_1 \bar{x} \\ \hat{\beta}_1 &= \frac{s_{xy}}{s_x^2} \\ \hat{\sigma}^2 &= \frac{1}{n} \sum_{i=1}^n (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2 \end{aligned} \quad (2)$$

where \bar{x} and \bar{y} are the sample means (\rightarrow I/1.12.2), s_x^2 is the sample variance (\rightarrow I/1.13.2) of x and s_{xy} is the sample covariance (\rightarrow I/1.15.2) between x and y .

Proof: Simple linear regression is a special case of multiple linear regression (\rightarrow III/1.4.2) with

$$X = \begin{bmatrix} 1_n & x \end{bmatrix} \quad \text{and} \quad \beta = \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} \quad (3)$$

and maximum likelihood estimates (\rightarrow III/1.5.23) are given by

$$\begin{aligned} \hat{\beta} &= (X^T V^{-1} X)^{-1} X^T V^{-1} y \\ \hat{\sigma}^2 &= \frac{1}{n} (y - X \hat{\beta})^T V^{-1} (y - X \hat{\beta}). \end{aligned} \quad (4)$$

Under independent observations, the covariance matrix is

$$V = I_n, \quad \text{such that} \quad V^{-1} = I_n. \quad (5)$$

Thus, we can write out the estimate of β

$$\begin{aligned} \hat{\beta} &= \left(\begin{bmatrix} 1_n^T \\ x^T \end{bmatrix} V^{-1} \begin{bmatrix} 1_n & x \end{bmatrix} \right)^{-1} \begin{bmatrix} 1_n^T \\ x^T \end{bmatrix} V^{-1} y \\ &= \left(\begin{bmatrix} 1_n^T \\ x^T \end{bmatrix} \begin{bmatrix} 1_n & x \end{bmatrix} \right)^{-1} \begin{bmatrix} 1_n^T \\ x^T \end{bmatrix} y \end{aligned} \quad (6)$$

which is equal to the ordinary least squares solution for simple linear regression (\rightarrow III/1.4.4):

$$\begin{aligned} \hat{\beta}_0 &= \bar{y} - \hat{\beta}_1 \bar{x} \\ \hat{\beta}_1 &= \frac{s_{xy}}{s_x^2}. \end{aligned} \quad (7)$$

Additionally, we can write out the estimate of σ^2 :

$$\begin{aligned} \hat{\sigma}^2 &= \frac{1}{n} (y - X\hat{\beta})^T V^{-1} (y - X\hat{\beta}) \\ &= \frac{1}{n} \left(y - \begin{bmatrix} 1_n & x \end{bmatrix} \begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \end{bmatrix} \right)^T \left(y - \begin{bmatrix} 1_n & x \end{bmatrix} \begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \end{bmatrix} \right) \\ &= \frac{1}{n} (y - \hat{\beta}_0 - \hat{\beta}_1 x)^T (y - \hat{\beta}_0 - \hat{\beta}_1 x) \\ &= \frac{1}{n} \sum_{i=1}^n (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2. \end{aligned} \quad (8)$$

■

1.4.20 t-test for intercept parameter

Theorem: Consider a simple linear regression model (\rightarrow III/1.4.1) with independent observations

$$y_i = \beta_0 + \beta_1 x_i + \varepsilon_i, \quad \varepsilon_i \sim \mathcal{N}(0, \sigma^2), \quad i = 1, \dots, n, \quad (1)$$

and the parameter estimates (\rightarrow III/1.4.18)

$$\begin{aligned} \hat{\beta}_0 &= \bar{y} - \hat{\beta}_1 \bar{x} \\ \hat{\beta}_1 &= \frac{s_{xy}}{s_x^2} \\ \hat{\sigma}^2 &= \frac{1}{n-2} \sum_{i=1}^n (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2. \end{aligned} \quad (2)$$

where \bar{x} and \bar{y} are the sample means (\rightarrow I/1.12.2) of the x_i and y_i , s_{xy} is the sample covariance (\rightarrow I/1.15.2) of the x_i and y_i and s_x^2 is the sample variance (\rightarrow I/1.13.2) of the x_i . Then, the test statistic (\rightarrow I/4.3.5)

$$t_0 = \frac{\bar{y} - \hat{\beta}_1 \bar{x}}{\sqrt{\hat{\sigma}^2} \sigma_0} \quad (3)$$

with σ_0 equal to the first diagonal element of the parameter covariance matrix (\rightarrow III/1.4.7)

$$\sigma_0 = \frac{x^T x / n}{(n-1) s_x^2} \quad \text{where} \quad s_x^2 = \frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x})^2 \quad (4)$$

follows a t-distribution (\rightarrow II/3.3.1)

$$t_0 \sim t(n-2) \quad (5)$$

under the null hypothesis (\rightarrow I/4.3.2) that the intercept parameter (\rightarrow III/1.4.1) is zero:

$$H_0 : \beta_0 = 0. \quad (6)$$

Proof: In multiple linear regression (\rightarrow III/1.5.1), the contrast-based t-test (\rightarrow III/1.5.28) is based on the t-statistic (\rightarrow I/4.3.5)

$$t = \frac{c^T \hat{\beta}}{\sqrt{\hat{\sigma}^2 c^T (X^T V^{-1} X)^{-1} c}} \quad (7)$$

which follows a t-distribution (\rightarrow II/3.3.1) under the null hypothesis (\rightarrow I/4.3.2) that the scalar product of the contrast vector (\rightarrow III/1.5.26) and the regression coefficients (\rightarrow III/1.5.1) is zero:

$$t \sim t(n-p), \quad \text{if} \quad c^T \beta = 0. \quad (8)$$

Since simple linear regression is a special case of multiple linear regression (\rightarrow III/1.4.2), in the present case we have the following quantities:

$$\beta = \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}, \quad \hat{\beta} = \begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \end{bmatrix}, \quad c_0 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad X = \begin{bmatrix} 1_n & x \end{bmatrix}, \quad V = I_n. \quad (9)$$

Thus, we have the null hypothesis

$$H_0 : c_0^T \beta = \begin{bmatrix} 1 \\ 0 \end{bmatrix}^T \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} = \beta_0 = 0 \quad (10)$$

and the contrast estimate

$$c_0^T \hat{\beta} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}^T \begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \end{bmatrix} = \hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}. \quad (11)$$

Moreover, when deriving the distribution of ordinary least squares parameter estimates for simple linear regression with independent observations (\rightarrow III/1.4.7), we have identified the parameter covariance matrix as

$$(X^T X)^{-1} = \frac{1}{(n-1)s_x^2} \cdot \begin{bmatrix} x^T x/n & -\bar{x} \\ -\bar{x} & 1 \end{bmatrix}. \quad (12)$$

Plugging (9), (11), (12) and (2) into (7), the test statistic becomes

$$\begin{aligned} t_0 &= \frac{c_0^T \hat{\beta}}{\sqrt{\hat{\sigma}^2 c_0^T (X^T X)^{-1} c_0}} \\ &= \frac{\begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} \hat{\beta}_0 & \hat{\beta}_1 \end{bmatrix}^T}{\sqrt{\hat{\sigma}^2 \begin{bmatrix} 1 & 0 \end{bmatrix} (X^T X)^{-1} \begin{bmatrix} 1 & 0 \end{bmatrix}^T}} \\ &= \frac{\begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} \hat{\beta}_0 & \hat{\beta}_1 \end{bmatrix}^T}{\sqrt{\hat{\sigma}^2 \begin{bmatrix} 1 & 0 \end{bmatrix} \left(\frac{1}{(n-1)s_x^2} \cdot \begin{bmatrix} x^T x/n & -\bar{x} \\ -\bar{x} & 1 \end{bmatrix} \right) \begin{bmatrix} 1 & 0 \end{bmatrix}^T}} \\ &= \frac{\hat{\beta}_0}{\sqrt{\hat{\sigma}^2 \left(\frac{x^T x/n}{(n-1)s_x^2} \right)}} \\ &= \frac{\bar{y} - \hat{\beta}_1 \bar{x}}{\sqrt{\hat{\sigma}^2} \sigma_0}. \end{aligned} \quad (13)$$

Finally, because $X = \begin{bmatrix} 1_n & x \end{bmatrix}$ is an $n \times 2$ matrix, we have $p = 2$, such that from (8), it follows that

$$t_0 \sim t(n-2), \quad \text{if } \beta_0 = 0. \quad (14)$$

■

1.4.21 t-test for slope parameter

Theorem: Consider a simple linear regression model (\rightarrow III/1.4.1) with independent observations

$$y_i = \beta_0 + \beta_1 x_i + \varepsilon_i, \quad \varepsilon_i \sim \mathcal{N}(0, \sigma^2), \quad i = 1, \dots, n, \quad (1)$$

and the parameter estimates (\rightarrow III/1.4.18)

$$\begin{aligned} \hat{\beta}_0 &= \bar{y} - \hat{\beta}_1 \bar{x} \\ \hat{\beta}_1 &= \frac{s_{xy}}{s_x^2} \\ \hat{\sigma}^2 &= \frac{1}{n-2} \sum_{i=1}^n (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2. \end{aligned} \quad (2)$$

where \bar{x} and \bar{y} are the sample means (\rightarrow I/1.12.2) of the x_i and y_i , s_{xy} is the sample covariance (\rightarrow I/1.15.2) of the x_i and y_i and s_x^2 is the sample variance (\rightarrow I/1.13.2) of the x_i .

Then, the test statistic (\rightarrow I/4.3.5)

$$t_1 = \frac{s_{xy}/s_x^2}{\sqrt{\hat{\sigma}^2} \sigma_1} \quad (3)$$

with σ_1 equal to the first diagonal element of the parameter covariance matrix (\rightarrow III/1.4.7)

$$\sigma_1 = \frac{1}{\sum_{i=1}^n (x_i - \bar{x})^2} \quad (4)$$

follows a t-distribution (\rightarrow II/3.3.1)

$$t_1 \sim t(n-2) \quad (5)$$

under the null hypothesis (\rightarrow I/4.3.2) that the slope parameter (\rightarrow III/1.4.1) is zero:

$$H_0 : \beta_1 = 0 . \quad (6)$$

Proof: In multiple linear regression (\rightarrow III/1.5.1), the contrast-based t-test (\rightarrow III/1.5.28) is based on the t-statistic (\rightarrow I/4.3.5)

$$t = \frac{c^T \hat{\beta}}{\sqrt{\hat{\sigma}^2 c^T (X^T V^{-1} X)^{-1} c}} \quad (7)$$

which follows a t-distribution (\rightarrow II/3.3.1) under the null hypothesis (\rightarrow I/4.3.2) that the scalar product of the contrast vector (\rightarrow III/1.5.26) and the regression coefficients (\rightarrow III/1.5.1) is zero:

$$t \sim t(n-p), \quad \text{if } c^T \beta = 0 . \quad (8)$$

Since simple linear regression is a special case of multiple linear regression (\rightarrow III/1.4.2), in the present case we have the following quantities:

$$\beta = \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}, \quad \hat{\beta} = \begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \end{bmatrix}, \quad c_1 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \quad X = \begin{bmatrix} 1_n & x \end{bmatrix}, \quad V = I_n . \quad (9)$$

Thus, we have the null hypothesis

$$H_0 : c_1^T \beta = \begin{bmatrix} 0 \\ 1 \end{bmatrix}^T \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} = \beta_1 = 0 \quad (10)$$

and the contrast estimate

$$c_1^T \hat{\beta} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}^T \begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \end{bmatrix} = \hat{\beta}_1 = \frac{s_{xy}}{s_x^2} . \quad (11)$$

Moreover, when deriving the distribution of ordinary least squares parameter estimates for simple linear regression with independent observations (\rightarrow III/1.4.7), we have identified the parameter covariance matrix as

$$(X^T X)^{-1} = \frac{1}{(n-1)s_x^2} \cdot \begin{bmatrix} x^T x/n & -\bar{x} \\ -\bar{x} & 1 \end{bmatrix}. \quad (12)$$

Plugging (9), (11), (12) and (2) into (7), the test statistic becomes

$$\begin{aligned} t_1 &= \frac{c_1^T \hat{\beta}}{\sqrt{\hat{\sigma}^2 c_1^T (X^T X)^{-1} c_1}} \\ &= \frac{\begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} \hat{\beta}_0 & \hat{\beta}_1 \end{bmatrix}^T}{\sqrt{\hat{\sigma}^2 \begin{bmatrix} 0 & 1 \end{bmatrix} (X^T X)^{-1} \begin{bmatrix} 0 & 1 \end{bmatrix}^T}} \\ &= \frac{\begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} \hat{\beta}_0 & \hat{\beta}_1 \end{bmatrix}^T}{\sqrt{\hat{\sigma}^2 \begin{bmatrix} 0 & 1 \end{bmatrix} \left(\frac{1}{(n-1)s_x^2} \cdot \begin{bmatrix} x^T x/n & -\bar{x} \\ -\bar{x} & 1 \end{bmatrix} \right) \begin{bmatrix} 0 & 1 \end{bmatrix}^T}} \\ &= \frac{\hat{\beta}_1}{\sqrt{\hat{\sigma}^2 \left(\frac{1}{(n-1)s_x^2} \right)}} \\ &= \frac{\hat{\beta}_1}{\sqrt{\hat{\sigma}^2 / \sum_{i=1}^n (x_i - \bar{x})^2}} \\ &= \frac{s_{xy}/s_x^2}{\sqrt{\hat{\sigma}^2} \sigma_1}. \end{aligned} \quad (13)$$

Finally, because $X = \begin{bmatrix} 1_n & x \end{bmatrix}$ is an $n \times 2$ matrix, we have $p = 2$, such that from (8) it follows that

$$t_1 \sim t(n-2), \quad \text{if } \beta_1 = 0. \quad (14)$$

■

1.4.22 F-test for model comparison

Theorem: Consider a simple linear regression model (\rightarrow III/1.4.1) with independent observations

$$y_i = \beta_0 + \beta_1 x_i + \varepsilon_i, \quad \varepsilon_i \sim \mathcal{N}(0, \sigma^2), \quad i = 1, \dots, n, \quad (1)$$

and the parameter estimates (\rightarrow III/1.4.18)

$$\begin{aligned} \hat{\beta}_0 &= \bar{y} - \hat{\beta}_1 \bar{x} \\ \hat{\beta}_1 &= \frac{s_{xy}}{s_x^2} \\ \hat{\sigma}^2 &= \frac{1}{n-2} \sum_{i=1}^n (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2. \end{aligned} \quad (2)$$

where \bar{x} and \bar{y} are the sample means (\rightarrow I/1.12.2) of the x_i and y_i , s_{xy} is the sample covariance (\rightarrow I/1.15.2) of the x_i and y_i and s_x^2 is the sample variance (\rightarrow I/1.13.2) of the x_i . Then, the test statistic (\rightarrow I/4.3.5)

$$F = \frac{s_{xy}^2/s_x^2}{\hat{\sigma}^2/(n-1)} \quad (3)$$

follows an F-distribution (\rightarrow II/3.8.1)

$$F \sim F(1, n-2) \quad (4)$$

under the scenario that the data were generated using a model in which the slope parameter (\rightarrow III/1.4.1) is zero:

$$H_0 : \beta_1 = 0. \quad (5)$$

Proof: In multiple linear regression (\rightarrow III/1.5.1), the contrast-based F-test (\rightarrow III/1.5.29) is based on the F-statistic (\rightarrow I/4.3.5)

$$F = \hat{\beta}^T C (\hat{\sigma}^2 C^T (X^T V^{-1} X)^{-1} C)^{-1} C^T \hat{\beta} / q \quad (6)$$

which follows an F-distribution (\rightarrow II/3.8.1) under the null hypothesis (\rightarrow I/4.3.2) that the product of the contrast matrix (\rightarrow III/1.5.27) $C \in \mathbb{R}^{p \times q}$ and the regression coefficients (\rightarrow III/1.5.1) is a zero vector:

$$F \sim F(q, n-p), \quad \text{if } C^T \beta = 0_q = [0, \dots, 0]^T. \quad (7)$$

Since simple linear regression is a special case of multiple linear regression (\rightarrow III/1.4.2), we have the following quantities, if we want to compare the regression model against a model without the slope parameter:

$$\beta = \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}, \quad \hat{\beta} = \begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \end{bmatrix}, \quad C = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \quad X = \begin{bmatrix} 1_n & x \end{bmatrix}, \quad V = I_n. \quad (8)$$

Thus, we have the null hypothesis

$$H_0 : C^T \beta = \begin{bmatrix} 0 \\ 1 \end{bmatrix}^T \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} = \beta_1 = 0 \quad (9)$$

and the contrast estimate

$$C^T \hat{\beta} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}^T \begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \end{bmatrix} = \hat{\beta}_1 = \frac{s_{xy}}{s_x^2}. \quad (10)$$

Moreover, when deriving the distribution of ordinary least squares parameter estimates for simple linear regression with independent observations (\rightarrow III/1.4.7), we have identified the parameter covariance matrix as

$$(X^T X)^{-1} = \frac{1}{(n-1)s_x^2} \cdot \begin{bmatrix} x^T x/n & -\bar{x} \\ -\bar{x} & 1 \end{bmatrix}. \quad (11)$$

Plugging (8), (10), (11) and (2) into (6), the test statistic becomes

$$\begin{aligned} F &= \hat{\beta}^T C (\hat{\sigma}^2 C^T (X^T V^{-1} X)^{-1} C)^{-1} C^T \hat{\beta} / q \\ &= \left(\frac{s_{xy}}{s_x^2} \right) \left(\hat{\sigma}^2 \begin{bmatrix} 0 & 1 \end{bmatrix} \left(\frac{1}{(n-1)s_x^2} \cdot \begin{bmatrix} x^T x/n & -\bar{x} \\ -\bar{x} & 1 \end{bmatrix} \right) \begin{bmatrix} 0 & 1 \end{bmatrix}^T \right)^{-1} \left(\frac{s_{xy}}{s_x^2} \right) / 1 \\ &= \frac{s_{xy}^2 / (s_x^2)^2}{\hat{\sigma}^2 / ((n-1)s_x^2)} \\ &= \frac{s_{xy}^2 / s_x^2}{\hat{\sigma}^2 / (n-1)}. \end{aligned} \quad (12)$$

Finally, because $C = \begin{bmatrix} 0 & 1 \end{bmatrix}^T \in \mathbb{R}^{2 \times 1}$ and $X = \begin{bmatrix} 1_n & x \end{bmatrix} \in \mathbb{R}^{n \times 2}$, we have $p = 2$ and $q = 1$, such that from (7) it follows that

$$F \sim F(1, n-2), \quad \text{if } \beta_1 = 0. \quad (13)$$

■

1.4.23 Sum of residuals is zero

Theorem: In simple linear regression (\rightarrow III/1.4.1), the sum of the residuals (\rightarrow III/1.5.9) is zero when estimated using ordinary least squares (\rightarrow III/1.4.3).

Proof: The residuals are defined as the estimated error terms (\rightarrow III/1.4.1)

$$\hat{\varepsilon}_i = y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i \quad (1)$$

where $\hat{\beta}_0$ and $\hat{\beta}_1$ are parameter estimates obtained using ordinary least squares (\rightarrow III/1.4.3):

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x} \quad \text{and} \quad \hat{\beta}_1 = \frac{s_{xy}}{s_x^2}. \quad (2)$$

With that, we can calculate the sum of the residuals:

$$\begin{aligned} \sum_{i=1}^n \hat{\varepsilon}_i &= \sum_{i=1}^n (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i) \\ &= \sum_{i=1}^n (y_i - \bar{y} + \hat{\beta}_1 \bar{x} - \hat{\beta}_1 x_i) \\ &= \sum_{i=1}^n y_i - n\bar{y} + \hat{\beta}_1 n\bar{x} - \hat{\beta}_1 \sum_{i=1}^n x_i \\ &= n\bar{y} - n\bar{y} + \hat{\beta}_1 n\bar{x} - \hat{\beta}_1 n\bar{x} \\ &= 0. \end{aligned} \quad (3)$$

Thus, the sum of the residuals (\rightarrow III/1.5.9) is zero under ordinary least squares (\rightarrow III/1.4.3), if the model (\rightarrow III/1.4.1) includes an intercept term β_0 . ■

Sources:

- Wikipedia (2021): “Simple linear regression”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-10-27; URL: https://en.wikipedia.org/wiki/Simple_linear_regression#Numerical_properties.

1.4.24 Correlation with covariate is zero

Theorem: In simple linear regression (\rightarrow III/1.4.1), the residuals (\rightarrow III/1.5.9) and the covariate (\rightarrow III/1.4.1) are uncorrelated (\rightarrow I/1.17.1) when estimated using ordinary least squares (\rightarrow III/1.4.3).

Proof: The residuals are defined as the estimated error terms (\rightarrow III/1.4.1)

$$\hat{\varepsilon}_i = y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i \quad (1)$$

where $\hat{\beta}_0$ and $\hat{\beta}_1$ are parameter estimates obtained using ordinary least squares (\rightarrow III/1.4.3):

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x} \quad \text{and} \quad \hat{\beta}_1 = \frac{s_{xy}}{s_x^2}. \quad (2)$$

With that, we can calculate the inner product of the covariate and the residuals vector:

$$\begin{aligned}
\sum_{i=1}^n x_i \hat{\varepsilon}_i &= \sum_{i=1}^n x_i (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i) \\
&= \sum_{i=1}^n (x_i y_i - \hat{\beta}_0 x_i - \hat{\beta}_1 x_i^2) \\
&= \sum_{i=1}^n (x_i y_i - x_i (\bar{y} - \hat{\beta}_1 \bar{x}) - \hat{\beta}_1 x_i^2) \\
&= \sum_{i=1}^n (x_i (y_i - \bar{y}) + \hat{\beta}_1 (\bar{x} x_i - x_i^2)) \\
&= \sum_{i=1}^n x_i y_i - \bar{y} \sum_{i=1}^n x_i - \hat{\beta}_1 \left(\sum_{i=1}^n x_i^2 - \bar{x} \sum_{i=1}^n x_i \right) \\
&= \left(\sum_{i=1}^n x_i y_i - n \bar{x} \bar{y} - n \bar{x} \bar{y} + n \bar{x} \bar{y} \right) - \hat{\beta}_1 \left(\sum_{i=1}^n x_i^2 - 2n \bar{x} \bar{x} + n \bar{x}^2 \right) \\
&= \left(\sum_{i=1}^n x_i y_i - \bar{y} \sum_{i=1}^n x_i - \bar{x} \sum_{i=1}^n y_i + n \bar{x} \bar{y} \right) - \hat{\beta}_1 \left(\sum_{i=1}^n x_i^2 - 2\bar{x} \sum_{i=1}^n x_i + n \bar{x}^2 \right) \\
&= \sum_{i=1}^n (x_i y_i - \bar{y} x_i - \bar{x} y_i + \bar{x} \bar{y}) - \hat{\beta}_1 \sum_{i=1}^n (x_i^2 - 2\bar{x} x_i + \bar{x}^2) \\
&= \sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y}) - \hat{\beta}_1 \sum_{i=1}^n (x_i - \bar{x})^2 \\
&= (n-1) s_{xy} - \frac{s_{xy}}{s_x^2} (n-1) s_x^2 \\
&= (n-1) s_{xy} - (n-1) s_{xy} \\
&= 0.
\end{aligned} \tag{3}$$

Because an inner product of zero also implies zero correlation (\rightarrow I/1.17.1), this demonstrates that residuals (\rightarrow III/1.5.9) and covariate (\rightarrow III/1.4.1) values are uncorrelated under ordinary least squares (\rightarrow III/1.4.3).

■

Sources:

- Wikipedia (2021): “Simple linear regression”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-10-27; URL: https://en.wikipedia.org/wiki/Simple_linear_regression#Numerical_properties.

1.4.25 Residual variance in terms of sample variance

Theorem: Assume a simple linear regression model (\rightarrow III/1.4.1) with independent observations

$$y = \beta_0 + \beta_1 x + \varepsilon, \quad \varepsilon_i \sim \mathcal{N}(0, \sigma^2), \quad i = 1, \dots, n \tag{1}$$

and consider estimation using ordinary least squares (\rightarrow III/1.4.3). Then, residual variance (\rightarrow IV/1.1.1) and sample variance (\rightarrow I/1.13.2) are related to each other via the correlation coefficient (\rightarrow I/1.17.1):

$$\hat{\sigma}^2 = (1 - r_{xy}^2) s_y^2. \quad (2)$$

Proof: The residual variance (\rightarrow IV/1.1.1) can be expressed in terms of the residual sum of squares (\rightarrow III/1.5.9):

$$\hat{\sigma}^2 = \frac{1}{n-1} \text{RSS}(\hat{\beta}_0, \hat{\beta}_1) \quad (3)$$

and the residual sum of squares for simple linear regression (\rightarrow III/1.4.13) is

$$\text{RSS}(\hat{\beta}_0, \hat{\beta}_1) = (n-1) \left(s_y^2 - \frac{s_{xy}^2}{s_x^2} \right). \quad (4)$$

Combining (3) and (4), we obtain:

$$\begin{aligned} \hat{\sigma}^2 &= \left(s_y^2 - \frac{s_{xy}^2}{s_x^2} \right) \\ &= \left(1 - \frac{s_{xy}^2}{s_x^2 s_y^2} \right) s_y^2 \\ &= \left(1 - \left(\frac{s_{xy}}{s_x s_y} \right)^2 \right) s_y^2. \end{aligned} \quad (5)$$

Using the relationship between correlation, covariance and standard deviation (\rightarrow I/1.17.1)

$$\text{Corr}(X, Y) = \frac{\text{Cov}(X, Y)}{\sqrt{\text{Var}(X)} \sqrt{\text{Var}(Y)}} \quad (6)$$

which also holds for sample correlation, sample covariance (\rightarrow I/1.15.2) and sample standard deviation (\rightarrow I/1.19.1)

$$r_{xy} = \frac{s_{xy}}{s_x s_y}, \quad (7)$$

we get the final result:

$$\hat{\sigma}^2 = (1 - r_{xy}^2) s_y^2. \quad (8)$$

■

Sources:

- Penny, William (2006): “Relation to correlation”; in: *Mathematics for Brain Imaging*, ch. 1.2.3, p. 18, eq. 1.28; URL: https://ueapsylabs.co.uk/sites/wpenny/mbi/mbi_course.pdf.
- Wikipedia (2021): “Simple linear regression”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-10-27; URL: https://en.wikipedia.org/wiki/Simple_linear_regression#Numerical_properties.

1.4.26 Correlation coefficient in terms of slope estimate

Theorem: Assume a simple linear regression model (\rightarrow III/1.4.1) with independent observations

$$y = \beta_0 + \beta_1 x + \varepsilon, \quad \varepsilon_i \sim \mathcal{N}(0, \sigma^2), \quad i = 1, \dots, n \quad (1)$$

and consider estimation using ordinary least squares (\rightarrow III/1.4.3). Then, correlation coefficient (\rightarrow I/1.17.4) and the estimated value of the slope parameter (\rightarrow III/1.4.1) are related to each other via the sample (\rightarrow I/1.13.2) standard deviations (\rightarrow I/1.19.1):

$$r_{xy} = \frac{s_x}{s_y} \hat{\beta}_1. \quad (2)$$

Proof: The ordinary least squares estimate of the slope (\rightarrow III/1.4.3) is given by

$$\hat{\beta}_1 = \frac{s_{xy}}{s_x^2}. \quad (3)$$

Using the relationship between covariance and correlation (\rightarrow I/1.15.8)

$$\text{Cov}(X, Y) = \sigma_X \text{Corr}(X, Y) \sigma_Y \quad (4)$$

which also holds for sample correlation (\rightarrow I/1.17.4) and sample covariance (\rightarrow I/1.15.2)

$$s_{xy} = s_x r_{xy} s_y, \quad (5)$$

we get the final result:

$$\begin{aligned} \hat{\beta}_1 &= \frac{s_{xy}}{s_x^2} \\ \hat{\beta}_1 &= \frac{s_x r_{xy} s_y}{s_x^2} \\ \hat{\beta}_1 &= \frac{s_y}{s_x} r_{xy} \\ \Leftrightarrow r_{xy} &= \frac{s_x}{s_y} \hat{\beta}_1. \end{aligned} \quad (6)$$

■

Sources:

- Penny, William (2006): “Relation to correlation”; in: *Mathematics for Brain Imaging*, ch. 1.2.3, p. 18, eq. 1.27; URL: https://ueapsylabs.co.uk/sites/wpenny/mbi/mbi_course.pdf.
- Wikipedia (2021): “Simple linear regression”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-10-27; URL: https://en.wikipedia.org/wiki/Simple_linear_regression#Fitting_the_regression_line.

1.4.27 Coefficient of determination in terms of correlation coefficient

Theorem: Assume a simple linear regression model (\rightarrow III/1.4.1) with independent observations

$$y = \beta_0 + \beta_1 x + \varepsilon, \quad \varepsilon_i \sim \mathcal{N}(0, \sigma^2), \quad i = 1, \dots, n \quad (1)$$

and consider estimation using ordinary least squares (\rightarrow III/1.4.3). Then, the coefficient of determination (\rightarrow IV/1.2.1) is equal to the squared correlation coefficient (\rightarrow I/1.17.4) between x and y :

$$R^2 = r_{xy}^2 . \quad (2)$$

Proof: The ordinary least squares estimates for simple linear regression (\rightarrow III/1.4.3) are

$$\begin{aligned} \hat{\beta}_0 &= \bar{y} - \hat{\beta}_1 \bar{x} \\ \hat{\beta}_1 &= \frac{s_{xy}}{s_x^2} . \end{aligned} \quad (3)$$

The coefficient of determination (\rightarrow IV/1.2.1) R^2 is defined as the proportion of the variance explained by the independent variables, relative to the total variance in the data. This can be quantified as the ratio of explained sum of squares (\rightarrow III/1.5.8) to total sum of squares (\rightarrow III/1.5.7):

$$R^2 = \frac{\text{ESS}}{\text{TSS}} . \quad (4)$$

Using the explained and total sum of squares for simple linear regression (\rightarrow III/1.4.13), we have:

$$\begin{aligned} R^2 &= \frac{\sum_{i=1}^n (\hat{y}_i - \bar{y})^2}{\sum_{i=1}^n (y_i - \bar{y})^2} \\ &= \frac{\sum_{i=1}^n (\hat{\beta}_0 + \hat{\beta}_1 x_i - \bar{y})^2}{\sum_{i=1}^n (y_i - \bar{y})^2} . \end{aligned} \quad (5)$$

By applying (3), we can further develop the coefficient of determination:

$$\begin{aligned} R^2 &= \frac{\sum_{i=1}^n (\bar{y} - \hat{\beta}_1 \bar{x} + \hat{\beta}_1 x_i - \bar{y})^2}{\sum_{i=1}^n (y_i - \bar{y})^2} \\ &= \frac{\sum_{i=1}^n \left(\hat{\beta}_1 (x_i - \bar{x}) \right)^2}{\sum_{i=1}^n (y_i - \bar{y})^2} \\ &= \hat{\beta}_1^2 \frac{\frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x})^2}{\frac{1}{n-1} \sum_{i=1}^n (y_i - \bar{y})^2} \\ &= \hat{\beta}_1^2 \frac{s_x^2}{s_y^2} \\ &= \left(\frac{s_x}{s_y} \hat{\beta}_1 \right)^2 . \end{aligned} \quad (6)$$

Using the relationship between correlation coefficient and slope estimate (\rightarrow III/1.4.26), we conclude:

$$R^2 = \left(\frac{s_x}{s_y} \hat{\beta}_1 \right)^2 = r_{xy}^2 . \quad (7)$$

■

Sources:

- Wikipedia (2021): “Simple linear regression”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-10-27; URL: https://en.wikipedia.org/wiki/Simple_linear_regression#Fitting_the_regression_line.
- Wikipedia (2021): “Coefficient of determination”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-10-27; URL: https://en.wikipedia.org/wiki/Coefficient_of_determination#As_squared_correlation_coefficient.
- Wikipedia (2021): “Correlation”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-10-27; URL: https://en.wikipedia.org/wiki/Correlation#Sample_correlation_coefficient.

1.5 Multiple linear regression

1.5.1 Definition

Definition: Let y be an $n \times 1$ vector and let X be an $n \times p$ matrix. Then, a statement asserting a linear combination of X into y

$$y = X\beta + \varepsilon, \quad (1)$$

together with a statement asserting a normal distribution (\rightarrow II/4.1.1) for ε

$$\varepsilon \sim \mathcal{N}(0, \sigma^2 V) \quad (2)$$

is called a univariate linear regression model or simply, “multiple linear regression”.

- y is called “measured data”, “dependent variable” or “measurements”;
- X is called “design matrix”, “set of independent variables” or “predictors”;
- V is called “covariance matrix” or “covariance structure”;
- β are called “regression coefficients” or “weights”;
- ε is called “noise”, “errors” or “error terms”;
- σ^2 is called “noise variance” or “error variance”;
- n is the number of observations;
- p is the number of predictors.

Alternatively, the linear combination may also be written as

$$y = \sum_{i=1}^p \beta_i x_i + \varepsilon \quad (3)$$

or, when the model includes an intercept term, as

$$y = \beta_0 + \sum_{i=1}^p \beta_i x_i + \varepsilon \quad (4)$$

which is equivalent to adding a constant regressor $x_0 = 1_n$ to the design matrix X .

When the covariance structure V is equal to the $n \times n$ identity matrix, this is called multiple linear regression with independent and identically distributed (\rightarrow I/1.2.8) (i.i.d.) observations:

$$V = I_n \quad \Rightarrow \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 I_n) \quad \Rightarrow \quad \varepsilon_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2). \quad (5)$$

Otherwise, it is called multiple linear regression with correlated observations (\rightarrow I/1.17.1).

Sources:

- Wikipedia (2020): “Linear regression”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-03-21; URL: https://en.wikipedia.org/wiki/Linear_regression#Simple_and_multiple_linear_regression.

1.5.2 Special case of general linear model

Theorem: Multiple linear regression (\rightarrow III/1.5.1) is a special case of the general linear model (\rightarrow III/2.2.1) with number of measurements $v = 1$, such that data matrix Y , regression coefficients B , noise matrix E and noise covariance Σ equate as

$$Y = y, \quad B = \beta, \quad E = \varepsilon \quad \text{and} \quad \Sigma = \sigma^2 \quad (1)$$

where y , β , ε and σ^2 are the data vector, regression coefficients, noise vector and noise variance from multiple linear regression (\rightarrow III/1.5.1).

Proof: The linear regression model with correlated errors (\rightarrow III/1.5.1) is given by:

$$y = X\beta + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 V) . \quad (2)$$

Because ε is an n -dimensional vector and σ^2 is scalar, we have the following identities:

$$\begin{aligned} \text{vec}(\varepsilon) &= \varepsilon \\ \sigma^2 \otimes V &= \sigma^2 V . \end{aligned} \quad (3)$$

Thus, using the relationship between multivariate normal and matrix normal distribution (\rightarrow II/5.1.2), equation (2) can also be written as

$$y = X\beta + \varepsilon, \quad \varepsilon \sim \mathcal{MN}(0, V, \sigma^2) . \quad (4)$$

Comparing with the general linear model with correlated observations (\rightarrow III/2.2.1)

$$Y = XB + E, \quad E \sim \mathcal{MN}(0, V, \Sigma) , \quad (5)$$

we finally note the equivalences given in equation (1). ■

Sources:

- Wikipedia (2022): “General linear model”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-07-21; URL: https://en.wikipedia.org/wiki/General_linear_model#Comparison_to_multiple_linear_regression.

1.5.3 Ordinary least squares

Theorem: Given a linear regression model (\rightarrow III/1.5.1) with independent observations

$$y = X\beta + \varepsilon, \quad \varepsilon_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2) , \quad (1)$$

the parameters minimizing the residual sum of squares (\rightarrow III/1.5.9) are given by

$$\hat{\beta} = (X^T X)^{-1} X^T y . \quad (2)$$

Proof: Let $\hat{\beta}$ be the ordinary least squares (OLS) solution and let $\hat{\varepsilon} = y - X\hat{\beta}$ be the resulting vector of residuals. Then, this vector must be orthogonal to the design matrix,

$$X^T \hat{\varepsilon} = 0, \quad (3)$$

because if it wasn't, there would be another solution $\tilde{\beta}$ giving another vector $\tilde{\varepsilon}$ with a smaller residual sum of squares. From (3), the OLS formula can be directly derived:

$$\begin{aligned} X^T \hat{\varepsilon} &= 0 \\ X^T (y - X\hat{\beta}) &= 0 \\ X^T y - X^T X \hat{\beta} &= 0 \\ X^T X \hat{\beta} &= X^T y \\ \hat{\beta} &= (X^T X)^{-1} X^T y. \end{aligned} \quad (4)$$

■

Sources:

- Stephan, Klaas Enno (2010): “The General Linear Model (GLM)” in: *Methods and models for fMRI data analysis in neuroeconomics*, Lecture 3, Slides 10/11; URL: <http://www.socialbehavior.uzh.ch/teaching/methodspring10.html>.

1.5.4 Ordinary least squares

Theorem: Given a linear regression model (\rightarrow III/1.5.1) with independent observations

$$y = X\beta + \varepsilon, \quad \varepsilon_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2), \quad (1)$$

the parameters minimizing the residual sum of squares (\rightarrow III/1.5.9) are given by

$$\hat{\beta} = (X^T X)^{-1} X^T y. \quad (2)$$

Proof: The residual sum of squares (\rightarrow III/1.5.9) is defined as

$$\text{RSS}(\beta) = \sum_{i=1}^n \varepsilon_i^2 = \varepsilon^T \varepsilon = (y - X\beta)^T (y - X\beta) \quad (3)$$

which can be developed into

$$\begin{aligned} \text{RSS}(\beta) &= y^T y - y^T X\beta - \beta^T X^T y + \beta^T X^T X \beta \\ &= y^T y - 2\beta^T X^T y + \beta^T X^T X \beta. \end{aligned} \quad (4)$$

The derivative of $\text{RSS}(\beta)$ with respect to β is

$$\frac{d\text{RSS}(\beta)}{d\beta} = -2X^T y + 2X^T X \beta \quad (5)$$

and setting this derivative to zero, we obtain:

$$\begin{aligned}
\frac{d\text{RSS}(\hat{\beta})}{d\beta} &= 0 \\
0 &= -2X^T y + 2X^T X \hat{\beta} \\
X^T X \hat{\beta} &= X^T y \\
\hat{\beta} &= (X^T X)^{-1} X^T y .
\end{aligned} \tag{6}$$

Since the quadratic form $y^T y$ in (4) is positive, $\hat{\beta}$ minimizes $\text{RSS}(\beta)$. ■

Sources:

- Wikipedia (2020): “Proofs involving ordinary least squares”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-02-03; URL: https://en.wikipedia.org/wiki/Proofs_involving_ordinary_least_squares#Least_squares_estimator_for_%CE%B2.
- ad (2015): “Derivation of the Least Squares Estimator for Beta in Matrix Notation”; in: *Economic Theory Blog*, retrieved on 2021-05-27; URL: https://economytheoryblog.com/2015/02/19/ols_estimator/.

1.5.5 Ordinary least squares

Theorem: Given a linear regression model (\rightarrow III/1.5.1) with independent observations

$$y = X\beta + \varepsilon, \quad \varepsilon_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2), \tag{1}$$

the parameters minimizing the residual sum of squares (\rightarrow III/1.5.9) are given by

$$\hat{\beta} = (X^T X)^{-1} X^T y. \tag{2}$$

Proof: We consider the sum of squared differences between y and $X\beta$:

$$\sum_{i=1}^n \varepsilon_i^2 = \varepsilon^T \varepsilon = (y - X\beta)^T (y - X\beta). \tag{3}$$

First, we note that the residual vector $\hat{\varepsilon}$ implied by the ordinary least squares solution $\hat{\beta}$ is orthogonal to the columns of the design matrix, such that the result of their multiplication is the p -dimensional zero vector (where $X \in \mathbb{R}^{n \times p}$):

$$\begin{aligned}
X^T (y - X\hat{\beta}) &= X^T y - X^T X \hat{\beta} \\
&= X^T y - X^T X (X^T X)^{-1} X^T y \\
&= X^T y - X^T y \\
&= 0_p .
\end{aligned} \tag{4}$$

Second, since $X^T X$ is a positive semi-definite matrix (\rightarrow I/1.16.5), the following product is non-negative for each p -dimensional real vector z :

$$z^T X^T X z \geq 0 \quad \text{for each } z \in \mathbb{R}^p. \tag{5}$$

We continue developping the sum of squared differences from (3):

$$\begin{aligned}
 (y - X\beta)^T(y - X\beta) &= (y - X\hat{\beta} + X\hat{\beta} - X\beta)^T(y - X\hat{\beta} + X\hat{\beta} - X\beta) \\
 &= \left((y - X\hat{\beta}) + X(\hat{\beta} - \beta) \right)^T \left((y - X\hat{\beta}) + X(\hat{\beta} - \beta) \right) \\
 &= (y - X\hat{\beta})^T(y - X\hat{\beta}) + (y - X\hat{\beta})^T X(\hat{\beta} - \beta) + (\hat{\beta} - \beta)^T X^T(y - X\hat{\beta}) + (\hat{\beta} - \beta)^T X^T X(\hat{\beta} - \beta) \\
 &\stackrel{(4)}{=} (y - X\hat{\beta})^T(y - X\hat{\beta}) + 0_p^T(\hat{\beta} - \beta) + (\hat{\beta} - \beta)^T 0_p + (\hat{\beta} - \beta)^T X^T X(\hat{\beta} - \beta) \\
 &= (y - X\hat{\beta})^T(y - X\hat{\beta}) + (\hat{\beta} - \beta)^T X^T X(\hat{\beta} - \beta) .
 \end{aligned} \tag{6}$$

By virtue of (5), the second term on the right-hand side must be non-zero:

$$(\hat{\beta} - \beta)^T X^T X(\hat{\beta} - \beta) \geq 0 . \tag{7}$$

Thus, the residual sum of squares must be greater than or equal to the first term

$$(y - X\beta)^T(y - X\beta) \geq (y - X\hat{\beta})^T(y - X\hat{\beta}) \tag{8}$$

and its minimum value is reached when the the second term is zero:

$$\begin{aligned}
 (\hat{\beta} - \beta)^T X^T X(\hat{\beta} - \beta) &= 0 \\
 \Leftrightarrow (\hat{\beta} - \beta) &= 0 \\
 \Leftrightarrow \beta &= \hat{\beta} .
 \end{aligned} \tag{9}$$

Thus, the residual sum of squares is minimized when $\beta = \hat{\beta}$:

$$\hat{\beta} = (X^T X)^{-1} X^T y = \arg \min_{\beta} (y - X\beta)^T(y - X\beta) . \tag{10}$$

■

Sources:

- Ostwald, Dirk (2023): “Parameterschätzung”; in: *Allgemeines Lineares Modell*, Einheit (6), Folien 10-12; URL: https://www.ipsy.ovgu.de/ipsy_media/Methodenlehre+I/Sommersemester+2023/Allgemeines+Lineares+Modell/6_Parametersch%C3%A4tzung.pdf.

1.5.6 Ordinary least squares for two regressors

Theorem: Consider a linear regression model (\rightarrow III/1.5.1) in which the design matrix (\rightarrow III/1.5.1) has two columns:

$$y = X\beta + \varepsilon \quad \text{where} \quad y \in \mathbb{R}^{n \times 1} \quad \text{and} \quad X = \begin{bmatrix} x_1 & x_2 \end{bmatrix} \in \mathbb{R}^{n \times 2} . \tag{1}$$

Then,

1) the ordinary least squares (\rightarrow III/1.5.3) estimates for β_1 and β_2 are given by

$$\hat{\beta}_1 = \frac{x_2^T x_2 x_1^T y - x_1^T x_2 x_2^T y}{x_1^T x_1 x_2^T x_2 - x_1^T x_2 x_2^T x_1} \quad \text{and} \quad \hat{\beta}_2 = \frac{x_1^T x_1 x_2^T y - x_2^T x_1 x_1^T y}{x_1^T x_1 x_2^T x_2 - x_1^T x_2 x_2^T x_1} \tag{2}$$

2) and, if the two regressors are orthogonal to each other, they simplify to

$$\hat{\beta}_1 = \frac{x_1^T y}{x_1^T x_1} \quad \text{and} \quad \hat{\beta}_2 = \frac{x_2^T y}{x_2^T x_2} . \quad (3)$$

Proof: The model in (1) is a special case of multiple linear regression (\rightarrow III/1.5.1) and the ordinary least squares solution for multiple linear regression (\rightarrow III/1.5.3) is:

$$\hat{\beta} = (X^T X)^{-1} X^T y . \quad (4)$$

1) Plugging $X = \begin{bmatrix} x_1 & x_2 \end{bmatrix}$ into this equation, we obtain:

$$\begin{aligned} \hat{\beta} &= \left(\begin{bmatrix} x_1^T \\ x_2^T \end{bmatrix} \begin{bmatrix} x_1 & x_2 \end{bmatrix} \right)^{-1} \begin{bmatrix} x_1^T \\ x_2^T \end{bmatrix} y \\ &= \begin{pmatrix} x_1^T x_1 & x_1^T x_2 \\ x_2^T x_1 & x_2^T x_2 \end{pmatrix}^{-1} \begin{pmatrix} x_1^T y \\ x_2^T y \end{pmatrix} . \end{aligned} \quad (5)$$

Using the inverse of of a 2×2 matrix

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix}^{-1} = \frac{1}{ad - bc} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix} , \quad (6)$$

this can be further developped into

$$\begin{aligned} \hat{\beta} &= \frac{1}{x_1^T x_1 x_2^T x_2 - x_1^T x_2 x_2^T x_1} \begin{pmatrix} x_2^T x_2 & -x_1^T x_2 \\ -x_2^T x_1 & x_1^T x_1 \end{pmatrix} \begin{pmatrix} x_1^T y \\ x_2^T y \end{pmatrix} \\ &= \frac{1}{x_1^T x_1 x_2^T x_2 - x_1^T x_2 x_2^T x_1} \begin{pmatrix} x_2^T x_2 x_1^T y - x_1^T x_2 x_2^T y \\ x_1^T x_1 x_2^T y - x_2^T x_1 x_1^T y \end{pmatrix} \end{aligned} \quad (7)$$

which can also be written as

$$\begin{aligned} \hat{\beta}_1 &= \frac{x_2^T x_2 x_1^T y - x_1^T x_2 x_2^T y}{x_1^T x_1 x_2^T x_2 - x_1^T x_2 x_2^T x_1} \\ \hat{\beta}_2 &= \frac{x_1^T x_1 x_2^T y - x_2^T x_1 x_1^T y}{x_1^T x_1 x_2^T x_2 - x_1^T x_2 x_2^T x_1} . \end{aligned} \quad (8)$$

2) If two regressors are orthogonal to each other, this means that the inner product of the corresponding vectors is zero:

$$x_1 \perp x_2 \quad \Leftrightarrow \quad x_1^T x_2 = x_2^T x_1 = 0 . \quad (9)$$

Applying this to equation (8), we obtain:

$$\begin{aligned}\hat{\beta}_1 &= \frac{x_2^T x_2 x_1^T y}{x_1^T x_1 x_2^T x_2} = \frac{x_1^T y}{x_1^T x_1} \\ \hat{\beta}_2 &= \frac{x_1^T x_1 x_2^T y}{x_1^T x_1 x_2^T x_2} = \frac{x_2^T y}{x_2^T x_2}.\end{aligned}\tag{10}$$

■

1.5.7 Total sum of squares

Definition: Let there be a multiple linear regression with independent observations (\rightarrow III/1.5.1) using measured data y and design matrix X :

$$y = X\beta + \varepsilon, \quad \varepsilon_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2). \tag{1}$$

Then, the total sum of squares (TSS) is defined as the sum of squared deviations of the measured signal from the average signal:

$$\text{TSS} = \sum_{i=1}^n (y_i - \bar{y})^2 \quad \text{where} \quad \bar{y} = \frac{1}{n} \sum_{i=1}^n y_i. \tag{2}$$

Sources:

- Wikipedia (2020): “Total sum of squares”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-03-21; URL: https://en.wikipedia.org/wiki/Total_sum_of_squares.

1.5.8 Explained sum of squares

Definition: Let there be a multiple linear regression with independent observations (\rightarrow III/1.5.1) using measured data y and design matrix X :

$$y = X\beta + \varepsilon, \quad \varepsilon_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2). \tag{1}$$

Then, the explained sum of squares (ESS) is defined as the sum of squared deviations of the fitted signal from the average signal:

$$\text{ESS} = \sum_{i=1}^n (\hat{y}_i - \bar{y})^2 \quad \text{where} \quad \hat{y} = X\hat{\beta} \quad \text{and} \quad \bar{y} = \frac{1}{n} \sum_{i=1}^n y_i \tag{2}$$

with estimated regression coefficients $\hat{\beta}$, e.g. obtained via ordinary least squares (\rightarrow III/1.5.3).

Sources:

- Wikipedia (2020): “Explained sum of squares”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-03-21; URL: https://en.wikipedia.org/wiki/Explained_sum_of_squares.

1.5.9 Residual sum of squares

Definition: Let there be a multiple linear regression with independent observations (\rightarrow III/1.5.1) using measured data y and design matrix X :

$$y = X\beta + \varepsilon, \quad \varepsilon_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2). \quad (1)$$

Then, the residual sum of squares (RSS) is defined as the sum of squared deviations of the measured signal from the fitted signal:

$$\text{RSS} = \sum_{i=1}^n (y_i - \hat{y}_i)^2 \quad \text{where} \quad \hat{y} = X\hat{\beta} \quad (2)$$

with estimated regression coefficients $\hat{\beta}$, e.g. obtained via ordinary least squares (\rightarrow III/1.5.3).

Sources:

- Wikipedia (2020): “Residual sum of squares”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-03-21; URL: https://en.wikipedia.org/wiki/Residual_sum_of_squares.

1.5.10 Total, explained and residual sum of squares

Theorem: Assume a linear regression model (\rightarrow III/1.5.1) with independent observations

$$y = X\beta + \varepsilon, \quad \varepsilon_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2) \quad (1)$$

and let X contain a constant regressor 1_n modelling the intercept term. Then, it holds that

$$\text{TSS} = \text{ESS} + \text{RSS} \quad (2)$$

where TSS is the total sum of squares (\rightarrow III/1.5.7), ESS is the explained sum of squares (\rightarrow III/1.5.8) and RSS is the residual sum of squares (\rightarrow III/1.5.9).

Proof: The total sum of squares (\rightarrow III/1.5.7) is given by

$$\text{TSS} = \sum_{i=1}^n (y_i - \bar{y})^2 \quad (3)$$

where \bar{y} is the mean across all y_i . The TSS can be rewritten as

$$\begin{aligned}
\text{TSS} &= \sum_{i=1}^n (y_i - \bar{y} + \hat{y}_i - \hat{y}_i)^2 \\
&= \sum_{i=1}^n ((\hat{y}_i - \bar{y}) + (y_i - \hat{y}_i))^2 \\
&= \sum_{i=1}^n ((\hat{y}_i - \bar{y}) + \hat{\varepsilon}_i)^2 \\
&= \sum_{i=1}^n ((\hat{y}_i - \bar{y})^2 + 2\hat{\varepsilon}_i(\hat{y}_i - \bar{y}) + \hat{\varepsilon}_i^2) \\
&= \sum_{i=1}^n (\hat{y}_i - \bar{y})^2 + \sum_{i=1}^n \hat{\varepsilon}_i^2 + 2 \sum_{i=1}^n \hat{\varepsilon}_i(\hat{y}_i - \bar{y}) \\
&= \sum_{i=1}^n (\hat{y}_i - \bar{y})^2 + \sum_{i=1}^n \hat{\varepsilon}_i^2 + 2 \sum_{i=1}^n \hat{\varepsilon}_i(x_i\hat{\beta} - \bar{y}) \\
&= \sum_{i=1}^n (\hat{y}_i - \bar{y})^2 + \sum_{i=1}^n \hat{\varepsilon}_i^2 + 2 \sum_{i=1}^n \hat{\varepsilon}_i \left(\sum_{j=1}^p x_{ij}\hat{\beta}_j \right) - 2 \sum_{i=1}^n \hat{\varepsilon}_i \bar{y} \\
&= \sum_{i=1}^n (\hat{y}_i - \bar{y})^2 + \sum_{i=1}^n \hat{\varepsilon}_i^2 + 2 \sum_{j=1}^p \hat{\beta}_j \sum_{i=1}^n \hat{\varepsilon}_i x_{ij} - 2\bar{y} \sum_{i=1}^n \hat{\varepsilon}_i
\end{aligned} \tag{4}$$

The fact that the design matrix includes a constant regressor ensures that

$$\sum_{i=1}^n \hat{\varepsilon}_i = \hat{\varepsilon}^T \mathbf{1}_n = 0 \tag{5}$$

and because the residuals are orthogonal to the design matrix (\rightarrow III/1.5.3), we have

$$\sum_{i=1}^n \hat{\varepsilon}_i x_{ij} = \hat{\varepsilon}^T x_j = 0. \tag{6}$$

Applying (5) and (6) to (4), this becomes

$$\text{TSS} = \sum_{i=1}^n (\hat{y}_i - \bar{y})^2 + \sum_{i=1}^n \hat{\varepsilon}_i^2 \tag{7}$$

and, with the definitions of explained (\rightarrow III/1.5.8) and residual sum of squares (\rightarrow III/1.5.9), it is

$$\text{TSS} = \text{ESS} + \text{RSS}. \tag{8}$$

■

Sources:

- Wikipedia (2020): “Partition of sums of squares”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-03-09; URL: https://en.wikipedia.org/wiki/Partition_of_sums_of_squares#Partitioning_the_sum_of_squares_in_linear_regression.

1.5.11 Estimation matrix

Definition: In multiple linear regression (\rightarrow III/1.5.1), the estimation matrix is the matrix E that results in ordinary least squares (\rightarrow III/1.5.3) or weighted least squares (\rightarrow III/1.5.21) parameter estimates when right-multiplied with the measured data:

$$Ey = \hat{\beta} . \quad (1)$$

1.5.12 Projection matrix

Definition: In multiple linear regression (\rightarrow III/1.5.1), the projection matrix is the matrix P that results in the fitted signal explained by estimated parameters (\rightarrow III/1.5.11) when right-multiplied with the measured data:

$$Py = \hat{y} = X\hat{\beta} . \quad (1)$$

Sources:

- Wikipedia (2020): “Projection matrix”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-07-22; URL: https://en.wikipedia.org/wiki/Projection_matrix#Overview.

1.5.13 Residual-forming matrix

Definition: In multiple linear regression (\rightarrow III/1.5.1), the residual-forming matrix is the matrix R that results in the vector of residuals left over by estimated parameters (\rightarrow III/1.5.11) when right-multiplied with the measured data:

$$Ry = \hat{\varepsilon} = y - \hat{y} = y - X\hat{\beta} . \quad (1)$$

Sources:

- Wikipedia (2020): “Projection matrix”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-07-22; URL: https://en.wikipedia.org/wiki/Projection_matrix#Properties.

1.5.14 Estimation, projection and residual-forming matrix

Theorem: Assume a linear regression model (\rightarrow III/1.5.1) with independent observations

$$y = X\beta + \varepsilon, \varepsilon_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2) \quad (1)$$

and consider estimation using ordinary least squares (\rightarrow III/1.5.3). Then, the estimated parameters, fitted signal and residuals are given by

$$\begin{aligned} \hat{\beta} &= Ey \\ \hat{y} &= Py \\ \hat{\varepsilon} &= Ry \end{aligned} \quad (2)$$

where

$$\begin{aligned}
E &= (X^T X)^{-1} X^T \\
P &= X(X^T X)^{-1} X^T \\
R &= I_n - X(X^T X)^{-1} X^T
\end{aligned} \tag{3}$$

are the estimation matrix (\rightarrow III/1.5.11), projection matrix (\rightarrow III/1.5.12) and residual-forming matrix (\rightarrow III/1.5.13) and n is the number of observations.

Proof:

1) Ordinary least squares parameter estimates of β are defined as minimizing the residual sum of squares (\rightarrow III/1.5.9)

$$\hat{\beta} = \arg \min_{\beta} [(y - X\beta)^T (y - X\beta)] \tag{4}$$

and the solution to this (\rightarrow III/1.5.3) is given by

$$\begin{aligned}
\hat{\beta} &= (X^T X)^{-1} X^T y \\
&\stackrel{(3)}{=} Ey .
\end{aligned} \tag{5}$$

2) The fitted signal is given by multiplying the design matrix with the estimated regression coefficients

$$\hat{y} = X\hat{\beta} \tag{6}$$

and using (5), this becomes

$$\begin{aligned}
\hat{y} &= X(X^T X)^{-1} X^T y \\
&\stackrel{(3)}{=} Py .
\end{aligned} \tag{7}$$

3) The residuals of the model are calculated by subtracting the fitted signal from the measured signal

$$\hat{\varepsilon} = y - \hat{y} \tag{8}$$

and using (7), this becomes

$$\begin{aligned}
\hat{\varepsilon} &= y - X(X^T X)^{-1} X^T y \\
&= (I_n - X(X^T X)^{-1} X^T) y \\
&\stackrel{(3)}{=} Ry .
\end{aligned} \tag{9}$$

■

Sources:

- Stephan, Klaas Enno (2010): “The General Linear Model (GLM)”; in: *Methods and models for fMRI data analysis in neuroeconomics*, Lecture 3, Slide 10; URL: <http://www.socialbehavior.uzh.ch/teaching/methodspring10.html>.

1.5.15 Symmetry of projection and residual-forming matrix

Theorem: The projection matrix (\rightarrow III/1.5.12) and the residual-forming matrix (\rightarrow III/1.5.13) are symmetric:

$$\begin{aligned} P^T &= P \\ R^T &= R . \end{aligned} \tag{1}$$

Proof: Let X be the design matrix from the linear regression model (\rightarrow III/1.5.1). Then, the matrix $X^T X$ is symmetric, because

$$(X^T X)^T = X^T X^{TT} = X^T X . \tag{2}$$

Thus, the inverse of $X^T X$ is also symmetric, i.e.

$$((X^T X)^{-1})^T = (X^T X)^{-1} . \tag{3}$$

1) The projection matrix for ordinary least squares is given by (\rightarrow III/1.5.14)

$$P = X(X^T X)^{-1} X^T , \tag{4}$$

such that

$$\begin{aligned} P^T &= (X(X^T X)^{-1} X^T)^T \\ &= X^{TT} ((X^T X)^{-1})^T X^T \\ &= X(X^T X)^{-1} X^T \\ &\stackrel{(4)}{=} P . \end{aligned} \tag{5}$$

2) The residual-forming matrix for ordinary least squares is given by (\rightarrow III/1.5.14)

$$R = I_n - X(X^T X)^{-1} X^T = I_n - P , \tag{6}$$

such that

$$\begin{aligned} R^T &= (I_n - P)^T \\ &= I_n^T - P^T \\ &\stackrel{(5)}{=} I_n - P \\ &\stackrel{(6)}{=} R . \end{aligned} \tag{7}$$

■

Sources:

- Wikipedia (2020): “Projection matrix”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-12-22; URL: https://en.wikipedia.org/wiki/Projection_matrix#Properties.

1.5.16 Idempotence of projection and residual-forming matrix

Theorem: The projection matrix (\rightarrow III/1.5.12) and the residual-forming matrix (\rightarrow III/1.5.13) are idempotent:

$$\begin{aligned} P^2 &= P \\ R^2 &= R. \end{aligned} \tag{1}$$

Proof:

1) The projection matrix for ordinary least squares is given by (\rightarrow III/1.5.14)

$$P = X(X^T X)^{-1} X^T, \tag{2}$$

such that

$$\begin{aligned} P^2 &= X(X^T X)^{-1} X^T X(X^T X)^{-1} X^T \\ &= X(X^T X)^{-1} X^T \\ &\stackrel{(2)}{=} P. \end{aligned} \tag{3}$$

2) The residual-forming matrix for ordinary least squares is given by (\rightarrow III/1.5.14)

$$R = I_n - X(X^T X)^{-1} X^T = I_n - P, \tag{4}$$

such that

$$\begin{aligned} R^2 &= (I_n - P)(I_n - P) \\ &= I_n - P - P + P^2 \\ &\stackrel{(3)}{=} I_n - 2P + P \\ &= I_n - P \\ &\stackrel{(4)}{=} R. \end{aligned} \tag{5}$$

■

Sources:

- Wikipedia (2020): “Projection matrix”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-07-22; URL: https://en.wikipedia.org/wiki/Projection_matrix#Properties.

1.5.17 Independence of estimated parameters and residuals

Theorem: Assume a linear regression model (\rightarrow III/1.5.1) with correlated observations

$$y = X\beta + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 V) \tag{1}$$

and consider estimation using weighted least squares (\rightarrow III/1.5.21). Then, the estimated parameters and the vector of residuals (\rightarrow III/1.5.19) are independent from each other:

$$\begin{aligned}\hat{\beta} &= (X^T V^{-1} X)^{-1} X^T V^{-1} y \quad \text{and} \\ \hat{\varepsilon} &= y - X \hat{\beta} \quad \text{ind.}\end{aligned}\tag{2}$$

Proof: Equation (1) implies the following distribution (\rightarrow III/1.5.19) for the random vector (\rightarrow I/1.2.3) y :

$$\begin{aligned}y &\sim \mathcal{N}(X\beta, \sigma^2 V) \\ &\sim \mathcal{N}(X\beta, \Sigma) \\ \text{with } \Sigma &= \sigma^2 V.\end{aligned}\tag{3}$$

Note that the estimated parameters and residuals can be written as projections from the same random vector (\rightarrow III/1.5.14) y :

$$\begin{aligned}\hat{\beta} &= (X^T V^{-1} X)^{-1} X^T V^{-1} y \\ &= Ay \\ \text{with } A &= (X^T V^{-1} X)^{-1} X^T V^{-1}\end{aligned}\tag{4}$$

$$\begin{aligned}\hat{\varepsilon} &= y - X \hat{\beta} \\ &= (I_n - X(X^T V^{-1} X)^{-1} X^T V^{-1}) y \\ &= By \\ \text{with } B &= (I_n - X(X^T V^{-1} X)^{-1} X^T V^{-1}).\end{aligned}\tag{5}$$

Two projections AZ and BZ from the same multivariate normal (\rightarrow II/4.1.1) random vector (\rightarrow I/1.2.3) $Z \sim \mathcal{N}(\mu, \Sigma)$ are independent, if and only if the following condition holds (\rightarrow II/4.1.18):

$$A \Sigma B^T = 0.\tag{6}$$

Combining (3), (4) and (5), we check whether this is fulfilled in the present case:

$$\begin{aligned}A \Sigma B^T &= (X^T V^{-1} X)^{-1} X^T V^{-1} (\sigma^2 V) (I_n - X(X^T V^{-1} X)^{-1} X^T V^{-1})^T \\ &= \sigma^2 [(X^T V^{-1} X)^{-1} X^T V^{-1} V - (X^T V^{-1} X)^{-1} X^T V^{-1} V V^{-1} X (X^T V^{-1} X)^{-1} X^T] \\ &= \sigma^2 [(X^T V^{-1} X)^{-1} X^T - (X^T V^{-1} X)^{-1} X^T] \\ &= \sigma^2 \cdot 0_{pn} \\ &= 0.\end{aligned}\tag{7}$$

This demonstrates that $\hat{\beta}$ and $\hat{\varepsilon}$ – and likewise, all pairs of terms separately derived (\rightarrow III/1.5.28) from $\hat{\beta}$ and $\hat{\varepsilon}$ – are statistically independent (\rightarrow I/1.3.6). ■

Sources:

- jld (2018): “Understanding t-test for linear regression”; in: *StackExchange CrossValidated*, retrieved on 2022-12-13; URL: <https://stats.stackexchange.com/a/344008>.

1.5.18 Distribution of OLS estimates, signal and residuals

Theorem: Assume a linear regression model (\rightarrow III/1.5.1) with independent observations

$$y = X\beta + \varepsilon, \varepsilon_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2) \quad (1)$$

and consider estimation using ordinary least squares (\rightarrow III/1.5.3). Then, the estimated parameters, fitted signal and residuals are distributed as

$$\begin{aligned} \hat{\beta} &\sim \mathcal{N}(\beta, \sigma^2(X^T X)^{-1}) \\ \hat{y} &\sim \mathcal{N}(X\beta, \sigma^2 P) \\ \hat{\varepsilon} &\sim \mathcal{N}(0, \sigma^2(I_n - P)) \end{aligned} \quad (2)$$

where P is the projection matrix (\rightarrow III/1.5.12) for ordinary least squares (\rightarrow III/1.5.3)

$$P = X(X^T X)^{-1} X^T. \quad (3)$$

Proof: We will use the linear transformation theorem for the multivariate normal distribution (\rightarrow II/4.1.14):

$$x \sim \mathcal{N}(\mu, \Sigma) \Rightarrow y = Ax + b \sim \mathcal{N}(A\mu + b, A\Sigma A^T). \quad (4)$$

The distributional assumption in (1) is equivalent to (\rightarrow II/4.1.17):

$$y = X\beta + \varepsilon, \varepsilon \sim \mathcal{N}(0, \sigma^2 I_n). \quad (5)$$

Applying (4) to (5), the measured data are distributed as

$$y \sim \mathcal{N}(X\beta, \sigma^2 I_n). \quad (6)$$

1) The parameter estimates from ordinary least squares (\rightarrow III/1.5.3) are given by

$$\hat{\beta} = (X^T X)^{-1} X^T y \quad (7)$$

and thus, by applying (4) to (7), they are distributed as

$$\begin{aligned} \hat{\beta} &\sim \mathcal{N}([(X^T X)^{-1} X^T] X\beta, \sigma^2 [(X^T X)^{-1} X^T] I_n [X(X^T X)^{-1}]) \\ &\sim \mathcal{N}(\beta, \sigma^2 (X^T X)^{-1}). \end{aligned} \quad (8)$$

2) The fitted signal in multiple linear regression (\rightarrow III/1.5.14) is given by

$$\hat{y} = X\hat{\beta} = X(X^T X)^{-1} X^T y = Py \quad (9)$$

and thus, by applying (4) to (9), they are distributed as

$$\begin{aligned} \hat{y} &\sim \mathcal{N}(X\beta, \sigma^2 X(X^T X)^{-1} X^T) \\ &\sim \mathcal{N}(X\beta, \sigma^2 P). \end{aligned} \quad (10)$$

3) The residuals of the linear regression model (\rightarrow III/1.5.14) are given by

$$\hat{\varepsilon} = y - X\hat{\beta} = (I_n - X(X^T X)^{-1} X^T) y = (I_n - P) y \quad (11)$$

and thus, by applying (4) to (11), they are distributed as

$$\begin{aligned} \hat{\varepsilon} &\sim \mathcal{N} \left([I_n - X(X^T X)^{-1} X^T] X\beta, \sigma^2 [I_n - P] I_n [I_n - P]^T \right) \\ &\sim \mathcal{N} \left(X\beta - X\beta, \sigma^2 [I_n - P] [I_n - P]^T \right) . \end{aligned} \quad (12)$$

Because the residual-forming matrix (\rightarrow III/1.5.13) is symmetric (\rightarrow III/1.5.15) and idempotent (\rightarrow III/1.5.16), this becomes:

$$\hat{\varepsilon} \sim \mathcal{N} (0, \sigma^2 (I_n - P)) . \quad (13)$$

■

Sources:

- Koch, Karl-Rudolf (2007): “Linear Model”; in: *Introduction to Bayesian Statistics*, Springer, Berlin/Heidelberg, 2007, ch. 4, eqs. 4.2, 4.30; URL: <https://www.springer.com/de/book/9783540727231>; DOI: 10.1007/978-3-540-72726-2.
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- Ostwald, Dirk (2023): “Modellformulierung”; in: *Allgemeines Lineares Modell*, Einheit (5), Folie 14; URL: https://www.ipsy.ovgu.de/ipsy_media/Methodenlehre+I/Sommersemester+2023/Allgemeines+Lineares+Modell/5_Modellformulierung.pdf.
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1.5.19 Distribution of WLS estimates, signal and residuals

Theorem: Assume a linear regression model (\rightarrow III/1.5.1) with correlated observations

$$y = X\beta + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 V) \quad (1)$$

and consider estimation using weighted least squares (\rightarrow III/1.5.21). Then, the estimated parameters, fitted signal and residuals are distributed as

$$\begin{aligned} \hat{\beta} &\sim \mathcal{N} (\beta, \sigma^2 (X^T V^{-1} X)^{-1}) \\ \hat{y} &\sim \mathcal{N} (X\beta, \sigma^2 (P V)) \\ \hat{\varepsilon} &\sim \mathcal{N} (0, \sigma^2 (I_n - P) V) \end{aligned} \quad (2)$$

where P is the projection matrix (\rightarrow III/1.5.12) for weighted least squares (\rightarrow III/1.5.21)

$$P = X(X^T V^{-1} X)^{-1} X^T V^{-1} . \quad (3)$$

Proof: We will use the linear transformation theorem for the multivariate normal distribution (\rightarrow II/4.1.14):

$$x \sim \mathcal{N}(\mu, \Sigma) \Rightarrow y = Ax + b \sim \mathcal{N}(A\mu + b, A\Sigma A^T) . \quad (4)$$

Applying (4) to (1), the measured data are distributed as

$$y \sim \mathcal{N}(X\beta, \sigma^2 V) . \quad (5)$$

1) The parameter estimates from weighted least squares (\rightarrow III/1.5.21) are given by

$$\hat{\beta} = (X^T V^{-1} X)^{-1} X^T V^{-1} y \quad (6)$$

and thus, by applying (4) to (6), they are distributed as

$$\begin{aligned} \hat{\beta} &\sim \mathcal{N}([(X^T V^{-1} X)^{-1} X^T V^{-1}] X\beta, \sigma^2 [(X^T V^{-1} X)^{-1} X^T V^{-1}] V [V^{-1} X (X^T V^{-1} X)^{-1}]) \\ &\sim \mathcal{N}(\beta, \sigma^2 (X^T V^{-1} X)^{-1}) . \end{aligned} \quad (7)$$

2) The fitted signal in multiple linear regression (\rightarrow III/1.5.14) is given by

$$\hat{y} = X\hat{\beta} = X(X^T V^{-1} X)^{-1} X^T V^{-1} y = Py \quad (8)$$

and thus, by applying (4) to (8), they are distributed as

$$\begin{aligned} \hat{y} &\sim \mathcal{N}(X\beta, \sigma^2 X(X^T V^{-1} X)^{-1} X^T) \\ &\sim \mathcal{N}(X\beta, \sigma^2 (PV)) . \end{aligned} \quad (9)$$

3) The residuals of the linear regression model (\rightarrow III/1.5.14) are given by

$$\hat{\varepsilon} = y - X\hat{\beta} = (I_n - X(X^T V^{-1} X)^{-1} X^T V^{-1}) y = (I_n - P) y \quad (10)$$

and thus, by applying (4) to (10), they are distributed as

$$\begin{aligned} \hat{\varepsilon} &\sim \mathcal{N}([I_n - X(X^T V^{-1} X)^{-1} X^T V^{-1}] X\beta, \sigma^2 [I_n - P] V [I_n - P]^T) \\ &\sim \mathcal{N}(X\beta - X\beta, \sigma^2 [V - V P^T - P V + P V P^T]) \\ &\sim \mathcal{N}(0, \sigma^2 [V - V V^{-1} X (X^T V^{-1} X)^{-1} X^T - X (X^T V^{-1} X)^{-1} X^T V^{-1} V + P V P^T]) \\ &\sim \mathcal{N}(0, \sigma^2 [V - 2PV + X (X^T V^{-1} X)^{-1} X^T V^{-1} V V^{-1} X (X^T V^{-1} X)^{-1} X^T]) \\ &\sim \mathcal{N}(0, \sigma^2 [V - 2PV + PV]) \\ &\sim \mathcal{N}(0, \sigma^2 [V - PV]) \\ &\sim \mathcal{N}(0, \sigma^2 [I_n - P] V) . \end{aligned} \quad (11)$$

■

Sources:

- Koch, Karl-Rudolf (2007): “Linear Model”; in: *Introduction to Bayesian Statistics*, Springer, Berlin/Heidelberg, 2007, ch. 4, eqs. 4.2, 4.30; URL: <https://www.springer.com/de/book/9783540727231>; DOI: 10.1007/978-3-540-72726-2.
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1.5.20 Distribution of residual sum of squares

Theorem: Assume a linear regression model (\rightarrow III/1.5.1) with correlated observations

$$y = X\beta + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 V) \quad (1)$$

and consider estimation using weighted least squares (\rightarrow III/1.5.21). Then, the residual sum of squares (\rightarrow III/1.5.9) $\hat{\varepsilon}^T \hat{\varepsilon}$, divided by the true error variance (\rightarrow III/1.5.1) σ^2 , follows a chi-squared distribution (\rightarrow II/3.7.1) with $n - p$ degrees of freedom (\rightarrow I/1.5.12)

$$\frac{\hat{\varepsilon}^T \hat{\varepsilon}}{\sigma^2} \sim \chi^2(n - p) \quad (2)$$

where n and p are the dimensions of the $n \times p$ design matrix (\rightarrow III/1.5.1) X .

Proof: Consider an $n \times n$ square matrix W , such that

$$WVW^T = I_n. \quad (3)$$

Then, left-multiplying the regression model in (1) with W gives

$$Wy = WX\beta + W\varepsilon, \quad W\varepsilon \sim \mathcal{N}(0, \sigma^2 WVW^T) \quad (4)$$

which can be rewritten as

$$\tilde{y} = \tilde{X}\beta + \tilde{\varepsilon}, \quad \tilde{\varepsilon} \sim \mathcal{N}(0, \sigma^2 I_n) \quad (5)$$

where $\tilde{y} = Wy$, $\tilde{X} = WX$ and $\tilde{\varepsilon} = W\varepsilon$. This implies the distribution (\rightarrow II/4.1.14)

$$\tilde{y} \sim \mathcal{N}(\tilde{X}\beta, \sigma^2 I_n). \quad (6)$$

With that, we have obtained a linear regression model (\rightarrow III/1.5.1) with independent observations. Cochran’s theorem for multivariate normal variables states that, for an n -dimensional normal random vector (\rightarrow II/4.1.1) whose covariance matrix (\rightarrow I/1.16.1) is a scalar multiple of the identity matrix, a specific squared form will follow a non-central chi-squared distribution where the degrees of freedom and the non-centrality parameter depend on the matrix in the quadratic form:

$$x \sim \mathcal{N}(\mu, \sigma^2 I_n) \quad \Rightarrow \quad y = x^T A x / \sigma^2 \sim \chi^2(\text{rk}(A), \mu^T A \mu). \quad (7)$$

First, we formulate the residuals (\rightarrow III/1.5.14) in terms of transformed measurements \tilde{y} :

$$\begin{aligned}
\hat{\varepsilon} &= \tilde{y} - \tilde{X}\hat{\beta} & \text{where} & \quad \hat{\beta} = (\tilde{X}^T \tilde{X})^{-1} \tilde{X}^T \tilde{y} \\
&= (I_n - \tilde{P})\tilde{y} & \text{where} & \quad \tilde{P} = \tilde{X}(\tilde{X}^T \tilde{X})^{-1} \tilde{X}^T \\
&= \tilde{R}\tilde{y} & \text{where} & \quad \tilde{R} = I_n - \tilde{P} .
\end{aligned} \tag{8}$$

Next, we observe that the residual sum of squares can be represented as a quadratic form:

$$\frac{1}{\sigma^2} \sum_{i=1}^n \hat{\varepsilon}_i^2 = \frac{\hat{\varepsilon}^T \hat{\varepsilon}}{\sigma^2} = \tilde{y}^T \tilde{R}^T \tilde{R} \tilde{y} / \sigma^2 \tag{9}$$

Because the residual-forming matrix (\rightarrow III/1.5.13) \tilde{R} is symmetric (\rightarrow III/1.5.15) and idempotent (\rightarrow III/1.5.16), we have $\tilde{R}^T = \tilde{R}$ and $\tilde{R}^2 = \tilde{R}$, such that:

$$\frac{\hat{\varepsilon}^T \hat{\varepsilon}}{\sigma^2} = \tilde{y}^T \tilde{R} \tilde{y} / \sigma^2 . \tag{10}$$

Since \tilde{R} is idempotent, its rank is equal to its trace, such that:

$$\text{rk}(\tilde{R}) = \text{tr}(\tilde{R}) . \tag{11}$$

With that, we can apply Cochran's theorem given by (7) which yields

$$\begin{aligned}
\frac{\hat{\varepsilon}^T \hat{\varepsilon}}{\sigma^2} &\sim \chi^2 \left(\text{rk}(\tilde{R}), \beta^T \tilde{X}^T \tilde{R} \tilde{X} \beta \right) \\
&\sim \chi^2 \left(\text{tr}(I_n - \tilde{P}), \beta^T \tilde{X}^T (I_n - \tilde{P}) \tilde{X} \beta \right) \\
&\sim \chi^2 \left(\text{tr}(I_n) - \text{tr}(\tilde{X}(\tilde{X}^T \tilde{X})^{-1} \tilde{X}^T), \beta^T (\tilde{X}^T \tilde{X} - \tilde{X}^T \tilde{X}(\tilde{X}^T \tilde{X})^{-1} \tilde{X}^T) \beta \right) \\
&\sim \chi^2 \left(\text{tr}(I_n) - \text{tr}(\tilde{X}^T \tilde{X}(\tilde{X}^T \tilde{X})^{-1}), \beta^T (\tilde{X}^T \tilde{X} - \tilde{X}^T \tilde{X}) \beta \right) \\
&\sim \chi^2 \left(\text{tr}(I_n) - \text{tr}(I_p), \beta^T 0_{pp} \beta \right) \\
&\sim \chi^2 (n - p, 0) .
\end{aligned} \tag{12}$$

Because a non-central chi-squared distribution with non-centrality parameter of zero reduces to the central chi-squared distribution, we obtain our final result:

$$\frac{\hat{\varepsilon}^T \hat{\varepsilon}}{\sigma^2} \sim \chi^2(n - p) . \tag{13}$$

■

Sources:

- Koch, Karl-Rudolf (2007): “Estimation of the Variance Factor in Traditional Statistics”; in: *Introduction to Bayesian Statistics*, Springer, Berlin/Heidelberg, 2007, ch. 4.2.3, eq. 4.37; URL: <https://www.springer.com/de/book/9783540727231>; DOI: 10.1007/978-3-540-72726-2.
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1.5.21 Weighted least squares

Theorem: Given a linear regression model (\rightarrow III/1.5.1) with correlated observations

$$y = X\beta + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 V), \quad (1)$$

the parameters minimizing the weighted residual sum of squares (\rightarrow III/1.5.9) are given by

$$\hat{\beta} = (X^T V^{-1} X)^{-1} X^T V^{-1} y. \quad (2)$$

Proof: Let there be an $n \times n$ square matrix W , such that

$$WVW^T = I_n. \quad (3)$$

Since V is a covariance matrix and thus symmetric (\rightarrow I/1.15.4), W is also symmetric and can be expressed as the matrix square root of the inverse of V :

$$WVW = I_n \quad \Leftrightarrow \quad V = W^{-1}W^{-1} \quad \Leftrightarrow \quad V^{-1} = WW \quad \Leftrightarrow \quad W = V^{-1/2}. \quad (4)$$

Left-multiplying the linear regression equation (1) with W , the linear transformation theorem (\rightarrow II/4.1.14) implies that

$$Wy = WX\beta + W\varepsilon, \quad W\varepsilon \sim \mathcal{N}(0, \sigma^2 WVW^T). \quad (5)$$

Applying (3), we see that (5) is actually a linear regression model (\rightarrow III/1.5.1) with independent observations

$$\tilde{y} = \tilde{X}\beta + \tilde{\varepsilon}, \quad \tilde{\varepsilon} \sim \mathcal{N}(0, \sigma^2 I_n) \quad (6)$$

where $\tilde{y} = Wy$, $\tilde{X} = WX$ and $\tilde{\varepsilon} = W\varepsilon$, such that we can apply the ordinary least squares solution (\rightarrow III/1.5.3) giving

$$\begin{aligned} \hat{\beta} &= (\tilde{X}^T \tilde{X})^{-1} \tilde{X}^T \tilde{y} \\ &= ((WX)^T WX)^{-1} (WX)^T Wy \\ &= (X^T W^T WX)^{-1} X^T W^T Wy \\ &= (X^T WWX)^{-1} X^T WWy \\ &\stackrel{(4)}{=} (X^T V^{-1} X)^{-1} X^T V^{-1} y \end{aligned} \quad (7)$$

which corresponds to the weighted least squares solution (2). ■

Sources:

- Stephan, Klaas Enno (2010): “The General Linear Model (GLM)”; in: *Methods and models for fMRI data analysis in neuroeconomics*, Lecture 3, Slides 20/23; URL: <http://www.socialbehavior.uzh.ch/teaching/methodspring10.html>.
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1.5.22 Weighted least squares

Theorem: Given a linear regression model (\rightarrow III/1.5.1) with correlated observations

$$y = X\beta + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 V), \quad (1)$$

the parameters minimizing the weighted residual sum of squares (\rightarrow III/1.5.9) are given by

$$\hat{\beta} = (X^T V^{-1} X)^{-1} X^T V^{-1} y. \quad (2)$$

Proof: Let there be an $n \times n$ square matrix W , such that

$$WVW^T = I_n. \quad (3)$$

Since V is a covariance matrix and thus symmetric (\rightarrow I/1.15.4), W is also symmetric and can be expressed the matrix square root of the inverse of V :

$$WVW = I_n \quad \Leftrightarrow \quad V = W^{-1}W^{-1} \quad \Leftrightarrow \quad V^{-1} = WW \quad \Leftrightarrow \quad W = V^{-1/2}. \quad (4)$$

Left-multiplying the linear regression equation (1) with W , the linear transformation theorem (\rightarrow II/4.1.14) implies that

$$Wy = WX\beta + W\varepsilon, \quad W\varepsilon \sim \mathcal{N}(0, \sigma^2 WVW^T). \quad (5)$$

Applying (3), we see that (5) is actually a linear regression model (\rightarrow III/1.5.1) with independent observations

$$Wy = WX\beta + W\varepsilon, \quad W\varepsilon \sim \mathcal{N}(0, \sigma^2 I_n). \quad (6)$$

With this, we can express the weighted residual sum of squares (\rightarrow III/1.5.9) as

$$\text{wRSS}(\beta) = \sum_{i=1}^n (W\varepsilon)_i^2 = (W\varepsilon)^T (W\varepsilon) = (Wy - WX\beta)^T (Wy - WX\beta) \quad (7)$$

which can be developed into

$$\begin{aligned} \text{wRSS}(\beta) &= y^T W^T W y - y^T W^T W X \beta - \beta^T X^T W^T W y + \beta^T X^T W^T W X \beta \\ &= y^T W W y - 2\beta^T X^T W W y + \beta^T X^T W W X \beta \\ &\stackrel{(4)}{=} y^T V^{-1} y - 2\beta^T X^T V^{-1} y + \beta^T X^T V^{-1} X \beta. \end{aligned} \quad (8)$$

The derivative of $\text{wRSS}(\beta)$ with respect to β is

$$\frac{d\text{wRSS}(\beta)}{d\beta} = -2X^T V^{-1} y + 2X^T V^{-1} X \beta \quad (9)$$

and setting this derivative to zero, we obtain:

$$\begin{aligned} \frac{d\text{wRSS}(\hat{\beta})}{d\beta} &= 0 \\ 0 &= -2X^T V^{-1} y + 2X^T V^{-1} X \hat{\beta} \\ X^T V^{-1} X \hat{\beta} &= X^T V^{-1} y \\ \hat{\beta} &= (X^T V^{-1} X)^{-1} X^T V^{-1} y. \end{aligned} \quad (10)$$

Since the quadratic form $y^T V^{-1} y$ in (8) is positive, $\hat{\beta}$ minimizes $\text{wRSS}(\beta)$. ■

1.5.23 Maximum likelihood estimation

Theorem: Given a linear regression model (\rightarrow III/1.5.1) with correlated observations

$$y = X\beta + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 V), \quad (1)$$

the maximum likelihood estimates (\rightarrow I/4.1.3) of β and σ^2 are given by

$$\begin{aligned} \hat{\beta} &= (X^T V^{-1} X)^{-1} X^T V^{-1} y \\ \hat{\sigma}^2 &= \frac{1}{n} (y - X\hat{\beta})^T V^{-1} (y - X\hat{\beta}). \end{aligned} \quad (2)$$

Proof: With the probability density function of the multivariate normal distribution (\rightarrow II/4.1.4), the linear regression equation (1) implies the following likelihood function (\rightarrow I/5.1.2)

$$\begin{aligned} p(y|\beta, \sigma^2) &= \mathcal{N}(y; X\beta, \sigma^2 V) \\ &= \sqrt{\frac{1}{(2\pi)^n |\sigma^2 V|}} \cdot \exp \left[-\frac{1}{2} (y - X\beta)^T (\sigma^2 V)^{-1} (y - X\beta) \right] \end{aligned} \quad (3)$$

and, using $|\sigma^2 V| = (\sigma^2)^n |V|$, the log-likelihood function (\rightarrow I/4.1.2)

$$\begin{aligned} \text{LL}(\beta, \sigma^2) &= \log p(y|\beta, \sigma^2) \\ &= -\frac{n}{2} \log(2\pi) - \frac{n}{2} \log(\sigma^2) - \frac{1}{2} \log |V| \\ &\quad - \frac{1}{2\sigma^2} (y - X\beta)^T V^{-1} (y - X\beta). \end{aligned} \quad (4)$$

Substituting the precision matrix $P = V^{-1}$ into (4) to ease notation, we have:

$$\begin{aligned} \text{LL}(\beta, \sigma^2) &= -\frac{n}{2} \log(2\pi) - \frac{n}{2} \log(\sigma^2) - \frac{1}{2} \log(|V|) \\ &\quad - \frac{1}{2\sigma^2} (y^T P y - 2\beta^T X^T P y + \beta^T X^T P X \beta). \end{aligned} \quad (5)$$

The derivative of the log-likelihood function (5) with respect to β is

$$\begin{aligned} \frac{d\text{LL}(\beta, \sigma^2)}{d\beta} &= \frac{d}{d\beta} \left(-\frac{1}{2\sigma^2} (y^T P y - 2\beta^T X^T P y + \beta^T X^T P X \beta) \right) \\ &= \frac{1}{2\sigma^2} \frac{d}{d\beta} (2\beta^T X^T P y - \beta^T X^T P X \beta) \\ &= \frac{1}{2\sigma^2} (2X^T P y - 2X^T P X \beta) \\ &= \frac{1}{\sigma^2} (X^T P y - X^T P X \beta) \end{aligned} \quad (6)$$

and setting this derivative to zero gives the MLE for β :

$$\begin{aligned}
 \frac{dLL(\hat{\beta}, \sigma^2)}{d\beta} &= 0 \\
 0 &= \frac{1}{\sigma^2} \left(X^T P y - X^T P X \hat{\beta} \right) \\
 0 &= X^T P y - X^T P X \hat{\beta} \\
 X^T P X \hat{\beta} &= X^T P y \\
 \hat{\beta} &= (X^T P X)^{-1} X^T P y
 \end{aligned} \tag{7}$$

The derivative of the log-likelihood function (4) at $\hat{\beta}$ with respect to σ^2 is

$$\begin{aligned}
 \frac{dLL(\hat{\beta}, \sigma^2)}{d\sigma^2} &= \frac{d}{d\sigma^2} \left(-\frac{n}{2} \log(\sigma^2) - \frac{1}{2\sigma^2} (y - X\hat{\beta})^T V^{-1} (y - X\hat{\beta}) \right) \\
 &= -\frac{n}{2} \frac{1}{\sigma^2} + \frac{1}{2(\sigma^2)^2} (y - X\hat{\beta})^T V^{-1} (y - X\hat{\beta}) \\
 &= -\frac{n}{2\sigma^2} + \frac{1}{2(\sigma^2)^2} (y - X\hat{\beta})^T V^{-1} (y - X\hat{\beta})
 \end{aligned} \tag{8}$$

and setting this derivative to zero gives the MLE for σ^2 :

$$\begin{aligned}
 \frac{dLL(\hat{\beta}, \hat{\sigma}^2)}{d\sigma^2} &= 0 \\
 0 &= -\frac{n}{2\hat{\sigma}^2} + \frac{1}{2(\hat{\sigma}^2)^2} (y - X\hat{\beta})^T V^{-1} (y - X\hat{\beta}) \\
 \frac{n}{2\hat{\sigma}^2} &= \frac{1}{2(\hat{\sigma}^2)^2} (y - X\hat{\beta})^T V^{-1} (y - X\hat{\beta}) \\
 \frac{2(\hat{\sigma}^2)^2}{n} \cdot \frac{n}{2\hat{\sigma}^2} &= \frac{2(\hat{\sigma}^2)^2}{n} \cdot \frac{1}{2(\hat{\sigma}^2)^2} (y - X\hat{\beta})^T V^{-1} (y - X\hat{\beta}) \\
 \hat{\sigma}^2 &= \frac{1}{n} (y - X\hat{\beta})^T V^{-1} (y - X\hat{\beta})
 \end{aligned} \tag{9}$$

Together, (7) and (9) constitute the MLE for multiple linear regression.

■

1.5.24 Maximum log-likelihood

Theorem: Consider a linear regression model (\rightarrow III/1.5.1) m with correlation structure (\rightarrow I/1.17.6) V

$$m : y = X\beta + \varepsilon, \varepsilon \sim \mathcal{N}(0, \sigma^2 V). \tag{1}$$

Then, the maximum log-likelihood (\rightarrow I/4.1.4) for this model is

$$\text{MLL}(m) = -\frac{n}{2} \log \left(\frac{\text{RSS}}{n} \right) - \frac{n}{2} [1 + \log(2\pi)] \quad (2)$$

under uncorrelated observations (\rightarrow III/1.5.1), i.e. if $V = I_n$, and

$$\text{MLL}(m) = -\frac{n}{2} \log \left(\frac{\text{wRSS}}{n} \right) - \frac{n}{2} [1 + \log(2\pi)] - \frac{1}{2} \log |V|, \quad (3)$$

in the general case, i.e. if $V \neq I_n$, where RSS is the residual sum of squares (\rightarrow III/1.5.9) and wRSS is the weighted residual sum of squares (\rightarrow III/1.5.22).

Proof: The likelihood function (\rightarrow I/5.1.2) for multiple linear regression is given by (\rightarrow III/1.5.23)

$$\begin{aligned} p(y|\beta, \sigma^2) &= \mathcal{N}(y; X\beta, \sigma^2 V) \\ &= \sqrt{\frac{1}{(2\pi)^n |\sigma^2 V|}} \cdot \exp \left[-\frac{1}{2} (y - X\beta)^T (\sigma^2 V)^{-1} (y - X\beta) \right], \end{aligned} \quad (4)$$

such that, with $|\sigma^2 V| = (\sigma^2)^n |V|$, the log-likelihood function (\rightarrow I/4.1.2) for this model becomes (\rightarrow III/1.5.23)

$$\begin{aligned} \text{LL}(\beta, \sigma^2) &= \log p(y|\beta, \sigma^2) \\ &= -\frac{n}{2} \log(2\pi) - \frac{n}{2} \log(\sigma^2) - \frac{1}{2} \log |V| - \frac{1}{2\sigma^2} (y - X\beta)^T V^{-1} (y - X\beta). \end{aligned} \quad (5)$$

The maximum likelihood estimate for the noise variance (\rightarrow III/1.5.23) is

$$\hat{\sigma}^2 = \frac{1}{n} (y - X\hat{\beta})^T V^{-1} (y - X\hat{\beta}) \quad (6)$$

which can also be expressed in terms of the (weighted) residual sum of squares (\rightarrow III/1.5.9) as

$$\frac{1}{n} (y - X\hat{\beta})^T V^{-1} (y - X\hat{\beta}) = \frac{1}{n} (Wy - WX\hat{\beta})^T (Wy - WX\hat{\beta}) = \frac{1}{n} \sum_{i=1}^n (W\hat{\varepsilon})_i^2 = \frac{\text{wRSS}}{n} \quad (7)$$

where $W = V^{-1/2}$. Plugging (6) into (5), we obtain the maximum log-likelihood (\rightarrow I/4.1.4) as

$$\begin{aligned} \text{MLL}(m) &= \text{LL}(\hat{\beta}, \hat{\sigma}^2) \\ &= -\frac{n}{2} \log(2\pi) - \frac{n}{2} \log(\hat{\sigma}^2) - \frac{1}{2} \log |V| - \frac{1}{2\hat{\sigma}^2} (y - X\hat{\beta})^T V^{-1} (y - X\hat{\beta}) \\ &= -\frac{n}{2} \log(2\pi) - \frac{n}{2} \log \left(\frac{\text{wRSS}}{n} \right) - \frac{1}{2} \log |V| - \frac{1}{2} \cdot \frac{n}{\text{wRSS}} \cdot \text{wRSS} \\ &= -\frac{n}{2} \log \left(\frac{\text{wRSS}}{n} \right) - \frac{n}{2} [1 + \log(2\pi)] - \frac{1}{2} \log |V| \end{aligned} \quad (8)$$

which proves the result in (3). Assuming $V = I_n$, we have

$$\hat{\sigma}^2 = \frac{1}{n} (y - X\hat{\beta})^T (y - X\hat{\beta}) = \frac{1}{n} \sum_{i=1}^n \hat{\varepsilon}_i^2 = \frac{\text{RSS}}{n} \quad (9)$$

and

$$\frac{1}{2} \log |V| = \frac{1}{2} \log |I_n| = \frac{1}{2} \log 1 = 0, \quad (10)$$

such that

$$\text{MLL}(m) = -\frac{n}{2} \log \left(\frac{\text{RSS}}{n} \right) - \frac{n}{2} [1 + \log(2\pi)] \quad (11)$$

which proves the result in (2). This completes the proof. ■

Sources:

- Claeskens G, Hjort NL (2008): “Akaike’s information criterion”; in: *Model Selection and Model Averaging*, ex. 2.2, p. 66; URL: <https://www.cambridge.org/core/books/model-selection-and-model-averaging/E6F1EC77279D1223423BB64FC3A12C37>; DOI: 10.1017/CBO9780511790485.

1.5.25 Log-likelihood ratio

Theorem: Let $y = [y_1, \dots, y_n]^T$ be an n -dimensional data vector (\rightarrow I/1.1.5) and consider a linear regression model (\rightarrow III/1.5.1) m_1 with design matrix (\rightarrow III/1.5.1) $X = [X_0, X_1] \in \mathbb{R}^{n \times p}$ as well as a reduced linear regression model (\rightarrow III/1.5.1) m_0 with design matrix (\rightarrow III/1.5.1) $X_0 \in \mathbb{R}^{n \times p_0}$:

$$\begin{aligned} m_1 : y &= X\beta + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 V) \\ m_0 : y &= X_0\beta_0 + \varepsilon_0, \quad \varepsilon_0 \sim \mathcal{N}(0, \sigma_0^2 V). \end{aligned} \quad (1)$$

Both models use the same covariance matrix (\rightarrow III/1.5.1) $V \in \mathbb{R}^{n \times n}$, but entail potentially different regression coefficients (\rightarrow III/1.5.1) β, β_0 and noise variances (\rightarrow III/1.5.1) σ^2, σ_0^2 . Then, the log-likelihood ratio (\rightarrow I/4.1.7) for comparing m_0 vs. m_1 is given by

$$\ln \Lambda_{01} = \frac{n}{2} \ln \left(\frac{\hat{\sigma}^2}{\hat{\sigma}_0^2} \right) \quad (2)$$

where $\hat{\sigma}^2$ and $\hat{\sigma}_0^2$ are the maximum likelihood estimates (\rightarrow I/4.1.3) of the noise variance (\rightarrow III/1.5.1) based on the full model m_1 and the reduced model m_0 , respectively.

Proof: The likelihood ratio (\rightarrow I/4.1.6) between two models m_1 and m_2 with model parameters θ_1 and θ_2 and parameter spaces Θ_1 and Θ_2 is defined as the quotient of their maximized (\rightarrow I/4.1.3) likelihood functions (\rightarrow I/5.1.2):

$$\Lambda_{12} = \frac{\max_{\theta_1 \in \Theta_1} p(y|\theta_1, m_1)}{\max_{\theta_2 \in \Theta_2} p(y|\theta_2, m_2)}. \quad (3)$$

The likelihood function (\rightarrow I/5.1.2) of multiple linear regression (\rightarrow III/1.5.1) is a multivariate normal probability density function (\rightarrow II/4.1.4):

$$\begin{aligned} p(y|\beta, \sigma^2) &= \mathcal{N}(y; X\beta, \sigma^2 V) \\ &= \sqrt{\frac{1}{(2\pi)^n |\sigma^2 V|}} \cdot \exp \left[-\frac{1}{2} (y - X\beta)^T (\sigma^2 V)^{-1} (y - X\beta) \right] \\ &= \sqrt{\frac{1}{(2\pi\sigma^2)^n |V|}} \cdot \exp \left[-\frac{1}{2\sigma^2} (y - X\beta)^T V^{-1} (y - X\beta) \right] \end{aligned} \quad (4)$$

and the maximum likelihood estimates for multiple linear regression (\rightarrow III/1.5.23) are given by

$$\begin{aligned}\hat{\beta} &= (X^T V^{-1} X)^{-1} X^T V^{-1} y \\ \hat{\sigma}^2 &= \frac{1}{n} (y - X \hat{\beta})^T V^{-1} (y - X \hat{\beta}) .\end{aligned}\quad (5)$$

Thus, the likelihood ratio comparing m_0 vs. m_1 is equal to

$$\begin{aligned}\Lambda_{01} &= \frac{p(y|\hat{\beta}_0, \hat{\sigma}_0^2, m_0)}{p(y|\hat{\beta}, \hat{\sigma}^2, m_1)} \\ &= \frac{\sqrt{\frac{1}{(2\pi\hat{\sigma}_0^2)^n |V|}} \cdot \exp \left[-\frac{1}{2\hat{\sigma}_0^2} (y - X_0 \hat{\beta}_0)^T V^{-1} (y - X_0 \hat{\beta}_0) \right]}{\sqrt{\frac{1}{(2\pi\hat{\sigma}^2)^n |V|}} \cdot \exp \left[-\frac{1}{2\hat{\sigma}^2} (y - X \hat{\beta})^T V^{-1} (y - X \hat{\beta}) \right]} \\ &= \frac{(2\pi)^{-n/2} (\hat{\sigma}_0^2)^{-n/2} |V|^{-n/2} \cdot \exp \left[-\frac{1}{2\hat{\sigma}_0^2} (y - X_0 \hat{\beta}_0)^T V^{-1} (y - X_0 \hat{\beta}_0) \right]}{(2\pi)^{-n/2} (\hat{\sigma}^2)^{-n/2} |V|^{-n/2} \cdot \exp \left[-\frac{1}{2\hat{\sigma}^2} (y - X \hat{\beta})^T V^{-1} (y - X \hat{\beta}) \right]} \\ &= \left(\frac{\hat{\sigma}_0^2}{\hat{\sigma}^2} \right)^{-n/2} \cdot \frac{\exp \left[-\frac{n}{2} \frac{(y - X_0 \hat{\beta}_0)^T V^{-1} (y - X_0 \hat{\beta}_0)}{(y - X_0 \hat{\beta}_0)^T V^{-1} (y - X_0 \hat{\beta}_0)} \right]}{\exp \left[-\frac{n}{2} \frac{(y - X \hat{\beta})^T V^{-1} (y - X \hat{\beta})}{(y - X \hat{\beta})^T V^{-1} (y - X \hat{\beta})} \right]} \\ &= \left(\frac{\hat{\sigma}_0^2}{\hat{\sigma}^2} \right)^{-n/2} \cdot \frac{\exp \left[-\frac{n}{2} \right]}{\exp \left[-\frac{n}{2} \right]} \\ &= \left(\frac{\hat{\sigma}_0^2}{\hat{\sigma}^2} \right)^{-n/2} .\end{aligned}\quad (6)$$

Logarithmizing both sides, the log-likelihood ratio is obtained as

$$\ln \Lambda_{01} = \ln \left(\frac{\hat{\sigma}_0^2}{\hat{\sigma}^2} \right)^{-n/2} = -\frac{n}{2} \ln \left(\frac{\hat{\sigma}_0^2}{\hat{\sigma}^2} \right) = \frac{n}{2} \ln \left(\frac{\hat{\sigma}^2}{\hat{\sigma}_0^2} \right) . \quad (7)$$

■

Sources:

- Ostwald, Dirk (2023): “F-Statistiken”; in: *Allgemeines Lineares Modell*, Einheit (8), Folien 20-22;
URL: https://www.ipsy.ovgu.de/ipsy_media/Methodenlehre+I/Sommersemester+2023/Allgemeines+Lineares+Modell/8_F_Statistiken-p-9972.pdf.

1.5.26 t-contrast

Definition: Consider a linear regression model (\rightarrow III/1.5.1) with $n \times p$ design matrix X and $p \times 1$ regression coefficients β :

$$y = X\beta + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 V) . \quad (1)$$

Then, a t-contrast is specified by a $p \times 1$ vector c and it entails the null hypothesis (\rightarrow I/4.3.2) that the product of this vector and the regression coefficients is zero:

$$H_0 : c^T \beta = 0 . \quad (2)$$

Consequently, the alternative hypothesis (\rightarrow I/4.3.3) of a two-tailed t-test (\rightarrow I/4.2.4) is

$$H_1 : c^T \beta \neq 0 \quad (3)$$

and the alternative hypothesis (\rightarrow I/4.3.3) of a one-sided t-test (\rightarrow I/4.2.4) would be

$$H_1 : c^T \beta < 0 \quad \text{or} \quad H_1 : c^T \beta > 0 . \quad (4)$$

Here, c is called the “contrast vector” and $c^T \beta$ is called the “contrast value”. With estimated regression coefficients, $c^T \hat{\beta}$ is called the “estimated contrast value”.

Sources:

- Stephan, Klaas Enno (2010): “Classical (frequentist) inference”; in: *Methods and models for fMRI data analysis in neuroeconomics*, Lecture 4, Slides 7/9; URL: <http://www.socialbehavior.uzh.ch/teaching/methodspring10.html>.

1.5.27 F-contrast

Definition: Consider a linear regression model (\rightarrow III/1.5.1) with $n \times p$ design matrix X and $p \times 1$ regression coefficients β :

$$y = X\beta + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 V) . \quad (1)$$

Then, an F-contrast is specified by a $p \times q$ matrix C , yielding a $q \times 1$ vector $\gamma = C^T \beta$, and it entails the null hypothesis (\rightarrow I/4.3.2) that each value in this vector is zero:

$$H_0 : \gamma_1 = 0 \wedge \dots \wedge \gamma_q = 0 . \quad (2)$$

Consequently, the alternative hypothesis (\rightarrow I/4.3.3) of the statistical test (\rightarrow I/4.3.1) would be that at least one entry of this vector is non-zero:

$$H_1 : \gamma_1 \neq 0 \vee \dots \vee \gamma_q \neq 0 . \quad (3)$$

Here, C is called the “contrast matrix” and $C^T \beta$ are called the “contrast values”. With estimated regression coefficients, $C^T \hat{\beta}$ are called the “estimated contrast values”.

Sources:

- Stephan, Klaas Enno (2010): “Classical (frequentist) inference”; in: *Methods and models for fMRI data analysis in neuroeconomics*, Lecture 4, Slides 23/25; URL: <http://www.socialbehavior.uzh.ch/teaching/methodspring10.html>.

1.5.28 Contrast-based t-test

Theorem: Consider a linear regression model (\rightarrow III/1.5.1)

$$y = X\beta + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 V) \quad (1)$$

and a t-contrast (\rightarrow III/1.5.26) on the model parameters

$$\gamma = c^T \beta \quad \text{where} \quad c \in \mathbb{R}^{p \times 1} . \quad (2)$$

Then, the test statistic (\rightarrow I/4.3.5)

$$t = \frac{c^T \hat{\beta}}{\sqrt{\hat{\sigma}^2 c^T (X^T V^{-1} X)^{-1} c}} \quad (3)$$

with the parameter estimates (\rightarrow III/1.5.23)

$$\begin{aligned} \hat{\beta} &= (X^T V^{-1} X)^{-1} X^T V^{-1} y \\ \hat{\sigma}^2 &= \frac{1}{n-p} (y - X\hat{\beta})^T V^{-1} (y - X\hat{\beta}) \end{aligned} \quad (4)$$

follows a t-distribution (\rightarrow II/3.3.1)

$$t \sim t(n-p) \quad (5)$$

under the null hypothesis (\rightarrow I/4.3.2)

$$\begin{aligned} H_0 &: c^T \beta = 0 \\ H_1 &: c^T \beta > 0 . \end{aligned} \quad (6)$$

Proof:

1) We know that the estimated regression coefficients in linear regression follow a multivariate normal distribution (\rightarrow III/1.5.19):

$$\hat{\beta} \sim \mathcal{N}(\beta, \sigma^2 (X^T V^{-1} X)^{-1}) . \quad (7)$$

Thus, the estimated contrast value (\rightarrow III/1.5.26) $\hat{\gamma} = c^T \hat{\beta}$ is distributed according to a univariate normal distribution (\rightarrow II/4.1.14):

$$\hat{\gamma} \sim \mathcal{N}(c^T \beta, \sigma^2 c^T (X^T V^{-1} X)^{-1} c) . \quad (8)$$

Now, define the random variable z by dividing $\hat{\gamma}$ by its standard deviation:

$$z = \frac{c^T \hat{\beta}}{\sqrt{\sigma^2 c^T (X^T V^{-1} X)^{-1} c}} . \quad (9)$$

Again applying the linear transformation theorem (\rightarrow II/4.1.14), this is distributed as

$$z \sim \mathcal{N}\left(\frac{c^T \beta}{\sqrt{\sigma^2 c^T (X^T V^{-1} X)^{-1} c}}, 1\right) \quad (10)$$

and thus follows a standard normal distribution (\rightarrow II/3.2.3) under the null hypothesis (\rightarrow I/4.3.2):

$$z \sim \mathcal{N}(0, 1), \quad \text{if } H_0 . \quad (11)$$

2) We also know that the residual sum of squares (\rightarrow III/1.5.9), divided the true error variance (\rightarrow III/1.5.1)

$$v = \frac{1}{\sigma^2} \sum_{i=1}^n \hat{\varepsilon}_i^2 = \frac{\hat{\varepsilon}^T \hat{\varepsilon}}{\sigma^2} = \frac{1}{\sigma^2} (y - X\hat{\beta})^T V^{-1} (y - X\hat{\beta}) \quad (12)$$

is following a chi-squared distribution (\rightarrow III/1.5.20):

$$v \sim \chi^2(n - p) . \quad (13)$$

3) Because the estimated regression coefficients and the vector of residuals are independent from each other (\rightarrow III/1.5.17)

$$\hat{\beta} \quad \text{and} \quad \hat{\varepsilon} \quad \text{ind.} \quad (14)$$

and thus, the estimated contrast values are also independent from the function of the residual sum of squares

$$z = \frac{c^T \hat{\beta}}{\sqrt{\sigma^2 c^T (X^T V^{-1} X)^{-1} c}} \quad \text{and} \quad v = \frac{\hat{\varepsilon}^T \hat{\varepsilon}}{\sigma^2} \quad \text{ind.} , \quad (15)$$

the following quantity is, by definition, t-distributed (\rightarrow II/3.3.1)

$$t = \frac{z}{\sqrt{v/(n - p)}} \sim t(n - p), \quad \text{if } H_0 \quad (16)$$

and the quantity can be evaluated as:

$$\begin{aligned} t &\stackrel{(16)}{=} \frac{z}{\sqrt{v/(n - p)}} \\ &\stackrel{(15)}{=} \frac{c^T \hat{\beta}}{\sqrt{\sigma^2 c^T (X^T V^{-1} X)^{-1} c}} \cdot \sqrt{\frac{n - p}{\hat{\varepsilon}^T \hat{\varepsilon} / \sigma^2}} \\ &= \frac{c^T \hat{\beta}}{\sqrt{\frac{\hat{\varepsilon}^T \hat{\varepsilon}}{n - p} \cdot c^T (X^T V^{-1} X)^{-1} c}} \\ &\stackrel{(12)}{=} \frac{c^T \hat{\beta}}{\sqrt{\frac{(y - X \hat{\beta})^T V^{-1} (y - X \hat{\beta})}{n - p} \cdot c^T (X^T V^{-1} X)^{-1} c}} \\ &\stackrel{(4)}{=} \frac{c^T \hat{\beta}}{\sqrt{\hat{\sigma}^2 c^T (X^T V^{-1} X)^{-1} c}} . \end{aligned} \quad (17)$$

This means that the null hypothesis (\rightarrow I/4.3.2) in (6) can be rejected when t from (17) is as extreme or more extreme than the critical value (\rightarrow I/4.3.9) obtained from Student's t-distribution (\rightarrow II/3.3.1) with $n - p$ degrees of freedom (\rightarrow I/1.5.12) using a significance level (\rightarrow I/4.3.8) α .

■

Sources:

- Stephan, Klaas Enno (2010): “Classical (frequentist) inference”; in: *Methods and models for fMRI data analysis in neuroeconomics*, Lecture 4, Slides 7/9; URL: <http://www.socialbehavior.uzh.ch/teaching/methodspring10.html>.
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- jld (2018): “Understanding t-test for linear regression”; in: *StackExchange CrossValidated*, retrieved on 2022-12-13; URL: <https://stats.stackexchange.com/a/344008>.

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1.5.29 Contrast-based F-test

Theorem: Consider a linear regression model (\rightarrow III/1.5.1)

$$y = X\beta + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 V) \quad (1)$$

and an F-contrast (\rightarrow III/1.5.27) on the model parameters

$$\gamma = C^T \beta \quad \text{where} \quad C \in \mathbb{R}^{p \times q} . \quad (2)$$

Then, the test statistic (\rightarrow I/4.3.5)

$$F = \hat{\beta}^T C (\hat{\sigma}^2 C^T (X^T V^{-1} X)^{-1} C)^{-1} C^T \hat{\beta} / q \quad (3)$$

with the parameter estimates (\rightarrow III/1.5.23)

$$\begin{aligned} \hat{\beta} &= (X^T V^{-1} X)^{-1} X^T V^{-1} y \\ \hat{\sigma}^2 &= \frac{1}{n-p} (y - X\hat{\beta})^T V^{-1} (y - X\hat{\beta}) \end{aligned} \quad (4)$$

follows an F-distribution (\rightarrow II/3.8.1)

$$F \sim F(q, n-p) \quad (5)$$

under the null hypothesis (\rightarrow I/4.3.2)

$$\begin{aligned} H_0 &: \gamma_1 = 0 \wedge \dots \wedge \gamma_q = 0 \\ H_1 &: \gamma_1 \neq 0 \vee \dots \vee \gamma_q \neq 0 . \end{aligned} \quad (6)$$

Proof:

1) We know that the estimated regression coefficients in linear regression follow a multivariate normal distribution (\rightarrow III/1.5.19):

$$\hat{\beta} \sim \mathcal{N}(\beta, \sigma^2 (X^T V^{-1} X)^{-1}) . \quad (7)$$

Thus, the estimated contrast vector (\rightarrow III/1.5.27) $\hat{\gamma} = C^T \hat{\beta}$ is also distributed according to a multivariate normal distribution (\rightarrow II/4.1.14):

$$\hat{\gamma} \sim \mathcal{N}(C^T \beta, \sigma^2 C^T (X^T V^{-1} X)^{-1} C) . \quad (8)$$

Substituting the noise variance σ^2 with the noise precision $\tau = 1/\sigma^2$, we can also write this down as a conditional distribution (\rightarrow I/1.5.4):

$$\hat{\gamma} | \tau \sim \mathcal{N}(C^T \beta, (\tau Q)^{-1}) \quad \text{with} \quad Q = (C^T (X^T V^{-1} X)^{-1} C)^{-1} . \quad (9)$$

2) We also know that the residual sum of squares (\rightarrow III/1.5.9), divided the true error variance (\rightarrow III/1.5.1)

$$\frac{1}{\sigma^2} \sum_{i=1}^n \hat{\varepsilon}_i^2 = \frac{\hat{\varepsilon}^T \hat{\varepsilon}}{\sigma^2} = \frac{1}{\sigma^2} (y - X\hat{\beta})^T V^{-1} (y - X\hat{\beta}) \quad (10)$$

is following a chi-squared distribution (\rightarrow III/1.5.20):

$$\frac{\hat{\varepsilon}^T \hat{\varepsilon}}{\sigma^2} = \tau \hat{\varepsilon}^T \hat{\varepsilon} \sim \chi^2(n-p) . \quad (11)$$

The chi-squared distribution is a special case of the gamma distribution (\rightarrow II/3.7.2)

$$X \sim \chi^2(k) \quad \Rightarrow \quad X \sim \text{Gam}\left(\frac{k}{2}, \frac{1}{2}\right) \quad (12)$$

and the gamma distribution changes under multiplication (\rightarrow II/3.4.6) in the following way:

$$X \sim \text{Gam}(a, b) \quad \Rightarrow \quad cX \sim \text{Gam}\left(a, \frac{b}{c}\right) . \quad (13)$$

Thus, combining (12) and (13) with (11), we obtain the marginal distribution (\rightarrow I/1.5.3) of τ as:

$$\frac{1}{\hat{\varepsilon}^T \hat{\varepsilon}} (\tau \hat{\varepsilon}^T \hat{\varepsilon}) = \tau \sim \text{Gam}\left(\frac{n-p}{2}, \frac{\hat{\varepsilon}^T \hat{\varepsilon}}{2}\right) . \quad (14)$$

3) Note that the joint distribution (\rightarrow I/1.5.2) of $\hat{\gamma}$ and τ is, following from (9) and (14) and by definition, a normal-gamma distribution (\rightarrow II/4.4.1):

$$\hat{\gamma}, \tau \sim \text{NG}\left(C^T \beta, Q, \frac{n-p}{2}, \frac{\hat{\varepsilon}^T \hat{\varepsilon}}{2}\right) . \quad (15)$$

The marginal distribution of a normal-gamma distribution with respect to the normal random variable, is a multivariate t-distribution (\rightarrow II/4.4.8):

$$X, Y \sim \text{NG}(\mu, \Lambda, a, b) \quad \Rightarrow \quad X \sim t\left(\mu, \left(\frac{a}{b}\Lambda\right)^{-1}, 2a\right) . \quad (16)$$

Thus, the marginal distribution (\rightarrow I/1.5.3) of $\hat{\gamma}$ is:

$$\hat{\gamma} \sim t\left(C^T \beta, \left(\frac{n-p}{\hat{\varepsilon}^T \hat{\varepsilon}} Q\right)^{-1}, n-p\right) . \quad (17)$$

4) Because of the following relationship between the multivariate t-distribution and the F-distribution (\rightarrow II/4.3.3)

$$X \sim t(\mu, \Sigma, \nu) \quad \Rightarrow \quad (X - \mu)^T \Sigma^{-1} (X - \mu) / \nu \sim F(n, \nu) , \quad (18)$$

the following quantity is, by definition, F-distributed (\rightarrow II/3.8.1)

$$F = (\hat{\gamma} - C^T \beta)^T \left(\frac{n-p}{\hat{\varepsilon}^T \hat{\varepsilon}} Q\right) (\hat{\gamma} - C^T \beta) / q \sim F(q, n-p) \quad (19)$$

and under the null hypothesis (\rightarrow I/4.3.2) (6), it can be evaluated as:

$$\begin{aligned}
F &\stackrel{(19)}{=} (\hat{\gamma} - C^T \beta)^T \left(\frac{n-p}{\hat{\varepsilon}^T \hat{\varepsilon}} Q \right) (\hat{\gamma} - C^T \beta) / q \\
&\stackrel{(6)}{=} \hat{\gamma}^T \left(\frac{n-p}{\hat{\varepsilon}^T \hat{\varepsilon}} Q \right) \hat{\gamma} / q \\
&\stackrel{(2)}{=} \hat{\beta}^T C \left(\frac{n-p}{\hat{\varepsilon}^T \hat{\varepsilon}} Q \right) C^T \hat{\beta} / q \\
&\stackrel{(9)}{=} \hat{\beta}^T C \left(\frac{n-p}{\hat{\varepsilon}^T \hat{\varepsilon}} (C^T (X^T V^{-1} X)^{-1} C)^{-1} \right) C^T \hat{\beta} / q \\
&\stackrel{(10)}{=} \hat{\beta}^T C \left(\frac{n-p}{(y - X\hat{\beta})^T V^{-1} (y - X\hat{\beta})} (C^T (X^T V^{-1} X)^{-1} C)^{-1} \right) C^T \hat{\beta} / q \\
&\stackrel{(4)}{=} \hat{\beta}^T C \left(\frac{1}{\hat{\sigma}^2} (C^T (X^T V^{-1} X)^{-1} C)^{-1} \right) C^T \hat{\beta} / q \\
&= \hat{\beta}^T C (\hat{\sigma}^2 C^T (X^T V^{-1} X)^{-1} C)^{-1} C^T \hat{\beta} / q .
\end{aligned} \tag{20}$$

This means that the null hypothesis (\rightarrow I/4.3.2) in (6) can be rejected when F from (20) is as extreme or more extreme than the critical value (\rightarrow I/4.3.9) obtained from Fisher's F-distribution (\rightarrow II/3.8.1) with q numerator and $n - p$ denominator degrees of freedom (\rightarrow I/1.5.12) using a significance level (\rightarrow I/4.3.8) α .

■

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1.5.30 t-test for single regressor

Theorem: Consider a linear regression model (\rightarrow III/1.5.1)

$$y = X\beta + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 V) \tag{1}$$

using the $n \times p$ design matrix X and the parameter estimates (\rightarrow III/1.5.23)

$$\begin{aligned}
\hat{\beta} &= (X^T V^{-1} X)^{-1} X^T V^{-1} y \\
\hat{\sigma}^2 &= \frac{1}{n-p} (y - X\hat{\beta})^T V^{-1} (y - X\hat{\beta}) .
\end{aligned} \tag{2}$$

Then, the test statistic (\rightarrow I/4.3.5)

$$t_j = \frac{\hat{\beta}_j}{\sqrt{(\hat{\varepsilon}^T V^{-1} \hat{\varepsilon}) / (n - p) \sigma_{jj}}} \quad (3)$$

with the n -dimensional vector of residuals (\rightarrow III/1.5.14)

$$\hat{\varepsilon} = y - X\hat{\beta} \quad (4)$$

and σ_{jj} equal to the j -th diagonal element of the parameter covariance matrix (\rightarrow III/1.5.19)

$$\sigma_{jj} = \left[(X^T V^{-1} X)^{-1} \right]_{jj} \quad (5)$$

follows a t-distribution (\rightarrow II/3.3.1)

$$t_j \sim t(n - p) \quad (6)$$

under the null hypothesis (\rightarrow I/4.3.2) that the j -th regression coefficient (\rightarrow III/1.5.1) is zero:

$$H_0 : \beta_j = 0 . \quad (7)$$

Proof: This is a special case of the contrast-based t-test for multiple linear regression (\rightarrow III/1.5.28) based on the following t-statistic (\rightarrow II/3.3.1):

$$t = \frac{c^T \hat{\beta}}{\sqrt{\hat{\sigma}^2 c^T (X^T V^{-1} X)^{-1} c}} \sim t(n - p) . \quad (8)$$

In this special case, the contrast vector (\rightarrow III/1.5.26) is equal to the j -th elementary vector e_j (a $p \times 1$ vector of zeros, with a single 1 in the j -th entry)

$$c = e_j = [0, \dots, 0, 1, 0, \dots, 0]^T , \quad (9)$$

such that the null hypothesis is given by

$$H_0 : c^T \beta = e_j^T \beta = \beta_j = 0 \quad (10)$$

and the test statistic becomes

$$\begin{aligned} t_j &= \frac{e_j^T \hat{\beta}}{\sqrt{\hat{\sigma}^2 e_j^T (X^T V^{-1} X)^{-1} e_j}} \\ &= \frac{[0, \dots, 0, 1, 0, \dots, 0] \left[\hat{\beta}_1, \dots, \hat{\beta}_{j-1}, \hat{\beta}_j, \hat{\beta}_{j+1}, \dots, \hat{\beta}_p \right]^T}{\sqrt{\frac{1}{n-p} (y - X\hat{\beta})^T V^{-1} (y - X\hat{\beta}) [0, \dots, 1, \dots, 0] (X^T V^{-1} X)^{-1} [0, \dots, 1, \dots, 0]^T}} \\ &= \frac{\hat{\beta}_j}{\sqrt{\frac{1}{n-p} (\hat{\varepsilon}^T V^{-1} \hat{\varepsilon}) \left[(X^T V^{-1} X)^{-1} \right]_{jj}}} \\ &= \frac{\hat{\beta}_j}{\sqrt{(\hat{\varepsilon}^T V^{-1} \hat{\varepsilon}) / (n - p) \sigma_{jj}}} . \end{aligned} \quad (11)$$

■

Sources:

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1.5.31 F-test for multiple regressors

Theorem: Consider a linear regression model (\rightarrow III/1.5.1)

$$y = X\beta + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 V) \quad (1)$$

the design matrix and regression coefficients of which are partitioned as

$$\begin{aligned} X &= \begin{bmatrix} X_0 & X_1 \end{bmatrix} \in \mathbb{R}^{n \times p} \quad \text{where} \quad X_0 \in \mathbb{R}^{n \times p_0} \quad \text{and} \quad X_1 \in \mathbb{R}^{n \times p_1} \\ \beta &= \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} \in \mathbb{R}^{p \times 1} \quad \text{where} \quad \beta_0 \in \mathbb{R}^{p_0 \times 1} \quad \text{and} \quad \beta_1 \in \mathbb{R}^{p_1 \times 1} \end{aligned} \quad (2)$$

with $p = p_0 + p_1$. Then, the test statistic (\rightarrow I/4.3.5)

$$F = \frac{(\hat{\varepsilon}_0^T V^{-1} \hat{\varepsilon}_0 - \hat{\varepsilon}^T V^{-1} \hat{\varepsilon})/p_1}{\hat{\varepsilon}^T V^{-1} \hat{\varepsilon}/(n - p)} \quad (3)$$

follows an F-distribution (\rightarrow II/3.8.1)

$$F \sim F(p_1, n - p) \quad (4)$$

under the null hypothesis (\rightarrow I/4.3.2) that all regression coefficients (\rightarrow III/1.5.1) β_1 are zero:

$$H_0 : \beta_1 = 0_{p_1} \quad \Leftrightarrow \quad \beta_{1j} = 0 \quad \text{for all} \quad j = 1, \dots, p_1. \quad (5)$$

In (3), $\hat{\varepsilon}$ and $\hat{\varepsilon}_0$ are the residual vectors (\rightarrow III/1.5.14) when using either the full design matrix X or the reduced design matrix X_0 :

$$\begin{aligned} \hat{\varepsilon} &= y - X\hat{\beta} \quad \text{with} \quad \hat{\beta} = (X^T V^{-1} X)^{-1} X^T V^{-1} y \\ \hat{\varepsilon}_0 &= y - X_0 \hat{\beta}_0 \quad \text{with} \quad \hat{\beta}_0 = (X_0^T V^{-1} X_0)^{-1} X_0^T V^{-1} y. \end{aligned} \quad (6)$$

Proof: This is a special case of the contrast-based F-test for multiple linear regression (\rightarrow III/1.5.29) based on the F-statistic (\rightarrow I/4.3.5)

$$F = \hat{\beta}^T C (\hat{\sigma}^2 C^T (X^T V^{-1} X)^{-1} C)^{-1} C^T \hat{\beta} / q \quad (7)$$

which follows an F-distribution (\rightarrow II/3.8.1) under the null hypothesis (\rightarrow I/4.3.2) that the product of the contrast matrix (\rightarrow III/1.5.27) $C \in \mathbb{R}^{p \times q}$ and the regression coefficients (\rightarrow III/1.5.1) equals zero:

$$F \sim F(q, n-p), \quad \text{if } C^T \beta = 0_q = \begin{bmatrix} 0 \\ \vdots \\ 0 \end{bmatrix}. \quad (8)$$

In (7), $\hat{\sigma}^2$ is an estimate of the noise variance (\rightarrow III/1.5.1) calculated as the weighted (\rightarrow III/1.5.21) residual sum of squares (\rightarrow III/1.5.9), divided by $n-p$:

$$\hat{\sigma}^2 = \frac{1}{n-p} (y - X\hat{\beta})^T V^{-1} (y - X\hat{\beta}). \quad (9)$$

In the present case, in order to compare the full model specified by X against the reduced model specified by X_0 , we have to define the contrast matrix (\rightarrow III/1.5.27) as a vertical concatenation of a zero matrix on the first p_0 components and an identity matrix on the last p_1 components of β ,

$$C_1 = \begin{bmatrix} 0_{p_0, p_1} \\ I_{p_1} \end{bmatrix} \in \mathbb{R}^{p \times p_1}, \quad (10)$$

i.e. specify an omnibus F-contrast that tests the alternative hypothesis (\rightarrow I/4.3.3) that any of the coefficients β_1 associated with the regressors X_1 is different from zero against the null hypothesis (\rightarrow I/4.3.2) that all those coefficients are zero:

$$\begin{aligned} H_0 : C_1^T \beta &= \begin{bmatrix} 0_{p_0, p_1} \\ I_{p_1} \end{bmatrix}^T \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} = \beta_1 = 0_{p_1} \quad \Leftrightarrow \quad \beta_{1j} = 0 \quad \text{for all } j = 1, \dots, p_1 \\ \Rightarrow H_1 &\Leftrightarrow \neg H_0 : C_1^T \beta = \beta_1 \neq 0_{p_1} \quad \Leftrightarrow \quad \beta_{1j} \neq 0 \quad \text{for at least one } j = 1, \dots, p_1. \end{aligned} \quad (11)$$

Thus, plugging $C = C_1$ and $q = p_1$ into (7) and noting that $\hat{\sigma}^2$ from (9) is a scalar, we obtain:

$$\begin{aligned} F &= \hat{\beta}^T C_1 (\hat{\sigma}^2 C_1^T (X^T V^{-1} X)^{-1} C_1)^{-1} C_1^T \hat{\beta} / p_1 \\ &\stackrel{(9)}{=} \frac{\hat{\beta}^T C_1 (C_1^T (X^T V^{-1} X)^{-1} C_1)^{-1} C_1^T \hat{\beta} / p_1}{(y - X\hat{\beta})^T V^{-1} (y - X\hat{\beta}) / (n-p)}. \end{aligned} \quad (12)$$

Here, we take note of the fact that the denominator in (12) is already equal to the denominator in (3):

$$(y - X\hat{\beta})^T V^{-1} (y - X\hat{\beta}) / (n-p) \stackrel{(6)}{=} \hat{\varepsilon}^T V^{-1} \hat{\varepsilon} / (n-p). \quad (13)$$

Therefore, what remains to be shown is that the numerator in (12) is equal to the numerator in (3):

$$\hat{\beta}^T C_1 (C_1^T (X^T V^{-1} X)^{-1} C_1)^{-1} C_1^T \hat{\beta} / p_1 = (\hat{\varepsilon}_0^T V^{-1} \hat{\varepsilon}_0 - \hat{\varepsilon}^T V^{-1} \hat{\varepsilon}) / p_1. \quad (14)$$

To do this, we start with the inner-most matrix:

$$\begin{aligned}
X^T V^{-1} X &\stackrel{(2)}{=} \begin{bmatrix} X_0 & X_1 \end{bmatrix}^T V^{-1} \begin{bmatrix} X_0 & X_1 \end{bmatrix} \\
&= \begin{bmatrix} X_0^T \\ X_1^T \end{bmatrix} V^{-1} \begin{bmatrix} X_0 & X_1 \end{bmatrix} \\
&= \begin{bmatrix} X_0^T V^{-1} X_0 & X_0^T V^{-1} X_1 \\ X_1^T V^{-1} X_0 & X_1^T V^{-1} X_1 \end{bmatrix}.
\end{aligned} \tag{15}$$

The inverse of a block matrix is:

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix}^{-1} = \begin{bmatrix} A^{-1} + A^{-1}B(D - CA^{-1}B)^{-1}CA^{-1} & -A^{-1}B(D - CA^{-1}B)^{-1} \\ -(D - CA^{-1}B)^{-1}CA^{-1} & (D - CA^{-1}B)^{-1} \end{bmatrix}. \tag{16}$$

Note that, with the contrast matrix C_1 , we only extract the lower-right part of the inverse block matrix, so that we have:

$$\begin{aligned}
(C_1^T (X^T V^{-1} X)^{-1} C_1)^{-1} &\stackrel{(10)}{=} \left(\begin{bmatrix} 0_{p_1, p_0} & I_{p_1} \end{bmatrix} (X^T V^{-1} X)^{-1} \begin{bmatrix} 0_{p_0, p_1} \\ I_{p_1} \end{bmatrix} \right)^{-1} \\
&\stackrel{(16)}{=} \left((X_1^T V^{-1} X_1 - X_1^T V^{-1} X_0 (X_0^T V^{-1} X_0)^{-1} X_0^T V^{-1} X_1)^{-1} \right)^{-1} \\
&= X_1^T V^{-1} X_1 - X_1^T V^{-1} X_0 (X_0^T V^{-1} X_0)^{-1} X_0^T V^{-1} X_1.
\end{aligned} \tag{17}$$

We call this $p_1 \times p_1$ matrix E and note that it can be written as

$$\begin{aligned}
E &\stackrel{(17)}{=} X_1^T (V^{-1} - V^{-1} X_0 (X_0^T V^{-1} X_0)^{-1} X_0^T V^{-1}) X_1 \\
&= X_1^T (V^{-1} - F) X_1
\end{aligned} \tag{18}$$

where the $n \times n$ matrix F is given as follows:

$$F = V^{-1} X_0 (X_0^T V^{-1} X_0)^{-1} X_0^T V^{-1}. \tag{19}$$

Let $\hat{\beta}_{0(X)}$ denote the first p_0 entries of $\hat{\beta}$, i.e. estimates of the coefficients belonging to X_0 , but estimated with X (as opposed to $\hat{\beta}_0$ estimated with X_0 given by (6)):

$$\hat{\beta} = \begin{bmatrix} \hat{\beta}_{0(X)} \\ \hat{\beta}_1 \end{bmatrix}. \tag{20}$$

Then, it obviously holds that

$$\begin{aligned}
X \hat{\beta} &\stackrel{(20)}{=} \begin{bmatrix} X_0 & X_1 \end{bmatrix} \begin{bmatrix} \hat{\beta}_{0(X)} \\ \hat{\beta}_1 \end{bmatrix} \\
&= X_0 \hat{\beta}_{0(X)} + X_1 \hat{\beta}_1 \\
&\Leftrightarrow \\
X_1 \hat{\beta}_1 &= X \hat{\beta} - X_0 \hat{\beta}_{0(X)}.
\end{aligned} \tag{21}$$

Next, we focus on $C_1^T \hat{\beta}$ which simply extracts $\hat{\beta}_1$:

$$\begin{aligned} C_1^T \hat{\beta} &\stackrel{(20)}{=} \begin{bmatrix} 0_{p_1, p_0} & I_{p_1} \end{bmatrix} \begin{bmatrix} \hat{\beta}_{0(X)} \\ \hat{\beta}_1 \end{bmatrix} \\ &= \hat{\beta}_1 . \end{aligned} \quad (22)$$

With these identities in mind, we can get back to our main quantity of interest from (14):

$$\begin{aligned} &\hat{\beta}^T C_1 (C_1^T (X^T V^{-1} X)^{-1} C_1)^{-1} C_1^T \hat{\beta} \\ &\stackrel{(22)}{=} \hat{\beta}_1^T E \hat{\beta}_1 \\ &\stackrel{(18)}{=} \hat{\beta}_1^T X_1^T (V^{-1} - V^{-1} X_0 (X_0^T V^{-1} X_0)^{-1} X_0^T V^{-1}) X_1 \hat{\beta}_1 \\ &\stackrel{(21)}{=} (\hat{\beta}^T X^T - \hat{\beta}_{0(X)}^T X_0^T) (V^{-1} - V^{-1} X_0 (X_0^T V^{-1} X_0)^{-1} X_0^T V^{-1}) (X \hat{\beta} - X_0 \hat{\beta}_{0(X)}) \\ &\stackrel{(19)}{=} (\hat{\beta}^T X^T V^{-1} - \hat{\beta}^T X^T F - \hat{\beta}_{0(X)}^T X_0^T V^{-1} + \hat{\beta}_{0(X)}^T X_0^T V^{-1} X_0 (X_0^T V^{-1} X_0)^{-1} X_0^T V^{-1}) (X \hat{\beta} - X_0 \hat{\beta}_{0(X)}) \\ &= (\hat{\beta}^T X^T V^{-1} - \hat{\beta}^T X^T F - \hat{\beta}_{0(X)}^T X_0^T V^{-1} + \hat{\beta}_{0(X)}^T X_0^T V^{-1}) (X \hat{\beta} - X_0 \hat{\beta}_{0(X)}) \\ &= (\hat{\beta}^T X^T V^{-1} - \hat{\beta}^T X^T F) (X \hat{\beta} - X_0 \hat{\beta}_{0(X)}) \\ &\stackrel{(19)}{=} \hat{\beta}^T X^T V^{-1} X \hat{\beta} - \hat{\beta}^T X^T V^{-1} X_0 \hat{\beta}_{0(X)} - \hat{\beta}^T X^T F X \hat{\beta} + \hat{\beta}^T X^T V^{-1} X_0 (X_0^T V^{-1} X_0)^{-1} X_0^T V^{-1} X_0 \hat{\beta}_{0(X)} \\ &= \hat{\beta}^T X^T V^{-1} X \hat{\beta} - \hat{\beta}^T X^T V^{-1} X_0 \hat{\beta}_{0(X)} - \hat{\beta}^T X^T F X \hat{\beta} + \hat{\beta}^T X^T V^{-1} X_0 \hat{\beta}_{0(X)} \\ &= \hat{\beta}^T X^T V^{-1} X \hat{\beta} - \hat{\beta}^T X^T F X \hat{\beta} \\ &\stackrel{(19)}{=} \hat{\beta}^T X^T V^{-1} X \hat{\beta} - \hat{\beta}^T X^T V^{-1} X_0 (X_0^T V^{-1} X_0)^{-1} X_0^T V^{-1} X \hat{\beta} . \end{aligned} \quad (23)$$

Let the residual vector of the full model be defined as given by (6)

$$\hat{\varepsilon} = y - X \hat{\beta} \quad \Leftrightarrow \quad y = X \hat{\beta} + \hat{\varepsilon} \quad (24)$$

and consider the term $X^T V^{-1} \hat{\varepsilon}$. Using the residual-forming matrix expression of the residual vector (\rightarrow III/1.5.14), we can show that this matrix product is zero:

$$\begin{aligned} X^T V^{-1} \hat{\varepsilon} &= X^T V^{-1} (I_n - X (X^T V^{-1} X)^{-1} X^T V^{-1}) y \\ &= X^T V^{-1} y - X^T V^{-1} X (X^T V^{-1} X)^{-1} X^T V^{-1} y \\ &= X^T V^{-1} y - X^T V^{-1} y \\ &= 0_p . \end{aligned} \quad (25)$$

From this, it follows that the product $X_0^T V^{-1} \hat{\varepsilon}$ is also zero:

$$\begin{aligned}
X^T V^{-1} \hat{\varepsilon} &= 0_p \\
\begin{bmatrix} X_0^T \\ X_1^T \end{bmatrix} V^{-1} \hat{\varepsilon} &= 0_p \\
\begin{bmatrix} X_0^T V^{-1} \hat{\varepsilon} \\ X_1^T V^{-1} \hat{\varepsilon} \end{bmatrix} &= \begin{bmatrix} 0_{p_0} \\ 0_{p_1} \end{bmatrix} \\
&\Leftrightarrow \\
X_0^T V^{-1} \hat{\varepsilon} &= 0_{p_0} .
\end{aligned} \tag{26}$$

Thus, any term containing $X_0^T V^{-1} \hat{\varepsilon} = 0_{p_0}$ can be added to a sum without changing the value of this sum. Continuing from above, we therefore write:

$$\begin{aligned}
&\hat{\beta}^T C_1 (C_1^T (X^T V^{-1} X)^{-1} C_1)^{-1} C_1^T \hat{\beta} \\
&\stackrel{(23)}{=} \hat{\beta}^T X^T V^{-1} X \hat{\beta} - \hat{\beta}^T X^T V^{-1} X_0 (X_0^T V^{-1} X_0)^{-1} X_0^T V^{-1} X \hat{\beta} \\
&\stackrel{(26)}{=} \hat{\beta}^T X^T V^{-1} X \hat{\beta} - \hat{\beta}^T X^T V^{-1} X_0 (X_0^T V^{-1} X_0)^{-1} X_0^T V^{-1} X \hat{\beta} \\
&\quad + 2 \hat{\beta}^T X^T V^{-1} X_0 (X_0^T V^{-1} X_0)^{-1} X_0^T V^{-1} \hat{\varepsilon} + \hat{\varepsilon}^T V^{-1} X_0 (X_0^T V^{-1} X_0)^{-1} X_0^T V^{-1} \hat{\varepsilon} \\
&= \hat{\beta}^T X^T V^{-1} X \hat{\beta} - (X \hat{\beta} + \hat{\varepsilon})^T V^{-1} X_0 (X_0^T V^{-1} X_0)^{-1} X_0^T V^{-1} (X \hat{\beta} + \hat{\varepsilon}) \\
&\stackrel{(24)}{=} \hat{\beta}^T X^T V^{-1} X \hat{\beta} - y^T V^{-1} X_0 (X_0^T V^{-1} X_0)^{-1} X_0^T V^{-1} y .
\end{aligned} \tag{27}$$

In the next transformations, we will make use of the weighted least squares parameter estimates (\rightarrow III/1.5.21)

$$\begin{aligned}
\hat{\beta} &= (X^T V^{-1} X)^{-1} X^T V^{-1} y \\
\hat{\beta}_0 &= (X_0^T V^{-1} X_0)^{-1} X_0^T V^{-1} y
\end{aligned} \tag{28}$$

and the fact that matrices and their inverses cancel out:

$$\begin{aligned}
X^T V^{-1} X (X^T V^{-1} X)^{-1} &= (X^T V^{-1} X)^{-1} X^T V^{-1} X = I_p \\
X_0^T V^{-1} X_0 (X_0^T V^{-1} X_0)^{-1} &= (X_0^T V^{-1} X_0)^{-1} X_0^T V^{-1} X_0 = I_{p_0} .
\end{aligned} \tag{29}$$

Continuing from above, we have:

$$\begin{aligned}
& \hat{\beta}^T C_1 (C_1^T (X^T V^{-1} X)^{-1} C_1)^{-1} C_1^T \hat{\beta} \\
& \stackrel{(27)}{=} \hat{\beta}^T X^T V^{-1} X \hat{\beta} - y^T V^{-1} X_0 (X_0^T V^{-1} X_0)^{-1} X_0^T V^{-1} y \\
& \stackrel{(28)}{=} y^T V^{-1} X (X^T V^{-1} X)^{-1} X^T V^{-1} X (X^T V^{-1} X)^{-1} X^T V^{-1} y - y^T V^{-1} X_0 (X_0^T V^{-1} X_0)^{-1} X_0^T V^{-1} y \\
& = y^T V^{-1} X (X^T V^{-1} X)^{-1} X^T V^{-1} y - y^T V^{-1} X_0 (X_0^T V^{-1} X_0)^{-1} X_0^T V^{-1} y \\
& = y^T V^{-1} X_0 (X_0^T V^{-1} X_0)^{-1} X_0^T V^{-1} y - 2y^T V^{-1} X_0 (X_0^T V^{-1} X_0)^{-1} X_0^T V^{-1} y \\
& - y^T V^{-1} X (X^T V^{-1} X)^{-1} X^T V^{-1} y + 2y^T V^{-1} X (X^T V^{-1} X)^{-1} X^T V^{-1} y \\
& \stackrel{(29)}{=} y^T V^{-1} X_0 (X_0^T V^{-1} X_0)^{-1} X_0^T V^{-1} X_0 (X_0^T V^{-1} X_0)^{-1} X_0^T V^{-1} y - 2y^T V^{-1} X_0 (X_0^T V^{-1} X_0)^{-1} X_0^T V^{-1} y \\
& - y^T V^{-1} X (X^T V^{-1} X)^{-1} X^T V^{-1} X (X^T V^{-1} X)^{-1} X^T V^{-1} y + 2y^T V^{-1} X (X^T V^{-1} X)^{-1} X^T V^{-1} y \\
& \stackrel{(28)}{=} \hat{\beta}_0^T X_0^T V^{-1} X_0 \hat{\beta}_0 - 2y^T V^{-1} X_0 \hat{\beta}_0 - \hat{\beta}^T X^T V^{-1} X \hat{\beta} + 2y^T V^{-1} X \hat{\beta} \\
& = y^T V^{-1} y - 2y^T V^{-1} X_0 \hat{\beta}_0 + \hat{\beta}_0^T X_0^T V^{-1} X_0 \hat{\beta}_0 - y^T V^{-1} y + 2y^T V^{-1} X \hat{\beta} - \hat{\beta}^T X^T V^{-1} X \hat{\beta} \\
& = \left(y^T V^{-1} y - 2y^T V^{-1} X_0 \hat{\beta}_0 + \hat{\beta}_0^T X_0^T V^{-1} X_0 \hat{\beta}_0 \right) - \left(y^T V^{-1} y - 2y^T V^{-1} X \hat{\beta} + \hat{\beta}^T X^T V^{-1} X \hat{\beta} \right) \\
& = (y - X_0 \hat{\beta}_0)^T V^{-1} (y - X_0 \hat{\beta}_0) - (y - X \hat{\beta})^T V^{-1} (y - X \hat{\beta}) \\
& \stackrel{(6)}{=} \hat{\varepsilon}_0^T V^{-1} \hat{\varepsilon}_0 - \hat{\varepsilon}^T V^{-1} \hat{\varepsilon} .
\end{aligned} \tag{30}$$

With that, it is shown that (14) is true which, together with (13), finally demonstrates that the F-value in (12) is equal to the test statistic given by (3). This completes the proof. ■

Sources:

- Ostwald, Dirk (2023): “F-Statistiken”; in: *Allgemeines Lineares Modell*, Einheit (8), Folien 20, 24; URL: https://www.ipsy.ovgu.de/ipsy_media/Methodenlehre+I/Sommersemester+2023/Allgemeines+Lineares+Modell/8_F_Statistiken-p-9972.pdf.

1.5.32 Deviance function

Theorem: Consider a linear regression model (\rightarrow III/1.5.1) m with correlation structure (\rightarrow I/1.17.6) V

$$m : y = X\beta + \varepsilon, \varepsilon \sim \mathcal{N}(0, \sigma^2 V) . \tag{1}$$

Then, the deviance (\rightarrow IV/2.3.2) for this model is

$$D(\beta, \sigma^2) = \text{RSS}/\sigma^2 + n \cdot [\log(\sigma^2) + \log(2\pi)] \tag{2}$$

under uncorrelated observations (\rightarrow III/1.5.1), i.e. if $V = I_n$, and

$$D(\beta, \sigma^2) = \text{wRSS}/\sigma^2 + n \cdot [\log(\sigma^2) + \log(2\pi)] + \log |V| , \tag{3}$$

in the general case, i.e. if $V \neq I_n$, where RSS is the residual sum of squares (\rightarrow III/1.5.9) and wRSS is the weighted residual sum of squares (\rightarrow III/1.5.22).

Proof: The likelihood function (\rightarrow I/5.1.2) for multiple linear regression is given by (\rightarrow III/1.5.23)

$$\begin{aligned}
p(y|\beta, \sigma^2) &= \mathcal{N}(y; X\beta, \sigma^2 V) \\
&= \sqrt{\frac{1}{(2\pi)^n |\sigma^2 V|}} \cdot \exp \left[-\frac{1}{2} (y - X\beta)^T (\sigma^2 V)^{-1} (y - X\beta) \right], \tag{4}
\end{aligned}$$

such that, with $|\sigma^2 V| = (\sigma^2)^n |V|$, the log-likelihood function (\rightarrow I/4.1.2) for this model becomes (\rightarrow III/1.5.23)

$$\begin{aligned}
\text{LL}(\beta, \sigma^2) &= \log p(y|\beta, \sigma^2) \\
&= -\frac{n}{2} \log(2\pi) - \frac{n}{2} \log(\sigma^2) - \frac{1}{2} \log |V| - \frac{1}{2\sigma^2} (y - X\beta)^T V^{-1} (y - X\beta). \tag{5}
\end{aligned}$$

The last term can be expressed in terms of the (weighted) residual sum of squares (\rightarrow III/1.5.9) as

$$\begin{aligned}
-\frac{1}{2\sigma^2} (y - X\beta)^T V^{-1} (y - X\beta) &= -\frac{1}{2\sigma^2} (Wy - WX\beta)^T (Wy - WX\beta) \\
&= -\frac{1}{2\sigma^2} \left(\frac{1}{n} \sum_{i=1}^n (W\varepsilon_i)^2 \right) = -\frac{\text{wRSS}}{2\sigma^2} \tag{6}
\end{aligned}$$

where $W = V^{-1/2}$. Plugging (6) into (5) and multiplying with -2 , we obtain the deviance (\rightarrow IV/2.3.2) as

$$\begin{aligned}
D(\beta, \sigma^2) &= -2 \text{LL}(\beta, \sigma^2) \\
&= -2 \left(-\frac{\text{wRSS}}{2\sigma^2} - \frac{n}{2} \log(\sigma^2) - \frac{n}{2} \log(2\pi) - \frac{1}{2} \log |V| \right) \\
&= \text{wRSS}/\sigma^2 + n \cdot [\log(\sigma^2) + \log(2\pi)] + \log |V| \tag{7}
\end{aligned}$$

which proves the result in (3). Assuming $V = I_n$, we have

$$\begin{aligned}
-\frac{1}{2\sigma^2} (y - X\beta)^T V^{-1} (y - X\beta) &= -\frac{1}{2\sigma^2} (y - X\beta)^T (y - X\beta) \\
&= -\frac{1}{2\sigma^2} \left(\frac{1}{n} \sum_{i=1}^n \varepsilon_i^2 \right) = -\frac{\text{RSS}}{2\sigma^2} \tag{8}
\end{aligned}$$

and

$$\frac{1}{2} \log |V| = \frac{1}{2} \log |I_n| = \frac{1}{2} \log 1 = 0, \tag{9}$$

such that

$$D(\beta, \sigma^2) = \text{RSS}/\sigma^2 + n \cdot [\log(\sigma^2) + \log(2\pi)] \tag{10}$$

which proves the result in (2). This completes the proof. ■

1.5.33 Akaike information criterion

Theorem: Consider a linear regression model (\rightarrow III/1.5.1) m

$$m : y = X\beta + \varepsilon, \varepsilon \sim \mathcal{N}(0, \sigma^2 V) . \quad (1)$$

Then, the Akaike information criterion (\rightarrow IV/2.1.1) for this model is

$$\text{AIC}(m) = n \log \left(\frac{\text{wRSS}}{n} \right) + n [1 + \log(2\pi)] + \log |V| + 2(p + 1) \quad (2)$$

where wRSS is the weighted residual sum of squares (\rightarrow III/1.5.9), p is the number of regressors (\rightarrow III/1.5.1) in the design matrix X and n is the number of observations (\rightarrow III/1.5.1) in the data vector y .

Proof: The Akaike information criterion (\rightarrow IV/2.1.1) is defined as

$$\text{AIC}(m) = -2 \text{MLL}(m) + 2k \quad (3)$$

where $\text{MLL}(m)$ is the maximum log-likelihood (\rightarrow I/4.1.4) is k is the number of free parameters in m .

The maximum log-likelihood for multiple linear regression (\rightarrow III/1.5.24) is given by

$$\text{MLL}(m) = -\frac{n}{2} \log \left(\frac{\text{wRSS}}{n} \right) - \frac{n}{2} [1 + \log(2\pi)] - \frac{1}{2} \log |V| \quad (4)$$

and the number of free parameters in multiple linear regression (\rightarrow III/1.5.1) is $k = p + 1$, i.e. one for each regressor in the design matrix (\rightarrow III/1.5.1) X , plus one for the noise variance (\rightarrow III/1.5.1) σ^2 .

Thus, the AIC of m follows from (3) and (4) as

$$\text{AIC}(m) = n \log \left(\frac{\text{wRSS}}{n} \right) + n [1 + \log(2\pi)] + \log |V| + 2(p + 1) . \quad (5)$$

■

Sources:

- Claeskens G, Hjort NL (2008): “Akaike’s information criterion”; in: *Model Selection and Model Averaging*, ex. 2.2, p. 66; URL: <https://www.cambridge.org/core/books/model-selection-and-model-averaging/E6F1EC77279D1223423BB64FC3A12C37>; DOI: 10.1017/CBO9780511790485.

1.5.34 Bayesian information criterion

Theorem: Consider a linear regression model (\rightarrow III/1.5.1) m

$$m : y = X\beta + \varepsilon, \varepsilon \sim \mathcal{N}(0, \sigma^2 V) . \quad (1)$$

Then, the Bayesian information criterion (\rightarrow IV/2.2.1) for this model is

$$\text{BIC}(m) = n \log \left(\frac{\text{wRSS}}{n} \right) + n [1 + \log(2\pi)] + \log |V| + \log(n) (p + 1) \quad (2)$$

where wRSS is the weighted residual sum of squares (\rightarrow III/1.5.9), p is the number of regressors (\rightarrow III/1.5.1) in the design matrix X and n is the number of observations (\rightarrow III/1.5.1) in the data vector y .

Proof: The Bayesian information criterion (\rightarrow IV/2.2.1) is defined as

$$\text{BIC}(m) = -2 \text{MLL}(m) + k \log(n) \quad (3)$$

where $\text{MLL}(m)$ is the maximum log-likelihood (\rightarrow I/4.1.4), k is the number of free parameters in m and n is the number of observations.

The maximum log-likelihood for multiple linear regression (\rightarrow III/1.5.24) is given by

$$\text{MLL}(m) = -\frac{n}{2} \log \left(\frac{\text{wRSS}}{n} \right) - \frac{n}{2} [1 + \log(2\pi)] - \frac{1}{2} \log |V| \quad (4)$$

and the number of free parameters in multiple linear regression (\rightarrow III/1.5.1) is $k = p + 1$, i.e. one for each regressor in the design matrix (\rightarrow III/1.5.1) X , plus one for the noise variance (\rightarrow III/1.5.1) σ^2 .

Thus, the BIC of m follows from (3) and (4) as

$$\text{BIC}(m) = n \log \left(\frac{\text{wRSS}}{n} \right) + n [1 + \log(2\pi)] + \log |V| + \log(n) (p + 1) . \quad (5)$$

■

1.5.35 Corrected Akaike information criterion

Theorem: Consider a linear regression model (\rightarrow III/1.5.1) m

$$m : y = X\beta + \varepsilon, \varepsilon \sim \mathcal{N}(0, \sigma^2 V) . \quad (1)$$

Then, the corrected Akaike information criterion (\rightarrow IV/2.1.2) for this model is

$$\text{AIC}_c(m) = n \log \left(\frac{\text{wRSS}}{n} \right) + n [1 + \log(2\pi)] + \log |V| + \frac{2n(p+1)}{n-p-2} \quad (2)$$

where wRSS is the weighted residual sum of squares (\rightarrow III/1.5.9), p is the number of regressors (\rightarrow III/1.5.1) in the design matrix X and n is the number of observations (\rightarrow III/1.5.1) in the data vector y .

Proof: The corrected Akaike information criterion (\rightarrow IV/2.1.2) is defined as

$$\text{AIC}_c(m) = \text{AIC}(m) + \frac{2k^2 + 2k}{n - k - 1} \quad (3)$$

where $\text{AIC}(m)$ is the Akaike information criterion (\rightarrow IV/2.1.1), k is the number of free parameters in m and n is the number of observations.

The Akaike information criterion for multiple linear regression (\rightarrow III/1.5.33) is given by

$$\text{AIC}(m) = n \log \left(\frac{\text{wRSS}}{n} \right) + n [1 + \log(2\pi)] + \log |V| + 2(p + 1) \quad (4)$$

and the number of free parameters in multiple linear regression (\rightarrow III/1.5.1) is $k = p + 1$, i.e. one for each regressor in the design matrix (\rightarrow III/1.5.1) X , plus one for the noise variance (\rightarrow III/1.5.1) σ^2 .

Thus, the corrected AIC of m follows from (3) and (4) as

$$\begin{aligned}
\text{AIC}_c(m) &= n \log \left(\frac{\text{wRSS}}{n} \right) + n [1 + \log(2\pi)] + \log |V| + 2k + \frac{2k^2 + 2k}{n - k - 1} \\
&= n \log \left(\frac{\text{wRSS}}{n} \right) + n [1 + \log(2\pi)] + \log |V| + \frac{2nk - 2k^2 - 2k}{n - k - 1} + \frac{2k^2 + 2k}{n - k - 1} \\
&= n \log \left(\frac{\text{wRSS}}{n} \right) + n [1 + \log(2\pi)] + \log |V| + \frac{2nk}{n - k - 1} \\
&= n \log \left(\frac{\text{wRSS}}{n} \right) + n [1 + \log(2\pi)] + \log |V| + \frac{2n(p+1)}{n - p - 2}
\end{aligned} \tag{5}$$

Sources:

- Claeskens G, Hjort NL (2008): “Akaike’s information criterion”; in: *Model Selection and Model Averaging*, ex. 2.5, p. 67; URL: <https://www.cambridge.org/core/books/model-selection-and-model-averaging/E6F1EC77279D1223423BB64FC3A12C37>; DOI: 10.1017/CBO9780511790485.

1.6 Bayesian linear regression

1.6.1 Conjugate prior distribution

Theorem: Let

$$y = X\beta + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 V) \tag{1}$$

be a linear regression model (\rightarrow III/1.5.1) with measured n -dimensional data vector y , known $n \times p$ design matrix X , known $n \times n$ covariance structure V as well as unknown $p \times 1$ regression coefficients β and unknown noise variance σ^2 .

Then, the conjugate prior (\rightarrow I/5.2.5) for this model is a normal-gamma distribution (\rightarrow II/4.4.1)

$$p(\beta, \tau) = \mathcal{N}(\beta; \mu_0, (\tau \Lambda_0)^{-1}) \cdot \text{Gam}(\tau; a_0, b_0) \tag{2}$$

where $\tau = 1/\sigma^2$ is the inverse noise variance or noise precision.

Proof: By definition, a conjugate prior (\rightarrow I/5.2.5) is a prior distribution (\rightarrow I/5.1.3) that, when combined with the likelihood function (\rightarrow I/5.1.2), leads to a posterior distribution (\rightarrow I/5.1.9) that belongs to the same family of probability distributions (\rightarrow I/1.5.1). This is fulfilled when the prior density and the likelihood function are proportional to the model parameters in the same way, i.e. the model parameters appear in the same functional form in both.

Equation (1) implies the following likelihood function (\rightarrow I/5.1.2)

$$p(y|\beta, \sigma^2) = \mathcal{N}(y; X\beta, \sigma^2 V) = \sqrt{\frac{1}{(2\pi)^n |\sigma^2 V|}} \exp \left[-\frac{1}{2\sigma^2} (y - X\beta)^T V^{-1} (y - X\beta) \right] \tag{3}$$

which, for mathematical convenience, can also be parametrized as

$$p(y|\beta, \tau) = \mathcal{N}(y; X\beta, (\tau P)^{-1}) = \sqrt{\frac{|\tau P|}{(2\pi)^n}} \exp \left[-\frac{\tau}{2} (y - X\beta)^T P (y - X\beta) \right] \tag{4}$$

using the noise precision $\tau = 1/\sigma^2$ and the $n \times n$ precision matrix $P = V^{-1}$.

Separating constant and variable terms, we have:

$$p(y|\beta, \tau) = \sqrt{\frac{|P|}{(2\pi)^n}} \cdot \tau^{n/2} \cdot \exp \left[-\frac{\tau}{2} (y - X\beta)^T P (y - X\beta) \right] . \quad (5)$$

Expanding the product in the exponent, we have:

$$p(y|\beta, \tau) = \sqrt{\frac{|P|}{(2\pi)^n}} \cdot \tau^{n/2} \cdot \exp \left[-\frac{\tau}{2} (y^T P y - y^T P X \beta - \beta^T X^T P y + \beta^T X^T P X \beta) \right] . \quad (6)$$

Completing the square over β , finally gives

$$p(y|\beta, \tau) = \sqrt{\frac{|P|}{(2\pi)^n}} \cdot \tau^{n/2} \cdot \exp \left[-\frac{\tau}{2} \left((\beta - \tilde{X}y)^T X^T P X (\beta - \tilde{X}y) - y^T Q y + y^T P y \right) \right] \quad (7)$$

where $\tilde{X} = (X^T P X)^{-1} X^T P$ and $Q = \tilde{X}^T (X^T P X) \tilde{X}$.

In other words, the likelihood function (\rightarrow I/5.1.2) is proportional to a power of τ , times an exponential of τ and an exponential of a squared form of β , weighted by τ :

$$p(y|\beta, \tau) \propto \tau^{n/2} \cdot \exp \left[-\frac{\tau}{2} (y^T P y - y^T Q y) \right] \cdot \exp \left[-\frac{\tau}{2} (\beta - \tilde{X}y)^T X^T P X (\beta - \tilde{X}y) \right] . \quad (8)$$

The same is true for a normal-gamma distribution (\rightarrow II/4.4.1) over β and τ

$$p(\beta, \tau) = \mathcal{N}(\beta; \mu_0, (\tau \Lambda_0)^{-1}) \cdot \text{Gam}(\tau; a_0, b_0) \quad (9)$$

the probability density function of which (\rightarrow II/4.4.3)

$$p(\beta, \tau) = \sqrt{\frac{|\tau \Lambda_0|}{(2\pi)^p}} \exp \left[-\frac{\tau}{2} (\beta - \mu_0)^T \Lambda_0 (\beta - \mu_0) \right] \cdot \frac{b_0^{a_0}}{\Gamma(a_0)} \tau^{a_0-1} \exp[-b_0 \tau] \quad (10)$$

exhibits the same proportionality

$$p(\beta, \tau) \propto \tau^{a_0+p/2-1} \cdot \exp[-\tau b_0] \cdot \exp \left[-\frac{\tau}{2} (\beta - \mu_0)^T \Lambda_0 (\beta - \mu_0) \right] \quad (11)$$

and is therefore conjugate relative to the likelihood. ■

Sources:

- Bishop CM (2006): “Bayesian Linear Regression”; in: *Pattern Recognition for Machine Learning*, pp. 152-161, ex. 3.12, eq. 3.112; URL: <https://www.springer.com/gp/book/9780387310732>.

1.6.2 Posterior distribution

Theorem: Let

$$y = X\beta + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 V) \quad (1)$$

be a linear regression model (\rightarrow III/1.5.1) with measured n -dimensional data vector y , known $n \times p$ design matrix X , known $n \times n$ covariance structure V as well as unknown $p \times 1$ regression coefficients β and unknown noise variance σ^2 . Moreover, assume a normal-gamma prior distribution (\rightarrow III/1.6.1) over the model parameters β and $\tau = 1/\sigma^2$:

$$p(\beta, \tau) = \mathcal{N}(\beta; \mu_0, (\tau \Lambda_0)^{-1}) \cdot \text{Gam}(\tau; a_0, b_0) . \quad (2)$$

Then, the posterior distribution (\rightarrow I/5.1.9) is also a normal-gamma distribution (\rightarrow II/4.4.1)

$$p(\beta, \tau|y) = \mathcal{N}(\beta; \mu_n, (\tau \Lambda_n)^{-1}) \cdot \text{Gam}(\tau; a_n, b_n) \quad (3)$$

and the posterior hyperparameters (\rightarrow I/5.1.9) are given by

$$\begin{aligned} \mu_n &= \Lambda_n^{-1} (X^T P y + \Lambda_0 \mu_0) \\ \Lambda_n &= X^T P X + \Lambda_0 \\ a_n &= a_0 + \frac{n}{2} \\ b_n &= b_0 + \frac{1}{2} (y^T P y + \mu_0^T \Lambda_0 \mu_0 - \mu_n^T \Lambda_n \mu_n) . \end{aligned} \quad (4)$$

Proof: According to Bayes' theorem (\rightarrow I/5.3.2), the posterior distribution (\rightarrow I/5.1.9) is given by

$$p(\beta, \tau|y) = \frac{p(y|\beta, \tau) p(\beta, \tau)}{p(y)} . \quad (5)$$

Since $p(y)$ is just a normalization factor, the posterior is proportional (\rightarrow I/5.1.10) to the numerator:

$$p(\beta, \tau|y) \propto p(y|\beta, \tau) p(\beta, \tau) = p(y, \beta, \tau) . \quad (6)$$

Equation (1) implies the following likelihood function (\rightarrow I/5.1.2)

$$p(y|\beta, \sigma^2) = \mathcal{N}(y; X\beta, \sigma^2 V) = \sqrt{\frac{1}{(2\pi)^n |\sigma^2 V|}} \exp \left[-\frac{1}{2\sigma^2} (y - X\beta)^T V^{-1} (y - X\beta) \right] \quad (7)$$

which, for mathematical convenience, can also be parametrized as

$$p(y|\beta, \tau) = \mathcal{N}(y; X\beta, (\tau P)^{-1}) = \sqrt{\frac{|\tau P|}{(2\pi)^n}} \exp \left[-\frac{\tau}{2} (y - X\beta)^T P (y - X\beta) \right] \quad (8)$$

using the noise precision $\tau = 1/\sigma^2$ and the $n \times n$ precision matrix (\rightarrow I/1.16.12) $P = V^{-1}$.

Combining the likelihood function (\rightarrow I/5.1.2) (8) with the prior distribution (\rightarrow I/5.1.3) (2), the joint likelihood (\rightarrow I/5.1.7) of the model is given by

$$\begin{aligned}
p(y, \beta, \tau) &= p(y|\beta, \tau) p(\beta, \tau) \\
&= \sqrt{\frac{|\tau P|}{(2\pi)^n}} \exp \left[-\frac{\tau}{2} (y - X\beta)^T P (y - X\beta) \right] \cdot \\
&\quad \sqrt{\frac{|\tau \Lambda_0|}{(2\pi)^p}} \exp \left[-\frac{\tau}{2} (\beta - \mu_0)^T \Lambda_0 (\beta - \mu_0) \right] \cdot \\
&\quad \frac{b_0^{a_0}}{\Gamma(a_0)} \tau^{a_0-1} \exp[-b_0 \tau] .
\end{aligned} \tag{9}$$

Collecting identical variables gives:

$$\begin{aligned}
p(y, \beta, \tau) &= \sqrt{\frac{\tau^{n+p}}{(2\pi)^{n+p}} |P| |\Lambda_0|} \frac{b_0^{a_0}}{\Gamma(a_0)} \tau^{a_0-1} \exp[-b_0 \tau] \cdot \\
&\quad \exp \left[-\frac{\tau}{2} \left((y - X\beta)^T P (y - X\beta) + (\beta - \mu_0)^T \Lambda_0 (\beta - \mu_0) \right) \right] .
\end{aligned} \tag{10}$$

Expanding the products in the exponent gives:

$$\begin{aligned}
p(y, \beta, \tau) &= \sqrt{\frac{\tau^{n+p}}{(2\pi)^{n+p}} |P| |\Lambda_0|} \frac{b_0^{a_0}}{\Gamma(a_0)} \tau^{a_0-1} \exp[-b_0 \tau] \cdot \\
&\quad \exp \left[-\frac{\tau}{2} \left(y^T P y - y^T P X \beta - \beta^T X^T P y + \beta^T X^T P X \beta + \right. \right. \\
&\quad \left. \left. \beta^T \Lambda_0 \beta - \beta^T \Lambda_0 \mu_0 - \mu_0^T \Lambda_0 \beta + \mu_0^T \Lambda_0 \mu_0 \right) \right] .
\end{aligned} \tag{11}$$

Completing the square over β , we finally have

$$\begin{aligned}
p(y, \beta, \tau) &= \sqrt{\frac{\tau^{n+p}}{(2\pi)^{n+p}} |P| |\Lambda_0|} \frac{b_0^{a_0}}{\Gamma(a_0)} \tau^{a_0-1} \exp[-b_0 \tau] \cdot \\
&\quad \exp \left[-\frac{\tau}{2} \left((\beta - \mu_n)^T \Lambda_n (\beta - \mu_n) + (y^T P y + \mu_0^T \Lambda_0 \mu_0 - \mu_n^T \Lambda_n \mu_n) \right) \right]
\end{aligned} \tag{12}$$

with the posterior hyperparameters (\rightarrow I/5.1.9)

$$\begin{aligned}
\mu_n &= \Lambda_n^{-1} (X^T P y + \Lambda_0 \mu_0) \\
\Lambda_n &= X^T P X + \Lambda_0 .
\end{aligned} \tag{13}$$

Ergo, the joint likelihood is proportional to

$$p(y, \beta, \tau) \propto \tau^{p/2} \cdot \exp \left[-\frac{\tau}{2} (\beta - \mu_n)^T \Lambda_n (\beta - \mu_n) \right] \cdot \tau^{a_n-1} \cdot \exp[-b_n \tau] \tag{14}$$

with the posterior hyperparameters (\rightarrow I/5.1.9)

$$\begin{aligned}
a_n &= a_0 + \frac{n}{2} \\
b_n &= b_0 + \frac{1}{2} (y^T P y + \mu_0^T \Lambda_0 \mu_0 - \mu_n^T \Lambda_n \mu_n) .
\end{aligned} \tag{15}$$

From the term in (14), we can isolate the posterior distribution over β given τ :

$$p(\beta|\tau, y) = \mathcal{N}(\beta; \mu_n, (\tau\Lambda_n)^{-1}) . \quad (16)$$

From the remaining term, we can isolate the posterior distribution over τ :

$$p(\tau|y) = \text{Gam}(\tau; a_n, b_n) . \quad (17)$$

Together, (16) and (17) constitute the joint (\rightarrow I/1.3.2) posterior distribution (\rightarrow I/5.1.9) of β and τ . ■

Sources:

- Bishop CM (2006): “Bayesian Linear Regression”; in: *Pattern Recognition for Machine Learning*, pp. 152-161, ex. 3.12, eq. 3.113; URL: <https://www.springer.com/gp/book/9780387310732>.

1.6.3 Log model evidence

Theorem: Let

$$m : y = X\beta + \varepsilon, \varepsilon \sim \mathcal{N}(0, \sigma^2 V) \quad (1)$$

be a linear regression model (\rightarrow III/1.5.1) with measured n -dimensional data vector y , known $n \times p$ design matrix X , known $n \times n$ covariance structure V as well as unknown $p \times 1$ regression coefficients β and unknown noise variance σ^2 . Moreover, assume a normal-gamma prior distribution (\rightarrow III/1.6.1) over the model parameters β and $\tau = 1/\sigma^2$:

$$p(\beta, \tau) = \mathcal{N}(\beta; \mu_0, (\tau\Lambda_0)^{-1}) \cdot \text{Gam}(\tau; a_0, b_0) . \quad (2)$$

Then, the log model evidence (\rightarrow IV/3.1.3) for this model is

$$\begin{aligned} \log p(y|m) = & \frac{1}{2} \log |P| - \frac{n}{2} \log(2\pi) + \frac{1}{2} \log |\Lambda_0| - \frac{1}{2} \log |\Lambda_n| + \\ & \log \Gamma(a_n) - \log \Gamma(a_0) + a_0 \log b_0 - a_n \log b_n \end{aligned} \quad (3)$$

where the posterior hyperparameters (\rightarrow I/5.1.9) are given by

$$\begin{aligned} \mu_n &= \Lambda_n^{-1}(X^T P y + \Lambda_0 \mu_0) \\ \Lambda_n &= X^T P X + \Lambda_0 \\ a_n &= a_0 + \frac{n}{2} \\ b_n &= b_0 + \frac{1}{2}(y^T P y + \mu_0^T \Lambda_0 \mu_0 - \mu_n^T \Lambda_n \mu_n) . \end{aligned} \quad (4)$$

Proof: According to the law of marginal probability (\rightarrow I/1.3.3), the model evidence (\rightarrow I/5.1.15) for this model is:

$$p(y|m) = \iint p(y|\beta, \tau) p(\beta, \tau) d\beta d\tau . \quad (5)$$

According to the law of conditional probability (\rightarrow I/1.3.4), the integrand is equivalent to the joint likelihood (\rightarrow I/5.1.7):

$$p(y|m) = \iint p(y, \beta, \tau) d\beta d\tau . \quad (6)$$

Equation (1) implies the following likelihood function (\rightarrow I/5.1.2)

$$p(y|\beta, \sigma^2) = \mathcal{N}(y; X\beta, \sigma^2 V) = \sqrt{\frac{1}{(2\pi)^n |\sigma^2 V|}} \exp \left[-\frac{1}{2\sigma^2} (y - X\beta)^T V^{-1} (y - X\beta) \right] \quad (7)$$

which, for mathematical convenience, can also be parametrized as

$$p(y|\beta, \tau) = \mathcal{N}(y; X\beta, (\tau P)^{-1}) = \sqrt{\frac{|\tau P|}{(2\pi)^n}} \exp \left[-\frac{\tau}{2} (y - X\beta)^T P (y - X\beta) \right] \quad (8)$$

using the noise precision $\tau = 1/\sigma^2$ and the $n \times n$ precision matrix $P = V^{-1}$.

When deriving the posterior distribution (\rightarrow III/1.6.2) $p(\beta, \tau|y)$, the joint likelihood $p(y, \beta, \tau)$ is obtained as

$$p(y, \beta, \tau) = \sqrt{\frac{\tau^n |P|}{(2\pi)^n}} \sqrt{\frac{\tau^p |\Lambda_0|}{(2\pi)^p}} \frac{b_0^{a_0}}{\Gamma(a_0)} \tau^{a_0-1} \exp[-b_0 \tau] \cdot \exp \left[-\frac{\tau}{2} ((\beta - \mu_n)^T \Lambda_n (\beta - \mu_n) + (y^T P y + \mu_0^T \Lambda_0 \mu_0 - \mu_n^T \Lambda_n \mu_n)) \right] . \quad (9)$$

Using the probability density function of the multivariate normal distribution (\rightarrow II/4.1.4), we can rewrite this as

$$p(y, \beta, \tau) = \sqrt{\frac{\tau^n |P|}{(2\pi)^n}} \sqrt{\frac{\tau^p |\Lambda_0|}{(2\pi)^p}} \sqrt{\frac{(2\pi)^p}{\tau^p |\Lambda_n|}} \frac{b_0^{a_0}}{\Gamma(a_0)} \tau^{a_0-1} \exp[-b_0 \tau] \cdot \mathcal{N}(\beta; \mu_n, (\tau \Lambda_n)^{-1}) \exp \left[-\frac{\tau}{2} (y^T P y + \mu_0^T \Lambda_0 \mu_0 - \mu_n^T \Lambda_n \mu_n) \right] . \quad (10)$$

Now, β can be integrated out easily:

$$\int p(y, \beta, \tau) d\beta = \sqrt{\frac{\tau^n |P|}{(2\pi)^n}} \sqrt{\frac{|\Lambda_0|}{|\Lambda_n|}} \frac{b_0^{a_0}}{\Gamma(a_0)} \tau^{a_0-1} \exp[-b_0 \tau] \cdot \exp \left[-\frac{\tau}{2} (y^T P y + \mu_0^T \Lambda_0 \mu_0 - \mu_n^T \Lambda_n \mu_n) \right] . \quad (11)$$

Using the probability density function of the gamma distribution (\rightarrow II/3.4.7), we can rewrite this as

$$\int p(y, \beta, \tau) d\beta = \sqrt{\frac{|P|}{(2\pi)^n}} \sqrt{\frac{|\Lambda_0|}{|\Lambda_n|}} \frac{b_0^{a_0}}{\Gamma(a_0)} \frac{\Gamma(a_n)}{b_n^{a_n}} \text{Gam}(\tau; a_n, b_n) . \quad (12)$$

Finally, τ can also be integrated out:

$$\iint p(y, \beta, \tau) d\beta d\tau = \sqrt{\frac{|P|}{(2\pi)^n}} \sqrt{\frac{|\Lambda_0|}{|\Lambda_n|}} \frac{\Gamma(a_n)}{\Gamma(a_0)} \frac{b_0^{a_0}}{b_n^{a_n}} = p(y|m) . \quad (13)$$

Thus, the log model evidence (\rightarrow IV/3.1.3) of this model is given by

$$\begin{aligned} \log p(y|m) = & \frac{1}{2} \log |P| - \frac{n}{2} \log(2\pi) + \frac{1}{2} \log |\Lambda_0| - \frac{1}{2} \log |\Lambda_n| + \\ & \log \Gamma(a_n) - \log \Gamma(a_0) + a_0 \log b_0 - a_n \log b_n . \end{aligned} \quad (14)$$

■

Sources:

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1.6.4 Accuracy and complexity

Theorem: Let

$$m : y = X\beta + \varepsilon, \varepsilon \sim \mathcal{N}(0, \sigma^2 V) \quad (1)$$

be a linear regression model (\rightarrow III/1.5.1) with measured n -dimensional data vector y , known $n \times p$ design matrix X , known $n \times n$ covariance structure V as well as unknown $p \times 1$ regression coefficients β and unknown noise variance σ^2 . Moreover, assume a normal-gamma prior distribution (\rightarrow III/1.6.1) over the model parameters β and $\tau = 1/\sigma^2$:

$$p(\beta, \tau) = \mathcal{N}(\beta; \mu_0, (\tau \Lambda_0)^{-1}) \cdot \text{Gam}(\tau; a_0, b_0) . \quad (2)$$

Then, accuracy and complexity (\rightarrow IV/3.1.6) of this model are

$$\begin{aligned} \text{Acc}(m) = & -\frac{1}{2} \frac{a_n}{b_n} (y - X\mu_n)^T P (y - X\mu_n) - \frac{1}{2} \text{tr}(X^T P X \Lambda_n^{-1}) \\ & + \frac{1}{2} \log |P| - \frac{n}{2} \log(2\pi) + \frac{n}{2} (\psi(a_n) - \log(b_n)) \\ \text{Com}(m) = & \frac{1}{2} \frac{a_n}{b_n} [(\mu_0 - \mu_n)^T \Lambda_0 (\mu_0 - \mu_n) - 2(b_n - b_0)] + \frac{1}{2} \text{tr}(\Lambda_0 \Lambda_n^{-1}) - \frac{1}{2} \log \frac{|\Lambda_0|}{|\Lambda_n|} - \frac{p}{2} \\ & + a_0 \log \frac{b_n}{b_0} - \log \frac{\Gamma(a_n)}{\Gamma(a_0)} + (a_n - a_0) \psi(a_n) . \end{aligned} \quad (3)$$

where μ_n , Λ_n , a_n and b_n are the posterior hyperparameters for Bayesian linear regression (\rightarrow III/1.6.2) and P is the data precision matrix (\rightarrow I/1.16.12): $P = V^{-1}$.

Proof: Model accuracy and complexity are defined as (\rightarrow IV/3.1.6)

$$\begin{aligned} \text{LME}(m) &= \text{Acc}(m) - \text{Com}(m) \\ \text{Acc}(m) &= \langle \log p(y|\beta, \tau, m) \rangle_{p(\beta, \tau|y, m)} \\ \text{Com}(m) &= \text{KL} [p(\beta, \tau|y, m) || p(\beta, \tau|m)] . \end{aligned} \quad (4)$$

1) The accuracy term is the expectation (\rightarrow I/1.12.1) of the log-likelihood function (\rightarrow I/4.1.2) $\log p(y|\beta, \tau)$ with respect to the posterior distribution (\rightarrow I/5.1.9) $p(\beta, \tau|y)$. This expectation can be rewritten as:

$$\begin{aligned} \text{Acc}(m) &= \iint p(\beta, \tau|y) \log p(y|\beta, \tau) d\beta d\tau \\ &= \int p(\tau|y) \int p(\beta|\tau, y) \log p(y|\beta, \tau) d\beta d\tau \\ &= \left\langle \left\langle \log p(y|\beta, \tau) \right\rangle_{p(\beta|\tau, y)} \right\rangle_{p(\tau|y)}. \end{aligned} \quad (5)$$

With the log-likelihood function for multiple linear regression (\rightarrow III/1.5.23), we have:

$$\begin{aligned} \text{Acc}(m) &= \left\langle \left\langle \log \left(\sqrt{\frac{1}{(2\pi)^n |\sigma^2 V|}} \cdot \exp \left[-\frac{1}{2} (y - X\beta)^T (\sigma^2 V)^{-1} (y - X\beta) \right] \right) \right\rangle_{p(\beta|\tau, y)} \right\rangle_{p(\tau|y)} \\ &= \left\langle \left\langle \log \left(\sqrt{\frac{\tau^n |P|}{(2\pi)^n}} \cdot \exp \left[-\frac{1}{2} (y - X\beta)^T (\tau P) (y - X\beta) \right] \right) \right\rangle_{p(\beta|\tau, y)} \right\rangle_{p(\tau|y)} \\ &= \left\langle \left\langle \frac{1}{2} \log |P| + \frac{n}{2} \log \tau - \frac{n}{2} \log(2\pi) - \frac{1}{2} (y - X\beta)^T (\tau P) (y - X\beta) \right\rangle_{p(\beta|\tau, y)} \right\rangle_{p(\tau|y)} \\ &= \left\langle \left\langle \frac{1}{2} \log |P| + \frac{n}{2} \log \tau - \frac{n}{2} \log(2\pi) - \frac{\tau}{2} [y^T P y - 2y^T P X \beta + \beta^T X^T P X \beta] \right\rangle_{p(\beta|\tau, y)} \right\rangle_{p(\tau|y)}. \end{aligned} \quad (6)$$

With the posterior distribution for Bayesian linear regression (\rightarrow III/1.6.2), this becomes:

$$\text{Acc}(m) = \left\langle \left\langle \frac{1}{2} \log |P| + \frac{n}{2} \log \tau - \frac{n}{2} \log(2\pi) - \frac{\tau}{2} [y^T P y - 2y^T P X \beta + \beta^T X^T P X \beta] \right\rangle_{\mathcal{N}(\beta; \mu_n, (\tau \Lambda_n)^{-1})} \right\rangle_{\text{Gam}(\tau; a_n, b_n)} \quad (7)$$

If $x \sim \mathcal{N}(\mu, \Sigma)$, then its expected value is (\rightarrow II/4.1.6)

$$\langle x \rangle = \mu \quad (8)$$

and the expectation of a quadratic form is given by (\rightarrow I/1.12.17)

$$\langle x^T A x \rangle = \mu^T A \mu + \text{tr}(A \Sigma). \quad (9)$$

Thus, the model accuracy of m evaluates to:

$$\begin{aligned} \text{Acc}(m) &= \left\langle \frac{1}{2} \log |P| + \frac{n}{2} \log \tau - \frac{n}{2} \log(2\pi) - \right. \\ &\quad \left. \frac{\tau}{2} \left[y^T P y - 2y^T P X \mu_n + \mu_n^T X^T P X \mu_n + \frac{1}{\tau} \text{tr}(X^T P X \Lambda_n^{-1}) \right] \right\rangle_{\text{Gam}(\tau; a_n, b_n)} \\ &= \left\langle \frac{1}{2} \log |P| + \frac{n}{2} \log \tau - \frac{n}{2} \log(2\pi) - \frac{\tau}{2} (y - X \mu_n)^T P (y - X \mu_n) - \frac{1}{2} \text{tr}(X^T P X \Lambda_n^{-1}) \right\rangle_{\text{Gam}(\tau; a_n, b_n)}. \end{aligned} \quad (10)$$

If $x \sim \text{Gam}(a, b)$, then its expected value is (\rightarrow II/3.4.11)

$$\langle x \rangle = \frac{a}{b} \quad (11)$$

and its logarithmic expectation is given by (\rightarrow II/3.4.15)

$$\langle \log x \rangle = \psi(a) - \log(b) . \quad (12)$$

Thus, the model accuracy of m evaluates to

$$\begin{aligned} \text{Acc}(m) = & -\frac{1}{2} \frac{a_n}{b_n} (y - X\mu_n)^T P (y - X\mu_n) - \frac{1}{2} \text{tr}(X^T P X \Lambda_n^{-1}) \\ & + \frac{1}{2} \log |P| - \frac{n}{2} \log(2\pi) + \frac{n}{2} (\psi(a_n) - \log(b_n)) \end{aligned} \quad (13)$$

which proofs the first part of (3).

2) The complexity penalty is the Kullback-Leibler divergence (\rightarrow I/2.5.1) of the posterior distribution (\rightarrow I/5.1.9) $p(\beta, \tau|y)$ from the prior distribution (\rightarrow I/5.1.3) $p(\beta, \tau)$. This can be rewritten as follows:

$$\begin{aligned} \text{Com}(m) &= \iint p(\beta, \tau|y) \log \frac{p(\beta, \tau|y)}{p(\beta, \tau)} d\beta d\tau \\ &= \iint p(\beta|\tau, y) p(\tau|y) \log \left[\frac{p(\beta|\tau, y)}{p(\beta|\tau)} \frac{p(\tau|y)}{p(\tau)} \right] d\beta d\tau \\ &= \int p(\tau|y) \int p(\beta|\tau, y) \log \frac{p(\beta|\tau, y)}{p(\beta|\tau)} d\beta d\tau + \int p(\tau|y) \log \frac{p(\tau|y)}{p(\tau)} \int p(\beta|\tau, y) d\beta d\tau \\ &= \langle \text{KL} [p(\beta|\tau, y) || p(\beta|\tau)] \rangle_{p(\tau|y)} + \text{KL} [p(\tau|y) || p(\tau)] . \end{aligned} \quad (14)$$

With the prior distribution (\rightarrow III/1.6.1) given by (2) and the posterior distribution for Bayesian linear regression (\rightarrow III/1.6.2), this becomes:

$$\begin{aligned} \text{Com}(m) &= \langle \text{KL} [\mathcal{N}(\beta; \mu_n, (\tau\Lambda_n)^{-1}) || \mathcal{N}(\beta; \mu_0, (\tau\Lambda_0)^{-1})] \rangle_{\text{Gam}(\tau; a_n, b_n)} \\ &\quad + \text{KL} [\text{Gam}(\tau; a_n, b_n) || \text{Gam}(\tau; a_0, b_0)] . \end{aligned} \quad (15)$$

With the Kullback-Leibler divergence for the multivariate normal distribution (\rightarrow II/4.1.12)

$$\text{KL}[\mathcal{N}(\mu_1, \Sigma_1) || \mathcal{N}(\mu_2, \Sigma_2)] = \frac{1}{2} \left[(\mu_2 - \mu_1)^T \Sigma_2^{-1} (\mu_2 - \mu_1) + \text{tr}(\Sigma_2^{-1} \Sigma_1) - \ln \frac{|\Sigma_1|}{|\Sigma_2|} - n \right] \quad (16)$$

and the Kullback-Leibler divergence for the gamma distribution (\rightarrow II/3.4.18)

$$\text{KL}[\text{Gam}(a_1, b_1) || \text{Gam}(a_2, b_2)] = a_2 \ln \frac{b_1}{b_2} - \ln \frac{\Gamma(a_1)}{\Gamma(a_2)} + (a_1 - a_2) \psi(a_1) - (b_1 - b_2) \frac{a_1}{b_1} , \quad (17)$$

the model complexity of m evaluates to:

$$\begin{aligned} \text{Com}(m) &= \left\langle \frac{1}{2} \left[(\mu_0 - \mu_n)^T (\tau\Lambda_0) (\mu_0 - \mu_n) + \text{tr}((\tau\Lambda_0)(\tau\Lambda_n)^{-1}) - \log \frac{|(\tau\Lambda_n)^{-1}|}{|(\tau\Lambda_0)^{-1}|} - p \right] \right\rangle_{p(\tau|y)} \\ &\quad + a_0 \log \frac{b_n}{b_0} - \log \frac{\Gamma(a_n)}{\Gamma(a_0)} + (a_n - a_0) \psi(a_n) - (b_n - b_0) \frac{a_n}{b_n} . \end{aligned} \quad (18)$$

Using $x \sim \text{Gam}(a, b) \Rightarrow \langle x \rangle = a/b$ from (11) again, it follows that

$$\begin{aligned} \text{Com}(m) = & \frac{1}{2} \frac{a_n}{b_n} [(\mu_0 - \mu_n)^T \Lambda_0 (\mu_0 - \mu_n)] + \frac{1}{2} \text{tr}(\Lambda_0 \Lambda_n^{-1}) - \frac{1}{2} \log \frac{|\Lambda_0|}{|\Lambda_n|} - \frac{p}{2} \\ & + a_0 \log \frac{b_n}{b_0} - \log \frac{\Gamma(a_n)}{\Gamma(a_0)} + (a_n - a_0) \psi(a_n) - (b_n - b_0) \frac{a_n}{b_n}. \end{aligned} \quad (19)$$

Thus, the model complexity of m evaluates to

$$\begin{aligned} \text{Com}(m) = & \frac{1}{2} \frac{a_n}{b_n} [(\mu_0 - \mu_n)^T \Lambda_0 (\mu_0 - \mu_n) - 2(b_n - b_0)] + \frac{1}{2} \text{tr}(\Lambda_0 \Lambda_n^{-1}) - \frac{1}{2} \log \frac{|\Lambda_0|}{|\Lambda_n|} - \frac{p}{2} \\ & + a_0 \log \frac{b_n}{b_0} - \log \frac{\Gamma(a_n)}{\Gamma(a_0)} + (a_n - a_0) \psi(a_n) \end{aligned} \quad (20)$$

which proofs the second part of (3).

3) A control calculation confirms that

$$\text{Acc}(m) - \text{Com}(m) = \text{LME}(m) \quad (21)$$

where $\text{LME}(m)$ is the log model evidence for Bayesian linear regression (\rightarrow III/1.6.3):

$$\begin{aligned} \log p(y|m) = & \frac{1}{2} \log |P| - \frac{n}{2} \log(2\pi) + \frac{1}{2} \log |\Lambda_0| - \frac{1}{2} \log |\Lambda_n| + \\ & \log \Gamma(a_n) - \log \Gamma(a_0) + a_0 \log b_0 - a_n \log b_n \end{aligned} \quad (22)$$

This requires to recognize that

$$-\frac{1}{2} \text{tr}(X^T P X \Lambda_n^{-1}) - \frac{1}{2} \text{tr}(\Lambda_0 \Lambda_n^{-1}) + \frac{p}{2} = 0 \quad (23)$$

and

$$\frac{n}{2} (\psi(a_n) - \log(b_n)) - a_0 \log \frac{b_n}{b_0} - (a_n - a_0) \psi(a_n) = a_0 \log b_0 - a_n \log b_n \quad (24)$$

thanks to the nature of the posterior hyperparameters for Bayesian linear regression (\rightarrow III/1.6.2). ■

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1.6.5 Deviance information criterion

Theorem: Consider a linear regression model (\rightarrow III/1.5.1) m

$$m : y = X\beta + \varepsilon, \varepsilon \sim \mathcal{N}(0, \sigma^2 V), \sigma^2 V = (\tau P)^{-1} \quad (1)$$

with a normal-gamma prior distribution (\rightarrow III/1.6.1)

$$p(\beta, \tau) = \mathcal{N}(\beta; \mu_0, (\tau \Lambda_0)^{-1}) \cdot \text{Gam}(\tau; a_0, b_0) . \quad (2)$$

Then, the deviance information criterion (\rightarrow IV/2.3.1) for this model is

$$\begin{aligned} \text{DIC}(m) = & n \cdot \log(2\pi) - n [2\psi(a_n) - \log(a_n) - \log(b_n)] - \log |P| \\ & + \frac{a_n}{b_n} (y - X\mu_n)^T P (y - X\mu_n) + \text{tr} (X^T P X \Lambda_n^{-1}) \end{aligned} \quad (3)$$

where μ_n and Λ_n as well as a_n and b_n are posterior parameters (\rightarrow I/5.1.9) describing the posterior distribution in Bayesian linear regression (\rightarrow III/1.6.2).

Proof: The deviance for multiple linear regression (\rightarrow III/1.5.32) is

$$D(\beta, \sigma^2) = n \cdot \log(2\pi) + n \cdot \log(\sigma^2) + \log |V| + \frac{1}{\sigma^2} (y - X\beta)^T V^{-1} (y - X\beta) \quad (4)$$

which, applying the equalities $\tau = 1/\sigma^2$ and $P = V^{-1}$, becomes

$$D(\beta, \tau) = n \cdot \log(2\pi) - n \cdot \log(\tau) - \log |P| + \tau \cdot (y - X\beta)^T P (y - X\beta) . \quad (5)$$

The deviance information criterion (\rightarrow IV/2.3.1) (DIC) is defined as

$$\text{DIC}(m) = -2 \log p(y | \langle \beta \rangle, \langle \tau \rangle, m) + 2 p_D \quad (6)$$

where $\log p(y | \langle \beta \rangle, \langle \tau \rangle, m)$ is the log-likelihood function (\rightarrow III/1.5.24) at the posterior expectations (\rightarrow I/1.12.1) and the “effective number of parameters” p_D is the difference between the expectation of the deviance and the deviance at the expectation (\rightarrow IV/2.3.1):

$$p_D = \langle D(\beta, \tau) \rangle - D(\langle \beta \rangle, \langle \tau \rangle) . \quad (7)$$

With that, the DIC for multiple linear regression becomes:

$$\begin{aligned} \text{DIC}(m) &= -2 \log p(y | \langle \beta \rangle, \langle \tau \rangle, m) + 2 p_D \\ &= D(\langle \beta \rangle, \langle \tau \rangle) + 2 [\langle D(\beta, \tau) \rangle - D(\langle \beta \rangle, \langle \tau \rangle)] \\ &= 2 \langle D(\beta, \tau) \rangle - D(\langle \beta \rangle, \langle \tau \rangle) . \end{aligned} \quad (8)$$

The posterior distribution for multiple linear regression (\rightarrow III/1.6.2) is

$$p(\beta, \tau | y) = \mathcal{N}(\beta; \mu_n, (\tau \Lambda_n)^{-1}) \cdot \text{Gam}(\tau; a_n, b_n) \quad (9)$$

where the posterior hyperparameters (\rightarrow I/5.1.9) are given by

$$\begin{aligned}
\mu_n &= \Lambda_n^{-1}(X^T P y + \Lambda_0 \mu_0) \\
\Lambda_n &= X^T P X + \Lambda_0 \\
a_n &= a_0 + \frac{n}{2} \\
b_n &= b_0 + \frac{1}{2}(y^T P y + \mu_0^T \Lambda_0 \mu_0 - \mu_n^T \Lambda_n \mu_n) .
\end{aligned} \tag{10}$$

Thus, we have the following posterior expectations:

$$\langle \beta \rangle_{\beta, \tau | y} = \mu_n \tag{11}$$

$$\langle \tau \rangle_{\beta, \tau | y} = \frac{a_n}{b_n} \tag{12}$$

$$\langle \log \tau \rangle_{\beta, \tau | y} = \psi(a_n) - \log(b_n) \tag{13}$$

$$\begin{aligned}
\langle \beta^T A \beta \rangle_{\beta | \tau, y} &= \mu_n^T A \mu_n + \text{tr} (A(\tau \Lambda_n)^{-1}) \\
&= \mu_n^T A \mu_n + \frac{1}{\tau} \text{tr} (A \Lambda_n^{-1}) .
\end{aligned} \tag{14}$$

In these identities, we have used the mean of the multivariate normal distribution (\rightarrow II/4.1.6), the mean of the gamma distribution (\rightarrow II/3.4.11), the logarithmic expectation of the gamma distribution (\rightarrow II/3.4.15), the expectation of a quadratic form (\rightarrow I/1.12.17) and the covariance of the multivariate normal distribution (\rightarrow II/4.1.8).

With that, the deviance at the expectation is:

$$\begin{aligned}
D(\langle \beta \rangle, \langle \tau \rangle) &\stackrel{(5)}{=} n \cdot \log(2\pi) - n \cdot \log(\langle \tau \rangle) - \log |P| + \tau \cdot (y - X \langle \beta \rangle)^T P (y - X \langle \beta \rangle) \\
&\stackrel{(11)}{=} n \cdot \log(2\pi) - n \cdot \log(\langle \tau \rangle) - \log |P| + \tau \cdot (y - X \mu_n)^T P (y - X \mu_n) \\
&\stackrel{(12)}{=} n \cdot \log(2\pi) - n \cdot \log \left(\frac{a_n}{b_n} \right) - \log |P| + \frac{a_n}{b_n} \cdot (y - X \mu_n)^T P (y - X \mu_n) .
\end{aligned} \tag{15}$$

Moreover, the expectation of the deviance is:

$$\begin{aligned}
\langle D(\beta, \tau) \rangle &\stackrel{(5)}{=} \langle n \cdot \log(2\pi) - n \cdot \log(\tau) - \log |P| + \tau \cdot (y - X\beta)^T P (y - X\beta) \rangle \\
&= n \cdot \log(2\pi) - n \cdot \langle \log(\tau) \rangle - \log |P| + \langle \tau \cdot (y - X\beta)^T P (y - X\beta) \rangle \\
&\stackrel{(13)}{=} n \cdot \log(2\pi) - n \cdot [\psi(a_n) - \log(b_n)] - \log |P| \\
&\quad + \left\langle \tau \cdot \langle (y - X\beta)^T P (y - X\beta) \rangle_{\beta|\tau, y} \right\rangle_{\tau|y} \\
&= n \cdot \log(2\pi) - n \cdot [\psi(a_n) - \log(b_n)] - \log |P| \\
&\quad + \left\langle \tau \cdot \langle y^T P y - y^T P X \mu_n - \mu_n^T X^T P y + \mu_n^T X^T P X \mu_n \rangle_{\beta|\tau, y} \right\rangle_{\tau|y} \\
&\stackrel{(14)}{=} n \cdot \log(2\pi) - n \cdot [\psi(a_n) - \log(b_n)] - \log |P| \\
&\quad + \left\langle \tau \cdot \left[y^T P y - y^T P X \mu_n - \mu_n^T X^T P y + \mu_n^T X^T P X \mu_n + \frac{1}{\tau} \text{tr} (X^T P X \Lambda_n^{-1}) \right] \right\rangle_{\tau|y} \\
&= n \cdot \log(2\pi) - n \cdot [\psi(a_n) - \log(b_n)] - \log |P| \\
&\quad + \langle \tau \cdot (y - X\mu_n)^T P (y - X\mu_n) \rangle_{\tau|y} + \text{tr} (X^T P X \Lambda_n^{-1}) \\
&\stackrel{(12)}{=} n \cdot \log(2\pi) - n \cdot [\psi(a_n) - \log(b_n)] - \log |P| \\
&\quad + \frac{a_n}{b_n} \cdot (y - X\mu_n)^T P (y - X\mu_n) + \text{tr} (X^T P X \Lambda_n^{-1}) .
\end{aligned} \tag{16}$$

Finally, combining the two terms, we have:

$$\begin{aligned}
\text{DIC}(m) &\stackrel{(8)}{=} 2 \langle D(\beta, \tau) \rangle - D(\langle \beta \rangle, \langle \tau \rangle) \\
&\stackrel{(16)}{=} 2 [n \cdot \log(2\pi) - n \cdot [\psi(a_n) - \log(b_n)] - \log |P| \\
&\quad + \frac{a_n}{b_n} \cdot (y - X\mu_n)^T P (y - X\mu_n) + \text{tr} (X^T P X \Lambda_n^{-1})] \\
&\stackrel{(15)}{=} \left[n \cdot \log(2\pi) - n \cdot \log \left(\frac{a_n}{b_n} \right) - \log |P| + \frac{a_n}{b_n} \cdot (y - X\mu_n)^T P (y - X\mu_n) \right] \\
&= n \cdot \log(2\pi) - 2n\psi(a_n) + 2n \log(b_n) + n \log(a_n) - \log(b_n) - \log |P| \\
&\quad + \frac{a_n}{b_n} (y - X\mu_n)^T P (y - X\mu_n) + \text{tr} (X^T P X \Lambda_n^{-1}) \\
&= n \cdot \log(2\pi) - n [2\psi(a_n) - \log(a_n) - \log(b_n)] - \log |P| \\
&\quad + \frac{a_n}{b_n} (y - X\mu_n)^T P (y - X\mu_n) + \text{tr} (X^T P X \Lambda_n^{-1}) .
\end{aligned} \tag{17}$$

This conforms to equation (3). ■

1.6.6 Maximum-a-posteriori estimation

Theorem: Let there be a linear regression model (\rightarrow III/1.5.1)

$$y = X\beta + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 V), \quad \sigma^2 V = (\tau P)^{-1} \tag{1}$$

and assume a normal-gamma prior distribution (\rightarrow III/1.6.1) over the model parameters β and $\tau = 1/\sigma^2$

$$p(\beta, \tau) = \mathcal{N}(\beta; \mu_0, (\tau \Lambda_0)^{-1}) \cdot \text{Gam}(\tau; a_0, b_0) . \quad (2)$$

Then, the maximum-a-posteriori estimates (\rightarrow I/5.1.14) of β and τ are

$$\begin{aligned} \hat{\beta}_{\text{MAP}} &= (X^T P X + \Lambda_0)^{-1} (X^T P y + \Lambda_0 \mu_0) \\ \hat{\tau}_{\text{MAP}} &= (2a_0 + n - 2) \left(2b_0 + (y - X \hat{\beta}_{\text{MAP}})^T P (y - X \hat{\beta}_{\text{MAP}}) + (\hat{\beta}_{\text{MAP}} - \mu_0)^T \Lambda_0 (\hat{\beta}_{\text{MAP}} - \mu_0) \right)^{-1} \end{aligned} \quad (3)$$

where n is the number of data points (\rightarrow III/1.5.1).

Proof: Given the generative model (\rightarrow I/5.1.1) in (1) and the prior distribution (\rightarrow I/5.1.3) in (2), the posterior distribution (\rightarrow I/5.1.9) for multiple linear regression (\rightarrow III/1.5.1) is also a normal-gamma distribution (\rightarrow III/1.6.2)

$$p(\beta, \tau | y) = \mathcal{N}(\beta; \mu_n, (\tau \Lambda_n)^{-1}) \cdot \text{Gam}(\tau; a_n, b_n) \quad (4)$$

where the posterior hyperparameters (\rightarrow I/5.1.9) are equal to

$$\begin{aligned} \mu_n &= \Lambda_n^{-1} (X^T P y + \Lambda_0 \mu_0) \\ \Lambda_n &= X^T P X + \Lambda_0 \\ a_n &= a_0 + \frac{n}{2} \\ b_n &= b_0 + \frac{1}{2} (y^T P y + \mu_0^T \Lambda_0 \mu_0 - \mu_n^T \Lambda_n \mu_n) . \end{aligned} \quad (5)$$

From this, the conditional posterior distribution over β follows as (\rightarrow II/4.4.1)

$$p(\beta | \tau, y) = \mathcal{N}(\beta; \mu_n, (\tau \Lambda_n)^{-1}) \quad (6)$$

and the marginal posterior distribution over τ follows as (\rightarrow II/4.4.1)

$$p(\tau | y) = \text{Gam}(\tau; a_n, b_n) . \quad (7)$$

The mode of the multivariate normal distribution (\rightarrow II/4.1.7) is given by

$$X \sim \mathcal{N}(\mu, \Sigma) \quad \Rightarrow \quad \text{mode}(X) = \mu \quad (8)$$

and the mode of the gamma distribution (\rightarrow II/3.4.13) is given by

$$X \sim \text{Gam}(a, b) \quad \Rightarrow \quad \text{mode}(X) = \frac{a-1}{b} . \quad (9)$$

Applying (8) to (6), the maximum-a-posteriori estimate (\rightarrow I/5.1.14) of β follows as

$$\begin{aligned} \hat{\beta}_{\text{MAP}} &= \mu_n \\ &= \Lambda_n^{-1} (X^T P y + \Lambda_0 \mu_0) \\ &= (X^T P X + \Lambda_0)^{-1} (X^T P y + \Lambda_0 \mu_0) \end{aligned} \quad (10)$$

and applying (9) to (7), the maximum-a-posteriori estimate (\rightarrow I/5.1.14) of τ follows as

$$\begin{aligned}
 \hat{\tau}_{\text{MAP}} &= \frac{a_n - 1}{b_n} \\
 &= \left(a_0 + \frac{n}{2} - 1 \right) \left(b_0 + \frac{1}{2} (y^T P y + \mu_0^T \Lambda_0 \mu_0 - \mu_n^T \Lambda_n \mu_n) \right)^{-1} \\
 &= (2a_0 + n - 2) (2b_0 + y^T P y + \mu_0^T \Lambda_0 \mu_0 - \mu_n^T \Lambda_n \mu_n)^{-1} \\
 &= (2a_0 + n - 2) \left(2b_0 + y^T P y + \mu_0^T \Lambda_0 \mu_0 - \hat{\beta}_{\text{MAP}}^T (X^T P X + \Lambda_0) \hat{\beta}_{\text{MAP}} \right)^{-1} \\
 &= (2a_0 + n - 2) \left(2b_0 + y^T P y + \mu_0^T \Lambda_0 \mu_0 - \hat{\beta}_{\text{MAP}}^T X^T P X \hat{\beta}_{\text{MAP}} - \hat{\beta}_{\text{MAP}}^T \Lambda_0 \hat{\beta}_{\text{MAP}} \right)^{-1} \\
 &= (2a_0 + n - 2) \left(2b_0 + (y - X \hat{\beta}_{\text{MAP}})^T P (y - X \hat{\beta}_{\text{MAP}}) + (\hat{\beta}_{\text{MAP}} - \mu_0)^T \Lambda_0 (\hat{\beta}_{\text{MAP}} - \mu_0) \right)^{-1}.
 \end{aligned} \tag{11}$$

■

1.6.7 Expression of posterior parameters using error terms

Theorem: Let there be a linear regression model (\rightarrow III/1.5.1)

$$y = X\beta + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 V), \quad \sigma^2 V = (\tau P)^{-1}, \tag{1}$$

assume a normal-gamma prior distribution (\rightarrow III/1.6.1) over the model parameters β and $\tau = 1/\sigma^2$

$$p(\beta, \tau) = \mathcal{N}(\beta; \mu_0, (\tau \Lambda_0)^{-1}) \cdot \text{Gam}(\tau; a_0, b_0) \tag{2}$$

and consider the Bayesian posterior distribution (\rightarrow III/1.6.2) over these model parameters:

$$p(\beta, \tau | y) = \mathcal{N}(\beta; \mu_n, (\tau \Lambda_n)^{-1}) \cdot \text{Gam}(\tau; a_n, b_n). \tag{3}$$

Then, the posterior hyperparameters (\rightarrow I/5.1.9) for the noise precision (\rightarrow III/1.6.1) τ can be expressed as

$$\begin{aligned}
 a_n &= a_0 + \frac{n}{2} \\
 b_n &= b_0 + \frac{1}{2} (\varepsilon_y^T P \varepsilon_y + \varepsilon_\beta^T \Lambda_0 \varepsilon_\beta)
 \end{aligned} \tag{4}$$

where ε_y and ε_β are the “prediction errors” and “parameter errors”

$$\begin{aligned}
 \varepsilon_y &= y - \hat{y} \\
 \varepsilon_\beta &= \mu_n - \mu_0
 \end{aligned} \tag{5}$$

where \hat{y} is the predicted signal (\rightarrow III/1.5.12) at the posterior mean (\rightarrow III/1.6.2) regression coefficients (\rightarrow III/1.5.1) μ_n :

$$\hat{y} = X \mu_n. \tag{6}$$

Proof: The posterior hyperparameter for Bayesian linear regression (\rightarrow III/1.6.2) are:

$$\begin{aligned}\mu_n &= \Lambda_n^{-1}(X^T P y + \Lambda_0 \mu_0) \\ \Lambda_n &= X^T P X + \Lambda_0 \\ a_n &= a_0 + \frac{n}{2} \\ b_n &= b_0 + \frac{1}{2}(y^T P y + \mu_0^T \Lambda_0 \mu_0 - \mu_n^T \Lambda_n \mu_n) .\end{aligned}\tag{7}$$

The shape parameter (\rightarrow II/3.4.1) a_n is given by this equation. The rate parameter (\rightarrow II/3.4.1) b_n of the posterior distribution (\rightarrow I/5.1.9) can be developed as follows:

$$\begin{aligned}b_n &\stackrel{(7)}{=} b_0 + \frac{1}{2}(y^T P y + \mu_0^T \Lambda_0 \mu_0 - \mu_n^T \Lambda_n \mu_n) \\ &\stackrel{(7)}{=} b_0 + \frac{1}{2}(y^T P y + \mu_0^T \Lambda_0 \mu_0 - \mu_n^T (X^T P X + \Lambda_0) \mu_n) \\ &= b_0 + \frac{1}{2}(y^T P y + \mu_0^T \Lambda_0 \mu_0 - \mu_n^T X^T P X \mu_n - \mu_n^T \Lambda_0 \mu_n) \\ &= b_0 + \frac{1}{2}((y^T P y - \mu_n^T X^T P X \mu_n) + (\mu_0^T \Lambda_0 \mu_0 - \mu_n^T \Lambda_0 \mu_n)) \\ &= b_0 + \frac{1}{2}((y - X \mu_n)^T P (y - X \mu_n) + (\mu_0 - \mu_n)^T \Lambda_0 (\mu_0 - \mu_n)) \\ &\stackrel{(6)}{=} b_0 + \frac{1}{2}((y - \hat{y})^T P (y - \hat{y}) + (\mu_n - \mu_0)^T \Lambda_0 (\mu_n - \mu_0)) \\ &\stackrel{(5)}{=} b_0 + \frac{1}{2}(\varepsilon_y^T P \varepsilon_y + \varepsilon_\beta^T \Lambda_0 \varepsilon_\beta) .\end{aligned}\tag{8}$$

Together with equation a_n from (7), this completes the proof. ■

1.6.8 Posterior probability of alternative hypothesis

Theorem: Let there be a linear regression model (\rightarrow III/1.5.1) with normally distributed (\rightarrow II/4.1.1) errors:

$$y = X\beta + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 V)\tag{1}$$

and assume a normal-gamma (\rightarrow II/4.4.1) prior distribution (\rightarrow I/5.1.3) over the model parameters β and $\tau = 1/\sigma^2$:

$$p(\beta, \tau) = \mathcal{N}(\beta; \mu_0, (\tau \Lambda_0)^{-1}) \cdot \text{Gam}(\tau; a_0, b_0) .\tag{2}$$

Then, the posterior (\rightarrow I/5.1.9) probability (\rightarrow I/1.3.1) of the alternative hypothesis (\rightarrow I/4.3.3)

$$H_1 : c^T \beta > 0\tag{3}$$

is given by

$$\Pr(H_1 | y) = 1 - T\left(-\frac{c^T \mu}{\sqrt{c^T \Sigma c}}; \nu\right)\tag{4}$$

where c is a $p \times 1$ contrast vector (\rightarrow III/1.5.26), $T(x; \nu)$ is the cumulative distribution function (\rightarrow I/1.8.1) of the t-distribution (\rightarrow II/3.3.1) with ν degrees of freedom (\rightarrow I/1.5.12) and μ , Σ and ν can be obtained from the posterior hyperparameters (\rightarrow I/5.1.9) of Bayesian linear regression.

Proof: The posterior distribution for Bayesian linear regression (\rightarrow III/1.6.2) is given by a normal-gamma distribution (\rightarrow II/4.4.1) over β and $\tau = 1/\sigma^2$

$$p(\beta, \tau|y) = \mathcal{N}(\beta; \mu_n, (\tau \Lambda_n)^{-1}) \cdot \text{Gam}(\tau; a_n, b_n) \quad (5)$$

with the posterior hyperparameters (\rightarrow I/5.1.9)

$$\begin{aligned} \mu_n &= \Lambda_n^{-1}(X^T P y + \Lambda_0 \mu_0) \\ \Lambda_n &= X^T P X + \Lambda_0 \\ a_n &= a_0 + \frac{n}{2} \\ b_n &= b_0 + \frac{1}{2}(y^T P y + \mu_0^T \Lambda_0 \mu_0 - \mu_n^T \Lambda_n \mu_n) . \end{aligned} \quad (6)$$

The marginal distribution of a normal-gamma distribution is a multivariate t-distribution (\rightarrow II/4.4.8), such that the marginal (\rightarrow I/1.5.3) posterior (\rightarrow I/5.1.9) distribution of β is

$$p(\beta|y) = t(\beta; \mu, \Sigma, \nu) \quad (7)$$

with the posterior hyperparameters (\rightarrow I/5.1.9)

$$\begin{aligned} \mu &= \mu_n \\ \Sigma &= \left(\frac{a_n}{b_n} \Lambda_n \right)^{-1} \\ \nu &= 2 a_n . \end{aligned} \quad (8)$$

Define the quantity $\gamma = c^T \beta$. According to the linear transformation theorem for the multivariate t-distribution, γ also follows a multivariate t-distribution (\rightarrow II/4.3.1):

$$p(\gamma|y) = t(\gamma; c^T \mu, c^T \Sigma c, \nu) . \quad (9)$$

Because c^T is a $1 \times p$ vector, γ is a scalar and actually has a non-standardized t-distribution (\rightarrow II/3.3.3). Therefore, the posterior probability of H_1 can be calculated using a one-dimensional integral:

$$\begin{aligned} \Pr(H_1|y) &= p(\gamma > 0|y) \\ &= \int_0^{+\infty} p(\gamma|y) d\gamma \\ &= 1 - \int_{-\infty}^0 p(\gamma|y) d\gamma \\ &= 1 - T_{\text{nst}}(0; c^T \mu, c^T \Sigma c, \nu) . \end{aligned} \quad (10)$$

Using the relation between non-standardized t-distribution and standard t-distribution (\rightarrow II/3.3.4), we can finally write:

$$\begin{aligned}\Pr(H_1|y) &= 1 - T\left(\frac{(0 - c^T\mu)}{\sqrt{c^T\Sigma c}}; \nu\right) \\ &= 1 - T\left(-\frac{c^T\mu}{\sqrt{c^T\Sigma c}}; \nu\right).\end{aligned}\tag{11}$$

■

Sources:

- Koch, Karl-Rudolf (2007): “Multivariate t-distribution”; in: *Introduction to Bayesian Statistics*, Springer, Berlin/Heidelberg, 2007, eqs. 2.235, 2.236, 2.213, 2.210, 2.188; URL: <https://www.springer.com/de/book/9783540727231>; DOI: 10.1007/978-3-540-72726-2.

1.6.9 Posterior credibility region excluding null hypothesis

Theorem: Let there be a linear regression model (\rightarrow III/1.5.1) with normally distributed (\rightarrow II/4.1.1) errors:

$$y = X\beta + \varepsilon, \varepsilon \sim \mathcal{N}(0, \sigma^2 V) \tag{1}$$

and assume a normal-gamma (\rightarrow II/4.4.1) prior distribution (\rightarrow I/5.1.3) over the model parameters β and $\tau = 1/\sigma^2$:

$$p(\beta, \tau) = \mathcal{N}(\beta; \mu_0, (\tau\Lambda_0)^{-1}) \cdot \text{Gam}(\tau; a_0, b_0). \tag{2}$$

Then, the largest posterior (\rightarrow I/5.1.9) credibility region that does not contain the omnibus null hypothesis (\rightarrow I/4.3.2)

$$H_0 : C^T\beta = 0 \tag{3}$$

is given by the credibility level

$$(1 - \alpha) = F\left([\mu^T C (C^T \Sigma C)^{-1} C^T \mu] / q; q, \nu\right) \tag{4}$$

where C is a $p \times q$ contrast matrix (\rightarrow III/1.5.27), $F(x; v, w)$ is the cumulative distribution function (\rightarrow I/1.8.1) of the F-distribution (\rightarrow II/3.8.1) with v numerator degrees of freedom (\rightarrow I/1.5.12), w denominator degrees of freedom (\rightarrow I/1.5.12) and μ , Σ and ν can be obtained from the posterior hyperparameters (\rightarrow I/5.1.9) of Bayesian linear regression.

Proof: The posterior distribution for Bayesian linear regression (\rightarrow III/1.6.2) is given by a normal-gamma distribution (\rightarrow II/4.4.1) over β and $\tau = 1/\sigma^2$

$$p(\beta, \tau|y) = \mathcal{N}(\beta; \mu_n, (\tau\Lambda_n)^{-1}) \cdot \text{Gam}(\tau; a_n, b_n) \tag{5}$$

with the posterior hyperparameters (\rightarrow I/5.1.9)

$$\begin{aligned}\mu_n &= \Lambda_n^{-1}(X^T P y + \Lambda_0 \mu_0) \\ \Lambda_n &= X^T P X + \Lambda_0 \\ a_n &= a_0 + \frac{n}{2} \\ b_n &= b_0 + \frac{1}{2}(y^T P y + \mu_0^T \Lambda_0 \mu_0 - \mu_n^T \Lambda_n \mu_n).\end{aligned}\tag{6}$$

The marginal distribution of a normal-gamma distribution is a multivariate t-distribution (\rightarrow II/4.4.8), such that the marginal (\rightarrow I/1.5.3) posterior (\rightarrow I/5.1.9) distribution of β is

$$p(\beta|y) = t(\beta; \mu, \Sigma, \nu) \quad (7)$$

with the posterior hyperparameters (\rightarrow I/5.1.9)

$$\begin{aligned} \mu &= \mu_n \\ \Sigma &= \left(\frac{a_n}{b_n} \Lambda_n \right)^{-1} \\ \nu &= 2 a_n . \end{aligned} \quad (8)$$

Define the quantity $\gamma = C^T \beta$. According to the linear transformation theorem for the multivariate t-distribution, γ also follows a multivariate t-distribution (\rightarrow II/4.3.1):

$$p(\gamma|y) = t(\gamma; C^T \mu, C^T \Sigma C, \nu) . \quad (9)$$

Because C^T is a $q \times p$ matrix, γ is a $q \times 1$ vector. The quadratic form of a multivariate t-distributed random variable has an F-distribution (\rightarrow II/4.3.3), such that we can write:

$$\text{QF}(\gamma) = (\gamma - C^T \mu)^T (C^T \Sigma C)^{-1} (\gamma - C^T \mu) / q \sim F(q, \nu) . \quad (10)$$

Therefore, the largest posterior credibility region for γ which does not contain $\gamma = 0_q$ (i.e. only touches this origin point) can be obtained by plugging $\text{QF}(0)$ into the cumulative distribution function of the F-distribution:

$$\begin{aligned} (1 - \alpha) &= F(\text{QF}(0); q, \nu) \\ &= F([\mu^T C (C^T \Sigma C)^{-1} C^T \mu] / q; q, \nu) . \end{aligned} \quad (11)$$

■

Sources:

- Koch, Karl-Rudolf (2007): “Multivariate t-distribution”; in: *Introduction to Bayesian Statistics*, Springer, Berlin/Heidelberg, 2007, eqs. 2.235, 2.236, 2.213, 2.210, 2.211, 2.183; URL: <https://www.springer.com/de/book/9783540727231>; DOI: 10.1007/978-3-540-72726-2.

1.6.10 Combined posterior distribution from independent data sets

Theorem: Let $y = \{y_1, \dots, y_S\}$ be a set of S conditionally independent data sets (\rightarrow I/1.3.7) assumed to follow linear regression models (\rightarrow III/1.5.1) with design matrices (\rightarrow III/1.5.1) X_1, \dots, X_S , number of data points (\rightarrow III/1.5.1) n_1, \dots, n_S and precision matrices (\rightarrow III/1.6.1) P_1, \dots, P_n , governed by identical regression coefficients (\rightarrow III/1.5.1) β and identical noise precision (\rightarrow III/1.6.1) τ :

$$\begin{aligned} y_1 &= X_1 \beta + \varepsilon_1, \quad \varepsilon_1 \sim \mathcal{N}(0, \sigma^2 V_1), \quad \sigma^2 V_1 = (\tau P_1)^{-1} \\ &\vdots \\ y_S &= X_S \beta + \varepsilon_S, \quad \varepsilon_S \sim \mathcal{N}(0, \sigma^2 V_S), \quad \sigma^2 V_S = (\tau P_S)^{-1} . \end{aligned} \quad (1)$$

Moreover, assume a normal-gamma prior distribution (\rightarrow III/1.6.1) over the model parameters β and $\tau = 1/\sigma^2$:

$$p(\beta, \tau) = \mathcal{N}(\beta; \mu_0, (\tau \Lambda_0)^{-1}) \cdot \text{Gam}(\tau; a_0, b_0) . \quad (2)$$

Then, the combined posterior distribution (\rightarrow I/5.1.11) from observing these conditionally independent data sets (\rightarrow I/1.3.7) is also given by a normal-gamma distribution (\rightarrow II/4.4.1)

$$p(\beta, \tau | y) = \mathcal{N}(\beta; \mu_n, (\tau \Lambda_n)^{-1}) \cdot \text{Gam}(\tau; a_n, b_n) \quad (3)$$

with the posterior hyperparameters (\rightarrow I/5.1.9)

$$\begin{aligned} \mu_n &= \Lambda_n^{-1} \left(\sum_{i=1}^S X_i^T P_i y_i + \Lambda_0 \mu_0 \right) \\ \Lambda_n &= \sum_{i=1}^S X_i^T P_i X_i + \Lambda_0 \\ a_n &= a_0 + \frac{1}{2} \sum_{i=1}^S n_i \\ b_n &= b_0 + \frac{1}{2} \left(\sum_{i=1}^S y_i^T P_i y_i + \mu_0^T \Lambda_0 \mu_0 - \mu_n^T \Lambda_n \mu_n \right) . \end{aligned} \quad (4)$$

Proof: This can be seen by sequentially applying Bayes' theorem (\rightarrow I/5.3.2) for calculating the posterior distribution (\rightarrow I/5.1.10), while using the posterior after one iteration as the prior for the next iteration.

Let $\mu_0^{(i)}, \Lambda_0^{(i)}, a_0^{(i)}, b_0^{(i)}$ denote the prior hyperparameters (\rightarrow I/5.1.3) before analyzing the i -th data set, such that e.g. $\mu_0^{(1)}$ is identical to μ_0 in (2):

$$\begin{aligned} \mu_0^{(1)} &= \mu_0 \\ \Lambda_0^{(1)} &= \Lambda_0 \\ a_0^{(1)} &= a_0 \\ b_0^{(1)} &= b_0 . \end{aligned} \quad (5)$$

Moreover, let $\mu_n^{(i)}, \Lambda_n^{(i)}, a_n^{(i)}, b_n^{(i)}$ denote the posterior hyperparameters (\rightarrow I/5.1.9) after analyzing the i -th data set, such that e.g. $\mu_n^{(S)}$ is identical to μ_n in (3):

$$\begin{aligned} \mu_n^{(S)} &= \mu_n \\ \Lambda_n^{(S)} &= \Lambda_n \\ a_n^{(S)} &= a_n \\ b_n^{(S)} &= b_n . \end{aligned} \quad (6)$$

The posterior (\rightarrow I/5.1.9) after seeing the i -th data set is equal to the prior (\rightarrow I/5.1.3) before seeing the $(i+1)$ -th data set, so we have the relation:

$$\begin{aligned}
\mu_0^{(i+1)} &= \mu_n^{(i)} \\
\Lambda_0^{(i+1)} &= \Lambda_n^{(i)} \\
a_0^{(i+1)} &= a_n^{(i)} \\
b_0^{(i+1)} &= b_n^{(i)} .
\end{aligned} \tag{7}$$

The posterior distribution for Bayesian linear regression when observing a single data set is given by the following hyperparameter equations (\rightarrow III/1.6.2):

$$\begin{aligned}
\mu_n &= \Lambda_n^{-1}(X^T P y + \Lambda_0 \mu_0) \\
\Lambda_n &= X^T P X + \Lambda_0 \\
a_n &= a_0 + \frac{n}{2} \\
b_n &= b_0 + \frac{1}{2}(y^T P y + \mu_0^T \Lambda_0 \mu_0 - \mu_n^T \Lambda_n \mu_n) .
\end{aligned} \tag{8}$$

We can apply (8) to calculate the posterior hyperparameters after seeing the first data set:

$$\begin{aligned}
\mu_n^{(1)} &= \Lambda_n^{(1)-1} \left(X_1^T P_1 y_1 + \Lambda_0^{(1)} \mu_0^{(1)} \right) \\
&= \Lambda_n^{(1)-1} \left(X_1^T P_1 y_1 + \Lambda_0 \mu_0 \right) \\
\Lambda_n^{(1)} &= X_1^T P_1 X_1 + \Lambda_0^{(1)} \\
&= X_1^T P_1 X_1 + \Lambda_0 \\
a_n^{(1)} &= a_0^{(1)} + \frac{1}{2} n_1 \\
&= a_0 + \frac{1}{2} n_1 \\
b_n^{(1)} &= b_0^{(1)} + \frac{1}{2} \left(y_1^T P_1 y_1 + \mu_0^{(1)T} \Lambda_0^{(1)} \mu_0^{(1)} - \mu_n^{(1)T} \Lambda_n^{(1)} \mu_n^{(1)} \right) \\
&= b_0 + \frac{1}{2} \left(y_1^T P_1 y_1 + \mu_0^T \Lambda_0 \mu_0 - \mu_n^{(1)T} \Lambda_n^{(1)} \mu_n^{(1)} \right) .
\end{aligned} \tag{9}$$

These are the prior hyperparameters before seeing the second data set:

$$\begin{aligned}
\mu_0^{(2)} &= \mu_n^{(1)} \\
\Lambda_0^{(2)} &= \Lambda_n^{(1)} \\
a_0^{(2)} &= a_n^{(1)} \\
b_0^{(2)} &= b_n^{(1)} .
\end{aligned} \tag{10}$$

Thus, we can again use (8) to calculate the posterior hyperparameters after seeing the second data set:

$$\begin{aligned}
\mu_n^{(2)} &= \Lambda_n^{(2)-1} \left(X_2^T P_2 y_2 + \Lambda_0^{(2)} \mu_0^{(2)} \right) \\
&= \Lambda_n^{(2)-1} \left(X_2^T P_2 y_2 + \Lambda_n^{(1)} \Lambda_n^{(1)-1} (X_1^T P_1 y_1 + \Lambda_0 \mu_0) \right) \\
&= \Lambda_n^{(2)-1} (X_1^T P_1 y_1 + X_2^T P_2 y_2 + \Lambda_0 \mu_0) \\
\Lambda_n^{(2)} &= X_2^T P_2 X_2 + \Lambda_0^{(2)} \\
&= X_2^T P_2 X_2 + X_1^T P_1 X_1 + \Lambda_0 \\
&= X_1^T P_1 X_1 + X_2^T P_2 X_2 + \Lambda_0 \\
a_n^{(2)} &= a_0^{(2)} + \frac{1}{2} n_2 \\
&= a_0 + \frac{1}{2} n_1 + \frac{1}{2} n_2 \\
&= a_0 + \frac{1}{2} (n_1 + n_2) \\
b_n^{(2)} &= b_0^{(2)} + \frac{1}{2} \left(y_2^T P_2 y_2 + \mu_0^{(2)T} \Lambda_0^{(2)} \mu_0^{(2)} - \mu_n^{(2)T} \Lambda_n^{(2)} \mu_n^{(2)} \right) \\
&= b_0 + \frac{1}{2} \left(y_1^T P_1 y_1 + \mu_0^T \Lambda_0 \mu_0 - \mu_n^{(1)T} \Lambda_n^{(1)} \mu_n^{(1)} \right) + \frac{1}{2} \left(y_2^T P_2 y_2 + \mu_n^{(1)T} \Lambda_n^{(1)} \mu_n^{(1)} - \mu_n^{(2)T} \Lambda_n^{(2)} \mu_n^{(2)} \right) \\
&= b_0 + \frac{1}{2} \left(y_1^T P_1 y_1 + y_2^T P_2 y_2 + \mu_0^T \Lambda_0 \mu_0 - \mu_n^{(2)T} \Lambda_n^{(2)} \mu_n^{(2)} \right) .
\end{aligned} \tag{11}$$

These are the prior hyperparameters before seeing the third data set:

$$\begin{aligned}
\mu_0^{(3)} &= \mu_n^{(2)} \\
\Lambda_0^{(3)} &= \Lambda_n^{(2)} \\
a_0^{(3)} &= a_n^{(2)} \\
b_0^{(3)} &= b_n^{(2)} .
\end{aligned} \tag{12}$$

Generalizing this, we have after observing the j -th data set:

$$\begin{aligned}
\mu_n^{(j)} &= \Lambda_n^{(j)-1} \left(\sum_{i=1}^j X_i^T P_i y_i + \Lambda_0 \mu_0 \right) \\
\Lambda_n^{(j)} &= \sum_{i=1}^j X_i^T P_i X_i + \Lambda_0 \\
a_n^{(j)} &= a_0 + \frac{1}{2} \sum_{i=1}^j n_i \\
b_n^{(j)} &= b_0 + \frac{1}{2} \left(\sum_{i=1}^j y_i^T P_i y_i + \mu_0^T \Lambda_0 \mu_0 - \mu_n^{(j)T} \Lambda_n^{(j)} \mu_n^{(j)} \right) .
\end{aligned} \tag{13}$$

Plugging in $j = S$, we obtain the final posterior distribution:

$$\begin{aligned}
\mu_n &= \mu_n^{(S)} = \Lambda_n^{(S)-1} \left(\sum_{i=1}^S X_i^T P_i y_i + \Lambda_0 \mu_0 \right) = \Lambda_n^{-1} \left(\sum_{i=1}^S X_i^T P_i y_i + \Lambda_0 \mu_0 \right) \\
\Lambda_n &= \Lambda_n^{(S)} = \sum_{i=1}^S X_i^T P_i X_i + \Lambda_0 \\
a_n &= a_n^{(S)} = a_0 + \frac{1}{2} \sum_{i=1}^S n_i \\
b_n &= b_n^{(S)} = b_0 + \frac{1}{2} \left(\sum_{i=1}^S y_i^T P_i y_i + \mu_0^T \Lambda_0 \mu_0 - \mu_n^{(S)T} \Lambda_n^{(S)} \mu_n^{(S)} \right) \\
&= b_0 + \frac{1}{2} \left(\sum_{i=1}^S y_i^T P_i y_i + \mu_0^T \Lambda_0 \mu_0 - \mu_n^T \Lambda_n \mu_n \right) .
\end{aligned} \tag{14}$$

This result is also compatible with the general theorem about combined posterior distributions in terms of individual posterior distributions (\rightarrow I/5.1.11) when analyzing independent data sets. ■

1.6.11 Log Bayes factor for comparison of two regression models

Theorem: Let $y = [y_1, \dots, y_n]^T$ be an n -dimensional vector of a measured univariate signal (\rightarrow I/1.1.5) and consider two linear regression models (\rightarrow III/1.5.1) with design matrices (\rightarrow III/1.5.1) X_1, X_2 and precision matrices (\rightarrow III/1.6.1) P_1, P_2 , entailing potentially different regression coefficients (\rightarrow III/1.5.1) β_1, β_2 and noise precisions (\rightarrow III/1.6.1) τ_1, τ_2 :

$$\begin{aligned}
m_1 : y &= X_1 \beta_1 + \varepsilon_1, \quad \varepsilon_1 \sim \mathcal{N}(0, \sigma_1^2 V_1), \quad \sigma_1^2 V_1 = (\tau_1 P_1)^{-1} \\
m_2 : y &= X_2 \beta_2 + \varepsilon_2, \quad \varepsilon_2 \sim \mathcal{N}(0, \sigma_2^2 V_2), \quad \sigma_2^2 V_2 = (\tau_2 P_2)^{-1} .
\end{aligned} \tag{1}$$

Moreover, assume normal-gamma prior distributions (\rightarrow III/1.6.1) over the model parameters β_1 and $\tau_1 = 1/\sigma_1^2$ as well as β_2 and $\tau_2 = 1/\sigma_2^2$:

$$\begin{aligned}
p(\beta_1, \tau_1) &= \mathcal{N} \left(\beta_1; \mu_0^{(1)}, \left(\tau_1 \Lambda_0^{(1)} \right)^{-1} \right) \cdot \text{Gam} \left(\tau_1; a_0^{(1)}, b_0^{(1)} \right) \\
p(\beta_2, \tau_2) &= \mathcal{N} \left(\beta_2; \mu_0^{(2)}, \left(\tau_2 \Lambda_0^{(2)} \right)^{-1} \right) \cdot \text{Gam} \left(\tau_2; a_0^{(2)}, b_0^{(2)} \right) .
\end{aligned} \tag{2}$$

Then, the log Bayes factor (\rightarrow IV/3.3.6) in favor of m_1 against m_2 is

$$\begin{aligned}
\text{LBF}_{12} &= \frac{1}{2} \log \frac{|P_1|}{|P_2|} + \frac{1}{2} \log \frac{|\Lambda_0^{(1)}|}{|\Lambda_0^{(2)}|} - \frac{1}{2} \log \frac{|\Lambda_n^{(1)}|}{|\Lambda_n^{(2)}|} \\
&\quad + \log \frac{\Gamma(a_n^{(1)})}{\Gamma(a_0^{(1)})} + a_0^{(1)} \log b_0^{(1)} - a_n^{(1)} \log b_n^{(1)} \\
&\quad + \log \frac{\Gamma(a_n^{(2)})}{\Gamma(a_0^{(2)})} - a_0^{(2)} \log b_0^{(2)} + a_n^{(2)} \log b_n^{(2)}
\end{aligned} \tag{3}$$

where $\mu_n^{(1)}, \Lambda_n^{(1)}, a_n^{(1)}, b_n^{(1)}$ and $\mu_n^{(2)}, \Lambda_n^{(2)}, a_n^{(2)}, b_n^{(2)}$ are the posterior hyperparameters for Bayesian linear regression (\rightarrow III/1.6.2) for each of the two models which are functions of the design matrices, the precision matrices and the data vector.

Proof: For Bayesian linear regression with data vector y , design matrix X , precision matrix P and a normal-gamma prior distribution (\rightarrow III/1.6.1) over β and τ , the log model evidence is given by (\rightarrow III/1.6.3)

$$\begin{aligned} \log p(y|m) = & \frac{1}{2} \log |P| - \frac{n}{2} \log(2\pi) + \frac{1}{2} \log |\Lambda_0| - \frac{1}{2} \log |\Lambda_n| + \\ & \log \Gamma(a_n) - \log \Gamma(a_0) + a_0 \log b_0 - a_n \log b_n \end{aligned} \quad (4)$$

where the posterior hyperparameters are equal to (\rightarrow III/1.6.2)

$$\begin{aligned} \mu_n &= \Lambda_n^{-1}(X^T P y + \Lambda_0 \mu_0) \\ \Lambda_n &= X^T P X + \Lambda_0 \\ a_n &= a_0 + \frac{n}{2} \\ b_n &= b_0 + \frac{1}{2}(y^T P y + \mu_0^T \Lambda_0 \mu_0 - \mu_n^T \Lambda_n \mu_n) . \end{aligned} \quad (5)$$

Thus, the log model evidences (\rightarrow IV/3.1.3) for m_1 and m_2 are given by:

$$\begin{aligned} \text{LME}(m_1) &= \frac{1}{2} \log |P_1| - \frac{n}{2} \log(2\pi) + \frac{1}{2} \log |\Lambda_0^{(1)}| - \frac{1}{2} \log |\Lambda_n^{(1)}| + \\ & \quad \log \Gamma(a_n^{(1)}) - \log \Gamma(a_0^{(1)}) + a_0^{(1)} \log b_0^{(1)} - a_n^{(1)} \log b_n^{(1)} \\ \text{LME}(m_2) &= \frac{1}{2} \log |P_2| - \frac{n}{2} \log(2\pi) + \frac{1}{2} \log |\Lambda_0^{(2)}| - \frac{1}{2} \log |\Lambda_n^{(2)}| + \\ & \quad \log \Gamma(a_n^{(2)}) - \log \Gamma(a_0^{(2)}) + a_0^{(2)} \log b_0^{(2)} - a_n^{(2)} \log b_n^{(2)} . \end{aligned} \quad (6)$$

The log Bayes factor is equal to the difference of two log model evidences (\rightarrow IV/3.3.8):

$$\text{LBF}_{12} = \text{LME}(m_1) - \text{LME}(m_2) . \quad (7)$$

Plugging (6) into (7), this gives:

$$\begin{aligned} \text{LBF}_{12} &= \frac{1}{2} \log |P_1| - \frac{1}{2} \log |P_2| \\ & \quad + \frac{1}{2} \log |\Lambda_0^{(1)}| - \frac{1}{2} \log |\Lambda_0^{(2)}| \\ & \quad - \frac{1}{2} \log |\Lambda_n^{(1)}| + \frac{1}{2} \log |\Lambda_n^{(2)}| \\ & \quad + \log \Gamma(a_n^{(1)}) - \log \Gamma(a_0^{(1)}) + a_0^{(1)} \log b_0^{(1)} - a_n^{(1)} \log b_n^{(1)} \\ & \quad - \log \Gamma(a_n^{(2)}) + \log \Gamma(a_0^{(2)}) - a_0^{(2)} \log b_0^{(2)} + a_n^{(2)} \log b_n^{(2)} . \end{aligned} \quad (8)$$

Applying $\log a - \log b = \log(a/b)$, we obtain:

$$\begin{aligned}
\text{LBF}_{12} = & \frac{1}{2} \log \frac{|P_1|}{|P_2|} + \frac{1}{2} \log \frac{|\Lambda_0^{(1)}|}{|\Lambda_0^{(2)}|} - \frac{1}{2} \log \frac{|\Lambda_n^{(1)}|}{|\Lambda_n^{(2)}|} \\
& + \log \frac{\Gamma(a_n^{(1)})}{\Gamma(a_0^{(1)})} + a_0^{(1)} \log b_0^{(1)} - a_n^{(1)} \log b_n^{(1)} \\
& - \log \frac{\Gamma(a_n^{(2)})}{\Gamma(a_0^{(2)})} - a_0^{(2)} \log b_0^{(2)} + a_n^{(2)} \log b_n^{(2)} .
\end{aligned} \tag{9}$$

■

1.7 Bayesian linear regression with known covariance

1.7.1 Conjugate prior distribution

Theorem: Let

$$y = X\beta + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \Sigma) \tag{1}$$

be a linear regression model (\rightarrow III/1.5.1) with measured n -dimensional data vector y , known $n \times p$ design matrix X and known $n \times n$ covariance matrix Σ as well as unknown $p \times 1$ regression coefficients β .

Then, the conjugate prior (\rightarrow I/5.2.5) for this model is a multivariate normal distribution (\rightarrow II/4.1.1)

$$p(\beta) = \mathcal{N}(\beta; \mu_0, \Sigma_0) . \tag{2}$$

Proof: By definition, a conjugate prior (\rightarrow I/5.2.5) is a prior distribution (\rightarrow I/5.1.3) that, when combined with the likelihood function (\rightarrow I/5.1.2), leads to a posterior distribution (\rightarrow I/5.1.9) that belongs to the same family of probability distributions (\rightarrow I/1.5.1). This is fulfilled when the prior density and the likelihood function are proportional to the model parameters in the same way, i.e. the model parameters appear in the same functional form in both.

Equation (1) implies the following likelihood function (\rightarrow I/5.1.2):

$$p(y|\beta) = \mathcal{N}(y; X\beta, \Sigma) = \sqrt{\frac{1}{(2\pi)^n |\Sigma|}} \exp \left[-\frac{1}{2} (y - X\beta)^T \Sigma^{-1} (y - X\beta) \right] . \tag{3}$$

Expanding the product in the exponent, we have:

$$p(y|\beta) = \sqrt{\frac{1}{(2\pi)^n |\Sigma|}} \cdot \exp \left[-\frac{1}{2} (y^T \Sigma^{-1} y - y^T \Sigma^{-1} X\beta - \beta^T X^T \Sigma^{-1} y + \beta^T X^T \Sigma^{-1} X\beta) \right] . \tag{4}$$

Completing the square over β , one obtains

$$p(y|\beta) = \sqrt{\frac{1}{(2\pi)^n |\Sigma|}} \cdot \exp \left[-\frac{1}{2} \left((\beta - \tilde{X}y)^T X^T \Sigma^{-1} X (\beta - \tilde{X}y) - y^T Q y + y^T \Sigma^{-1} y \right) \right] \tag{5}$$

where $\tilde{X} = (X^T \Sigma^{-1} X)^{-1} X^T \Sigma^{-1}$ and $Q = \tilde{X}^T (X^T \Sigma^{-1} X) \tilde{X}$.

Separating constant and variable terms, we get:

$$p(y|\beta) = \sqrt{\frac{1}{(2\pi)^n |\Sigma|}} \cdot \exp \left[-\frac{1}{2} (y^T Q y + y^T \Sigma^{-1} y) \right] \cdot \exp \left[-\frac{1}{2} (\beta - \tilde{X} y)^T X^T \Sigma^{-1} X (\beta - \tilde{X} y) \right] . \quad (6)$$

In other words, the likelihood function (\rightarrow I/5.1.2) is proportional to an exponential of a squared form of β :

$$p(y|\beta) \propto \exp \left[-\frac{1}{2} (\beta - \tilde{X} y)^T X^T \Sigma^{-1} X (\beta - \tilde{X} y) \right] . \quad (7)$$

The same is true for a multivariate normal distribution (\rightarrow II/4.1.1) over β

$$p(\beta) = \mathcal{N}(\beta; \mu_0, \Sigma_0) \quad (8)$$

the probability density function of which (\rightarrow II/4.1.4)

$$p(\beta) = \sqrt{\frac{1}{(2\pi)^p |\Sigma_0|}} \cdot \exp \left[-\frac{1}{2} (\beta - \mu_0)^T \Sigma_0^{-1} (\beta - \mu_0) \right] \quad (9)$$

exhibits the same proportionality

$$p(\beta) \propto \exp \left[-\frac{1}{2} (\beta - \mu_0)^T \Sigma_0^{-1} (\beta - \mu_0) \right] \quad (10)$$

and is therefore conjugate relative to the likelihood. ■

Sources:

- Bishop CM (2006): “Bayesian Linear Regression”; in: *Pattern Recognition for Machine Learning*, pp. 152-161, eq. 3.48; URL: <https://www.springer.com/gp/book/9780387310732>.
- Penny WD (2012): “Comparing Dynamic Causal Models using AIC, BIC and Free Energy”; in: *NeuroImage*, vol. 59, iss. 2, pp. 319-330, eq. 9; URL: <https://www.sciencedirect.com/science/article/pii/S1053811911008160>; DOI: 10.1016/j.neuroimage.2011.07.039.

1.7.2 Posterior distribution

Theorem: Let

$$y = X\beta + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \Sigma) \quad (1)$$

be a linear regression model (\rightarrow III/1.5.1) with measured n -dimensional data vector y , known $n \times p$ design matrix X and known $n \times n$ covariance matrix Σ as well as unknown $p \times 1$ regression coefficients β . Moreover, assume a multivariate normal distribution (\rightarrow III/1.7.1) over the model parameter β :

$$p(\beta) = \mathcal{N}(\beta; \mu_0, \Sigma_0) . \quad (2)$$

Then, the posterior distribution (\rightarrow I/5.1.9) is also a multivariate normal distribution (\rightarrow II/4.1.1)

$$p(\beta|y) = \mathcal{N}(\beta; \mu_n, \Sigma_n) \quad (3)$$

and the posterior hyperparameters (\rightarrow I/5.1.9) are given by

$$\begin{aligned}\mu_n &= \Sigma_n(X^T \Sigma^{-1} y + \Sigma_0^{-1} \mu_0) \\ \Sigma_n &= (X^T \Sigma^{-1} X + \Sigma_0^{-1})^{-1}.\end{aligned}\tag{4}$$

Proof: According to Bayes' theorem (\rightarrow I/5.3.2), the posterior distribution (\rightarrow I/5.1.9) is given by

$$p(\beta|y) = \frac{p(y|\beta) p(\beta)}{p(y)}.\tag{5}$$

Since $p(y)$ is just a normalization factor, the posterior is proportional (\rightarrow I/5.1.10) to the numerator:

$$p(\beta|y) \propto p(y|\beta) p(\beta) = p(y, \beta).\tag{6}$$

Equation (1) implies the following likelihood function (\rightarrow I/5.1.2):

$$p(y|\beta) = \mathcal{N}(y; X\beta, \Sigma) = \sqrt{\frac{1}{(2\pi)^n |\Sigma|}} \exp \left[-\frac{1}{2} (y - X\beta)^T \Sigma^{-1} (y - X\beta) \right].\tag{7}$$

Combining the likelihood function (\rightarrow I/5.1.2) (7) with the prior distribution (\rightarrow I/5.1.3) (2) using the probability density function of the multivariate normal distribution (\rightarrow II/4.1.4), the joint likelihood (\rightarrow I/5.1.7) of the model is given by

$$\begin{aligned}p(y, \beta) &= p(y|\beta) p(\beta) \\ &= \sqrt{\frac{1}{(2\pi)^n |\Sigma|}} \exp \left[-\frac{1}{2} (y - X\beta)^T \Sigma^{-1} (y - X\beta) \right] \cdot \\ &\quad \sqrt{\frac{1}{(2\pi)^p |\Sigma_0|}} \exp \left[-\frac{1}{2} (\beta - \mu_0)^T \Sigma_0^{-1} (\beta - \mu_0) \right].\end{aligned}\tag{8}$$

Collecting identical variables gives:

$$\begin{aligned}p(y, \beta) &= \sqrt{\frac{1}{(2\pi)^{n+p} |\Sigma| |\Sigma_0|}} \cdot \\ &\quad \exp \left[-\frac{1}{2} ((y - X\beta)^T \Sigma^{-1} (y - X\beta) + (\beta - \mu_0)^T \Sigma_0^{-1} (\beta - \mu_0)) \right].\end{aligned}\tag{9}$$

Expanding the products in the exponent gives:

$$\begin{aligned}p(y, \beta) &= \sqrt{\frac{1}{(2\pi)^{n+p} |\Sigma| |\Sigma_0|}} \cdot \\ &\quad \exp \left[-\frac{1}{2} (y^T \Sigma^{-1} y - y^T \Sigma^{-1} X\beta - \beta^T X^T \Sigma^{-1} y + \beta^T X^T \Sigma^{-1} X\beta + \right. \\ &\quad \left. \beta^T \Sigma_0^{-1} \beta - \beta^T \Sigma_0^{-1} \mu_0 - \mu_0^T \Sigma_0^{-1} \beta + \mu_0^T \Sigma_0^{-1} \mu_0) \right].\end{aligned}\tag{10}$$

Regrouping the terms in the exponent gives:

$$\begin{aligned}
p(y, \beta) &= \sqrt{\frac{1}{(2\pi)^{n+p}|\Sigma||\Sigma_0|}} \cdot \\
&\exp \left[-\frac{1}{2} \left(\beta^T [X^T \Sigma^{-1} X + \Sigma_0^{-1}] \beta - 2\beta^T [X^T \Sigma^{-1} y + \Sigma_0^{-1} \mu_0] + \right. \right. \\
&\quad \left. \left. y^T \Sigma^{-1} y + \mu_0^T \Sigma_0^{-1} \mu_0 \right) \right] .
\end{aligned} \tag{11}$$

Completing the square over β , we finally have

$$\begin{aligned}
p(y, \beta) &= \sqrt{\frac{1}{(2\pi)^{n+p}|\Sigma||\Sigma_0|}} \cdot \\
&\exp \left[-\frac{1}{2} \left((\beta - \mu_n)^T \Sigma_n^{-1} (\beta - \mu_n) + (y^T \Sigma^{-1} y + \mu_0^T \Sigma_0^{-1} \mu_0 - \mu_n^T \Sigma_n^{-1} \mu_n) \right) \right]
\end{aligned} \tag{12}$$

with the posterior hyperparameters (\rightarrow I/5.1.9)

$$\begin{aligned}
\mu_n &= \Sigma_n (X^T \Sigma^{-1} y + \Sigma_0^{-1} \mu_0) \\
\Sigma_n &= (X^T \Sigma^{-1} X + \Sigma_0^{-1})^{-1} .
\end{aligned} \tag{13}$$

Ergo, the joint likelihood is proportional to

$$p(y, \beta) \propto \exp \left[-\frac{1}{2} (\beta - \mu_n)^T \Sigma_n^{-1} (\beta - \mu_n) \right] , \tag{14}$$

such that the posterior distribution over β is given by

$$p(\beta|y) = \mathcal{N}(\beta; \mu_n, \Sigma_n) \tag{15}$$

with the posterior hyperparameters given in (13). ■

Sources:

- Bishop CM (2006): “Bayesian Linear Regression”; in: *Pattern Recognition for Machine Learning*, pp. 152-161, eqs. 3.49-3.51, ex. 3.7; URL: <https://www.springer.com/gp/book/9780387310732>.
- Penny WD (2012): “Comparing Dynamic Causal Models using AIC, BIC and Free Energy”; in: *NeuroImage*, vol. 59, iss. 2, pp. 319-330, eq. 27; URL: <https://www.sciencedirect.com/science/article/pii/S1053811911008160>; DOI: 10.1016/j.neuroimage.2011.07.039.

1.7.3 Log model evidence

Theorem: Let

$$m : y = X\beta + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \Sigma) \tag{1}$$

be a linear regression model (\rightarrow III/1.5.1) with measured n -dimensional data vector y , known $n \times p$ design matrix X and known $n \times n$ covariance matrix Σ as well as unknown $p \times 1$ regression coefficients β . Moreover, assume a multivariate normal distribution (\rightarrow III/1.7.1) over the model parameter β :

$$p(\beta) = \mathcal{N}(\beta; \mu_0, \Sigma_0) . \quad (2)$$

Then, the log model evidence (\rightarrow IV/3.1.3) for this model is

$$\begin{aligned} \log p(y|m) = & -\frac{1}{2} e_y^T \Sigma^{-1} e_y - \frac{1}{2} \log |\Sigma| - \frac{n}{2} \log(2\pi) \\ & - \frac{1}{2} e_\beta^T \Sigma_0^{-1} e_\beta - \frac{1}{2} \log |\Sigma_0| + \frac{1}{2} \log |\Sigma_n| . \end{aligned} \quad (3)$$

with the “prediction error” and “parameter error” terms

$$\begin{aligned} e_y &= y - X\mu_n \\ e_\beta &= \mu_0 - \mu_n \end{aligned} \quad (4)$$

where the posterior hyperparameters (\rightarrow I/5.1.9) are given by

$$\begin{aligned} \mu_n &= \Sigma_n (X^T \Sigma^{-1} y + \Sigma_0^{-1} \mu_0) \\ \Sigma_n &= (X^T \Sigma^{-1} X + \Sigma_0^{-1})^{-1} . \end{aligned} \quad (5)$$

Proof: According to the law of marginal probability (\rightarrow I/1.3.3), the model evidence (\rightarrow I/5.1.15) for this model is:

$$p(y|m) = \int p(y|\beta) p(\beta) d\beta . \quad (6)$$

According to the law of conditional probability (\rightarrow I/1.3.4), the integrand is equivalent to the joint likelihood (\rightarrow I/5.1.7):

$$p(y|m) = \int p(y, \beta) d\beta . \quad (7)$$

Equation (1) implies the following likelihood function (\rightarrow I/5.1.2):

$$p(y|\beta) = \mathcal{N}(y; X\beta, \Sigma) = \sqrt{\frac{1}{(2\pi)^n |\Sigma|}} \exp \left[-\frac{1}{2} (y - X\beta)^T \Sigma^{-1} (y - X\beta) \right] . \quad (8)$$

When deriving the posterior distribution (\rightarrow III/1.7.2) $p(\beta|y)$, the joint likelihood $p(y, \beta)$ is obtained as

$$\begin{aligned} p(y, \beta) = & \sqrt{\frac{1}{(2\pi)^{n+p} |\Sigma| |\Sigma_0|}} \\ & \exp \left[-\frac{1}{2} ((\beta - \mu_n)^T \Sigma_n^{-1} (\beta - \mu_n) + (y^T \Sigma^{-1} y + \mu_0^T \Sigma_0^{-1} \mu_0 - \mu_n^T \Sigma_n^{-1} \mu_n)) \right] . \end{aligned} \quad (9)$$

Using the probability density function of the multivariate normal distribution (\rightarrow II/4.1.4), we can rewrite this as

$$p(y, \beta) = \sqrt{\frac{1}{(2\pi)^n |\Sigma|}} \sqrt{\frac{1}{(2\pi)^p |\Sigma_0|}} \sqrt{\frac{(2\pi)^p |\Sigma_n|}{1}} \cdot \mathcal{N}(\beta; \mu_n, \Sigma_n) \cdot \exp \left[-\frac{1}{2} (y^T \Sigma^{-1} y + \mu_0^T \Sigma_0^{-1} \mu_0 - \mu_n^T \Sigma_n^{-1} \mu_n) \right]. \quad (10)$$

With that, β can be integrated out easily:

$$\int p(y, \beta) d\beta = \sqrt{\frac{1}{(2\pi)^n |\Sigma|}} \sqrt{\frac{|\Sigma_n|}{|\Sigma_0|}} \cdot \exp \left[-\frac{1}{2} (y^T \Sigma^{-1} y + \mu_0^T \Sigma_0^{-1} \mu_0 - \mu_n^T \Sigma_n^{-1} \mu_n) \right]. \quad (11)$$

Now we turn to the intra-exponent term

$$y^T \Sigma^{-1} y + \mu_0^T \Sigma_0^{-1} \mu_0 - \mu_n^T \Sigma_n^{-1} \mu_n \quad (12)$$

and plug in the posterior covariance

$$\Sigma_n = (X^T \Sigma^{-1} X + \Sigma_0^{-1})^{-1}. \quad (13)$$

This gives

$$\begin{aligned} & y^T \Sigma^{-1} y + \mu_0^T \Sigma_0^{-1} \mu_0 - \mu_n^T \Sigma_n^{-1} \mu_n \\ &= y^T \Sigma^{-1} y + \mu_0^T \Sigma_0^{-1} \mu_0 - \mu_n^T (X^T \Sigma^{-1} X + \Sigma_0^{-1}) \mu_n \\ &= y^T \Sigma^{-1} y + \mu_0^T \Sigma_0^{-1} \mu_0 - \mu_n^T X^T \Sigma^{-1} X \mu_n - \mu_n^T \Sigma_0^{-1} \mu_n \\ &= (y - X \mu_n)^T \Sigma^{-1} (y - X \mu_n) + (\mu_0 - \mu_n)^T \Sigma_0^{-1} (\mu_0 - \mu_n) \\ &\stackrel{(4)}{=} e_y^T \Sigma^{-1} e_y + e_\beta^T \Sigma_0^{-1} e_\beta. \end{aligned} \quad (14)$$

Thus, the marginal likelihood (\rightarrow I/5.1.15) becomes

$$p(y|m) = \int p(y, \beta) d\beta \stackrel{(11)}{=} \sqrt{\frac{1}{(2\pi)^n |\Sigma|}} \sqrt{\frac{|\Sigma_n|}{|\Sigma_0|}} \cdot \exp \left[-\frac{1}{2} (e_y^T \Sigma^{-1} e_y + e_\beta^T \Sigma_0^{-1} e_\beta) \right] \quad (15)$$

and the log model evidence (\rightarrow IV/3.1.3) of this model is given by

$$\begin{aligned} \log p(y|m) &= -\frac{1}{2} e_y^T \Sigma^{-1} e_y - \frac{1}{2} \log |\Sigma| - \frac{n}{2} \log(2\pi) \\ &\quad - \frac{1}{2} e_\beta^T \Sigma_0^{-1} e_\beta - \frac{1}{2} \log |\Sigma_0| + \frac{1}{2} \log |\Sigma_n|. \end{aligned} \quad (16)$$

■

Sources:

- Penny WD (2012): “Comparing Dynamic Causal Models using AIC, BIC and Free Energy”; in: *NeuroImage*, vol. 59, iss. 2, pp. 319-330, eqs. 19-23; URL: <https://www.sciencedirect.com/science/article/pii/S1053811911008160>; DOI: 10.1016/j.neuroimage.2011.07.039.
- Bishop CM (2006): “Bayesian Linear Regression”; in: *Pattern Recognition for Machine Learning*, pp. 152-161; URL: <https://www.springer.com/gp/book/9780387310732>.

1.7.4 Accuracy and complexity

Theorem: Let

$$m : y = X\beta + \varepsilon, \varepsilon \sim \mathcal{N}(0, \Sigma) \quad (1)$$

be a linear regression model (\rightarrow III/1.5.1) with measured n -dimensional data vector y , known $n \times p$ design matrix X and known $n \times n$ covariance matrix Σ as well as unknown $p \times 1$ regression coefficients β . Moreover, assume a multivariate normal distribution (\rightarrow III/1.7.1) over the model parameter β :

$$p(\beta) = \mathcal{N}(\beta; \mu_0, \Sigma_0) . \quad (2)$$

Then, accuracy and complexity (\rightarrow IV/3.1.6) of this model are

$$\begin{aligned} \text{Acc}(m) &= -\frac{1}{2}e_y^T \Sigma^{-1} e_y - \frac{1}{2} \log |\Sigma| - \frac{n}{2} \log(2\pi) - \frac{1}{2} \text{tr}(X^T \Sigma^{-1} X \Sigma_n) \\ \text{Com}(m) &= \frac{1}{2}e_\beta^T \Sigma_0^{-1} e_\beta + \frac{1}{2} \log |\Sigma_0| - \frac{1}{2} \log |\Sigma_n| + \frac{1}{2} \text{tr}(\Sigma_0^{-1} \Sigma_n) - \frac{p}{2} \end{aligned} \quad (3)$$

with the “prediction error” and “parameter error” terms

$$\begin{aligned} e_y &= y - X\mu_n \\ e_\beta &= \mu_0 - \mu_n \end{aligned} \quad (4)$$

where the posterior hyperparameters (\rightarrow I/5.1.9) are given by

$$\begin{aligned} \mu_n &= \Sigma_n (X^T \Sigma^{-1} y + \Sigma_0^{-1} \mu_0) \\ \Sigma_n &= (X^T \Sigma^{-1} X + \Sigma_0^{-1})^{-1} . \end{aligned} \quad (5)$$

Proof: Model accuracy and complexity are defined as (\rightarrow IV/3.1.6)

$$\begin{aligned} \text{LME}(m) &= \text{Acc}(m) - \text{Com}(m) \\ \text{Acc}(m) &= \langle \log p(y|\beta, m) \rangle_{p(\beta|y, m)} \\ \text{Com}(m) &= \text{KL} [p(\beta|y, m) || p(\beta|m)] . \end{aligned} \quad (6)$$

1) The accuracy term is the expectation (\rightarrow I/1.12.1) of the log-likelihood function (\rightarrow I/4.1.2) $\log p(y|\beta)$ with respect to the posterior distribution (\rightarrow I/5.1.9) $p(\beta|y)$:

$$\text{Acc}(m) = \langle \log p(y|\beta) \rangle_{p(\beta|y)} . \quad (7)$$

With the likelihood function for Bayesian linear regression with known covariance (\rightarrow III/1.7.1), we have:

$$\begin{aligned} \text{Acc}(m) &= \left\langle \log \left(\sqrt{\frac{1}{(2\pi)^n |\Sigma|}} \exp \left[-\frac{1}{2} (y - X\beta)^T \Sigma^{-1} (y - X\beta) \right] \right) \right\rangle_{p(\beta|y)} \\ &= \left\langle -\frac{n}{2} \log(2\pi) - \frac{1}{2} \log |\Sigma| - \frac{1}{2} (y - X\beta)^T \Sigma^{-1} (y - X\beta) \right\rangle_{p(\beta|y)} \\ &= \left\langle -\frac{n}{2} \log(2\pi) - \frac{1}{2} \log |\Sigma| - \frac{1}{2} [y^T \Sigma^{-1} y - 2y^T \Sigma^{-1} X\beta + \beta^T X^T \Sigma^{-1} X\beta] \right\rangle_{p(\beta|y)} . \end{aligned} \quad (8)$$

With the posterior distribution for Bayesian linear regression with known covariance (\rightarrow III/1.7.2), this becomes:

$$\text{Acc}(m) = \left\langle -\frac{n}{2} \log(2\pi) - \frac{1}{2} \log |\Sigma| - \frac{1}{2} [y^T \Sigma^{-1} y - 2y^T \Sigma^{-1} X \beta + \beta^T X^T \Sigma^{-1} X \beta] \right\rangle_{\mathcal{N}(\beta; \mu_n, \Sigma_n)} . \quad (9)$$

If $x \sim \mathcal{N}(\mu, \Sigma)$, then its expected value is (\rightarrow II/4.1.6)

$$\langle x \rangle = \mu \quad (10)$$

and the expectation of a quadratic form is given by (\rightarrow I/1.12.17)

$$\langle x^T A x \rangle = \mu^T A \mu + \text{tr}(A \Sigma) . \quad (11)$$

Thus, the model accuracy of m evaluates to

$$\begin{aligned} \text{Acc}(m) &= -\frac{n}{2} \log(2\pi) - \frac{1}{2} \log |\Sigma| - \\ &\quad \frac{1}{2} [y^T \Sigma^{-1} y - 2y^T \Sigma^{-1} X \mu_n + \mu_n^T X^T \Sigma^{-1} X \mu_n + \text{tr}(X^T \Sigma^{-1} X \Sigma_n)] \\ &= -\frac{1}{2} (y - X \mu_n)^T \Sigma^{-1} (y - X \mu_n) - \frac{1}{2} \log |\Sigma| - \frac{n}{2} \log(2\pi) - \frac{1}{2} \text{tr}(X^T \Sigma^{-1} X \Sigma_n) \\ &\stackrel{(4)}{=} -\frac{1}{2} e_y^T \Sigma^{-1} e_y - \frac{1}{2} \log |\Sigma| - \frac{n}{2} \log(2\pi) - \frac{1}{2} \text{tr}(X^T \Sigma^{-1} X \Sigma_n) \end{aligned} \quad (12)$$

which proofs the first part of (3).

2) The complexity penalty is the Kullback-Leibler divergence (\rightarrow I/2.5.1) of the posterior distribution (\rightarrow I/5.1.9) $p(\beta|y)$ from the prior distribution (\rightarrow I/5.1.3) $p(\beta)$:

$$\text{Com}(m) = \text{KL} [p(\beta|y) || p(\beta)] . \quad (13)$$

With the prior distribution (\rightarrow III/1.7.1) given by (2) and the posterior distribution for Bayesian linear regression with known covariance (\rightarrow III/1.7.2), this becomes:

$$\text{Com}(m) = \text{KL} [\mathcal{N}(\beta; \mu_n, \Sigma_n) || \mathcal{N}(\beta; \mu_0, \Sigma_0)] . \quad (14)$$

With the Kullback-Leibler divergence for the multivariate normal distribution (\rightarrow II/4.1.12)

$$\text{KL}[\mathcal{N}(\mu_1, \Sigma_1) || \mathcal{N}(\mu_2, \Sigma_2)] = \frac{1}{2} \left[(\mu_2 - \mu_1)^T \Sigma_2^{-1} (\mu_2 - \mu_1) + \text{tr}(\Sigma_2^{-1} \Sigma_1) - \ln \frac{|\Sigma_1|}{|\Sigma_2|} - n \right] , \quad (15)$$

the model complexity of m evaluates to

$$\begin{aligned} \text{Com}(m) &= \frac{1}{2} \left[(\mu_0 - \mu_n)^T \Sigma_0^{-1} (\mu_0 - \mu_n) + \text{tr}(\Sigma_0^{-1} \Sigma_n) - \log \frac{|\Sigma_n|}{|\Sigma_0|} - p \right] \\ &= \frac{1}{2} (\mu_0 - \mu_n)^T \Sigma_0^{-1} (\mu_0 - \mu_n) + \frac{1}{2} \log |\Sigma_0| - \frac{1}{2} \log |\Sigma_n| + \frac{1}{2} \text{tr}(\Sigma_0^{-1} \Sigma_n) - \frac{p}{2} \\ &\stackrel{(4)}{=} \frac{1}{2} e_\beta^T \Sigma_0^{-1} e_\beta + \frac{1}{2} \log |\Sigma_0| - \frac{1}{2} \log |\Sigma_n| + \frac{1}{2} \text{tr}(\Sigma_0^{-1} \Sigma_n) - \frac{p}{2} \end{aligned} \quad (16)$$

which proofs the second part of (3).

3) A control calculation confirms that

$$\text{Acc}(m) - \text{Com}(m) = \text{LME}(m) \quad (17)$$

where $\text{LME}(m)$ is the log model evidence for Bayesian linear regression with known covariance (\rightarrow III/1.7.3):

$$\begin{aligned} \log p(y|m) = & -\frac{1}{2} e_y^T \Sigma^{-1} e_y - \frac{1}{2} \log |\Sigma| - \frac{n}{2} \log(2\pi) \\ & - \frac{1}{2} e_\beta^T \Sigma_0^{-1} e_\beta - \frac{1}{2} \log |\Sigma_0| + \frac{1}{2} \log |\Sigma_n| . \end{aligned} \quad (18)$$

This requires to recognize, based on (5), that

$$\begin{aligned} & -\frac{1}{2} \text{tr}(X^T \Sigma^{-1} X \Sigma_n) - \frac{1}{2} \text{tr}(\Sigma_0^{-1} \Sigma_n) + \frac{p}{2} \\ = & -\frac{1}{2} \text{tr}([X^T \Sigma^{-1} X + \Sigma_0^{-1}] \Sigma_n) + \frac{p}{2} \\ = & -\frac{1}{2} \text{tr}(\Sigma_n^{-1} \Sigma_n) + \frac{p}{2} \\ = & -\frac{1}{2} \text{tr}(I_p) + \frac{p}{2} \\ = & -\frac{p}{2} + \frac{p}{2} \\ = & 0 . \end{aligned} \quad (19)$$

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Sources:

- Penny WD (2012): “Comparing Dynamic Causal Models using AIC, BIC and Free Energy”; in: *NeuroImage*, vol. 59, iss. 2, pp. 319-330, eqs. 20-21; URL: <https://www.sciencedirect.com/science/article/pii/S1053811911008160>; DOI: 10.1016/j.neuroimage.2011.07.039.
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2 Multivariate normal data

2.1 Multivariate Gaussian

2.1.1 Bivariate normally distributed data

Definition: Bivariate normally distributed data are defined as a set of two-dimensional vectors $y = \{y_1, \dots, y_n\}$ with $y_i \in \mathbb{R}^2$, $i = 1, \dots, n$, independent and identically distributed (\rightarrow I/1.2.8) according to a bivariate normal distribution (\rightarrow II/4.2.1) with mean vector μ and covariance matrix Σ

$$y_i \sim \mathcal{N}(\mu, \Sigma), \quad i = 1, \dots, n \quad (1)$$

where μ and Σ can be parametrized (\rightarrow II/4.2.4) in terms of (\rightarrow II/4.2.3) means μ_1, μ_2 , variances σ_1^2, σ_2^2 and correlation ρ :

$$\mu = \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix} \quad \text{and} \quad \Sigma = \begin{bmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 \end{bmatrix}. \quad (2)$$

2.1.2 Multivariate normally distributed data

Definition: Multivariate normally distributed data are defined as a set of p -dimensional vectors $y = \{y_1, \dots, y_n\}$ with $y_i \in \mathbb{R}^p$, $i = 1, \dots, n$, independent and identically distributed (\rightarrow I/1.2.8) according to a multivariate normal distribution (\rightarrow II/4.1.1) with mean vector $\mu \in \mathbb{R}^p$ and covariance matrix $\Sigma \in \mathbb{R}^{p \times p}$

$$y_i \sim \mathcal{N}(\mu, \Sigma), \quad i = 1, \dots, n \quad (1)$$

where μ is a p -dimensional real vector and Σ is a $p \times p$ positive-definite matrix.

2.1.3 Maximum likelihood estimation ($p = 2$)

Theorem: Let there be a bivariate normally distributed data set (\rightarrow III/2.1.1) $y = \{y_1, \dots, y_n\}$:

$$y_i = \begin{bmatrix} y_{i1} \\ y_{i2} \end{bmatrix} \sim \mathcal{N} \left(\begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}, \begin{bmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 \end{bmatrix} \right), \quad i = 1, \dots, n. \quad (1)$$

Then, the maximum likelihood estimates (\rightarrow I/4.1.3) of $\mu_1, \mu_2, \sigma_1^2, \sigma_2^2$ and ρ are given by

$$\begin{aligned}
\hat{\mu}_1 &= \frac{1}{n} \sum_{i=1}^n y_{i1} \\
\hat{\mu}_2 &= \frac{1}{n} \sum_{i=1}^n y_{i2} \\
\hat{\sigma}_1^2 &= \frac{1}{n} \sum_{i=1}^n (y_{i1} - \hat{\mu}_1)^2 \\
\hat{\sigma}_2^2 &= \frac{1}{n} \sum_{i=1}^n (y_{i2} - \hat{\mu}_2)^2 \\
\hat{\rho} &= \frac{\frac{1}{n} \sum_{i=1}^n (y_{i1} - \hat{\mu}_1)(y_{i2} - \hat{\mu}_2)}{\sqrt{\hat{\sigma}_1^2} \sqrt{\hat{\sigma}_2^2}}.
\end{aligned} \tag{2}$$

Proof: This is a special case of multivariate normally distributed data (\rightarrow III/2.1.2)

$$y_i = \begin{bmatrix} y_{i1} \\ \vdots \\ y_{ip} \end{bmatrix} \sim \mathcal{N}(\mu, \Sigma), \quad i = 1, \dots, n \tag{3}$$

for which maximum likelihood estimates are given by (\rightarrow III/2.1.4)

$$\begin{aligned}
\hat{\mu} &= \frac{1}{n} \sum_{i=1}^n y_i \\
\hat{\Sigma} &= \frac{1}{n} \sum_{i=1}^n (y_i - \hat{\mu})(y_i - \hat{\mu})^T.
\end{aligned} \tag{4}$$

Applying this to (1) by setting $p = 2$, we obtain:

$$\begin{aligned}
\hat{\mu} &= \begin{bmatrix} \frac{1}{n} \sum_{i=1}^n y_{i1} \\ \frac{1}{n} \sum_{i=1}^n y_{i2} \end{bmatrix} \\
\hat{\Sigma} &= \begin{bmatrix} \frac{1}{n} \sum_{i=1}^n (y_{i1} - \hat{\mu}_1)(y_{i1} - \hat{\mu}_1) & \frac{1}{n} \sum_{i=1}^n (y_{i1} - \hat{\mu}_1)(y_{i2} - \hat{\mu}_2) \\ \frac{1}{n} \sum_{i=1}^n (y_{i2} - \hat{\mu}_2)(y_{i1} - \hat{\mu}_1) & \frac{1}{n} \sum_{i=1}^n (y_{i2} - \hat{\mu}_2)(y_{i2} - \hat{\mu}_2) \end{bmatrix}.
\end{aligned} \tag{5}$$

Equating this with the parametrized bivariate normal estimates (\rightarrow II/4.2.4)

$$\hat{\mu} = \begin{bmatrix} \hat{\mu}_1 \\ \hat{\mu}_2 \end{bmatrix} \quad \text{and} \quad \hat{\Sigma} = \begin{bmatrix} \hat{\sigma}_1^2 & \hat{\rho} \hat{\sigma}_1 \hat{\sigma}_2 \\ \hat{\rho} \hat{\sigma}_1 \hat{\sigma}_2 & \hat{\sigma}_2^2 \end{bmatrix}, \tag{6}$$

we obtain ML estimates for the means as

$$\begin{aligned}\hat{\mu}_1 &= \frac{1}{n} \sum_{i=1}^n y_{i1} \\ \hat{\mu}_2 &= \frac{1}{n} \sum_{i=1}^n y_{i2} ,\end{aligned}\tag{7}$$

we obtain ML estimates for the variances as

$$\begin{aligned}\hat{\sigma}_1^2 &= \frac{1}{n} \sum_{i=1}^n (y_{i1} - \hat{\mu}_1)^2 \\ \hat{\sigma}_2^2 &= \frac{1}{n} \sum_{i=1}^n (y_{i2} - \hat{\mu}_2)^2\end{aligned}\tag{8}$$

and we obtain an ML estimate for the correlation as:

$$\begin{aligned}\hat{\rho}\hat{\sigma}_1\hat{\sigma}_2 &= \frac{1}{n} \sum_{i=1}^n (y_{i1} - \hat{\mu}_1)(y_{i2} - \hat{\mu}_2) \\ \hat{\rho} &= \frac{\frac{1}{n} \sum_{i=1}^n (y_{i1} - \hat{\mu}_1)(y_{i2} - \hat{\mu}_2)}{\hat{\sigma}_1\hat{\sigma}_2} \\ \hat{\rho} &= \frac{\frac{1}{n} \sum_{i=1}^n (y_{i1} - \hat{\mu}_1)(y_{i2} - \hat{\mu}_2)}{\sqrt{\hat{\sigma}_1^2}\sqrt{\hat{\sigma}_2^2}} \\ \hat{\rho} &= \frac{\frac{1}{n} \sum_{i=1}^n (y_{i1} - \hat{\mu}_1)(y_{i2} - \hat{\mu}_2)}{\sqrt{\frac{1}{n} \sum_{i=1}^n (y_{i1} - \hat{\mu}_1)^2} \sqrt{\frac{1}{n} \sum_{i=1}^n (y_{i2} - \hat{\mu}_2)^2}} .\end{aligned}\tag{9}$$

Together, (7), (8) and (9) constitute the maximum likelihood estimates (\rightarrow I/4.1.3) for bivariate normally distributed data (\rightarrow III/2.1.1). ■

2.1.4 Maximum likelihood estimation ($p > 2$)

Theorem: Let there be a multivariate normally distributed data set (\rightarrow III/2.1.2) $y = \{y_1, \dots, y_n\}$:

$$y_i = \begin{bmatrix} y_{i1} \\ \vdots \\ y_{ip} \end{bmatrix} \sim \mathcal{N}(\mu, \Sigma), \quad i = 1, \dots, n .\tag{1}$$

Then, the maximum likelihood estimates (\rightarrow I/4.1.3) of μ and Σ are given by

$$\begin{aligned}\hat{\mu} &= \frac{1}{n} \sum_{i=1}^n y_i \\ \hat{\Sigma} &= \frac{1}{n} \sum_{i=1}^n (y_i - \hat{\mu})(y_i - \hat{\mu})^T .\end{aligned}\tag{2}$$

Proof: With the probability density function of the multivariate normal distribution (\rightarrow II/4.1.4), the likelihood function for a single data point (\rightarrow I/1.1.5) is

$$\begin{aligned} p(y_i|\mu, \Sigma) &= \mathcal{N}(y_i; \mu, \sigma^2) \\ &= \frac{1}{\sqrt{(2\pi)^p |\Sigma|}} \cdot \exp \left[-\frac{1}{2} (y_i - \mu)^T \Sigma^{-1} (y_i - \mu) \right] \end{aligned} \quad (3)$$

and all data points are independent (\rightarrow I/1.3.6), the total likelihood function is equal to the product (\rightarrow I/1.3.9) of the individual likelihood functions:

$$\begin{aligned} p(y|\mu, \Sigma) &= \prod_{i=1}^n p(y_i|\mu, \Sigma) \\ &= \frac{1}{\sqrt{(2\pi)^{np} |\Sigma|^n}} \cdot \exp \left[-\frac{1}{2} \sum_{i=1}^n (y_i - \mu)^T \Sigma^{-1} (y_i - \mu) \right] . \end{aligned} \quad (4)$$

Thus, the log-likelihood function (\rightarrow I/4.1.2) is

$$\begin{aligned} \text{LL}(\mu, \Sigma) &= \log p(y|\mu, \Sigma) \\ &= -\frac{np}{2} \log(2\pi) - \frac{n}{2} \log |\Sigma| - \frac{1}{2} \sum_{i=1}^n (y_i - \mu)^T \Sigma^{-1} (y_i - \mu) \\ &= -\frac{np}{2} \log(2\pi) - \frac{n}{2} \log |\Sigma| - \frac{1}{2} \sum_{i=1}^n (y_i^T \Sigma^{-1} y_i - 2\mu^T \Sigma^{-1} y_i + \mu^T \Sigma^{-1} \mu) . \end{aligned} \quad (5)$$

The derivative of the log-likelihood function (5) with respect to μ is

$$\begin{aligned} \frac{d\text{LL}(\mu, \Sigma)}{d\mu} &= \frac{d}{d\mu} \left[-\frac{1}{2} \sum_{i=1}^n (y_i^T \Sigma^{-1} y_i - 2\mu^T \Sigma^{-1} y_i + \mu^T \Sigma^{-1} \mu) \right] \\ &= -\frac{1}{2} \sum_{i=1}^n (-2\Sigma^{-1} y_i + 2\Sigma^{-1} \mu) \\ &= \sum_{i=1}^n (\Sigma^{-1} y_i - \Sigma^{-1} \mu) \end{aligned} \quad (6)$$

and setting this derivative to zero gives the MLE for μ :

$$\begin{aligned}
\frac{dLL(\hat{\mu}, \Sigma)}{d\mu} &= 0_p \\
0_p &= \sum_{i=1}^n (\Sigma^{-1}y_i - \Sigma^{-1}\hat{\mu}) \\
0_p &= \Sigma^{-1} \sum_{i=1}^n (y_i - \hat{\mu}) \\
0_p &= \sum_{i=1}^n y_i - n \cdot \hat{\mu} \\
\hat{\mu} &= \frac{1}{n} \sum_{i=1}^n y_i .
\end{aligned} \tag{7}$$

The derivative of the log-likelihood function (5) at $\hat{\mu}$ with respect to Σ is

$$\begin{aligned}
\frac{dLL(\hat{\mu}, \Sigma)}{d\Sigma} &= -\frac{n}{2} \frac{d}{d\Sigma} [\log |\Sigma|] - \frac{1}{2} \frac{d}{d\Sigma} \left[\sum_{i=1}^n (y_i - \mu)^T \Sigma^{-1} (y_i - \mu) \right] \\
&= -\frac{n}{2} (\Sigma^{-1})^T - \frac{1}{2} \sum_{i=1}^n \frac{d}{d\Sigma} [\text{tr} ((y_i - \mu)^T \Sigma^{-1} (y_i - \mu))] \\
&= -\frac{n}{2} \Sigma^{-1} - \frac{1}{2} \sum_{i=1}^n \frac{d}{d\Sigma} [\text{tr} (\Sigma^{-1} (y_i - \mu) (y_i - \mu)^T)] \\
&= -\frac{n}{2} \Sigma^{-1} - \frac{1}{2} \sum_{i=1}^n \left[-(\Sigma^{-1} (y_i - \mu) (y_i - \mu)^T \Sigma^{-1})^T \right] \\
&= -\frac{n}{2} \Sigma^{-1} + \frac{1}{2} \sum_{i=1}^n [\Sigma^{-1} (y_i - \mu) (y_i - \mu)^T \Sigma^{-1}]
\end{aligned} \tag{8}$$

and setting this derivative to zero gives the MLE for Σ :

$$\begin{aligned}
\frac{dLL(\hat{\mu}, \hat{\Sigma})}{d\Sigma} &= 0_{pp} \\
0_{pp} &= -\frac{n}{2} \hat{\Sigma}^{-1} + \frac{1}{2} \sum_{i=1}^n [\hat{\Sigma}^{-1} (y_i - \mu) (y_i - \mu)^T \hat{\Sigma}^{-1}] \\
\hat{\Sigma}^{-1} &= \frac{1}{n} \Sigma^{-1} \left(\sum_{i=1}^n (y_i - \mu) (y_i - \mu)^T \right) \Sigma^{-1} \\
\hat{\Sigma} \hat{\Sigma}^{-1} \hat{\Sigma} &= \frac{1}{n} \hat{\Sigma} \Sigma^{-1} \left(\sum_{i=1}^n (y_i - \mu) (y_i - \mu)^T \right) \Sigma^{-1} \hat{\Sigma} \\
I_p \hat{\Sigma} &= \frac{1}{n} I_p \left(\sum_{i=1}^n (y_i - \mu) (y_i - \mu)^T \right) I_p \\
\hat{\Sigma} &= \frac{1}{n} \sum_{i=1}^n (y_i - \mu) (y_i - \mu)^T
\end{aligned} \tag{9}$$

Together, (7) and (9) constitute the maximum likelihood estimates (\rightarrow I/4.1.3) for multivariate normally distributed data (\rightarrow III/2.1.2).

■

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2.2 General linear model

2.2.1 Definition

Definition: Let Y be an $n \times v$ matrix and let X be an $n \times p$ matrix. Then, a statement asserting a linear mapping from X to Y with parameters B and matrix-normally distributed (\rightarrow II/5.1.1) errors E

$$Y = XB + E, \quad E \sim \mathcal{MN}(0, V, \Sigma) \quad (1)$$

is called a multivariate linear regression model or simply, “general linear model”.

- Y is called “data matrix”, “set of dependent variables” or “measurements”;
- X is called “design matrix”, “set of independent variables” or “predictors”;
- B are called “regression coefficients” or “weights”;
- E is called “noise matrix” or “error terms”;
- V is called “covariance across rows”;
- Σ is called “covariance across columns”;
- n is the number of observations;
- v is the number of measurements;
- p is the number of predictors.

When rows of Y correspond to units of time, e.g. subsequent measurements, V is called “temporal covariance”. When columns of Y correspond to units of space, e.g. measurement channels, Σ is called “spatial covariance”.

When the covariance matrix V is a scalar multiple of the $n \times n$ identity matrix, this is called a general linear model with independent and identically distributed (\rightarrow I/1.2.8) (i.i.d.) observations:

$$V = \lambda I_n \quad \Rightarrow \quad E \sim \mathcal{MN}(0, \lambda I_n, \Sigma) \quad \Rightarrow \quad \varepsilon_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \lambda \Sigma) . \quad (2)$$

Otherwise, it is called a general linear model with correlated observations (\rightarrow I/1.17.1).

Sources:

- Wikipedia (2020): “General linear model”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-03-21; URL: https://en.wikipedia.org/wiki/General_linear_model.

2.2.2 Ordinary least squares

Theorem: Given a general linear model (\rightarrow III/2.2.1) with independent observations

$$Y = XB + E, \quad E \sim \mathcal{MN}(0, \sigma^2 I_n, \Sigma), \quad (1)$$

the ordinary least squares (\rightarrow III/1.5.3) parameters estimates are given by

$$\hat{B} = (X^T X)^{-1} X^T Y. \quad (2)$$

Proof: Let \hat{B} be the ordinary least squares (\rightarrow III/1.5.3) (OLS) solution and let $\hat{E} = Y - X\hat{B}$ be the resulting matrix of residuals. According to the exogeneity assumption of OLS, the errors have conditional mean (\rightarrow I/1.12.1) zero

$$E(E|X) = 0, \quad (3)$$

a direct consequence of which is that the regressors are uncorrelated with the errors

$$E(X^T E) = 0, \quad (4)$$

which, in the finite sample, means that the residual matrix must be orthogonal to the design matrix:

$$X^T \hat{E} = 0. \quad (5)$$

From (5), the OLS formula can be directly derived:

$$\begin{aligned} X^T \hat{E} &= 0 \\ X^T (Y - X\hat{B}) &= 0 \\ X^T Y - X^T X\hat{B} &= 0 \\ X^T X\hat{B} &= X^T Y \\ \hat{B} &= (X^T X)^{-1} X^T Y. \end{aligned} \quad (6)$$

■

Sources:

- Wikipedia (2025): “Ordinary least squares”; in: *Wikipedia, the free encyclopedia*, retrieved on 2025-12-19; URL: https://en.wikipedia.org/wiki/Ordinary_least_squares#Assumptions.

2.2.3 Weighted least squares

Theorem: Given a general linear model (\rightarrow III/2.2.1) with correlated observations

$$Y = XB + E, \quad E \sim \mathcal{MN}(0, V, \Sigma), \quad (1)$$

the weighted least squares (\rightarrow III/1.5.21) parameter estimates are given by

$$\hat{B} = (X^T V^{-1} X)^{-1} X^T V^{-1} Y. \quad (2)$$

Proof: Let there be an $n \times n$ square matrix W , such that

$$WVW^T = I_n . \quad (3)$$

Since V is a covariance matrix and thus symmetric (\rightarrow I/1.15.4), W is also symmetric and can be expressed as the matrix square root of the inverse of V :

$$WW = V^{-1} \Leftrightarrow W = V^{-1/2} . \quad (4)$$

Left-multiplying the linear regression equation (1) with W , the linear transformation theorem (\rightarrow II/5.1.9) implies that

$$WY = WXB + WE, \quad WE \sim \mathcal{MN}(0, WVW^T, \Sigma) . \quad (5)$$

Applying (3), we see that (5) is actually a general linear model (\rightarrow III/2.2.1) with independent observations

$$\tilde{Y} = \tilde{X}B + \tilde{E}, \quad \tilde{E} \sim \mathcal{N}(0, I_n, \Sigma) \quad (6)$$

where $\tilde{Y} = WY$, $\tilde{X} = WX$ and $\tilde{E} = WE$, such that we can apply the ordinary least squares solution (\rightarrow III/2.2.2) giving

$$\begin{aligned} \hat{B} &= (\tilde{X}^T \tilde{X})^{-1} \tilde{X}^T \tilde{Y} \\ &= ((WX)^T WX)^{-1} (WX)^T WY \\ &= (X^T W^T W X)^{-1} X^T W^T WY \\ &= (X^T W W X)^{-1} X^T W WY \\ &\stackrel{(4)}{=} (X^T V^{-1} X)^{-1} X^T V^{-1} Y \end{aligned} \quad (7)$$

which corresponds to the weighted least squares solution (2). ■

2.2.4 Maximum likelihood estimation

Theorem: Given a general linear model (\rightarrow III/2.2.1) with matrix-normally distributed (\rightarrow II/5.1.1) errors

$$Y = XB + E, \quad E \sim \mathcal{MN}(0, V, \Sigma) , \quad (1)$$

maximum likelihood estimates (\rightarrow I/4.1.3) for the unknown parameters B and Σ are given by

$$\begin{aligned} \hat{B} &= (X^T V^{-1} X)^{-1} X^T V^{-1} Y \\ \hat{\Sigma} &= \frac{1}{n} (Y - X\hat{B})^T V^{-1} (Y - X\hat{B}) . \end{aligned} \quad (2)$$

Proof: In (1), Y is an $n \times v$ matrix of measurements (n observations, v dependent variables), X is an $n \times p$ design matrix (n observations, p independent variables) and V is an $n \times n$ covariance matrix across observations. This multivariate GLM implies the following likelihood function (\rightarrow I/5.1.2)

$$\begin{aligned}
p(Y|B, \Sigma) &= \mathcal{MN}(Y; XB, V, \Sigma) \\
&= \sqrt{\frac{1}{(2\pi)^{nv} |\Sigma|^n |V|^v}} \cdot \exp \left[-\frac{1}{2} \text{tr} (\Sigma^{-1} (Y - XB)^T V^{-1} (Y - XB)) \right]
\end{aligned} \tag{3}$$

and the log-likelihood function (\rightarrow I/4.1.2)

$$\begin{aligned}
\text{LL}(B, \Sigma) &= \log p(Y|B, \Sigma) \\
&= -\frac{nv}{2} \log(2\pi) - \frac{n}{2} \log |\Sigma| - \frac{v}{2} \log |V| \\
&\quad - \frac{1}{2} \text{tr} [\Sigma^{-1} (Y - XB)^T V^{-1} (Y - XB)] .
\end{aligned} \tag{4}$$

Substituting V^{-1} by the precision matrix P to ease notation, we have:

$$\begin{aligned}
\text{LL}(B, \Sigma) &= -\frac{nv}{2} \log(2\pi) - \frac{n}{2} \log |\Sigma| + \frac{v}{2} \log |P| \\
&\quad - \frac{1}{2} \text{tr} [\Sigma^{-1} (Y^T P Y - Y^T P X B - B^T X^T P Y + B^T X^T P X B)] .
\end{aligned} \tag{5}$$

The derivative of the log-likelihood function (5) with respect to B is

$$\begin{aligned}
\frac{d\text{LL}(B, \Sigma)}{dB} &= \frac{d}{dB} \left(-\frac{1}{2} \text{tr} [\Sigma^{-1} (Y^T P Y - Y^T P X B - B^T X^T P Y + B^T X^T P X B)] \right) \\
&= \frac{d}{dB} \left(-\frac{1}{2} \text{tr} [-2 \Sigma^{-1} Y^T P X B] \right) + \frac{d}{dB} \left(-\frac{1}{2} \text{tr} [\Sigma^{-1} B^T X^T P X B] \right) \\
&= -\frac{1}{2} (-2 X^T P Y \Sigma^{-1}) - \frac{1}{2} (X^T P X B \Sigma^{-1} + (X^T P X)^T B (\Sigma^{-1})^T) \\
&= X^T P Y \Sigma^{-1} - X^T P X B \Sigma^{-1}
\end{aligned} \tag{6}$$

and setting this derivative to zero gives the MLE for B :

$$\begin{aligned}
\frac{d\text{LL}(\hat{B}, \Sigma)}{dB} &= 0 \\
0 &= X^T P Y \Sigma^{-1} - X^T P X \hat{B} \Sigma^{-1} \\
0 &= X^T P Y - X^T P X \hat{B} \\
X^T P X \hat{B} &= X^T P Y \\
\hat{B} &= (X^T P X)^{-1} X^T P Y .
\end{aligned} \tag{7}$$

The derivative of the log-likelihood function (4) at \hat{B} with respect to Σ is

$$\begin{aligned}
\frac{d\text{LL}(\hat{B}, \Sigma)}{d\Sigma} &= \frac{d}{d\Sigma} \left(-\frac{n}{2} \log |\Sigma| - \frac{1}{2} \text{tr} [\Sigma^{-1} (Y - X \hat{B})^T V^{-1} (Y - X \hat{B})] \right) \\
&= -\frac{n}{2} (\Sigma^{-1})^T + \frac{1}{2} \left(\Sigma^{-1} (Y - X \hat{B})^T V^{-1} (Y - X \hat{B}) \Sigma^{-1} \right)^T \\
&= -\frac{n}{2} \Sigma^{-1} + \frac{1}{2} \Sigma^{-1} (Y - X \hat{B})^T V^{-1} (Y - X \hat{B}) \Sigma^{-1}
\end{aligned} \tag{8}$$

and setting this derivative to zero gives the MLE for Σ :

$$\begin{aligned}
 \frac{dLL(\hat{B}, \hat{\Sigma})}{d\Sigma} &= 0 \\
 0 &= -\frac{n}{2} \hat{\Sigma}^{-1} + \frac{1}{2} \hat{\Sigma}^{-1} (Y - X\hat{B})^T V^{-1} (Y - X\hat{B}) \hat{\Sigma}^{-1} \\
 \frac{n}{2} \hat{\Sigma}^{-1} &= \frac{1}{2} \hat{\Sigma}^{-1} (Y - X\hat{B})^T V^{-1} (Y - X\hat{B}) \hat{\Sigma}^{-1} \\
 \hat{\Sigma}^{-1} &= \frac{1}{n} \hat{\Sigma}^{-1} (Y - X\hat{B})^T V^{-1} (Y - X\hat{B}) \hat{\Sigma}^{-1} \\
 I_v &= \frac{1}{n} (Y - X\hat{B})^T V^{-1} (Y - X\hat{B}) \hat{\Sigma}^{-1} \\
 \hat{\Sigma} &= \frac{1}{n} (Y - X\hat{B})^T V^{-1} (Y - X\hat{B}) .
 \end{aligned} \tag{9}$$

Together, (7) and (9) constitute the MLE for the GLM. ■

Sources:

- Petersen, Kaare Brandt; Pedersen, Michael Syskind (2012): “Derivatives”; in: *The Matrix Cookbook*, Section 2, eqs. (100), (117), (57), (124); URL: <https://www2.imm.dtu.dk/pubdb/pubs/3274-full.html>.

2.2.5 Maximum log-likelihood

Theorem: Consider a general linear model (\rightarrow III/2.2.1) m with $n \times v$ data matrix Y , $n \times p$ design matrix X and $n \times n$ covariance across rows (\rightarrow III/2.2.1) V

$$m : Y = XB + E, \quad E \sim \mathcal{MN}(0, V, \Sigma) . \tag{1}$$

Then, the maximum log-likelihood (\rightarrow I/4.1.4) for this model is

$$\text{MLL}(m) = -\frac{nv}{2} \ln(2\pi) - \frac{n}{2} \ln |\hat{\Sigma}| - \frac{nv}{2} \tag{2}$$

under uncorrelated observations (\rightarrow III/2.2.1), i.e. if $V = I_n$, and

$$\text{MLL}(m) = -\frac{nv}{2} \ln(2\pi) - \frac{n}{2} \ln |\hat{\Sigma}| - \frac{v}{2} \ln |V| - \frac{nv}{2} , \tag{3}$$

in the general case, i.e. if $V \neq I_n$, where $\hat{\Sigma}$ is the maximum likelihood estimate (\rightarrow I/4.1.3) of the $v \times v$ covariance across columns (\rightarrow III/2.2.1).

Proof: The likelihood function (\rightarrow I/5.1.2) for the general linear model is given by (\rightarrow III/2.2.4)

$$\begin{aligned}
 p(Y|B, \Sigma) &= \mathcal{MN}(Y; XB, V, \Sigma) \\
 &= \sqrt{\frac{1}{(2\pi)^{nv} |\Sigma|^n |V|^v}} \cdot \exp \left[-\frac{1}{2} \text{tr} (\Sigma^{-1} (Y - XB)^T V^{-1} (Y - XB)) \right] ,
 \end{aligned} \tag{4}$$

such that the log-likelihood function (\rightarrow I/4.1.2) for this model becomes (\rightarrow III/2.2.4)

$$\begin{aligned} \text{LL}(B, \Sigma) &= \log p(Y|B, \Sigma) \\ &= -\frac{nv}{2} \log(2\pi) - \frac{n}{2} \log |\Sigma| - \frac{v}{2} \log |V| - \frac{1}{2} \text{tr} [\Sigma^{-1}(Y - XB)^T V^{-1}(Y - XB)] . \end{aligned} \quad (5)$$

The maximum likelihood estimate for the noise covariance (\rightarrow III/2.2.4) is

$$\hat{\Sigma} = \frac{1}{n}(Y - X\hat{B})^T V^{-1}(Y - X\hat{B}) \quad (6)$$

Plugging (6) into (5), we obtain the maximum log-likelihood (\rightarrow I/4.1.4) as

$$\begin{aligned} \text{MLL}(m) &= \text{LL}(\hat{B}, \hat{\Sigma}) \\ &= -\frac{nv}{2} \log(2\pi) - \frac{n}{2} \log |\hat{\Sigma}| - \frac{v}{2} \log |V| - \frac{1}{2} \text{tr} [\hat{\Sigma}^{-1}(Y - X\hat{B})^T V^{-1}(Y - X\hat{B})] \\ &= -\frac{nv}{2} \log(2\pi) - \frac{n}{2} \log |\hat{\Sigma}| - \frac{v}{2} \log |V| \\ &\quad - \frac{1}{2} \text{tr} \left[\left(\frac{1}{n}(Y - X\hat{B})^T V^{-1}(Y - X\hat{B}) \right)^{-1} (Y - X\hat{B})^T V^{-1}(Y - X\hat{B}) \right] \\ &= -\frac{nv}{2} \log(2\pi) - \frac{n}{2} \log |\hat{\Sigma}| - \frac{v}{2} \log |V| - \frac{n}{2} \text{tr} [I_v] \\ &= -\frac{nv}{2} \log(2\pi) - \frac{n}{2} \log |\hat{\Sigma}| - \frac{v}{2} \log |V| - \frac{nv}{2} \end{aligned} \quad (7)$$

which proves the result in (3). Assuming $V = I_n$, we have

$$\hat{\Sigma} = \frac{1}{n}(Y - X\hat{B})^T (Y - X\hat{B}) \quad (8)$$

and

$$\frac{v}{2} \log |V| = \frac{v}{2} \log |I_n| = \frac{v}{2} \log 1 = 0 , \quad (9)$$

such that

$$\text{MLL}(m) = -\frac{nv}{2} \ln(2\pi) - \frac{n}{2} \ln |\hat{\Sigma}| - \frac{nv}{2} \quad (10)$$

which proves the result in (2). This completes the proof. ■

2.2.6 Log-likelihood ratio

Theorem: Let $Y = [y_1, \dots, y_v]$ be an $n \times v$ data matrix (\rightarrow I/1.1.5) and consider two general linear models (\rightarrow III/2.2.1) with design matrices (\rightarrow III/2.2.1) X_1, X_2 and row-by-row covariance matrices (\rightarrow III/2.2.1) V_1, V_2 , entailing potentially different regression coefficients (\rightarrow III/2.2.1) B_1, B_2 and column-by-column covariance matrices (\rightarrow III/2.2.1) Σ_1, Σ_2 :

$$\begin{aligned} m_1 : Y &= X_1 B_1 + E_1, \quad E_1 \sim \mathcal{MN}(0, V_1, \Sigma_1) \\ m_2 : Y &= X_2 B_2 + E_2, \quad E_2 \sim \mathcal{MN}(0, V_2, \Sigma_2) . \end{aligned} \quad (1)$$

Then, if the models assume the same covariance matrix across observations, i.e. if $V_1 = V_2$, the log-likelihood ratio (\rightarrow I/4.1.7) for comparing m_1 vs. m_2 is given by

$$\ln \Lambda_{12} = \frac{n}{2} \ln \frac{|\hat{\Sigma}_2|}{|\hat{\Sigma}_1|} \quad (2)$$

where $\hat{\Sigma}_1$ and $\hat{\Sigma}_2$ are the maximum likelihood estimates (\rightarrow I/4.1.3) of Σ_1 and Σ_2 .

Proof: The likelihood ratio (\rightarrow I/4.1.6) between two models m_1 and m_2 with model parameters θ_1 and θ_2 and parameter spaces Θ_1 and Θ_2 is defined as the quotient of their maximized (\rightarrow I/4.1.3) likelihood functions (\rightarrow I/5.1.2):

$$\Lambda_{12} = \frac{\max_{\theta_1 \in \Theta_1} p(y|\theta_1, m_1)}{\max_{\theta_2 \in \Theta_2} p(y|\theta_2, m_2)} . \quad (3)$$

Thus, the log-likelihood ratio (\rightarrow I/4.1.7) is equal to the difference of the maximum log-likelihoods (\rightarrow I/4.1.4) of the two models:

$$\ln \Lambda_{12} = \ln p(y|\hat{\theta}_1, m_1) - \ln p(y|\hat{\theta}_2, m_2) . \quad (4)$$

The likelihood function (\rightarrow I/5.1.2) of the general linear model (\rightarrow III/2.2.1) is a matrix-normal probability density function (\rightarrow II/5.1.3):

$$\begin{aligned} p(Y|B, \Sigma) &= \mathcal{MN}(Y; XB, V, \Sigma) \\ &= \sqrt{\frac{1}{(2\pi)^{nv} |\Sigma|^n |V|^v}} \cdot \exp \left[-\frac{1}{2} \text{tr} (\Sigma^{-1} (Y - XB)^T V^{-1} (Y - XB)) \right] . \end{aligned} \quad (5)$$

Thus, the log-likelihood function (\rightarrow I/4.1.2) is equal to a logarithmized matrix-normal (\rightarrow II/5.1.1) density (\rightarrow I/1.7.1):

$$\begin{aligned} \ln p(Y|B, \Sigma) &= \ln \mathcal{MN}(Y; XB, V, \Sigma) \\ &= -\frac{nv}{2} \ln(2\pi) - \frac{n}{2} \ln |\Sigma| - \frac{v}{2} \ln |V| - \frac{1}{2} \text{tr} [\Sigma^{-1} (Y - XB)^T V^{-1} (Y - XB)] . \end{aligned} \quad (6)$$

The maximum likelihood estimates for the general linear model (\rightarrow III/2.2.4) are given by

$$\begin{aligned} \hat{B} &= (X^T V^{-1} X)^{-1} X^T V^{-1} Y \\ \hat{\Sigma} &= \frac{1}{n} (Y - X\hat{B})^T V^{-1} (Y - X\hat{B}) . \end{aligned} \quad (7)$$

such that the last term in the maximum log-likelihood function (6) becomes

$$\begin{aligned}
& \frac{1}{2} \operatorname{tr} \left[\hat{\Sigma}^{-1} (Y - X\hat{B})^T V^{-1} (Y - X\hat{B}) \right] \\
&= \frac{1}{2} \operatorname{tr} \left[\left(\frac{1}{n} (Y - X\hat{B})^T V^{-1} (Y - X\hat{B}) \right)^{-1} (Y - X\hat{B})^T V^{-1} (Y - X\hat{B}) \right] \\
&= \frac{1}{2} \operatorname{tr} \left[n \left((Y - X\hat{B})^T V^{-1} (Y - X\hat{B}) \right)^{-1} \left((Y - X\hat{B})^T V^{-1} (Y - X\hat{B}) \right) \right] \\
&= \frac{n}{2} \operatorname{tr} [I_v] \\
&= \frac{nv}{2} .
\end{aligned} \tag{8}$$

Thus, the maximum log-likelihood for the general linear model (\rightarrow III/2.2.5) is equal to

$$\ln p(Y|\hat{B}, \hat{\Sigma}) = -\frac{nv}{2} \ln(2\pi) - \frac{n}{2} \ln |\hat{\Sigma}| - \frac{v}{2} \ln |V| - \frac{nv}{2} . \tag{9}$$

Evaluating (9) for m_1 and m_2 and plugging into (4), we obtain:

$$\begin{aligned}
\ln \Lambda_{12} &= \ln p(Y|\hat{B}_1, \hat{\Sigma}_1, m_1) - \ln p(Y|\hat{B}_2, \hat{\Sigma}_2, m_2) \\
&= \left(-\frac{nv}{2} \ln(2\pi) - \frac{n}{2} \ln |\hat{\Sigma}_1| - \frac{v}{2} \ln |V_1| - \frac{nv}{2} \right) \\
&\quad - \left(-\frac{nv}{2} \ln(2\pi) - \frac{n}{2} \ln |\hat{\Sigma}_2| - \frac{v}{2} \ln |V_2| - \frac{nv}{2} \right) \\
&= -\frac{n}{2} \ln \frac{|\hat{\Sigma}_1|}{|\hat{\Sigma}_2|} - \frac{v}{2} \ln \frac{|V_1|}{|V_2|} .
\end{aligned} \tag{10}$$

Thus, if $V_1 = V_2$, such that $\ln(|V_2|/|V_1|) = \ln(1) = 0$, the log-likelihood ratio is equal to

$$\ln \Lambda_{12} = -\frac{n}{2} \ln \frac{|\hat{\Sigma}_1|}{|\hat{\Sigma}_2|} . \tag{11}$$

■

2.2.7 Mutual information

Theorem: Consider a general linear model (\rightarrow III/2.2.1) m_1 with $n \times v$ data matrix Y , $n \times p$ design matrix X and uncorrelated observations (\rightarrow III/2.2.1), i.e. $V = I_n$,

$$m_1 : Y = XB + E_1, \quad E_1 \sim \mathcal{MN}(0, I_n, \Sigma_1) , \tag{1}$$

as well as another model m_0 in which X has no influence on Y :

$$m_0 : Y = E_0, \quad E_0 \sim \mathcal{MN}(0, I_n, \Sigma_0) . \tag{2}$$

Then, the mutual information (\rightarrow I/2.4.1) of Y and X is equal to

$$I(X, Y) = -\frac{n}{2} \ln \frac{|\Sigma_1|}{|\Sigma_0|} . \tag{3}$$

Proof: The continuous mutual information can be written in terms of marginal and conditional differential entropy (\rightarrow I/2.4.2) as follows:

$$I(X, Y) = h(Y) - h(Y|X) . \quad (4)$$

The marginal distribution of Y , unconditional on X , is given by model m_0

$$Y \sim \mathcal{MN}(0, I_n, \Sigma_0) \quad (5)$$

and the conditional distribution of Y given X is given by model m_1

$$Y \sim \mathcal{MN}(XB, I_n, \Sigma_1) . \quad (6)$$

Since X is constant (\rightarrow I/1.2.5) and thus only has one possible value (\rightarrow I/1.1.2), the conditional differential entropy (\rightarrow I/2.2.7) of Y given X is obtained by simply entering X into the probability distribution (\rightarrow I/1.5.1) for which the differential entropy (\rightarrow I/2.2.7) is calculated:

$$\begin{aligned} h(Y|X) &= \int_{x \in \mathcal{X}} p(x) \cdot h(Y|x) \, dx \\ &= p(X) \cdot h(Y|X) \\ &= h[p(Y|X, B, \Sigma_1)] . \end{aligned} \quad (7)$$

The differential entropy of the matrix-normal distribution (\rightarrow II/5.1.6) is

$$\begin{aligned} X &\sim \mathcal{MN}(M, U, V) \quad \text{where} \quad X \in \mathbb{R}^{n \times p} \\ \Rightarrow \quad h(X) &= \frac{np}{2} \ln(2\pi) + \frac{n}{2} \ln |V| + \frac{p}{2} \ln |U| + \frac{np}{2} , \end{aligned} \quad (8)$$

such that the mutual information of Y and X becomes

$$\begin{aligned} I(X, Y) &= h[p(Y|\Sigma_0)] - h[p(Y|X, B, \Sigma_1)] \\ &= h[\mathcal{MN}(0, I_n, \Sigma_0)] - h[\mathcal{MN}(XB, I_n, \Sigma_1)] \\ &= \left(\frac{nv}{2} \ln(2\pi) + \frac{n}{2} \ln |\Sigma_0| + \frac{v}{2} \ln |I_n| + \frac{nv}{2} \right) \\ &\quad - \left(\frac{nv}{2} \ln(2\pi) + \frac{n}{2} \ln |\Sigma_1| + \frac{v}{2} \ln |I_n| + \frac{nv}{2} \right) \\ &= \frac{n}{2} \ln |\Sigma_0| - \frac{n}{2} \ln |\Sigma_1| \\ &= \frac{n}{2} \ln \frac{|\Sigma_0|}{|\Sigma_1|} \\ &= -\frac{n}{2} \ln \frac{|\Sigma_1|}{|\Sigma_0|} . \end{aligned} \quad (9)$$

■

2.2.8 Log-likelihood ratio and estimated mutual information

Theorem: Consider a general linear model (\rightarrow III/2.2.1) m_1 with $n \times v$ data matrix Y , $n \times p$ design matrix X and uncorrelated observations (\rightarrow III/2.2.1), i.e. $V = I_n$,

$$m_1 : Y = XB + E_1, \quad E_1 \sim \mathcal{MN}(0, I_n, \Sigma_1), \quad (1)$$

as well as another model m_0 in which X has no influence on Y :

$$m_0 : Y = E_0, \quad E_0 \sim \mathcal{MN}(0, I_n, \Sigma_0). \quad (2)$$

Then, the log-likelihood ratio (\rightarrow I/4.1.7) of m_1 vs. m_0 is equal to the estimated (\rightarrow I/3.1.1) mutual information (\rightarrow I/2.4.1) of X and Y :

$$\ln \Lambda_{10} = \hat{I}(X, Y). \quad (3)$$

Proof: The maximum likelihood estimates for a general linear model (\rightarrow III/2.2.4) are

$$\begin{aligned} \hat{B} &= (X^T V^{-1} X)^{-1} X^T V^{-1} Y \\ \hat{\Sigma} &= \frac{1}{n} (Y - X \hat{B})^T V^{-1} (Y - X \hat{B}), \end{aligned} \quad (4)$$

such that, for the two models, the maximum likelihood estimates (\rightarrow I/4.1.3) are:

$$\begin{aligned} \hat{\Sigma}_1 &= \frac{1}{n} (Y - X \hat{B})^T (Y - X \hat{B}) \quad \text{with} \quad \hat{B} = (X^T X)^{-1} X^T Y \quad \text{and} \\ \hat{\Sigma}_0 &= \frac{1}{n} Y^T Y. \end{aligned} \quad (5)$$

The log-likelihood ratio for two general linear models (\rightarrow III/2.2.6) is

$$\ln \Lambda_{12} = -\frac{n}{2} \ln \frac{|\hat{\Sigma}_1|}{|\hat{\Sigma}_2|}, \quad (6)$$

such that in the present case, we have:

$$\ln \Lambda_{10} = -\frac{n}{2} \ln \frac{|\hat{\Sigma}_1|}{|\hat{\Sigma}_0|}. \quad (7)$$

The mutual information for the general linear model (\rightarrow III/2.2.7) is

$$I(X, Y) = -\frac{n}{2} \ln \frac{|\Sigma_1|}{|\Sigma_0|}, \quad (8)$$

such that with (5), the estimated mutual information is:

$$\hat{I}(X, Y) = -\frac{n}{2} \ln \frac{|\hat{\Sigma}_1|}{|\hat{\Sigma}_0|}, \quad (9)$$

Together, (7) and (9) show that

$$\ln \Lambda_{10} = \hat{I}(X, Y). \quad (10)$$

**Sources:**

- Friston K, Chu C, Mourão-Miranda J, Hulme O, Rees G, Penny W, Ashburner J (2008): “Bayesian decoding of brain images”; in: *NeuroImage*, vol. 39, pp. 181-205, eq. 6; URL: <https://www.sciencedirect.com/science/article/abs/pii/S1053811907007203>; DOI: 10.1016/j.neuroimage.2007.08.013.

2.3 Transformed general linear model**2.3.1 Definition**

Definition: Let there be two general linear models (\rightarrow III/2.2.1) of measured data $Y \in \mathbb{R}^{n \times v}$ using design matrices (\rightarrow III/2.2.1) $X \in \mathbb{R}^{n \times p}$ and $X_t \in \mathbb{R}^{n \times t}$

$$Y = XB + E, \quad E \sim \mathcal{MN}(0, V, \Sigma) \quad (1)$$

$$Y = X_t \Gamma + E_t, \quad E_t \sim \mathcal{MN}(0, V, \Sigma_t) \quad (2)$$

and assume that X_t can be transformed into X using a transformation matrix $T \in \mathbb{R}^{t \times p}$

$$X = X_t T \quad (3)$$

where $p < t$ and X , X_t and T have full ranks $\text{rk}(X) = p$, $\text{rk}(X_t) = t$ and $\text{rk}(T) = p$.

Then, a linear model (\rightarrow III/2.2.1) of the parameter estimates from (2), under the assumption of (1), is called a transformed general linear model.

Sources:

- Soch J, Allefeld C, Haynes JD (2020): “Inverse transformed encoding models – a solution to the problem of correlated trial-by-trial parameter estimates in fMRI decoding”; in: *NeuroImage*, vol. 209, art. 116449, Appendix A; URL: <https://www.sciencedirect.com/science/article/pii/S1053811919310407>; DOI: 10.1016/j.neuroimage.2019.116449.

2.3.2 Derivation of the distribution

Theorem: Let there be two general linear models (\rightarrow III/2.2.1) of measured data Y

$$Y = XB + E, \quad E \sim \mathcal{MN}(0, V, \Sigma) \quad (1)$$

$$Y = X_t \Gamma + E_t, \quad E_t \sim \mathcal{MN}(0, V, \Sigma_t) \quad (2)$$

and a matrix T transforming X_t into X :

$$X = X_t T. \quad (3)$$

Then, the transformed general linear model (\rightarrow III/2.3.1) is given by

$$\hat{\Gamma} = TB + H, \quad H \sim \mathcal{MN}(0, U, \Sigma) \quad (4)$$

where the covariance across rows (\rightarrow II/5.1.1) is $U = (X_t^T V^{-1} X_t)^{-1}$.

Proof: The linear transformation theorem for the matrix-normal distribution (\rightarrow II/5.1.9) states:

$$X \sim \mathcal{MN}(M, U, V) \Rightarrow Y = AXB + C \sim \mathcal{MN}(AMB + C, AUA^T, B^TVB) . \quad (5)$$

The weighted least squares parameter estimates (\rightarrow III/2.2.3) for (2) are given by

$$\hat{\Gamma} = (X_t^T V^{-1} X_t)^{-1} X_t^T V^{-1} Y . \quad (6)$$

Using (1) and (5), the distribution of Y is

$$Y \sim \mathcal{MN}(XB, V, \Sigma) \quad (7)$$

Combining (6) with (7), the distribution of $\hat{\Gamma}$ is

$$\begin{aligned} \hat{\Gamma} &\sim \mathcal{MN} \left([(X_t^T V^{-1} X_t)^{-1} X_t^T V^{-1}] XB, [(X_t^T V^{-1} X_t)^{-1} X_t^T V^{-1}] V [V^{-1} X_t (X_t^T V^{-1} X_t)^{-1}] , \Sigma \right) \\ &\sim \mathcal{MN} \left((X_t^T V^{-1} X_t)^{-1} X_t^T V^{-1} X_t TB, (X_t^T V^{-1} X_t)^{-1} X_t^T V^{-1} X_t (X_t^T V^{-1} X_t)^{-1}, \Sigma \right) \\ &\sim \mathcal{MN} \left(TB, (X_t^T V^{-1} X_t)^{-1}, \Sigma \right) . \end{aligned} \quad (8)$$

This can also be written as

$$\hat{\Gamma} = TB + H, \quad H \sim \mathcal{MN}(0, (X_t^T V^{-1} X_t)^{-1}, \Sigma) \quad (9)$$

which is equivalent to (4). ■

Sources:

- Soch J, Allefeld C, Haynes JD (2020): “Inverse transformed encoding models – a solution to the problem of correlated trial-by-trial parameter estimates in fMRI decoding”; in: *NeuroImage*, vol. 209, art. 116449, Appendix A, Theorem 1; URL: <https://www.sciencedirect.com/science/article/pii/S1053811919310407>; DOI: 10.1016/j.neuroimage.2019.116449.

2.3.3 Equivalence of parameter estimates

Theorem: Let there be a general linear model (\rightarrow III/2.2.1)

$$Y = XB + E, \quad E \sim \mathcal{MN}(0, V, \Sigma) \quad (1)$$

and the transformed general linear model (\rightarrow III/2.3.1)

$$\hat{\Gamma} = TB + H, \quad H \sim \mathcal{MN}(0, U, \Sigma) \quad (2)$$

which are linked to each other (\rightarrow III/2.3.2) via

$$\hat{\Gamma} = (X_t^T V^{-1} X_t)^{-1} X_t^T V^{-1} Y \quad (3)$$

and

$$X = X_t T . \quad (4)$$

Then, the parameter estimates for B from (1) and (2) are equivalent.

Proof: The weighted least squares parameter estimates (\rightarrow III/2.2.3) for (1) are given by

$$\hat{B} = (X^T V^{-1} X)^{-1} X^T V^{-1} Y \quad (5)$$

and the weighted least squares parameter estimates (\rightarrow III/2.2.3) for (2) are given by

$$\hat{B} = (T^T U^{-1} T)^{-1} T^T U^{-1} \hat{\Gamma} . \quad (6)$$

The covariance across rows for the transformed general linear model (\rightarrow III/2.3.2) is equal to

$$U = (X_t^T V^{-1} X_t)^{-1} . \quad (7)$$

Applying (7), (4) and (3), the estimates in (6) can be developed into

$$\begin{aligned} \hat{B} &\stackrel{(6)}{=} (T^T U^{-1} T)^{-1} T^T U^{-1} \hat{\Gamma} \\ &\stackrel{(7)}{=} (T^T [X_t^T V^{-1} X_t] T)^{-1} T^T [X_t^T V^{-1} X_t] \hat{\Gamma} \\ &\stackrel{(4)}{=} (X^T V^{-1} X)^{-1} T^T X_t^T V^{-1} X_t \hat{\Gamma} \\ &\stackrel{(3)}{=} (X^T V^{-1} X)^{-1} T^T X_t^T V^{-1} X_t [(X_t^T V^{-1} X_t)^{-1} X_t^T V^{-1} Y] \\ &= (X^T V^{-1} X)^{-1} T^T X_t^T V^{-1} Y \\ &\stackrel{(4)}{=} (X^T V^{-1} X)^{-1} X^T V^{-1} Y \end{aligned} \quad (8)$$

which is equivalent to the estimates in (5). ■

Sources:

- Soch J, Allefeld C, Haynes JD (2020): “Inverse transformed encoding models – a solution to the problem of correlated trial-by-trial parameter estimates in fMRI decoding”; in: *NeuroImage*, vol. 209, art. 116449, Appendix A, Theorem 2; URL: <https://www.sciencedirect.com/science/article/pii/S1053811919310407>; DOI: 10.1016/j.neuroimage.2019.116449.

2.4 Inverse general linear model

2.4.1 Definition

Definition: Let there be a general linear model (\rightarrow III/2.2.1) of measured data $Y \in \mathbb{R}^{n \times v}$ in terms of the design matrix (\rightarrow III/2.2.1) $X \in \mathbb{R}^{n \times p}$:

$$Y = XB + E, \quad E \sim \mathcal{MN}(0, V, \Sigma) . \quad (1)$$

Then, a linear model (\rightarrow III/2.2.1) of X in terms of Y , under the assumption of (1), is called an inverse general linear model.

Sources:

- Soch J, Allefeld C, Haynes JD (2020): “Inverse transformed encoding models – a solution to the problem of correlated trial-by-trial parameter estimates in fMRI decoding”; in: *NeuroImage*, vol. 209, art. 116449, Appendix C; URL: <https://www.sciencedirect.com/science/article/pii/S1053811919310407>; DOI: 10.1016/j.neuroimage.2019.116449.

2.4.2 Derivation of the distribution

Theorem: Let there be a general linear model (\rightarrow III/2.2.1) of $Y \in \mathbb{R}^{n \times v}$

$$Y = XB + E, \quad E \sim \mathcal{MN}(0, V, \Sigma) . \quad (1)$$

Then, the inverse general linear model (\rightarrow III/2.4.1) of $X \in \mathbb{R}^{n \times p}$ is given by

$$X = YW + N, \quad N \sim \mathcal{MN}(0, V, \Sigma_x) \quad (2)$$

where $W \in \mathbb{R}^{v \times p}$ is a matrix, such that $BW = I_p$, and the covariance across columns (\rightarrow II/5.1.1) is $\Sigma_x = W^T \Sigma W$.

Proof: The linear transformation theorem for the matrix-normal distribution (\rightarrow II/5.1.9) states:

$$X \sim \mathcal{MN}(M, U, V) \quad \Rightarrow \quad Y = AXB + C \sim \mathcal{MN}(AMB + C, AU A^T, B^T V B) . \quad (3)$$

The matrix W exists, if the rows of $B \in \mathbb{R}^{p \times v}$ are linearly independent, such that $\text{rk}(B) = p$. Then, right-multiplying the model (1) with W and applying (3) yields

$$YW = XBW + EW, \quad EW \sim \mathcal{MN}(0, V, W^T \Sigma W) . \quad (4)$$

Employing $BW = I_p$ and rearranging, we have

$$X = YW - EW, \quad EW \sim \mathcal{MN}(0, V, W^T \Sigma W) . \quad (5)$$

Substituting $N = -EW$, we get

$$X = YW + N, \quad N \sim \mathcal{MN}(0, V, W^T \Sigma W) \quad (6)$$

which is equivalent to (2). ■

Sources:

- Soch J, Allefeld C, Haynes JD (2020): “Inverse transformed encoding models – a solution to the problem of correlated trial-by-trial parameter estimates in fMRI decoding”; in: *NeuroImage*, vol. 209, art. 116449, Appendix C, Theorem 4; URL: <https://www.sciencedirect.com/science/article/pii/S1053811919310407>; DOI: 10.1016/j.neuroimage.2019.116449.

2.4.3 Best linear unbiased estimator

Theorem: Let there be a general linear model (\rightarrow III/2.2.1) of $Y \in \mathbb{R}^{n \times v}$

$$Y = XB + E, \quad E \sim \mathcal{MN}(0, V, \Sigma) \quad (1)$$

implying the inverse general linear model (\rightarrow III/2.4.2) of $X \in \mathbb{R}^{n \times p}$

$$X = YW + N, \quad N \sim \mathcal{MN}(0, V, \Sigma_x) . \quad (2)$$

where

$$BW = I_p \quad \text{and} \quad \Sigma_x = W^T \Sigma W . \quad (3)$$

Then, the weighted least squares solution (\rightarrow III/2.2.3) for W is the best linear unbiased estimator of W .

Proof: The linear transformation theorem for the matrix-normal distribution (\rightarrow II/5.1.9) states:

$$X \sim \mathcal{MN}(M, U, V) \Rightarrow Y = AXB + C \sim \mathcal{MN}(AMB + C, AU A^T, B^T V B). \quad (4)$$

The weighted least squares parameter estimates (\rightarrow III/2.2.3) for (2) are given by

$$\hat{W} = (Y^T V^{-1} Y)^{-1} Y^T V^{-1} X. \quad (5)$$

The best linear unbiased estimator $\hat{\theta}$ of a certain quantity θ estimated from measured data (\rightarrow I/1.1.5) y is 1) an estimator resulting from a linear operation $f(y)$, 2) whose expected value is equal to θ and 3) which has, among those satisfying 1) and 2), the minimum variance (\rightarrow I/1.13.1).

1) First, \hat{W} is a linear estimator, because it is of the form $\tilde{W} = MX$ where M is an arbitrary $v \times n$ matrix.

2) Second, \hat{W} is an unbiased estimator, if $\langle \hat{W} \rangle = W$. By applying (4) to (2), the distribution of \tilde{W} is

$$\tilde{W} = MX \sim \mathcal{MN}(MYW, MVM^T, \Sigma_x) \quad (6)$$

which requires (\rightarrow II/5.1.4) that $MY = I_v$. This is fulfilled by any matrix

$$M = (Y^T V^{-1} Y)^{-1} Y^T V^{-1} + D \quad (7)$$

where D is a $v \times n$ matrix which satisfies $DY = 0$.

3) Third, the best linear unbiased estimator is the one with minimum variance (\rightarrow I/1.13.1), i.e. the one that minimizes the expected Frobenius norm

$$\text{Var}(\tilde{W}) = \left\langle \text{tr} \left[(\tilde{W} - W)^T (\tilde{W} - W) \right] \right\rangle. \quad (8)$$

Using the matrix-normal distribution (\rightarrow II/5.1.1) of \tilde{W} from (6)

$$(\tilde{W} - W) \sim \mathcal{MN}(0, MVM^T, \Sigma_x) \quad (9)$$

and the property of the Wishart distribution (\rightarrow II/5.2.1)

$$X \sim \mathcal{MN}(0, U, V) \Rightarrow \langle XX^T \rangle = \text{tr}(V) U, \quad (10)$$

this variance (\rightarrow I/1.13.1) can be evaluated as a function of M :

$$\begin{aligned} \text{Var}[\tilde{W}(M)] &\stackrel{(8)}{=} \left\langle \text{tr} \left[(\tilde{W} - W)^T (\tilde{W} - W) \right] \right\rangle \\ &= \left\langle \text{tr} \left[(\tilde{W} - W)(\tilde{W} - W)^T \right] \right\rangle \\ &= \text{tr} \left[\left\langle (\tilde{W} - W)(\tilde{W} - W)^T \right\rangle \right] \\ &\stackrel{(10)}{=} \text{tr} [\text{tr}(\Sigma_x) MVM^T] \\ &= \text{tr}(\Sigma_x) \text{tr}(MVM^T). \end{aligned} \quad (11)$$

As a function of D and using $DY = 0$, it becomes:

$$\begin{aligned}
 \text{Var} \left[\tilde{W}(D) \right] &\stackrel{(7)}{=} \text{tr}(\Sigma_x) \text{tr} \left[\left((Y^T V^{-1} Y)^{-1} Y^T V^{-1} + D \right) V \left((Y^T V^{-1} Y)^{-1} Y^T V^{-1} + D \right)^T \right] \\
 &= \text{tr}(\Sigma_x) \text{tr} \left[(Y^T V^{-1} Y)^{-1} Y^T V^{-1} V V^{-1} Y (Y^T V^{-1} Y)^{-1} + \right. \\
 &\quad \left. (Y^T V^{-1} Y)^{-1} Y^T V^{-1} V D^T + D V V^{-1} Y (Y^T V^{-1} Y)^{-1} + D V D^T \right] \\
 &= \text{tr}(\Sigma_x) \left[\text{tr}((Y^T V^{-1} Y)^{-1}) + \text{tr}(D V D^T) \right].
 \end{aligned} \tag{12}$$

Since $D V D^T$ is a positive-semidefinite matrix, all its eigenvalues are non-negative. Because the trace of a square matrix is the sum of its eigenvalues, the minimum variance is achieved by $D = 0$, thus producing \hat{W} as in (5). ■

Sources:

- Soch J, Allefeld C, Haynes JD (2020): “Inverse transformed encoding models – a solution to the problem of correlated trial-by-trial parameter estimates in fMRI decoding”; in: *NeuroImage*, vol. 209, art. 116449, Appendix C, Theorem 5; URL: <https://www.sciencedirect.com/science/article/pii/S1053811919310407>; DOI: 10.1016/j.neuroimage.2019.116449.

2.4.4 Equivalence of log-likelihood ratios

Theorem: Consider two general linear models (\rightarrow III/2.2.1)

$$\begin{aligned}
 m_1^{(Y)} : Y &= X B + E_1, \quad E_1 \sim \mathcal{MN}(0, I_n, \Sigma_1^{(Y)}) \\
 m_0^{(Y)} : Y &= E_0, \quad E_0 \sim \mathcal{MN}(0, I_n, \Sigma_0^{(Y)})
 \end{aligned} \tag{1}$$

and two inverse general linear models (\rightarrow III/2.4.1)

$$\begin{aligned}
 m_1^{(X)} : X &= Y W + N_1, \quad N_1 \sim \mathcal{MN}(0, I_n, \Sigma_1^{(X)}) \\
 m_0^{(X)} : X &= N_0, \quad N_0 \sim \mathcal{MN}(0, I_n, \Sigma_0^{(X)})
 \end{aligned} \tag{2}$$

where $Y \in \mathbb{R}^{n \times v}$ and $X \in \mathbb{R}^{n \times p}$ are data matrices, such that $n > v$ and $n > p$. Then, the log-likelihood ratio (\rightarrow I/4.1.7) comparing the forward models (\rightarrow III/2.2.1) is equivalent to the log-likelihood ratio (\rightarrow I/4.1.7) comparing the backward models (\rightarrow III/2.4.1):

$$\ln \Lambda_{10}^{(Y)} = \ln \Lambda_{10}^{(X)}. \tag{3}$$

Proof: The maximum likelihood estimates for the general linear models (\rightarrow III/2.2.4) are

$$\begin{aligned}
 \hat{\Sigma}_1^{(Y)} &= \frac{1}{n} (Y - X \hat{B})^T (Y - X \hat{B}) \quad \text{with} \quad \hat{B} = (X^T X)^{-1} X^T Y \quad \text{and} \\
 \hat{\Sigma}_0^{(Y)} &= \frac{1}{n} Y^T Y
 \end{aligned} \tag{4}$$

as well as

$$\begin{aligned}\hat{\Sigma}_1^{(X)} &= \frac{1}{n}(X - Y\hat{W})^T(X - Y\hat{W}) \quad \text{with} \quad \hat{W} = (Y^T Y)^{-1}Y^T X \quad \text{and} \\ \hat{\Sigma}_0^{(X)} &= \frac{1}{n}X^T X.\end{aligned}\tag{5}$$

The likelihood ratio for two general linear models (\rightarrow III/2.2.6) m_1 and m_2 is:

$$\begin{aligned}\ln \Lambda_{12} &= -\frac{n}{2} \ln \frac{|\hat{\Sigma}_1|}{|\hat{\Sigma}_2|} \\ &= -\frac{n}{2} \ln \left(|\hat{\Sigma}_2^{-1}| |\hat{\Sigma}_1| \right) \\ &= -\frac{n}{2} \ln |\hat{\Sigma}_2^{-1} \hat{\Sigma}_1|.\end{aligned}\tag{6}$$

Thus, with (4), the log-likelihood ratio (\rightarrow I/4.1.7) of $m_1^{(Y)}$ vs. $m_0^{(Y)}$ is given as

$$\begin{aligned}\ln \Lambda_Y &= \ln \Lambda_{10}^{(Y)} \stackrel{(6)}{=} -\frac{n}{2} \ln \left| \left(\hat{\Sigma}_0^{(Y)} \right)^{-1} \hat{\Sigma}_1^{(Y)} \right| \\ &\stackrel{(4)}{=} -\frac{n}{2} \ln \left| \left(\frac{1}{n} Y^T Y \right)^{-1} \frac{1}{n} (Y - X\hat{B})^T (Y - X\hat{B}) \right| \\ &= -\frac{n}{2} \ln \left| (Y^T Y)^{-1} \left(Y^T Y - 2Y^T X\hat{B} + \hat{B}^T X^T X\hat{B} \right) \right| \\ &= -\frac{n}{2} \ln \left| \left((Y^T Y)^{-1} Y^T Y - 2(Y^T Y)^{-1} Y^T X\hat{B} + (Y^T Y)^{-1} \hat{B}^T X^T X\hat{B} \right) \right| \\ &\stackrel{(4)}{=} -\frac{n}{2} \ln \left| I_v - 2\hat{W}\hat{B} + (Y^T Y)^{-1} Y^T X (X^T X)^{-1} X^T X (X^T X)^{-1} X^T Y \right| \\ &= -\frac{n}{2} \ln \left| I_v - 2\hat{W}\hat{B} + (Y^T Y)^{-1} Y^T X (X^T X)^{-1} X^T Y \right| \\ &= -\frac{n}{2} \ln \left| I_v - 2\hat{W}\hat{B} + \hat{W}\hat{B} \right| \\ &= -\frac{n}{2} \ln \left| I_v - \hat{W}\hat{B} \right|.\end{aligned}\tag{7}$$

Similarly, with (5), the log-likelihood ratio (\rightarrow I/4.1.7) of $m_1^{(X)}$ vs. $m_0^{(X)}$ becomes

$$\begin{aligned}
\ln \Lambda_X &= \ln \Lambda_{10}^{(X)} \stackrel{(6)}{=} -\frac{n}{2} \ln \left| \left(\hat{\Sigma}_0^{(X)} \right)^{-1} \hat{\Sigma}_1^{(X)} \right| \\
&\stackrel{(5)}{=} -\frac{n}{2} \ln \left| \left(\frac{1}{n} X^T X \right)^{-1} \frac{1}{n} (X - Y\hat{W})^T (X - Y\hat{W}) \right| \\
&= -\frac{n}{2} \ln \left| (X^T X)^{-1} \left(X^T X - 2X^T Y\hat{W} + \hat{W}^T Y^T Y \hat{W} \right) \right| \\
&= -\frac{n}{2} \ln \left| \left((X^T X)^{-1} X^T X - 2(X^T X)^{-1} X^T Y\hat{W} + (X^T X)^{-1} \hat{W}^T Y^T Y \hat{W} \right) \right| \quad (8) \\
&\stackrel{(5)}{=} -\frac{n}{2} \ln \left| I_p - 2\hat{B}\hat{W} + (X^T X)^{-1} X^T Y (Y^T Y)^{-1} Y^T Y (Y^T Y)^{-1} Y^T X \right| \\
&= -\frac{n}{2} \ln \left| I_p - 2\hat{B}\hat{W} + (X^T X)^{-1} X^T Y (Y^T Y)^{-1} Y^T X \right| \\
&= -\frac{n}{2} \ln \left| I_p - 2\hat{B}\hat{W} + \hat{B}\hat{W} \right| \\
&= -\frac{n}{2} \ln \left| I_p - \hat{B}\hat{W} \right|.
\end{aligned}$$

Sylvester's determinant theorem (also known as the “Weinstein–Aronszajn identity”) states that, for two matrices $A \in \mathbb{R}^{m \times n}$ and $B \in \mathbb{R}^{n \times m}$, the following identity holds:

$$|I_m + AB| = |I_n + BA|. \quad (9)$$

Since $\hat{B} \in \mathbb{R}^{p \times v}$ and $(-\hat{W}) \in \mathbb{R}^{v \times p}$, it follows that

$$|I_p - \hat{B}\hat{W}| = |I_v - \hat{W}\hat{B}| \quad (10)$$

and thus, we finally have:

$$\ln \Lambda_Y = -\frac{n}{2} \ln |I_v - \hat{W}\hat{B}| = -\frac{n}{2} \ln |I_p - \hat{B}\hat{W}| = \ln \Lambda_X. \quad (11)$$

■

Sources:

- Friston K, Chu C, Mourão-Miranda J, Hulme O, Rees G, Penny W, Ashburner J (2008): “Bayesian decoding of brain images”; in: *NeuroImage*, vol. 39, pp. 181-205, p. 183; URL: <https://www.sciencedirect.com/science/article/abs/pii/S1053811907007203>; DOI: 10.1016/j.neuroimage.2007.08.013.
- Wikipedia (2024): “Weinstein–Aronszajn identity”; in: *Wikipedia, the free encyclopedia*, retrieved on 2024-06-28; URL: https://en.wikipedia.org/wiki/Weinstein%E2%80%93Aronszajn_identity.

2.4.5 Corresponding forward model

Definition: Let there be observations (\rightarrow I/1.1.5) $Y \in \mathbb{R}^{n \times v}$ and $X \in \mathbb{R}^{n \times p}$ and consider a weight matrix $W = f(Y, X) \in \mathbb{R}^{v \times p}$ estimated (\rightarrow I/3.1.1) from Y and X , such that right-multiplying Y with the weight matrix gives an estimate (\rightarrow I/3.1.1) or prediction of X :

$$\hat{X} = YW. \quad (1)$$

Given that the columns of \hat{X} are linearly independent, then

$$Y = \hat{X}A^T + E \quad \text{with} \quad \hat{X}^T E = 0 \quad (2)$$

is called the corresponding forward model relative to the weight matrix W .

Sources:

- Haufe S, Meinecke F, Gorgen K, Dhne S, Haynes JD, Blankertz B, Biemann F (2014): “On the interpretation of weight vectors of linear models in multivariate neuroimaging”; in: *NeuroImage*, vol. 87, pp. 96–110, eq. 3; URL: <https://www.sciencedirect.com/science/article/pii/S1053811913010914>; DOI: 10.1016/j.neuroimage.2013.10.067.

2.4.6 Derivation of parameters

Theorem: Let there be observations (\rightarrow I/1.1.5) $Y \in \mathbb{R}^{n \times v}$ and $X \in \mathbb{R}^{n \times p}$ and consider a weight matrix $W = f(Y, X) \in \mathbb{R}^{v \times p}$ predicting X from Y :

$$\hat{X} = YW . \quad (1)$$

Then, the parameter matrix of the corresponding forward model (\rightarrow III/2.4.5) is equal to

$$A = \Sigma_y W \Sigma_x^{-1} \quad (2)$$

with the “sample covariances (\rightarrow I/1.15.2)”

$$\begin{aligned} \Sigma_x &= \hat{X}^T \hat{X} \\ \Sigma_y &= Y^T Y . \end{aligned} \quad (3)$$

Proof: The corresponding forward model (\rightarrow III/2.4.5) is given by

$$Y = \hat{X} A^T + E , \quad (4)$$

subject to the constraint that predicted X and errors E are uncorrelated (\rightarrow I/1.17.1):

$$\hat{X}^T E = 0 . \quad (5)$$

With that, we can directly derive the parameter matrix A :

$$\begin{aligned} Y &\stackrel{(4)}{=} \hat{X} A^T + E \\ \hat{X} A^T &= Y - E \\ \hat{X}^T \hat{X} A^T &= \hat{X}^T (Y - E) \\ \hat{X}^T \hat{X} A^T &= \hat{X}^T Y - \hat{X}^T E \\ \hat{X}^T \hat{X} A^T &\stackrel{(5)}{=} \hat{X}^T Y \\ \hat{X}^T \hat{X} A^T &\stackrel{(1)}{=} W^T Y^T Y \\ \Sigma_x A^T &\stackrel{(3)}{=} W^T \Sigma_y \\ A^T &= \Sigma_x^{-1} W^T \Sigma_y \\ A &= \Sigma_y W \Sigma_x^{-1} . \end{aligned} \quad (6)$$

■

Sources:

- Haufe S, Meinecke F, Görgen K, Dähne S, Haynes JD, Blankertz B, Bießmann F (2014): “On the interpretation of weight vectors of linear models in multivariate neuroimaging”; in: *NeuroImage*, vol. 87, pp. 96–110, Theorem 1; URL: <https://www.sciencedirect.com/science/article/pii/S1053811913010914>; DOI: 10.1016/j.neuroimage.2013.10.067.

2.4.7 Proof of existence

Theorem: Let there be observations (\rightarrow I/1.1.5) $Y \in \mathbb{R}^{n \times v}$ and $X \in \mathbb{R}^{n \times p}$ and consider a weight matrix $W = f(Y, X) \in \mathbb{R}^{v \times p}$ predicting X from Y :

$$\hat{X} = YW . \quad (1)$$

Then, there exists a corresponding forward model (\rightarrow III/2.4.5).

Proof: The corresponding forward model (\rightarrow III/2.4.5) is defined as

$$Y = \hat{X}A^T + E \quad \text{with} \quad \hat{X}^T E = 0 \quad (2)$$

and the parameters of the corresponding forward model (\rightarrow III/2.4.6) are equal to

$$A = \Sigma_y W \Sigma_x^{-1} \quad \text{where} \quad \Sigma_x = \hat{X}^T \hat{X} \quad \text{and} \quad \Sigma_y = Y^T Y . \quad (3)$$

1) Because the columns of \hat{X} are assumed to be linearly independent by definition of the corresponding forward model (\rightarrow III/2.4.5), the matrix $\Sigma_x = \hat{X}^T \hat{X}$ is invertible, such that A in (3) is well-defined.

2) Moreover, the solution for the matrix A satisfies the constraint of the corresponding forward model (\rightarrow III/2.4.5) for predicted X and errors E to be uncorrelated (\rightarrow I/1.17.1) which can be shown as follows:

$$\begin{aligned} \hat{X}^T E &\stackrel{(2)}{=} \hat{X}^T (Y - \hat{X}A^T) \\ &\stackrel{(3)}{=} \hat{X}^T (Y - \hat{X} \Sigma_x^{-1} W^T \Sigma_y) \\ &= \hat{X}^T Y - \hat{X}^T \hat{X} \Sigma_x^{-1} W^T \Sigma_y \\ &\stackrel{(3)}{=} \hat{X}^T Y - \hat{X}^T \hat{X} (\hat{X}^T \hat{X})^{-1} W^T (Y^T Y) \\ &\stackrel{(1)}{=} (YW)^T Y - W^T (Y^T Y) \\ &= W^T Y^T Y - W^T Y^T Y \\ &= 0 . \end{aligned} \quad (4)$$

This completes the proof. ■

Sources:

- Haufe S, Meinecke F, Görgen K, Dähne S, Haynes JD, Blankertz B, Bießmann F (2014): “On the interpretation of weight vectors of linear models in multivariate neuroimaging”; in: *NeuroImage*, vol. 87, pp. 96–110, Appendix B; URL: <https://www.sciencedirect.com/science/article/pii/S1053811913010914>; DOI: 10.1016/j.neuroimage.2013.10.067.

2.5 Multivariate Bayesian linear regression

2.5.1 Conjugate prior distribution

Theorem: Let

$$Y = XB + E, \quad E \sim \mathcal{MN}(0, V, \Sigma) \quad (1)$$

be a general linear model (\rightarrow III/2.2.1) with measured $n \times v$ data matrix Y , known $n \times p$ design matrix X , known $n \times n$ covariance structure (\rightarrow II/5.1.1) V as well as unknown $p \times v$ regression coefficients B and unknown $v \times v$ noise covariance (\rightarrow II/5.1.1) Σ .

Then, the conjugate prior (\rightarrow I/5.2.5) for this model is a normal-Wishart distribution (\rightarrow II/5.3.1)

$$p(B, T) = \mathcal{MN}(B; M_0, \Lambda_0^{-1}, T^{-1}) \cdot \mathcal{W}(T; \Omega_0^{-1}, \nu_0) \quad (2)$$

where $T = \Sigma^{-1}$ is the inverse noise covariance (\rightarrow I/1.16.1) or noise precision matrix (\rightarrow I/1.16.12).

Proof: By definition, a conjugate prior (\rightarrow I/5.2.5) is a prior distribution (\rightarrow I/5.1.3) that, when combined with the likelihood function (\rightarrow I/5.1.2), leads to a posterior distribution (\rightarrow I/5.1.9) that belongs to the same family of probability distributions (\rightarrow I/1.5.1). This is fulfilled when the prior density and the likelihood function are proportional to the model parameters in the same way, i.e. the model parameters appear in the same functional form in both.

Equation (1) implies the following likelihood function (\rightarrow I/5.1.2)

$$p(Y|B, \Sigma) = \mathcal{MN}(Y; XB, V, \Sigma) = \sqrt{\frac{1}{(2\pi)^{nv} |\Sigma|^n |V|^v}} \exp \left[-\frac{1}{2} \text{tr} (\Sigma^{-1} (Y - XB)^T V^{-1} (Y - XB)) \right] \quad (3)$$

which, for mathematical convenience, can also be parametrized as

$$p(Y|B, T) = \mathcal{MN}(Y; XB, P^{-1}, T^{-1}) = \sqrt{\frac{|T|^n |P|^v}{(2\pi)^{nv}}} \exp \left[-\frac{1}{2} \text{tr} (T(Y - XB)^T P(Y - XB)) \right] \quad (4)$$

using the $v \times v$ precision matrix (\rightarrow I/1.16.12) $T = \Sigma^{-1}$ and the $n \times n$ precision matrix (\rightarrow I/1.16.12) $P = V^{-1}$.

Separating constant and variable terms, we have:

$$p(Y|B, T) = \sqrt{\frac{|P|^v}{(2\pi)^{nv}}} \cdot |T|^{n/2} \cdot \exp \left[-\frac{1}{2} \text{tr} (T(Y - XB)^T P(Y - XB)) \right]. \quad (5)$$

Expanding the product in the exponent, we have:

$$p(Y|B, T) = \sqrt{\frac{|P|^v}{(2\pi)^{nv}}} \cdot |T|^{n/2} \cdot \exp \left[-\frac{1}{2} \text{tr} (T [Y^T P Y - Y^T P X B - B^T X^T P Y + B^T X^T P X B]) \right]. \quad (6)$$

Completing the square over B , finally gives

$$p(Y|B, T) = \sqrt{\frac{|P|^v}{(2\pi)^{nv}}} \cdot |T|^{n/2} \cdot \exp \left[-\frac{1}{2} \text{tr} \left(T \left[(B - \tilde{X}Y)^T X^T P X (B - \tilde{X}Y) - Y^T Q Y + Y^T P Y \right] \right) \right] \quad (7)$$

where $\tilde{X} = (X^T P X)^{-1} X^T P$ and $Q = \tilde{X}^T (X^T P X) \tilde{X}$.

In other words, the likelihood function (\rightarrow I/5.1.2) is proportional to a power of the determinant of T , times an exponential of the trace of T and an exponential of the trace of a squared form of B , weighted by T :

$$p(Y|B, T) \propto |T|^{n/2} \cdot \exp \left[-\frac{1}{2} \text{tr} (T [Y^T P Y - Y^T Q Y]) \right] \cdot \exp \left[-\frac{1}{2} \text{tr} \left(T \left[(B - \tilde{X}Y)^T X^T P X (B - \tilde{X}Y) \right] \right) \right] . \quad (8)$$

The same is true for a normal-Wishart distribution (\rightarrow II/5.3.1) over B and T

$$p(B, T) = \mathcal{MN}(B; M_0, \Lambda_0^{-1}, T^{-1}) \cdot \mathcal{W}(T; \Omega_0^{-1}, \nu_0) \quad (9)$$

the probability density function of which (\rightarrow II/5.3.2)

$$p(B, T) = \sqrt{\frac{|T|^p |\Lambda_0|^v}{(2\pi)^{pv}}} \exp \left[-\frac{1}{2} \text{tr} (T (B - M_0)^T \Lambda_0 (B - M_0)) \right] \cdot \frac{1}{\Gamma_v(\frac{\nu_0}{2})} \sqrt{\frac{|\Omega_0|^{\nu_0}}{2^{\nu_0 v}}} |T|^{(\nu_0 - v - 1)/2} \exp \left[-\frac{1}{2} \text{tr} (\Omega_0 T) \right] \quad (10)$$

exhibits the same proportionality

$$p(B, T) \propto |T|^{(\nu_0 + p - v - 1)/2} \cdot \exp \left[-\frac{1}{2} \text{tr} (T \Omega_0) \right] \cdot \exp \left[-\frac{1}{2} \text{tr} (T [(B - M_0)^T \Lambda_0 (B - M_0)]) \right] \quad (11)$$

and is therefore conjugate relative to the likelihood. ■

Sources:

- Wikipedia (2020): “Bayesian multivariate linear regression”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-09-03; URL: https://en.wikipedia.org/wiki/Bayesian_multivariate_linear_regression#Conjugate_prior_distribution.

2.5.2 Posterior distribution

Theorem: Let

$$Y = XB + E, \quad E \sim \mathcal{MN}(0, V, \Sigma) \quad (1)$$

be a general linear model (\rightarrow III/2.2.1) with measured $n \times v$ data matrix Y , known $n \times p$ design matrix X , known $n \times n$ covariance structure (\rightarrow II/5.1.1) V as well as unknown $p \times v$ regression coefficients B and unknown $v \times v$ noise covariance (\rightarrow II/5.1.1) Σ . Moreover, assume a normal-Wishart prior distribution (\rightarrow III/2.5.1) over the model parameters B and $T = \Sigma^{-1}$:

$$p(B, T) = \mathcal{MN}(B; M_0, \Lambda_0^{-1}, T^{-1}) \cdot \mathcal{W}(T; \Omega_0^{-1}, \nu_0) . \quad (2)$$

Then, the posterior distribution (\rightarrow I/5.1.9) is also a normal-Wishart distribution (\rightarrow II/5.3.1)

$$p(B, T|Y) = \mathcal{MN}(B; M_n, \Lambda_n^{-1}, T^{-1}) \cdot \mathcal{W}(T; \Omega_n^{-1}, \nu_n) \quad (3)$$

and the posterior hyperparameters (\rightarrow I/5.1.9) are given by

$$\begin{aligned} M_n &= \Lambda_n^{-1}(X^T P Y + \Lambda_0 M_0) \\ \Lambda_n &= X^T P X + \Lambda_0 \\ \Omega_n &= \Omega_0 + Y^T P Y + M_0^T \Lambda_0 M_0 - M_n^T \Lambda_n M_n \\ \nu_n &= \nu_0 + n . \end{aligned} \quad (4)$$

Proof: According to Bayes' theorem (\rightarrow I/5.3.2), the posterior distribution (\rightarrow I/5.1.9) is given by

$$p(B, T|Y) = \frac{p(Y|B, T) p(B, T)}{p(Y)} . \quad (5)$$

Since $p(Y)$ is just a normalization factor, the posterior is proportional (\rightarrow I/5.1.10) to the numerator:

$$p(B, T|Y) \propto p(Y|B, T) p(B, T) = p(Y, B, T) . \quad (6)$$

Equation (1) implies the following likelihood function (\rightarrow I/5.1.2)

$$p(Y|B, \Sigma) = \mathcal{MN}(Y; XB, V, \Sigma) = \sqrt{\frac{1}{(2\pi)^{nv} |\Sigma|^n |V|^v}} \exp \left[-\frac{1}{2} \text{tr} (\Sigma^{-1} (Y - XB)^T V^{-1} (Y - XB)) \right] \quad (7)$$

which, for mathematical convenience, can also be parametrized as

$$p(Y|B, T) = \mathcal{MN}(Y; XB, P, T^{-1}) = \sqrt{\frac{|T|^n |P|^v}{(2\pi)^{nv}}} \exp \left[-\frac{1}{2} \text{tr} (T(Y - XB)^T P (Y - XB)) \right] \quad (8)$$

using the $v \times v$ precision matrix (\rightarrow I/1.16.12) $T = \Sigma^{-1}$ and the $n \times n$ precision matrix (\rightarrow I/1.16.12) $P = V^{-1}$.

Combining the likelihood function (\rightarrow I/5.1.2) (8) with the prior distribution (\rightarrow I/5.1.3) (2), the joint likelihood (\rightarrow I/5.1.7) of the model is given by

$$\begin{aligned} p(Y, B, T) &= p(Y|B, T) p(B, T) \\ &= \sqrt{\frac{|T|^n |P|^v}{(2\pi)^{nv}}} \exp \left[-\frac{1}{2} \text{tr} (T(Y - XB)^T P (Y - XB)) \right] \cdot \\ &\quad \sqrt{\frac{|T|^p |\Lambda_0|^v}{(2\pi)^{pv}}} \exp \left[-\frac{1}{2} \text{tr} (T(B - M_0)^T \Lambda_0 (B - M_0)) \right] \cdot \\ &\quad \frac{1}{\Gamma_v(\frac{\nu_0}{2})} \sqrt{\frac{|\Omega_0|^{\nu_0}}{2^{\nu_0 v}}} |T|^{(\nu_0 - v - 1)/2} \exp \left[-\frac{1}{2} \text{tr} (\Omega_0 T) \right] . \end{aligned} \quad (9)$$

Collecting identical variables gives:

$$p(Y, B, T) = \sqrt{\frac{|T|^n |P|^v}{(2\pi)^{nv}}} \sqrt{\frac{|T|^p |\Lambda_0|^v}{(2\pi)^{pv}}} \sqrt{\frac{|\Omega_0|^{\nu_0}}{2^{\nu_0 v}} \frac{1}{\Gamma_v\left(\frac{\nu_0}{2}\right)}} \cdot |T|^{(\nu_0 - v - 1)/2} \exp \left[-\frac{1}{2} \text{tr}(\Omega_0 T) \right] \cdot \exp \left[-\frac{1}{2} \text{tr} \left(T \left[(Y - XB)^T P (Y - XB) + (B - M_0)^T \Lambda_0 (B - M_0) \right] \right) \right]. \quad (10)$$

Expanding the products in the exponent gives:

$$p(Y, B, T) = \sqrt{\frac{|T|^n |P|^v}{(2\pi)^{nv}}} \sqrt{\frac{|T|^p |\Lambda_0|^v}{(2\pi)^{pv}}} \sqrt{\frac{|\Omega_0|^{\nu_0}}{2^{\nu_0 v}} \frac{1}{\Gamma_v\left(\frac{\nu_0}{2}\right)}} \cdot |T|^{(\nu_0 - v - 1)/2} \exp \left[-\frac{1}{2} \text{tr}(\Omega_0 T) \right] \cdot \exp \left[-\frac{1}{2} \text{tr} \left(T \left[Y^T P Y - Y^T P X B - B^T X^T P Y + B^T X^T P X B + B^T \Lambda_0 B - B^T \Lambda_0 M_0 - M_0^T \Lambda_0 B + M_0^T \Lambda_0 \mu_0 \right] \right) \right]. \quad (11)$$

Completing the square over B , we finally have

$$p(Y, B, T) = \sqrt{\frac{|T|^n |P|^v}{(2\pi)^{nv}}} \sqrt{\frac{|T|^p |\Lambda_0|^v}{(2\pi)^{pv}}} \sqrt{\frac{|\Omega_0|^{\nu_0}}{2^{\nu_0 v}} \frac{1}{\Gamma_v\left(\frac{\nu_0}{2}\right)}} \cdot |T|^{(\nu_0 - v - 1)/2} \exp \left[-\frac{1}{2} \text{tr}(\Omega_0 T) \right] \cdot \exp \left[-\frac{1}{2} \text{tr} \left(T \left[(B - M_n)^T \Lambda_n (B - M_n) + (Y^T P Y + M_0^T \Lambda_0 M_0 - M_n^T \Lambda_n M_n) \right] \right) \right]. \quad (12)$$

with the posterior hyperparameters (\rightarrow I/5.1.9)

$$\begin{aligned} M_n &= \Lambda_n^{-1} (X^T P Y + \Lambda_0 M_0) \\ \Lambda_n &= X^T P X + \Lambda_0. \end{aligned} \quad (13)$$

Ergo, the joint likelihood is proportional to

$$p(Y, B, T) \propto |T|^{p/2} \cdot \exp \left[-\frac{1}{2} \text{tr} \left(T \left[(B - M_n)^T \Lambda_n (B - M_n) \right] \right) \right] \cdot |T|^{(\nu_n - v - 1)/2} \cdot \exp \left[-\frac{1}{2} \text{tr}(\Omega_n T) \right] \quad (14)$$

with the posterior hyperparameters (\rightarrow I/5.1.9)

$$\begin{aligned} \Omega_n &= \Omega_0 + Y^T P Y + M_0^T \Lambda_0 M_0 - M_n^T \Lambda_n M_n \\ \nu_n &= \nu_0 + n. \end{aligned} \quad (15)$$

From the term in (14), we can isolate the posterior distribution over B given T :

$$p(B|T, Y) = \mathcal{MN}(B; M_n, \Lambda_n^{-1}, T^{-1}). \quad (16)$$

From the remaining term, we can isolate the posterior distribution over T :

$$p(T|Y) = \mathcal{W}(T; \Omega_n^{-1}, \nu_n). \quad (17)$$

Together, (16) and (17) constitute the joint (\rightarrow I/1.3.2) posterior distribution (\rightarrow I/5.1.9) of B and T .

**Sources:**

- Wikipedia (2020): “Bayesian multivariate linear regression”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-09-03; URL: https://en.wikipedia.org/wiki/Bayesian_multivariate_linear_regression#Posterior_distribution.

2.5.3 Log model evidence**Theorem:** Let

$$Y = XB + E, \quad E \sim \mathcal{MN}(0, V, \Sigma) \quad (1)$$

be a general linear model (\rightarrow III/2.2.1) with measured $n \times v$ data matrix Y , known $n \times p$ design matrix X , known $n \times n$ covariance structure (\rightarrow II/5.1.1) V as well as unknown $p \times v$ regression coefficients B and unknown $v \times v$ noise covariance (\rightarrow II/5.1.1) Σ . Moreover, assume a normal-Wishart prior distribution (\rightarrow III/2.5.1) over the model parameters B and $T = \Sigma^{-1}$:

$$p(B, T) = \mathcal{MN}(B; M_0, \Lambda_0^{-1}, T^{-1}) \cdot \mathcal{W}(T; \Omega_0^{-1}, \nu_0) . \quad (2)$$

Then, the log model evidence (\rightarrow IV/3.1.3) for this model is

$$\begin{aligned} \log p(Y|m) = & \frac{v}{2} \log |P| - \frac{nv}{2} \log(2\pi) + \frac{v}{2} \log |\Lambda_0| - \frac{v}{2} \log |\Lambda_n| + \\ & \frac{\nu_0}{2} \log \left| \frac{1}{2} \Omega_0 \right| - \frac{\nu_n}{2} \log \left| \frac{1}{2} \Omega_n \right| + \log \Gamma_v \left(\frac{\nu_n}{2} \right) - \log \Gamma_v \left(\frac{\nu_0}{2} \right) \end{aligned} \quad (3)$$

where the posterior hyperparameters (\rightarrow I/5.1.9) are given by

$$\begin{aligned} M_n &= \Lambda_n^{-1} (X^T P Y + \Lambda_0 M_0) \\ \Lambda_n &= X^T P X + \Lambda_0 \\ \Omega_n &= \Omega_0 + Y^T P Y + M_0^T \Lambda_0 M_0 - M_n^T \Lambda_n M_n \\ \nu_n &= \nu_0 + n . \end{aligned} \quad (4)$$

Proof: According to the law of marginal probability (\rightarrow I/1.3.3), the model evidence (\rightarrow I/5.1.15) for this model is:

$$p(Y|m) = \iint p(Y|B, T) p(B, T) dB dT . \quad (5)$$

According to the law of conditional probability (\rightarrow I/1.3.4), the integrand is equivalent to the joint likelihood (\rightarrow I/5.1.7):

$$p(Y|m) = \iint p(Y, B, T) dB dT . \quad (6)$$

Equation (1) implies the following likelihood function (\rightarrow I/5.1.2)

$$p(Y|B, \Sigma) = \mathcal{MN}(Y; XB, V, \Sigma) = \sqrt{\frac{1}{(2\pi)^{nv} |\Sigma|^n |V|^v}} \exp \left[-\frac{1}{2} \text{tr} (\Sigma^{-1} (Y - XB)^T V^{-1} (Y - XB)) \right] \quad (7)$$

which, for mathematical convenience, can also be parametrized as

$$p(Y|B, T) = \mathcal{MN}(Y; XB, P, T^{-1}) = \sqrt{\frac{|T|^n |P|^v}{(2\pi)^{nv}}} \exp \left[-\frac{1}{2} \text{tr} (T(Y - XB)^T P(Y - XB)) \right] \quad (8)$$

using the $v \times v$ precision matrix (\rightarrow I/1.16.12) $T = \Sigma^{-1}$ and the $n \times n$ precision matrix (\rightarrow I/1.16.12) $P = V^{-1}$.

When deriving the posterior distribution (\rightarrow III/2.5.2) $p(B, T|Y)$, the joint likelihood $p(Y, B, T)$ is obtained as

$$p(Y, B, T) = \sqrt{\frac{|T|^n |P|^v}{(2\pi)^{nv}}} \sqrt{\frac{|T|^p |\Lambda_0|^v}{(2\pi)^{pv}}} \sqrt{\frac{|\Omega_0|^{\nu_0}}{2^{\nu_0 v}} \frac{1}{\Gamma_v(\frac{\nu_0}{2})}} \cdot |T|^{(\nu_0 - v - 1)/2} \exp \left[-\frac{1}{2} \text{tr} (\Omega_0 T) \right] \cdot \exp \left[-\frac{1}{2} \text{tr} (T [(B - M_n)^T \Lambda_n (B - M_n) + (Y^T P Y + M_0^T \Lambda_0 M_0 - M_n^T \Lambda_n M_n)]) \right] \quad (9)$$

Using the probability density function of the matrix-normal distribution (\rightarrow II/5.1.3), we can rewrite this as

$$p(Y, B, T) = \sqrt{\frac{|T|^n |P|^v}{(2\pi)^{nv}}} \sqrt{\frac{|T|^p |\Lambda_0|^v}{(2\pi)^{pv}}} \sqrt{\frac{(2\pi)^{pv}}{|T|^p |\Lambda_n|^v}} \sqrt{\frac{|\Omega_0|^{\nu_0}}{2^{\nu_0 v}} \frac{1}{\Gamma_v(\frac{\nu_0}{2})}} \cdot |T|^{(\nu_0 - v - 1)/2} \exp \left[-\frac{1}{2} \text{tr} (\Omega_0 T) \right] \cdot \mathcal{MN}(B; M_n, \Lambda_n^{-1}, T^{-1}) \cdot \exp \left[-\frac{1}{2} \text{tr} (T [Y^T P Y + M_0^T \Lambda_0 M_0 - M_n^T \Lambda_n M_n]) \right] \quad (10)$$

Now, B can be integrated out easily:

$$\int p(Y, B, T) dB = \sqrt{\frac{|T|^n |P|^v}{(2\pi)^{nv}}} \sqrt{\frac{|\Lambda_0|^v}{|\Lambda_n|^v}} \sqrt{\frac{|\Omega_0|^{\nu_0}}{2^{\nu_0 v}} \frac{1}{\Gamma_v(\frac{\nu_0}{2})}} \cdot |T|^{(\nu_0 - v - 1)/2} \cdot \exp \left[-\frac{1}{2} \text{tr} (T [\Omega_0 + Y^T P Y + M_0^T \Lambda_0 M_0 - M_n^T \Lambda_n M_n]) \right] \quad (11)$$

Using the probability density function of the Wishart distribution, we can rewrite this as

$$\int p(Y, B, T) dB = \sqrt{\frac{|P|^v}{(2\pi)^{nv}}} \sqrt{\frac{|\Lambda_0|^v}{|\Lambda_n|^v}} \sqrt{\frac{|\Omega_0|^{\nu_0}}{2^{\nu_0 v}}} \sqrt{\frac{2^{\nu_n v}}{|\Omega_n|^{\nu_n}} \frac{\Gamma_v(\frac{\nu_n}{2})}{\Gamma_v(\frac{\nu_0}{2})}} \cdot \mathcal{W}(T; \Omega_n^{-1}, \nu_n) \quad (12)$$

Finally, T can also be integrated out:

$$\iint p(Y, B, T) \, dB \, dT = \sqrt{\frac{|P|^v}{(2\pi)^{nv}}} \sqrt{\frac{|\Lambda_0|^v}{|\Lambda_n|^v}} \sqrt{\frac{|\frac{1}{2}\Omega_0|^{\nu_0}}{|\frac{1}{2}\Omega_n|^{\nu_n}}} \frac{\Gamma_v\left(\frac{\nu_n}{2}\right)}{\Gamma_v\left(\frac{\nu_0}{2}\right)} = p(y|m) . \quad (13)$$

Thus, the log model evidence (\rightarrow IV/3.1.3) of this model is given by

$$\begin{aligned} \log p(Y|m) = & \frac{v}{2} \log |P| - \frac{nv}{2} \log(2\pi) + \frac{v}{2} \log |\Lambda_0| - \frac{v}{2} \log |\Lambda_n| + \\ & \frac{\nu_0}{2} \log \left| \frac{1}{2} \Omega_0 \right| - \frac{\nu_n}{2} \log \left| \frac{1}{2} \Omega_n \right| + \log \Gamma_v \left(\frac{\nu_n}{2} \right) - \log \Gamma_v \left(\frac{\nu_0}{2} \right) . \end{aligned} \quad (14)$$

■

3 Count data

3.1 Binomial observations

3.1.1 Definition

Definition: An ordered pair (n, y) with $n \in \mathbb{N}$ and $y \in \mathbb{N}_0$, where y is the number of successes in n trials, constitutes a set of binomial observations.

3.1.2 Binomial test

Theorem: Let y be the number of successes resulting from n independent trials with unknown success probability p , such that y follows a binomial distribution (\rightarrow II/1.3.1):

$$y \sim \text{Bin}(n, p) . \quad (1)$$

Then, the null hypothesis (\rightarrow I/4.3.2)

$$H_0 : p = p_0 \quad (2)$$

is rejected (\rightarrow I/4.3.1) at significance level (\rightarrow I/4.3.8) α , if

$$y \leq c_1 \quad \text{or} \quad y \geq c_2 \quad (3)$$

where c_1 is the largest integer value, such that

$$\sum_{x=0}^{c_1} \text{Bin}(x; n, p_0) \leq \frac{\alpha}{2} , \quad (4)$$

and c_2 is the smallest integer value, such that

$$\sum_{x=c_2}^n \text{Bin}(x; n, p_0) \leq \frac{\alpha}{2} , \quad (5)$$

where $\text{Bin}(x; n, p)$ is the probability mass function of the binomial distribution (\rightarrow II/1.3.3):

$$\text{Bin}(x; n, p) = \binom{n}{x} p^x (1-p)^{n-x} . \quad (6)$$

Proof: The alternative hypothesis (\rightarrow I/4.3.3) relative to H_0 for a two-sided test (\rightarrow I/4.3.4) is

$$H_1 : p \neq p_0 . \quad (7)$$

We can use y as a test statistic (\rightarrow I/4.3.5). Its sampling distribution (\rightarrow I/1.5.6) is given by (1). The cumulative distribution function (\rightarrow I/1.8.1) (CDF) of the test statistic under the null hypothesis is thus equal to the cumulative distribution function of a binomial distribution (\rightarrow II/1.3.4) with success probability (\rightarrow II/1.3.1) p_0 :

$$\Pr(y \leq z | H_0) = \sum_{x=0}^z \text{Bin}(x; n, p_0) = \sum_{x=0}^z \binom{n}{x} p_0^x (1-p_0)^{n-x} . \quad (8)$$

The critical value (\rightarrow I/4.3.9) is the value of y , such that the probability of observing this or more extreme values of the test statistic is equal to or smaller than α . Since H_0 and H_1 define a two-tailed test, we need two critical values y_1 and y_2 that satisfy

$$\begin{aligned}\alpha &\geq \Pr(y \in \{0, \dots, y_1\} \cup \{y_2, \dots, n\} | H_0) \\ &= \Pr(y \leq y_1 | H_0) + \Pr(y \geq y_2 | H_0) \\ &= \Pr(y \leq y_1 | H_0) + (1 - \Pr(y \leq (y_2 - 1) | H_0)) .\end{aligned}\tag{9}$$

Given the test statistic's CDF in (8), this is fulfilled by the values c_1 and c_2 defined in (4) and (5). Thus, the null hypothesis H_0 can be rejected (\rightarrow I/4.3.9), if the observed test statistic is inside the rejection region (\rightarrow I/4.3.1):

$$y \in \{0, \dots, c_1\} \cup \{c_2, \dots, n\} .\tag{10}$$

This is equivalent to (3) and thus completes the proof. ■

Sources:

- Wikipedia (2023): “Binomial test”; in: *Wikipedia, the free encyclopedia*, retrieved on 2023-12-16; URL: https://en.wikipedia.org/wiki/Binomial_test#Usage.
- Wikipedia (2023): “Binomialtest”; in: *Wikipedia – Die freie Enzyklopädie*, retrieved on 2023-12-16; URL: https://de.wikipedia.org/wiki/Binomialtest#Signifikanzniveau_und_kritische_Werte.

3.1.3 Maximum likelihood estimation

Theorem: Let y be the number of successes resulting from n independent trials with unknown success probability p , such that y follows a binomial distribution (\rightarrow II/1.3.1):

$$y \sim \text{Bin}(n, p) .\tag{1}$$

Then, the maximum likelihood estimator (\rightarrow I/4.1.3) of p is

$$\hat{p} = \frac{y}{n} .\tag{2}$$

Proof: With the probability mass function of the binomial distribution (\rightarrow II/1.3.3), equation (1) implies the following likelihood function (\rightarrow I/5.1.2):

$$\begin{aligned}p(y|p) &= \text{Bin}(y; n, p) \\ &= \binom{n}{y} p^y (1 - p)^{n-y} .\end{aligned}\tag{3}$$

Thus, the log-likelihood function (\rightarrow I/4.1.2) is given by

$$\begin{aligned}\text{LL}(p) &= \log p(y|p) \\ &= \log \binom{n}{y} + y \log p + (n - y) \log(1 - p) .\end{aligned}\tag{4}$$

The derivative of the log-likelihood function (4) with respect to p is

$$\frac{dLL(p)}{dp} = \frac{y}{p} - \frac{n-y}{1-p} \quad (5)$$

and setting this derivative to zero gives the MLE for p :

$$\begin{aligned} \frac{dLL(p)}{d\hat{p}} &= 0 \\ 0 &= \frac{y}{\hat{p}} - \frac{n-y}{1-\hat{p}} \\ \frac{n-y}{1-\hat{p}} &= \frac{y}{\hat{p}} \\ (n-y)\hat{p} &= y(1-\hat{p}) \\ n\hat{p} - y\hat{p} &= y - y\hat{p} \\ n\hat{p} &= y \\ \hat{p} &= \frac{y}{n} . \end{aligned} \quad (6)$$

■

Sources:

- Wikipedia (2022): “Binomial distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-11-23; URL: https://en.wikipedia.org/wiki/Binomial_distribution#Statistical_inference.

3.1.4 Maximum log-likelihood

Theorem: Let y be the number of successes resulting from n independent trials with unknown success probability p , such that y follows a binomial distribution (\rightarrow II/1.3.1):

$$y \sim \text{Bin}(n, p) . \quad (1)$$

Then, the maximum log-likelihood (\rightarrow I/4.1.4) for this model is

$$\begin{aligned} \text{MLL} &= \log \Gamma(n+1) - \log \Gamma(y+1) - \log \Gamma(n-y+1) \\ &\quad - n \log(n) + y \log(y) + (n-y) \log(n-y) . \end{aligned} \quad (2)$$

Proof: The log-likelihood function for binomial data (\rightarrow III/3.1.3) is given by

$$LL(p) = \log \binom{n}{y} + y \log p + (n-y) \log(1-p) \quad (3)$$

and the maximum likelihood estimate of the success probability (\rightarrow III/3.1.3) p is

$$\hat{p} = \frac{y}{n} . \quad (4)$$

Plugging (4) into (3), we obtain the maximum log-likelihood (\rightarrow I/4.1.4) of the binomial observation model in (1) as

$$\begin{aligned}
\text{MLL} &= \text{LL}(\hat{p}) \\
&= \log \binom{n}{y} + y \log \left(\frac{y}{n} \right) + (n - y) \log \left(1 - \frac{y}{n} \right) \\
&= \log \binom{n}{y} + y \log \left(\frac{y}{n} \right) + (n - y) \log \left(\frac{n - y}{n} \right) \\
&= \log \binom{n}{y} + y \log(y) + (n - y) \log(n - y) - n \log(n) .
\end{aligned} \tag{5}$$

With the definition of the binomial coefficient

$$\binom{n}{k} = \frac{n!}{k! (n - k)!} \tag{6}$$

and the definition of the gamma function

$$\Gamma(n) = (n - 1)! , \tag{7}$$

the MLL finally becomes

$$\begin{aligned}
\text{MLL} &= \log \Gamma(n + 1) - \log \Gamma(y + 1) - \log \Gamma(n - y + 1) \\
&\quad - n \log(n) + y \log(y) + (n - y) \log(n - y) .
\end{aligned} \tag{8}$$

■

3.1.5 Maximum-a-posteriori estimation

Theorem: Let y be the number of successes resulting from n independent trials with unknown success probability p , such that y follows a binomial distribution (\rightarrow II/1.3.1):

$$y \sim \text{Bin}(n, p) . \tag{1}$$

Moreover, assume a beta prior distribution (\rightarrow III/3.1.6) over the model parameter p :

$$p(p) = \text{Bet}(p; \alpha_0, \beta_0) . \tag{2}$$

Then, the maximum-a-posteriori estimate (\rightarrow I/5.1.14) of p is

$$\hat{p}_{\text{MAP}} = \frac{\alpha_0 + y - 1}{\alpha_0 + \beta_0 + n - 2} . \tag{3}$$

Proof: Given the prior distribution (\rightarrow I/5.1.3) in (2), the posterior distribution (\rightarrow I/5.1.9) for binomial observations (\rightarrow III/3.1.1) is also a beta distribution (\rightarrow III/3.1.7)

$$p(p|y) = \text{Bet}(p; \alpha_n, \beta_n) \tag{4}$$

where the posterior hyperparameters (\rightarrow I/5.1.9) are equal to

$$\begin{aligned}
\alpha_n &= \alpha_0 + y \\
\beta_n &= \beta_0 + (n - y) .
\end{aligned} \tag{5}$$

The mode of the beta distribution (\rightarrow II/3.9.10) is given by:

$$X \sim \text{Bet}(\alpha, \beta) \quad \Rightarrow \quad \text{mode}(X) = \frac{\alpha - 1}{\alpha + \beta - 2} . \quad (6)$$

Applying (6) to (4) with (5), the maximum-a-posteriori estimate (\rightarrow I/5.1.14) of p follows as:

$$\begin{aligned} \hat{p}_{\text{MAP}} &= \frac{\alpha_n - 1}{\alpha_n + \beta_n - 2} \\ &\stackrel{(5)}{=} \frac{\alpha_0 + y - 1}{\alpha_0 + y + \beta_0 + (n - y) - 2} \\ &= \frac{\alpha_0 + y - 1}{\alpha_0 + \beta_0 + n - 2} . \end{aligned} \quad (7)$$

■

3.1.6 Conjugate prior distribution

Theorem: Let y be the number of successes resulting from n independent trials with unknown success probability p , such that y follows a binomial distribution (\rightarrow II/1.3.1):

$$y \sim \text{Bin}(n, p) . \quad (1)$$

Then, the conjugate prior (\rightarrow I/5.2.5) for the model parameter p is a beta distribution (\rightarrow II/3.9.1):

$$p(p) = \text{Bet}(p; \alpha_0, \beta_0) . \quad (2)$$

Proof: With the probability mass function of the binomial distribution (\rightarrow II/1.3.3), the likelihood function (\rightarrow I/5.1.2) implied by (1) is given by

$$p(y|p) = \binom{n}{y} p^y (1 - p)^{n-y} . \quad (3)$$

In other words, the likelihood function is proportional to a power of p times a power of $(1 - p)$:

$$p(y|p) \propto p^y (1 - p)^{n-y} . \quad (4)$$

The same is true for a beta distribution over p

$$p(p) = \text{Bet}(p; \alpha_0, \beta_0) \quad (5)$$

the probability density function of which (\rightarrow II/3.9.5)

$$p(p) = \frac{1}{B(\alpha_0, \beta_0)} p^{\alpha_0-1} (1 - p)^{\beta_0-1} \quad (6)$$

exhibits the same proportionality

$$p(p) \propto p^{\alpha_0-1} (1 - p)^{\beta_0-1} \quad (7)$$

and is therefore conjugate relative to the likelihood.

■

Sources:

- Wikipedia (2020): “Binomial distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-01-23; URL: https://en.wikipedia.org/wiki/Binomial_distribution#Estimation_of_parameters.

3.1.7 Posterior distribution

Theorem: Let y be the number of successes resulting from n independent trials with unknown success probability p , such that y follows a binomial distribution (\rightarrow II/1.3.1):

$$y \sim \text{Bin}(n, p) . \quad (1)$$

Moreover, assume a beta prior distribution (\rightarrow III/3.1.6) over the model parameter p :

$$p(p) = \text{Bet}(p; \alpha_0, \beta_0) . \quad (2)$$

Then, the posterior distribution (\rightarrow I/5.1.9) is also a beta distribution (\rightarrow II/3.9.1)

$$p(p|y) = \text{Bet}(p; \alpha_n, \beta_n) . \quad (3)$$

and the posterior hyperparameters (\rightarrow I/5.1.9) are given by

$$\begin{aligned} \alpha_n &= \alpha_0 + y \\ \beta_n &= \beta_0 + (n - y) . \end{aligned} \quad (4)$$

Proof: With the probability mass function of the binomial distribution (\rightarrow II/1.3.3), the likelihood function (\rightarrow I/5.1.2) implied by (1) is given by

$$p(y|p) = \binom{n}{y} p^y (1 - p)^{n-y} . \quad (5)$$

Combining the likelihood function (5) with the prior distribution (2), the joint likelihood (\rightarrow I/5.1.7) of the model is given by

$$\begin{aligned} p(y, p) &= p(y|p) p(p) \\ &= \binom{n}{y} p^y (1 - p)^{n-y} \cdot \frac{1}{B(\alpha_0, \beta_0)} p^{\alpha_0-1} (1 - p)^{\beta_0-1} \\ &= \frac{1}{B(\alpha_0, \beta_0)} \binom{n}{y} p^{\alpha_0+y-1} (1 - p)^{\beta_0+(n-y)-1} . \end{aligned} \quad (6)$$

Note that the posterior distribution is proportional to the joint likelihood (\rightarrow I/5.1.10):

$$p(p|y) \propto p(y, p) . \quad (7)$$

Setting $\alpha_n = \alpha_0 + y$ and $\beta_n = \beta_0 + (n - y)$, the posterior distribution is therefore proportional to

$$p(p|y) \propto p^{\alpha_n-1} (1 - p)^{\beta_n-1} \quad (8)$$

which, when normalized to one, results in the probability density function of the beta distribution (\rightarrow II/3.9.5):

$$p(p|y) = \frac{1}{B(\alpha_n, \beta_n)} p^{\alpha_n-1} (1 - p)^{\beta_n-1} = \text{Bet}(p; \alpha_n, \beta_n) . \quad (9)$$



Sources:

- Wikipedia (2020): “Binomial distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-01-23; URL: https://en.wikipedia.org/wiki/Binomial_distribution#Estimation_of_parameters.

3.1.8 Log model evidence

Theorem: Let y be the number of successes resulting from n independent trials with unknown success probability p , such that y follows a binomial distribution (\rightarrow II/1.3.1):

$$y \sim \text{Bin}(n, p) . \quad (1)$$

Moreover, assume a beta prior distribution (\rightarrow III/3.1.6) over the model parameter p :

$$p(p) = \text{Bet}(p; \alpha_0, \beta_0) . \quad (2)$$

Then, the log model evidence (\rightarrow IV/3.1.3) for this model is

$$\begin{aligned} \log p(y|m) &= \log \Gamma(n+1) - \log \Gamma(y+1) - \log \Gamma(n-y+1) \\ &\quad + \log B(\alpha_n, \beta_n) - \log B(\alpha_0, \beta_0) . \end{aligned} \quad (3)$$

where the posterior hyperparameters (\rightarrow I/5.1.9) are given by

$$\begin{aligned} \alpha_n &= \alpha_0 + y \\ \beta_n &= \beta_0 + (n - y) . \end{aligned} \quad (4)$$

Proof: With the probability mass function of the binomial distribution (\rightarrow II/1.3.3), the likelihood function (\rightarrow I/5.1.2) implied by (1) is given by

$$p(y|p) = \binom{n}{y} p^y (1-p)^{n-y} . \quad (5)$$

Combining the likelihood function (5) with the prior distribution (2), the joint likelihood (\rightarrow I/5.1.7) of the model is given by

$$\begin{aligned} p(y, p) &= p(y|p) p(p) \\ &= \binom{n}{y} p^y (1-p)^{n-y} \cdot \frac{1}{B(\alpha_0, \beta_0)} p^{\alpha_0-1} (1-p)^{\beta_0-1} \\ &= \binom{n}{y} \frac{1}{B(\alpha_0, \beta_0)} p^{\alpha_0+y-1} (1-p)^{\beta_0+(n-y)-1} . \end{aligned} \quad (6)$$

Note that the model evidence is the marginal density of the joint likelihood (\rightarrow I/5.1.15):

$$p(y) = \int p(y, p) dp . \quad (7)$$

Setting $\alpha_n = \alpha_0 + y$ and $\beta_n = \beta_0 + (n - y)$, the joint likelihood can also be written as

$$p(y, p) = \binom{n}{y} \frac{1}{B(\alpha_0, \beta_0)} \frac{B(\alpha_n, \beta_n)}{1} \frac{1}{B(\alpha_n, \beta_n)} p^{\alpha_n-1} (1-p)^{\beta_n-1} . \quad (8)$$

Using the probability density function of the beta distribution (\rightarrow II/3.9.5), p can now be integrated out easily

$$\begin{aligned} p(y) &= \int \binom{n}{y} \frac{1}{B(\alpha_0, \beta_0)} \frac{B(\alpha_n, \beta_n)}{1} \frac{1}{B(\alpha_n, \beta_n)} p^{\alpha_n-1} (1-p)^{\beta_n-1} dp \\ &= \binom{n}{y} \frac{B(\alpha_n, \beta_n)}{B(\alpha_0, \beta_0)} \int \text{Bet}(p; \alpha_n, \beta_n) dp \\ &= \binom{n}{y} \frac{B(\alpha_n, \beta_n)}{B(\alpha_0, \beta_0)} , \end{aligned} \quad (9)$$

such that the log model evidence (\rightarrow IV/3.1.3) (LME) is shown to be

$$\log p(y|m) = \log \binom{n}{y} + \log B(\alpha_n, \beta_n) - \log B(\alpha_0, \beta_0) . \quad (10)$$

With the definition of the binomial coefficient

$$\binom{n}{k} = \frac{n!}{k!(n-k)!} \quad (11)$$

and the definition of the gamma function

$$\Gamma(n) = (n-1)! , \quad (12)$$

the LME finally becomes

$$\begin{aligned} \log p(y|m) &= \log \Gamma(n+1) - \log \Gamma(y+1) - \log \Gamma(n-y+1) \\ &\quad + \log B(\alpha_n, \beta_n) - \log B(\alpha_0, \beta_0) . \end{aligned} \quad (13)$$

■

Sources:

- Wikipedia (2020): “Beta-binomial distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-01-24; URL: https://en.wikipedia.org/wiki/Beta-binomial_distribution#Motivation_and_derivation.

3.1.9 Log Bayes factor

Theorem: Let y be the number of successes resulting from n independent trials with unknown success probability p , such that y follows a binomial distribution (\rightarrow II/1.3.1):

$$y \sim \text{Bin}(n, p) . \quad (1)$$

Moreover, assume two statistical models (\rightarrow I/5.1.6), one assuming that p is 0.5 (null model (\rightarrow I/4.3.2)), the other imposing a beta distribution (\rightarrow III/3.1.6) as the prior distribution (\rightarrow I/5.1.3) on the model parameter p (alternative (\rightarrow I/4.3.3)):

$$\begin{aligned} m_0 : y &\sim \text{Bin}(n, p), \quad p = 0.5 \\ m_1 : y &\sim \text{Bin}(n, p), \quad p \sim \text{Bet}(\alpha_0, \beta_0) . \end{aligned} \quad (2)$$

Then, the log Bayes factor (\rightarrow IV/3.3.6) in favor of m_1 against m_0 is

$$\text{LBF}_{10} = \log B(\alpha_n, \beta_n) - \log B(\alpha_0, \beta_0) - n \log \left(\frac{1}{2} \right) \quad (3)$$

where $B(x, y)$ is the beta function and α_n and β_n are the posterior hyperparameters for binomial observations (\rightarrow III/3.1.7) which are functions of the number of trials (\rightarrow II/1.3.1) n and the number of successes (\rightarrow II/1.3.1) y .

Proof: The log Bayes factor is equal to the difference of two log model evidences (\rightarrow IV/3.3.8):

$$\text{LBF}_{12} = \text{LME}(m_1) - \text{LME}(m_2) . \quad (4)$$

The LME of the alternative m_1 is equal to the log model evidence for binomial observations (\rightarrow III/3.1.8):

$$\text{LME}(m_1) = \log p(y|m_1) = \log \binom{n}{y} + \log B(\alpha_n, \beta_n) - \log B(\alpha_0, \beta_0) . \quad (5)$$

Because the null model m_0 has no free parameter, its log model evidence (\rightarrow IV/3.1.3) (logarithmized marginal likelihood (\rightarrow I/5.1.15)) is equal to the log-likelihood function for binomial observations (\rightarrow III/3.1.3) at the value $p = 0.5$:

$$\begin{aligned} \text{LME}(m_0) &= \log p(y|p = 0.5) = \log \binom{n}{y} + y \log(0.5) + (n - y) \log(1 - 0.5) \\ &= \log \binom{n}{y} + n \log \left(\frac{1}{2} \right) . \end{aligned} \quad (6)$$

Subtracting the two LMEs from each other, the LBF emerges as

$$\text{LBF}_{10} = \log B(\alpha_n, \beta_n) - \log B(\alpha_0, \beta_0) - n \log \left(\frac{1}{2} \right) \quad (7)$$

where the posterior hyperparameters (\rightarrow I/5.1.9) are given by (\rightarrow III/3.1.7)

$$\begin{aligned} \alpha_n &= \alpha_0 + y \\ \beta_n &= \beta_0 + (n - y) \end{aligned} \quad (8)$$

with the number of trials (\rightarrow II/1.3.1) n and the number of successes (\rightarrow II/1.3.1) y .

■

3.1.10 Posterior probability

Theorem: Let y be the number of successes resulting from n independent trials with unknown success probability p , such that y follows a binomial distribution (\rightarrow II/1.3.1):

$$y \sim \text{Bin}(n, p) . \quad (1)$$

Moreover, assume two statistical models (\rightarrow I/5.1.6), one assuming that p is 0.5 (null model (\rightarrow I/4.3.2)), the other imposing a beta distribution (\rightarrow III/3.1.6) as the prior distribution (\rightarrow I/5.1.3) on the model parameter p (alternative (\rightarrow I/4.3.3)):

$$\begin{aligned} m_0 : y &\sim \text{Bin}(n, p), \quad p = 0.5 \\ m_1 : y &\sim \text{Bin}(n, p), \quad p \sim \text{Bet}(\alpha_0, \beta_0) . \end{aligned} \quad (2)$$

Then, the posterior probability (\rightarrow IV/3.4.1) of the alternative model (\rightarrow I/4.3.3) is given by

$$p(m_1|y) = \frac{1}{1 + 2^{-n} [B(\alpha_0, \beta_0)/B(\alpha_n, \beta_n)]} \quad (3)$$

where $B(x, y)$ is the beta function and α_n and β_n are the posterior hyperparameters for binomial observations (\rightarrow III/3.1.7) which are functions of the number of trials (\rightarrow II/1.3.1) n and the number of successes (\rightarrow II/1.3.1) y .

Proof: The posterior probability for one of two models is a function of the log Bayes factor in favor of this model (\rightarrow IV/3.4.4):

$$p(m_1|y) = \frac{\exp(\text{LBF}_{12})}{\exp(\text{LBF}_{12}) + 1} . \quad (4)$$

The log Bayes factor in favor of the alternative model for binomial observations (\rightarrow III/3.1.9) is given by

$$\text{LBF}_{10} = \log B(\alpha_n, \beta_n) - \log B(\alpha_0, \beta_0) - n \log \left(\frac{1}{2} \right) . \quad (5)$$

and the corresponding Bayes factor (\rightarrow IV/3.3.1), i.e. exponentiated log Bayes factor (\rightarrow IV/3.3.7), is equal to

$$\text{BF}_{10} = \exp(\text{LBF}_{10}) = 2^n \cdot \frac{B(\alpha_n, \beta_n)}{B(\alpha_0, \beta_0)} . \quad (6)$$

Thus, the posterior probability of the alternative, assuming a prior distribution over the probability p , compared to the null model, assuming a fixed probability $p = 0.5$, follows as

$$\begin{aligned} p(m_1|y) &\stackrel{(4)}{=} \frac{\exp(\text{LBF}_{10})}{\exp(\text{LBF}_{10}) + 1} \\ &\stackrel{(6)}{=} \frac{2^n \cdot \frac{B(\alpha_n, \beta_n)}{B(\alpha_0, \beta_0)}}{2^n \cdot \frac{B(\alpha_n, \beta_n)}{B(\alpha_0, \beta_0)} + 1} \\ &= \frac{2^n \cdot \frac{B(\alpha_n, \beta_n)}{B(\alpha_0, \beta_0)}}{2^n \cdot \frac{B(\alpha_n, \beta_n)}{B(\alpha_0, \beta_0)} \left(1 + 2^{-n} \frac{B(\alpha_0, \beta_0)}{B(\alpha_n, \beta_n)} \right)} \\ &= \frac{1}{1 + 2^{-n} [B(\alpha_0, \beta_0)/B(\alpha_n, \beta_n)]} \end{aligned} \quad (7)$$

where the posterior hyperparameters (\rightarrow I/5.1.9) are given by (\rightarrow III/3.1.7)

$$\begin{aligned}\alpha_n &= \alpha_0 + y \\ \beta_n &= \beta_0 + (n - y)\end{aligned}\tag{8}$$

with the number of trials (\rightarrow II/1.3.1) n and the number of successes (\rightarrow II/1.3.1) y . ■

3.1.11 Cross-validated log model evidence

Theorem: Let y be the number of successes resulting from n independent trials with unknown success probability p , such that y follows a binomial distribution:

$$y \sim \text{Bin}(n, p) . \tag{1}$$

Moreover, assume two statistical models (\rightarrow I/5.1.6), one assuming that p is 0.5 (null model (\rightarrow I/4.3.2)), the other imposing a beta distribution (\rightarrow III/3.1.6) as the prior distribution (\rightarrow I/5.1.3) on the model parameter p (alternative (\rightarrow I/4.3.3)):

$$\begin{aligned}m_0 : y &\sim \text{Bin}(n, p), p = 0.5 \\ m_1 : y &\sim \text{Bin}(n, p), p \sim \text{Bet}(\alpha_0, \beta_0) .\end{aligned}\tag{2}$$

Then, the cross-validated log model evidences (\rightarrow IV/3.1.9) of m_0 and m_1 are

$$\begin{aligned}\text{cvLME}(m_0) &= -n \log(2) + \sum_{i=1}^S \left[\log \binom{n_2}{y_2^{(i)}} \right] \\ \text{cvLME}(m_1) &= S \cdot \log B(y, n - y) + \sum_{i=1}^S \left[\log \binom{n_2}{y_2^{(i)}} - \log B(y_1^{(i)}, n_1 - y_1^{(i)}) \right]\end{aligned}\tag{3}$$

where $y_1^{(i)}$ and $y_2^{(i)}$ are the training and test data, respectively, in the i -th cross-validation fold with n_1 and n_2 data points, respectively, S is the number of data subsets (\rightarrow IV/3.1.9) and $B(x, y)$ is the beta function.

Proof: For evaluation of the cross-validated log model evidences (\rightarrow IV/3.1.9) (cvLME), we assume that n data points are divided into $S \mid n$ data subsets without remainder. Then, the number of training data points n_1 and test data points n_2 are given by

$$\begin{aligned}n &= n_1 + n_2 \\ n_1 &= \frac{S-1}{S}n \\ n_2 &= \frac{1}{S}n ,\end{aligned}\tag{4}$$

such that $y_1^{(i)}$ is the number of successes (\rightarrow II/1.3.1) from the n_1 trials of the training set (\rightarrow III/3.1.1) and $y_2^{(i)}$ is the number of successes (\rightarrow II/1.3.1) from the n_2 trials of the test set (\rightarrow III/3.1.1) in the i -th cross-validation fold and it holds that

$$y = y_1^{(i)} + y_2^{(i)} . \quad (5)$$

First, we consider the null model m_0 assuming $p = 0.5$. Because this model has no free parameter, nothing is estimated from the training data and the assumed parameter value is applied to the test data. Consequently, the out-of-sample log model evidence (\rightarrow IV/3.1.9) (oosLME) is equal to the log-likelihood function (\rightarrow III/3.1.3) of the test data at $p = 0.5$:

$$\begin{aligned} \text{oosLME}_i(m_0) &= \log p \left(y_2^{(i)} \middle| p = 0.5 \right) \\ &= \log \binom{n_2}{y_2^{(i)}} + y_2^{(i)} \log 0.5 + (n_2 - y_2^{(i)}) \log(1 - 0.5) \\ &= \log \binom{n_2}{y_2^{(i)}} + n_2 \log \frac{1}{2} . \end{aligned} \quad (6)$$

By definition, the cross-validated log model evidence is the sum of out-of-sample log model evidences (\rightarrow IV/3.1.9) over cross-validation folds, such that the cvLME of m_0 is:

$$\begin{aligned} \text{cvLME}(m_0) &= \sum_{i=1}^S \text{oosLME}_i(m_0) \\ &= \sum_{i=1}^S \left[\log \binom{n_2}{y_2^{(i)}} + n_2 \log \left(\frac{1}{2} \right) \right] \\ &= S \cdot n_2 \log \left(\frac{1}{2} \right) + \sum_{i=1}^S \left[\log \binom{n_2}{y_2^{(i)}} \right] \\ &= -n \log(2) + \sum_{i=1}^S \left[\log \binom{n_2}{y_2^{(i)}} \right] . \end{aligned} \quad (7)$$

Next, we have a look at the alternative m_1 assuming $p \neq 0.5$. First, the training data $y_1^{(i)}$ are analyzed using a non-informative prior distribution (\rightarrow I/5.2.3) and applying the posterior distribution for binomial observations (\rightarrow III/3.1.7):

$$\begin{aligned} \alpha_0^{(1)} = 0 &\Rightarrow \alpha_n^{(1)} = \alpha_0^{(1)} + y_1^{(i)} = y_1^{(i)} \\ \beta_0^{(1)} = 0 &\Rightarrow \beta_n^{(1)} = \beta_0^{(1)} + (n_1 - y_1^{(i)}) = n_1 - y_1^{(i)} . \end{aligned} \quad (8)$$

This results in a posterior characterized by $\alpha_n^{(1)}$ and $\beta_n^{(1)}$. Then, the test data $y_2^{(i)}$ are analyzed using this posterior as an informative prior distribution (\rightarrow I/5.2.3), again applying the posterior distribution for binomial observations (\rightarrow III/3.1.7):

$$\begin{aligned} \alpha_0^{(2)} = \alpha_n^{(1)} = y_1^{(i)} &\Rightarrow \alpha_n^{(2)} = \alpha_0^{(2)} + y_2^{(i)} = y \\ \beta_0^{(2)} = \beta_n^{(1)} = n_1 - y_1^{(i)} &\Rightarrow \beta_n^{(2)} = \beta_0^{(2)} + (n_2 - y_2^{(i)}) = n - y . \end{aligned} \quad (9)$$

In the test data, we now have a prior characterized by $\alpha_0^{(2)}$ and $\beta_0^{(2)}$ and a posterior characterized $\alpha_n^{(2)}$ and $\beta_n^{(2)}$. Applying the log model evidence for binomial observations (\rightarrow III/3.1.8), the out-of-sample log model evidence (\rightarrow IV/3.1.9) (oosLME) therefore follows as

$$\begin{aligned} \text{oosLME}_i(m_1) &= \log \binom{n_2}{y_2^{(i)}} + \log B(\alpha_n^{(2)}, \beta_n^{(2)}) - \log B(\alpha_0^{(2)}, \beta_0^{(2)}) \\ &= \log \binom{n_2}{y_2^{(i)}} + \log B(y, n - y) - \log B(y_1^{(i)}, n_1 - y_1^{(i)}) . \end{aligned} \quad (10)$$

Again, because the cross-validated log model evidence is the sum of out-of-sample log model evidences (\rightarrow IV/3.1.9) over cross-validation folds, the cvLME of m_1 becomes:

$$\begin{aligned} \text{cvLME}(m_1) &= \sum_{i=1}^S \text{oosLME}_i(m_1) \\ &= \sum_{i=1}^S \left[\log \binom{n_2}{y_2^{(i)}} + \log B(y, n - y) - \log B(y_1^{(i)}, n_1 - y_1^{(i)}) \right] \\ &= S \cdot \log B(y, n - y) + \sum_{i=1}^S \left[\log \binom{n_2}{y_2^{(i)}} - \log B(y_1^{(i)}, n_1 - y_1^{(i)}) \right] \end{aligned} \quad (11)$$

Together, (7) and (11) conform to the results given in (3). ■

3.2 Multinomial observations

3.2.1 Definition

Definition: An ordered pair (n, y) with $n \in \mathbb{N}$ and $y = [y_1, \dots, y_k] \in \mathbb{N}_0^{1 \times k}$, where y_i is the number of observations for the i -th out of k categories obtained in n trials, $i = 1, \dots, k$, constitutes a set of multinomial observations.

3.2.2 Multinomial test

Theorem: Let $y = [y_1, \dots, y_k]$ be the number of observations in k categories resulting from n independent trials with unknown category probabilities $p = [p_1, \dots, p_k]$, such that y follows a multinomial distribution (\rightarrow II/2.2.1):

$$y \sim \text{Mult}(n, p) . \quad (1)$$

Then, the null hypothesis (\rightarrow I/4.3.2)

$$H_0 : p = p_0 = [p_{01}, \dots, p_{0k}] \quad (2)$$

is rejected (\rightarrow I/4.3.1) at significance level (\rightarrow I/4.3.8) α , if

$$\text{Pr}_{\text{sig}} = \sum_{x: \text{Pr}_0(x) \leq \text{Pr}_0(y)} \text{Pr}_0(x) < \alpha \quad (3)$$

where $\Pr_0(x)$ is the probability of observing the numbers of occurrences $x = [x_1, \dots, x_k]$ under the null hypothesis:

$$\Pr_0(x) = n! \prod_{j=1}^k \frac{p_{0j}^{x_j}}{x_j!} . \quad (4)$$

Proof: The alternative hypothesis (\rightarrow I/4.3.3) relative to H_0 is

$$H_1 : p_j \neq p_{0j} \quad \text{for at least one } j = 1, \dots, k . \quad (5)$$

We can use y as a test statistic (\rightarrow I/4.3.5). Its sampling distribution (\rightarrow I/1.5.6) is given by (1). The probability mass function (\rightarrow I/1.6.1) (PMF) of the test statistic under the null hypothesis is thus equal to the probability mass function of the multinomial distribution (\rightarrow II/2.2.2) with category probabilities (\rightarrow II/2.2.1) p_0 :

$$\Pr(y = x | H_0) = \text{Mult}(x; n, p_0) = \binom{n}{x_1, \dots, x_k} \prod_{j=1}^k p_j^{x_j} . \quad (6)$$

The multinomial coefficient in this equation is equal to

$$\binom{n}{k_1, \dots, k_m} = \frac{n!}{k_1! \cdot \dots \cdot k_m!} , \quad (7)$$

such that the probability of observing the counts y , given H_0 , is

$$\Pr(y | H_0) = n! \prod_{j=1}^k \frac{p_{0j}^{y_j}}{y_j!} . \quad (8)$$

The probability of observing any other set of counts x , given H_0 , is

$$\Pr(x | H_0) = n! \prod_{j=1}^k \frac{p_{0j}^{x_j}}{x_j!} . \quad (9)$$

The p-value (\rightarrow I/4.3.10) is the probability of observing a value of the test statistic (\rightarrow I/4.3.5) that is as extreme or more extreme than the actually observed test statistic. Any set of counts x might be considered as extreme or more extreme than the actually observed counts y , if the former is equally probable or less probable than the latter according to the PMF:

$$\Pr_0(x) \leq \Pr_0(y) . \quad (10)$$

Thus, the p-value (\rightarrow I/4.3.10) for the data in (1) is equal to

$$p = \sum_{x: \Pr_0(x) \leq \Pr_0(y)} \Pr_0(x) \quad (11)$$

and the null hypothesis in (2) is rejected (\rightarrow I/4.3.1), if

$$p < \alpha . \quad (12)$$

■

Sources:

- Wikipedia (2023): “Multinomial test”; in: *Wikipedia, the free encyclopedia*, retrieved on 2023-12-23; URL: https://en.wikipedia.org/wiki/Multinomial_test.

3.2.3 Maximum likelihood estimation

Theorem: Let $y = [y_1, \dots, y_k]$ be the number of observations in k categories resulting from n independent trials with unknown category probabilities $p = [p_1, \dots, p_k]$, such that y follows a multinomial distribution (\rightarrow II/2.2.1):

$$y \sim \text{Mult}(n, p) . \quad (1)$$

Then, the maximum likelihood estimator (\rightarrow I/4.1.3) of p is

$$\hat{p} = \frac{1}{n}y, \quad \text{i.e.} \quad \hat{p}_j = \frac{y_j}{n} \quad \text{for all } j = 1, \dots, k . \quad (2)$$

Proof: Note that the marginal distribution of each element in a multinomial random vector is a binomial distribution (\rightarrow II/2.2.7)

$$X \sim \text{Mult}(n, p) \quad \Rightarrow \quad X_j \sim \text{Bin}(n, p_j) \quad \text{for all } j = 1, \dots, k . \quad (3)$$

Thus, combining (1) with (3), we have

$$y_j \sim \text{Bin}(n, p_j) \quad (4)$$

which implies the likelihood function (\rightarrow III/3.1.3)

$$p(y|p_j) = \text{Bin}(y_j; n, p_j) = \binom{n}{y_j} p_j^{y_j} (1 - p_j)^{n-y_j} . \quad (5)$$

To this, we can apply maximum likelihood estimation for binomial observations (\rightarrow III/3.1.3), such that the MLE for each p_j is

$$\hat{p}_j = \frac{y_j}{n} . \quad (6)$$

■

3.2.4 Maximum log-likelihood

Theorem: Let $y = [y_1, \dots, y_k]$ be the number of observations in k categories resulting from n independent trials with unknown category probabilities $p = [p_1, \dots, p_k]$, such that y follows a multinomial distribution (\rightarrow II/2.2.1):

$$y \sim \text{Mult}(n, p) . \quad (1)$$

Then, the maximum log-likelihood (\rightarrow I/4.1.4) for this model is

$$\text{MLL} = \log \Gamma(n+1) - \sum_{j=1}^k \log \Gamma(y_j+1) - n \log(n) + \sum_{j=1}^k y_j \log(y_j) . \quad (2)$$

Proof: With the probability mass function of the multinomial distribution (\rightarrow II/2.2.2), equation (1) implies the following likelihood function (\rightarrow I/5.1.2):

$$\begin{aligned} p(y|p) &= \text{Mult}(y; n, p) \\ &= \binom{n}{y_1, \dots, y_k} \prod_{j=1}^k p_j^{y_j} . \end{aligned} \quad (3)$$

Thus, the log-likelihood function (\rightarrow I/4.1.2) is given by

$$\begin{aligned} \text{LL}(p) &= \log p(y|p) \\ &= \log \binom{n}{y_1, \dots, y_k} + \sum_{j=1}^k y_j \log(p_j) . \end{aligned} \quad (4)$$

The maximum likelihood estimates of the category probabilities (\rightarrow III/3.2.3) p are

$$\hat{p} = [\hat{p}_1, \dots, \hat{p}_k] \quad \text{with} \quad \hat{p}_j = \frac{y_j}{n} \quad \text{for all} \quad j = 1, \dots, k . \quad (5)$$

Plugging (5) into (4), we obtain the maximum log-likelihood (\rightarrow I/4.1.4) of the multinomial observation model in (1) as

$$\begin{aligned} \text{MLL} &= \text{LL}(\hat{p}) \\ &= \log \binom{n}{y_1, \dots, y_k} + \sum_{j=1}^k y_j \log \left(\frac{y_j}{n} \right) \\ &= \log \binom{n}{y_1, \dots, y_k} + \sum_{j=1}^k [y_j \log(y_j) - y_j \log(n)] \\ &= \log \binom{n}{y_1, \dots, y_k} + \sum_{j=1}^k y_j \log(y_j) - \sum_{j=1}^k y_j \log(n) \\ &= \log \binom{n}{y_1, \dots, y_k} + \sum_{j=1}^k y_j \log(y_j) - n \log(n) . \end{aligned} \quad (6)$$

With the definition of the multinomial coefficient

$$\binom{n}{k_1, \dots, k_m} = \frac{n!}{k_1! \cdot \dots \cdot k_m!} \quad (7)$$

and the definition of the gamma function

$$\Gamma(n) = (n-1)! , \quad (8)$$

the MLL finally becomes

$$\text{MLL} = \log \Gamma(n+1) - \sum_{j=1}^k \log \Gamma(y_j+1) - n \log(n) + \sum_{j=1}^k y_j \log(y_j) . \quad (9)$$

■

3.2.5 Maximum-a-posteriori estimation

Theorem: Let $y = [y_1, \dots, y_k]$ be the number of observations in k categories resulting from n independent trials with unknown category probabilities $p = [p_1, \dots, p_k]$, such that y follows a multinomial distribution (\rightarrow II/2.2.1):

$$y \sim \text{Mult}(n, p) . \quad (1)$$

Moreover, assume a Dirichlet prior distribution (\rightarrow III/3.2.6) over the model parameter p :

$$p(p) = \text{Dir}(p; \alpha_0) . \quad (2)$$

Then, the maximum-a-posteriori estimates (\rightarrow I/5.1.14) of p are

$$\hat{p}_{\text{MAP}} = \frac{\alpha_0 + y - 1}{\sum_{j=1}^k \alpha_{0j} + n - k} . \quad (3)$$

Proof: Given the prior distribution (\rightarrow I/5.1.3) in (2), the posterior distribution (\rightarrow I/5.1.9) for multinomial observations (\rightarrow III/3.2.1) is also a Dirichlet distribution (\rightarrow III/3.2.7)

$$p(p|y) = \text{Dir}(p; \alpha_n) \quad (4)$$

where the posterior hyperparameters (\rightarrow I/5.1.9) are equal to

$$\alpha_{nj} = \alpha_{0j} + y_j, \quad j = 1, \dots, k . \quad (5)$$

The mode of the Dirichlet distribution is given by:

$$X \sim \text{Dir}(\alpha) \quad \Rightarrow \quad \text{mode}(X_i) = \frac{\alpha_i - 1}{\sum_j \alpha_j - k} . \quad (6)$$

Applying (6) to (4) with (5), the maximum-a-posteriori estimates (\rightarrow I/5.1.14) of p follow as

$$\begin{aligned} \hat{p}_{i,\text{MAP}} &= \frac{\alpha_{ni} - 1}{\sum_j \alpha_{nj} - k} \\ &\stackrel{(5)}{=} \frac{\alpha_{0i} + y_i - 1}{\sum_j (\alpha_{0j} + y_j) - k} \\ &= \frac{\alpha_{0i} + y_i - 1}{\sum_j \alpha_{0j} + \sum_j y_j - k} . \end{aligned} \quad (7)$$

Since $y_1 + \dots + y_k = n$ by definition (\rightarrow III/3.2.1), this becomes

$$\hat{p}_{i,\text{MAP}} = \frac{\alpha_{0i} + y_i - 1}{\sum_j \alpha_{0j} + n - k} \quad (8)$$

which, using the $1 \times k$ vectors (\rightarrow III/3.2.1) y , p and α_0 , can be written as:

$$\hat{p}_{\text{MAP}} = \frac{\alpha_0 + y - 1}{\sum_{j=1}^k \alpha_{0j} + n - k} . \quad (9)$$

■

3.2.6 Conjugate prior distribution

Theorem: Let $y = [y_1, \dots, y_k]$ be the number of observations in k categories resulting from n independent trials with unknown category probabilities $p = [p_1, \dots, p_k]$, such that y follows a multinomial distribution (\rightarrow II/2.2.1):

$$y \sim \text{Mult}(n, p) . \quad (1)$$

Then, the conjugate prior (\rightarrow I/5.2.5) for the model parameter p is a Dirichlet distribution (\rightarrow II/4.5.1):

$$p(p) = \text{Dir}(p; \alpha_0) . \quad (2)$$

Proof: With the probability mass function of the multinomial distribution (\rightarrow II/2.2.2), the likelihood function (\rightarrow I/5.1.2) implied by (1) is given by

$$p(y|p) = \binom{n}{y_1, \dots, y_k} \prod_{j=1}^k p_j^{y_j} . \quad (3)$$

In other words, the likelihood function is proportional to a product of powers of the entries of the vector p :

$$p(y|p) \propto \prod_{j=1}^k p_j^{y_j} . \quad (4)$$

The same is true for a Dirichlet distribution over p

$$p(p) = \text{Dir}(p; \alpha_0) \quad (5)$$

the probability density function of which (\rightarrow II/4.5.2)

$$p(p) = \frac{\Gamma\left(\sum_{j=1}^k \alpha_{0j}\right)}{\prod_{j=1}^k \Gamma(\alpha_{0j})} \prod_{j=1}^k p_j^{\alpha_{0j}-1} \quad (6)$$

exhibits the same proportionality

$$p(p) \propto \prod_{j=1}^k p_j^{\alpha_{0j}-1} \quad (7)$$

and is therefore conjugate relative to the likelihood. ■

Sources:

- Wikipedia (2020): “Dirichlet distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-03-11; URL: https://en.wikipedia.org/wiki/Dirichlet_distribution#Conjugate_to_categorical/multinomial

3.2.7 Posterior distribution

Theorem: Let $y = [y_1, \dots, y_k]$ be the number of observations in k categories resulting from n independent trials with unknown category probabilities $p = [p_1, \dots, p_k]$, such that y follows a multinomial distribution (\rightarrow II/2.2.1):

$$y \sim \text{Mult}(n, p) . \quad (1)$$

Moreover, assume a Dirichlet prior distribution (\rightarrow III/3.2.6) over the model parameter p :

$$p(p) = \text{Dir}(p; \alpha_0) . \quad (2)$$

Then, the posterior distribution (\rightarrow I/5.1.9) is also a Dirichlet distribution (\rightarrow II/4.5.1)

$$p(p|y) = \text{Dir}(p; \alpha_n) . \quad (3)$$

and the posterior hyperparameters (\rightarrow I/5.1.9) are given by

$$\alpha_{nj} = \alpha_{0j} + y_j, \quad j = 1, \dots, k . \quad (4)$$

Proof: With the probability mass function of the multinomial distribution (\rightarrow II/2.2.2), the likelihood function (\rightarrow I/5.1.2) implied by (1) is given by

$$p(y|p) = \binom{n}{y_1, \dots, y_k} \prod_{j=1}^k p_j^{y_j} . \quad (5)$$

Combining the likelihood function (5) with the prior distribution (2), the joint likelihood (\rightarrow I/5.1.7) of the model is given by

$$\begin{aligned} p(y, p) &= p(y|p) p(p) \\ &= \binom{n}{y_1, \dots, y_k} \prod_{j=1}^k p_j^{y_j} \cdot \frac{\Gamma(\sum_{j=1}^k \alpha_{0j})}{\prod_{j=1}^k \Gamma(\alpha_{0j})} \prod_{j=1}^k p_j^{\alpha_{0j}-1} \\ &= \frac{\Gamma(\sum_{j=1}^k \alpha_{0j})}{\prod_{j=1}^k \Gamma(\alpha_{0j})} \binom{n}{y_1, \dots, y_k} \prod_{j=1}^k p_j^{\alpha_{0j}+y_j-1} . \end{aligned} \quad (6)$$

Note that the posterior distribution is proportional to the joint likelihood (\rightarrow I/5.1.10):

$$p(p|y) \propto p(y, p) . \quad (7)$$

Setting $\alpha_{nj} = \alpha_{0j} + y_j$, the posterior distribution is therefore proportional to

$$p(p|y) \propto \prod_{j=1}^k p_j^{\alpha_{nj}-1} \quad (8)$$

which, when normalized to one, results in the probability density function of the Dirichlet distribution (\rightarrow II/4.5.2):

$$p(p|y) = \frac{\Gamma(\sum_{j=1}^k \alpha_{nj})}{\prod_{j=1}^k \Gamma(\alpha_{nj})} \prod_{j=1}^k p_j^{\alpha_{nj}-1} = \text{Dir}(p; \alpha_n) . \quad (9)$$

**Sources:**

- Wikipedia (2020): “Dirichlet distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-03-11; URL: https://en.wikipedia.org/wiki/Dirichlet_distribution#Conjugate_to_categorical/multinomial

3.2.8 Log model evidence

Theorem: Let $y = [y_1, \dots, y_k]$ be the number of observations in k categories resulting from n independent trials with unknown category probabilities $p = [p_1, \dots, p_k]$, such that y follows a multinomial distribution (\rightarrow II/2.2.1):

$$y \sim \text{Mult}(n, p) . \quad (1)$$

Moreover, assume a Dirichlet prior distribution (\rightarrow III/3.2.6) over the model parameter p :

$$p(p) = \text{Dir}(p; \alpha_0) . \quad (2)$$

Then, the log model evidence (\rightarrow IV/3.1.3) for this model is

$$\begin{aligned} \log p(y|m) &= \log \Gamma(n+1) - \sum_{j=1}^k \log \Gamma(y_j+1) \\ &\quad + \log \Gamma\left(\sum_{j=1}^k \alpha_{0j}\right) - \log \Gamma\left(\sum_{j=1}^k \alpha_{nj}\right) \\ &\quad + \sum_{j=1}^k \log \Gamma(\alpha_{nj}) - \sum_{j=1}^k \log \Gamma(\alpha_{0j}) . \end{aligned} \quad (3)$$

and the posterior hyperparameters (\rightarrow I/5.1.9) are given by

$$\alpha_{nj} = \alpha_{0j} + y_j, \quad j = 1, \dots, k . \quad (4)$$

Proof: With the probability mass function of the multinomial distribution (\rightarrow II/2.2.2), the likelihood function (\rightarrow I/5.1.2) implied by (1) is given by

$$p(y|p) = \binom{n}{y_1, \dots, y_k} \prod_{j=1}^k p_j^{y_j} . \quad (5)$$

Combining the likelihood function (5) with the prior distribution (2), the joint likelihood (\rightarrow I/5.1.7) of the model is given by

$$\begin{aligned} p(y, p) &= p(y|p) p(p) \\ &= \binom{n}{y_1, \dots, y_k} \prod_{j=1}^k p_j^{y_j} \cdot \frac{\Gamma\left(\sum_{j=1}^k \alpha_{0j}\right)}{\prod_{j=1}^k \Gamma(\alpha_{0j})} \prod_{j=1}^k p_j^{\alpha_{0j}-1} \\ &= \binom{n}{y_1, \dots, y_k} \frac{\Gamma\left(\sum_{j=1}^k \alpha_{0j}\right)}{\prod_{j=1}^k \Gamma(\alpha_{0j})} \prod_{j=1}^k p_j^{\alpha_{0j}+y_j-1} . \end{aligned} \quad (6)$$

Note that the model evidence is the marginal density of the joint likelihood:

$$p(y) = \int p(y, p) dp. \quad (7)$$

Setting $\alpha_{nj} = \alpha_{0j} + y_j$, the joint likelihood can also be written as

$$p(y, p) = \binom{n}{y_1, \dots, y_k} \frac{\Gamma\left(\sum_{j=1}^k \alpha_{0j}\right)}{\prod_{j=1}^k \Gamma(\alpha_{0j})} \frac{\prod_{j=1}^k \Gamma(\alpha_{nj})}{\Gamma\left(\sum_{j=1}^k \alpha_{nj}\right)} \frac{\Gamma\left(\sum_{j=1}^k \alpha_{nj}\right)}{\prod_{j=1}^k \Gamma(\alpha_{nj})} \prod_{j=1}^k p_j^{\alpha_{nj}-1}. \quad (8)$$

Using the probability density function of the Dirichlet distribution (\rightarrow II/4.5.2), p can now be integrated out easily

$$\begin{aligned} p(y) &= \int \binom{n}{y_1, \dots, y_k} \frac{\Gamma\left(\sum_{j=1}^k \alpha_{0j}\right)}{\prod_{j=1}^k \Gamma(\alpha_{0j})} \frac{\prod_{j=1}^k \Gamma(\alpha_{nj})}{\Gamma\left(\sum_{j=1}^k \alpha_{nj}\right)} \frac{\Gamma\left(\sum_{j=1}^k \alpha_{nj}\right)}{\prod_{j=1}^k \Gamma(\alpha_{nj})} \prod_{j=1}^k p_j^{\alpha_{nj}-1} dp \\ &= \binom{n}{y_1, \dots, y_k} \frac{\Gamma\left(\sum_{j=1}^k \alpha_{0j}\right)}{\prod_{j=1}^k \Gamma(\alpha_{0j})} \frac{\prod_{j=1}^k \Gamma(\alpha_{nj})}{\Gamma\left(\sum_{j=1}^k \alpha_{nj}\right)} \int \text{Dir}(p; \alpha_n) dp \\ &= \binom{n}{y_1, \dots, y_k} \frac{\Gamma\left(\sum_{j=1}^k \alpha_{0j}\right)}{\Gamma\left(\sum_{j=1}^k \alpha_{nj}\right)} \frac{\prod_{j=1}^k \Gamma(\alpha_{nj})}{\prod_{j=1}^k \Gamma(\alpha_{0j})}, \end{aligned} \quad (9)$$

such that the log model evidence (\rightarrow IV/3.1.3) (LME) is shown to be

$$\begin{aligned} \log p(y|m) &= \log \binom{n}{y_1, \dots, y_k} + \log \Gamma\left(\sum_{j=1}^k \alpha_{0j}\right) - \log \Gamma\left(\sum_{j=1}^k \alpha_{nj}\right) \\ &\quad + \sum_{j=1}^k \log \Gamma(\alpha_{nj}) - \sum_{j=1}^k \log \Gamma(\alpha_{0j}). \end{aligned} \quad (10)$$

With the definition of the multinomial coefficient

$$\binom{n}{k_1, \dots, k_m} = \frac{n!}{k_1! \cdot \dots \cdot k_m!} \quad (11)$$

and the definition of the gamma function

$$\Gamma(n) = (n-1)!, \quad (12)$$

the LME finally becomes

$$\begin{aligned}
\log p(y|m) &= \log \Gamma(n+1) - \sum_{j=1}^k \log \Gamma(y_j+1) \\
&\quad + \log \Gamma\left(\sum_{j=1}^k \alpha_{0j}\right) - \log \Gamma\left(\sum_{j=1}^k \alpha_{nj}\right) \\
&\quad + \sum_{j=1}^k \log \Gamma(\alpha_{nj}) - \sum_{j=1}^k \log \Gamma(\alpha_{0j}) .
\end{aligned} \tag{13}$$

■

3.2.9 Log Bayes factor

Theorem: Let $y = [y_1, \dots, y_k]$ be the number of observations in k categories resulting from n independent trials with unknown category probabilities $p = [p_1, \dots, p_k]$, such that y follows a multinomial distribution (\rightarrow II/2.2.1):

$$y \sim \text{Mult}(n, p) . \tag{1}$$

Moreover, assume two statistical models (\rightarrow I/5.1.6), one assuming that each p_j is $1/k$ (null model (\rightarrow I/4.3.2)), the other imposing a Dirichlet distribution (\rightarrow III/3.2.6) as the prior distribution (\rightarrow I/5.1.3) on the model parameters p_1, \dots, p_k (alternative (\rightarrow I/4.3.3)):

$$\begin{aligned}
m_0 : y &\sim \text{Mult}(n, p), \quad p = [1/k, \dots, 1/k] \\
m_1 : y &\sim \text{Mult}(n, p), \quad p \sim \text{Dir}(\alpha_0) .
\end{aligned} \tag{2}$$

Then, the log Bayes factor (\rightarrow IV/3.3.6) in favor of m_1 against m_0 is

$$\begin{aligned}
\text{LBF}_{10} &= \log \Gamma\left(\sum_{j=1}^k \alpha_{0j}\right) - \log \Gamma\left(\sum_{j=1}^k \alpha_{nj}\right) \\
&\quad + \sum_{j=1}^k \log \Gamma(\alpha_{nj}) - \sum_{j=1}^k \log \Gamma(\alpha_{0j}) - n \log\left(\frac{1}{k}\right)
\end{aligned} \tag{3}$$

where $\Gamma(x)$ is the gamma function and α_n are the posterior hyperparameters for multinomial observations (\rightarrow III/3.2.7) which are functions of the numbers of observations (\rightarrow II/2.2.1) y_1, \dots, y_k .

Proof: The log Bayes factor is equal to the difference of two log model evidences (\rightarrow IV/3.3.8):

$$\text{LBF}_{12} = \text{LME}(m_1) - \text{LME}(m_2) . \tag{4}$$

The LME of the alternative m_1 is equal to the log model evidence for multinomial observations (\rightarrow III/3.2.8):

$$\begin{aligned}
\text{LME}(m_1) = \log p(y|m_1) &= \log \Gamma(n+1) - \sum_{j=1}^k \log \Gamma(y_j+1) \\
&+ \log \Gamma\left(\sum_{j=1}^k \alpha_{0j}\right) - \log \Gamma\left(\sum_{j=1}^k \alpha_{nj}\right) \\
&+ \sum_{j=1}^k \log \Gamma(\alpha_{nj}) - \sum_{j=1}^k \log \Gamma(\alpha_{0j}) .
\end{aligned} \tag{5}$$

Because the null model m_0 has no free parameter, its log model evidence (\rightarrow IV/3.1.3) (logarithmized marginal likelihood (\rightarrow I/5.1.15)) is equal to the log-likelihood function for multinomial observations (\rightarrow III/3.2.3) at the value $p_0 = [1/k, \dots, 1/k]$:

$$\begin{aligned}
\text{LME}(m_0) = \log p(y|p=p_0) &= \log \binom{n}{y_1, \dots, y_k} + \sum_{j=1}^k y_j \log \left(\frac{1}{k}\right) \\
&= \log \binom{n}{y_1, \dots, y_k} + n \log \left(\frac{1}{k}\right) .
\end{aligned} \tag{6}$$

Subtracting the two LMEs from each other, the LBF emerges as

$$\begin{aligned}
\text{LBF}_{10} &= \log \Gamma\left(\sum_{j=1}^k \alpha_{0j}\right) - \log \Gamma\left(\sum_{j=1}^k \alpha_{nj}\right) \\
&+ \sum_{j=1}^k \log \Gamma(\alpha_{nj}) - \sum_{j=1}^k \log \Gamma(\alpha_{0j}) - n \log \left(\frac{1}{k}\right)
\end{aligned} \tag{7}$$

where the posterior hyperparameters (\rightarrow I/5.1.9) are given by (\rightarrow III/3.2.7)

$$\begin{aligned}
\alpha_n &= \alpha_0 + y \\
&= [\alpha_{01}, \dots, \alpha_{0k}] + [y_1, \dots, y_k] \\
&= [\alpha_{01} + y_1, \dots, \alpha_{0k} + y_k] \\
\text{i.e. } \alpha_{nj} &= \alpha_{0j} + y_j \quad \text{for all } j = 1, \dots, k
\end{aligned} \tag{8}$$

with the numbers of observations (\rightarrow II/2.2.1) y_1, \dots, y_k .

■

3.2.10 Posterior probability

Theorem: Let $y = [y_1, \dots, y_k]$ be the number of observations in k categories resulting from n independent trials with unknown category probabilities $p = [p_1, \dots, p_k]$, such that y follows a multinomial distribution (\rightarrow II/2.2.1):

$$y \sim \text{Mult}(n, p) . \tag{1}$$

Moreover, assume two statistical models (\rightarrow I/5.1.6), one assuming that each p_j is $1/k$ (null model (\rightarrow I/4.3.2)), the other imposing a Dirichlet distribution (\rightarrow III/3.2.6) as the prior distribution (\rightarrow I/5.1.3) on the model parameters p_1, \dots, p_k (alternative (\rightarrow I/4.3.3)):

$$\begin{aligned} m_0 : y &\sim \text{Mult}(n, p), \quad p = [1/k, \dots, 1/k] \\ m_1 : y &\sim \text{Mult}(n, p), \quad p \sim \text{Dir}(\alpha_0) . \end{aligned} \quad (2)$$

Then, the posterior probability (\rightarrow IV/3.4.1) of the alternative model (\rightarrow I/4.3.3) is given by

$$p(m_1|y) = \frac{1}{1 + k^{-n} \cdot \frac{\Gamma(\sum_{j=1}^k \alpha_{nj})}{\Gamma(\sum_{j=1}^k \alpha_{0j})} \cdot \frac{\prod_{j=1}^k \Gamma(\alpha_{0j})}{\prod_{j=1}^k \Gamma(\alpha_{nj})}} \quad (3)$$

where $\Gamma(x)$ is the gamma function and α_n are the posterior hyperparameters for multinomial observations (\rightarrow III/3.2.7) which are functions of the numbers of observations (\rightarrow II/2.2.1) y_1, \dots, y_k .

Proof: The posterior probability for one of two models is a function of the log Bayes factor in favor of this model (\rightarrow IV/3.4.4):

$$p(m_1|y) = \frac{\exp(\text{LBF}_{12})}{\exp(\text{LBF}_{12}) + 1} . \quad (4)$$

The log Bayes factor in favor of the alternative model for multinomial observations (\rightarrow III/3.2.9) is given by

$$\begin{aligned} \text{LBF}_{10} &= \log \Gamma \left(\sum_{j=1}^k \alpha_{0j} \right) - \log \Gamma \left(\sum_{j=1}^k \alpha_{nj} \right) \\ &\quad + \sum_{j=1}^k \log \Gamma(\alpha_{nj}) - \sum_{j=1}^k \log \Gamma(\alpha_{0j}) - n \log \left(\frac{1}{k} \right) \end{aligned} \quad (5)$$

and the corresponding Bayes factor (\rightarrow IV/3.3.1), i.e. exponentiated log Bayes factor (\rightarrow IV/3.3.7), is equal to

$$\text{BF}_{10} = \exp(\text{LBF}_{10}) = k^n \cdot \frac{\Gamma \left(\sum_{j=1}^k \alpha_{0j} \right)}{\Gamma \left(\sum_{j=1}^k \alpha_{nj} \right)} \cdot \frac{\prod_{j=1}^k \Gamma(\alpha_{nj})}{\prod_{j=1}^k \Gamma(\alpha_{0j})} . \quad (6)$$

Thus, the posterior probability of the alternative, assuming a prior distribution over the probabilities p_1, \dots, p_k , compared to the null model, assuming fixed probabilities $p = [1/k, \dots, 1/k]$, follows as

$$\begin{aligned}
p(m_1|y) &\stackrel{(4)}{=} \frac{\exp(\text{LBF}_{10})}{\exp(\text{LBF}_{10}) + 1} \\
&\stackrel{(6)}{=} \frac{k^n \cdot \frac{\Gamma(\sum_{j=1}^k \alpha_{0j})}{\Gamma(\sum_{j=1}^k \alpha_{nj})} \cdot \frac{\prod_{j=1}^k \Gamma(\alpha_{nj})}{\prod_{j=1}^k \Gamma(\alpha_{0j})}}{k^n \cdot \frac{\Gamma(\sum_{j=1}^k \alpha_{0j})}{\Gamma(\sum_{j=1}^k \alpha_{nj})} \cdot \frac{\prod_{j=1}^k \Gamma(\alpha_{nj})}{\prod_{j=1}^k \Gamma(\alpha_{0j})} + 1} \\
&= \frac{k^n \cdot \frac{\Gamma(\sum_{j=1}^k \alpha_{0j})}{\Gamma(\sum_{j=1}^k \alpha_{nj})} \cdot \frac{\prod_{j=1}^k \Gamma(\alpha_{nj})}{\prod_{j=1}^k \Gamma(\alpha_{0j})}}{1 + k^{-n} \cdot \frac{\Gamma(\sum_{j=1}^k \alpha_{nj})}{\Gamma(\sum_{j=1}^k \alpha_{0j})} \cdot \frac{\prod_{j=1}^k \Gamma(\alpha_{0j})}{\prod_{j=1}^k \Gamma(\alpha_{nj})}} \\
&= \frac{1}{1 + k^{-n} \cdot \frac{\Gamma(\sum_{j=1}^k \alpha_{nj})}{\Gamma(\sum_{j=1}^k \alpha_{0j})} \cdot \frac{\prod_{j=1}^k \Gamma(\alpha_{0j})}{\prod_{j=1}^k \Gamma(\alpha_{nj})}}
\end{aligned} \tag{7}$$

where the posterior hyperparameters (\rightarrow I/5.1.9) are given by (\rightarrow III/3.2.7)

$$\alpha_n = \alpha_0 + y, \quad \text{i.e.} \quad \alpha_{nj} = \alpha_{0j} + y_j \tag{8}$$

with the numbers of observations (\rightarrow II/2.2.1) y_1, \dots, y_k .

■

3.2.11 Cross-validated log model evidence

Theorem: Let $y = [y_1, \dots, y_k] \in \mathbb{N}_0^{1 \times k}$ be the number of observations in k categories resulting from n independent trials with unknown category probabilities $p = [p_1, \dots, p_k]$, such that y follows a multinomial distribution (\rightarrow II/2.2.1):

$$y \sim \text{Mult}(n, p) . \tag{1}$$

Moreover, assume two statistical models (\rightarrow I/5.1.6), one assuming that each p_j is $1/k$ (null model (\rightarrow I/4.3.2)), the other imposing a Dirichlet distribution (\rightarrow III/3.2.6) as the prior distribution (\rightarrow I/5.1.3) on the model parameters p_1, \dots, p_k (alternative (\rightarrow I/4.3.3)):

$$\begin{aligned}
m_0 : y &\sim \text{Mult}(n, p), \quad p = [1/k, \dots, 1/k] \\
m_1 : y &\sim \text{Mult}(n, p), \quad p \sim \text{Dir}(\alpha_0) .
\end{aligned} \tag{2}$$

Then, the cross-validated log model evidences (\rightarrow IV/3.1.9) of m_0 and m_1 are

$$\begin{aligned}
\text{cvLME}(m_0) &= -n \log(k) + \sum_{i=1}^S \left[\log \left(\binom{n_2}{y_{21}^{(i)}, \dots, y_{2k}^{(i)}} \right) \right] \\
\text{cvLME}(m_1) &= S \cdot \log \frac{\Gamma(n_1)}{\Gamma(y)} + \sum_{i=1}^S \left[\log \left(\binom{n_2}{y_{21}^{(i)}, \dots, y_{2k}^{(i)}} \right) - \sum_{j=1}^k \log \left(\frac{y_{1j}^{(i)}}{y_j} \right) \right] .
\end{aligned} \tag{3}$$

where $y_1^{(i)}$ and $y_2^{(i)}$ are the training and test data, respectively, in the i -th cross-validation fold with n_1 and n_2 data points, respectively, S is the number of data subsets (\rightarrow IV/3.1.9) and $\Gamma(x)$ is the gamma function.

Proof: For evaluation of the cross-validated log model evidences (\rightarrow IV/3.1.9) (cvLME), we assume that n data points are divided into $S \mid n$ data subsets without remainder. Then, the number of training data points n_1 and test data points n_2 are given by

$$\begin{aligned} n &= n_1 + n_2 \\ n_1 &= \frac{S-1}{S}n \\ n_2 &= \frac{1}{S}n, \end{aligned} \quad (4)$$

such that $y_1^{(i)}$ are the number of category observations (\rightarrow II/2.2.1) from the n_1 trials of the training set (\rightarrow III/3.2.1) and $y_2^{(i)}$ is the number of category observations (\rightarrow II/2.2.1) from the n_2 trials of the test set (\rightarrow III/3.2.1) in the i -th cross-validation fold and it holds that

$$y = y_1^{(i)} + y_2^{(i)} \quad (5)$$

as well as

$$\begin{aligned} n &= \sum_{j=1}^k y_j \\ n_1 &= \sum_{j=1}^k y_{1j}^{(i)} \\ n_2 &= \sum_{j=1}^k y_{2j}^{(i)}. \end{aligned} \quad (6)$$

First, we consider the null model m_0 assuming $p_j = 1/k$ for each $j = 1, \dots, k$. Because this model has no free parameter, nothing is estimated from the training data and the assumed parameter value is applied to the test data. Consequently, the out-of-sample log model evidence (\rightarrow IV/3.1.9) (oosLME) is equal to the log-likelihood function (\rightarrow III/3.2.3) of the test data at $p = [1/k, \dots, 1/k]$:

$$\begin{aligned} \text{oosLME}_i(m_0) &= \log p \left(y_2^{(i)} \mid p = [1/k, \dots, 1/k] \right) \\ &= \log \binom{n_2}{y_{21}^{(i)}, \dots, y_{2k}^{(i)}} + \sum_{j=1}^k y_{2j}^{(i)} \log(1/k) \\ &= \log \binom{n_2}{y_{21}^{(i)}, \dots, y_{2k}^{(i)}} + n_2 \log \frac{1}{k}. \end{aligned} \quad (7)$$

By definition, the cross-validated log model evidence is the sum of out-of-sample log model evidences (\rightarrow IV/3.1.9) over cross-validation folds, such that the cvLME of m_0 is:

$$\begin{aligned}
\text{cvLME}(m_0) &= \sum_{i=1}^S \text{oosLME}_i(m_0) \\
&= \sum_{i=1}^S \left[\log \binom{n_2}{y_{21}^{(i)}, \dots, y_{2k}^{(i)}} + n_2 \log \left(\frac{1}{k} \right) \right] \\
&= S \cdot n_2 \log \left(\frac{1}{k} \right) + \sum_{i=1}^S \left[\log \binom{n_2}{y_{21}^{(i)}, \dots, y_{2k}^{(i)}} \right] \\
&= -n \log(k) + \sum_{i=1}^S \left[\log \binom{n_2}{y_{21}^{(i)}, \dots, y_{2k}^{(i)}} \right].
\end{aligned} \tag{8}$$

Next, we have a look at the alternative m_1 assuming $p_j = 1/k$ for at least one $j = 1, \dots, k$. First, the training data $y_1^{(i)}$ are analyzed using a non-informative prior distribution (\rightarrow I/5.2.3) and applying the posterior distribution for multinomial observations (\rightarrow III/3.2.7):

$$\alpha_0^{(1)} = 0_{1k} \quad \Rightarrow \quad \alpha_n^{(1)} = \alpha_0^{(1)} + y_1^{(i)} = y_1^{(i)}. \tag{9}$$

This results in a posterior characterized by $\alpha_n^{(1)}$. Then, the test data $y_2^{(i)}$ are analyzed using this posterior as an informative prior distribution (\rightarrow I/5.2.3), again applying the posterior distribution for multinomial observations (\rightarrow III/3.2.7):

$$\alpha_0^{(2)} = \alpha_n^{(1)} = y_1^{(i)} \quad \Rightarrow \quad \alpha_n^{(2)} = \alpha_0^{(2)} + y_2^{(i)} = y. \tag{10}$$

In the test data, we now have a prior characterized by $\alpha_0^{(2)}$ and a posterior characterized $\alpha_n^{(2)}$. Applying the log model evidence for multinomial observations (\rightarrow III/3.2.8), the out-of-sample log model evidence (\rightarrow IV/3.1.9) (oosLME) therefore follows as

$$\begin{aligned}
\text{oosLME}_i(m_1) &= \log \binom{n_2}{y_{21}^{(i)}, \dots, y_{2k}^{(i)}} + \log \Gamma \left(\sum_{j=1}^k \alpha_{0j}^{(2)} \right) - \log \Gamma \left(\sum_{j=1}^k \alpha_{nj}^{(2)} \right) \\
&\quad + \sum_{j=1}^k \log \Gamma(\alpha_{nj}^{(2)}) - \sum_{j=1}^k \log \Gamma(\alpha_{0j}^{(2)}) \\
&= \log \binom{n_2}{y_{21}^{(i)}, \dots, y_{2k}^{(i)}} + \log \Gamma \left(\sum_{j=1}^k y_{1j}^{(i)} \right) - \log \Gamma \left(\sum_{j=1}^k y_j \right) \\
&\quad + \sum_{j=1}^k \log \Gamma(y_j) - \sum_{j=1}^k \log \Gamma(y_{1j}^{(i)}) \\
&= \log \binom{n_2}{y_{21}^{(i)}, \dots, y_{2k}^{(i)}} + \log \frac{\Gamma(n_1)}{\Gamma(y)} - \sum_{j=1}^k \log \left(\frac{y_{1j}^{(i)}}{y_j} \right).
\end{aligned} \tag{11}$$

Again, because the cross-validated log model evidence is the sum of out-of-sample log model evidences (\rightarrow IV/3.1.9) over cross-validation folds, the cvLME of m_1 becomes:

$$\begin{aligned}
\text{cvLME}(m_1) &= \sum_{i=1}^S \text{oosLME}_i(m_1) \\
&= \sum_{i=1}^S \left[\log \binom{n_2}{y_{21}^{(i)}, \dots, y_{2k}^{(i)}} + \log \frac{\Gamma(n_1)}{\Gamma(y)} - \sum_{j=1}^k \log \left(\frac{y_{1j}^{(i)}}{y_j} \right) \right] \\
&= S \cdot \log \frac{\Gamma(n_1)}{\Gamma(y)} + \sum_{i=1}^S \left[\log \binom{n_2}{y_{21}^{(i)}, \dots, y_{2k}^{(i)}} - \sum_{j=1}^k \log \left(\frac{y_{1j}^{(i)}}{y_j} \right) \right].
\end{aligned} \tag{12}$$

Together, (8) and (12) conform to the results given in (3). ■

3.3 Poisson-distributed data

3.3.1 Definition

Definition: Poisson-distributed data are defined as a set of observed counts $y = \{y_1, \dots, y_n\}$, independent and identically distributed (\rightarrow I/1.2.8) according to a Poisson distribution (\rightarrow II/1.5.1) with rate λ :

$$y_i \sim \text{Poiss}(\lambda), \quad i = 1, \dots, n. \tag{1}$$

Sources:

- Wikipedia (2020): “Poisson distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-03-22; URL: https://en.wikipedia.org/wiki/Poisson_distribution#Parameter_estimation.

3.3.2 Maximum likelihood estimation

Theorem: Let there be a Poisson-distributed data (\rightarrow III/3.3.1) set $y = \{y_1, \dots, y_n\}$:

$$y_i \sim \text{Poiss}(\lambda), \quad i = 1, \dots, n. \tag{1}$$

Then, the maximum likelihood estimate (\rightarrow I/4.1.3) for the rate parameter λ is given by

$$\hat{\lambda} = \bar{y} \tag{2}$$

where \bar{y} is the sample mean (\rightarrow I/1.12.2)

$$\bar{y} = \frac{1}{n} \sum_{i=1}^n y_i. \tag{3}$$

Proof: The likelihood function (\rightarrow I/5.1.2) for each observation is given by the probability mass function of the Poisson distribution (\rightarrow II/1.5.2)

$$p(y_i | \lambda) = \text{Poiss}(y_i; \lambda) = \frac{\lambda^{y_i} \cdot \exp(-\lambda)}{y_i!} \tag{4}$$

and because observations are independent (\rightarrow I/1.3.6), the likelihood function for all observations is the product of the individual ones:

$$p(y|\lambda) = \prod_{i=1}^n p(y_i|\lambda) = \prod_{i=1}^n \frac{\lambda^{y_i} \cdot \exp(-\lambda)}{y_i!} . \quad (5)$$

Thus, the log-likelihood function (\rightarrow I/4.1.2) is

$$\text{LL}(\lambda) = \log p(y|\lambda) = \log \left[\prod_{i=1}^n \frac{\lambda^{y_i} \cdot \exp(-\lambda)}{y_i!} \right] \quad (6)$$

which can be developed into

$$\begin{aligned} \text{LL}(\lambda) &= \sum_{i=1}^n \log \left[\frac{\lambda^{y_i} \cdot \exp(-\lambda)}{y_i!} \right] \\ &= \sum_{i=1}^n [y_i \cdot \log(\lambda) - \lambda - \log(y_i!)] \\ &= - \sum_{i=1}^n \lambda + \sum_{i=1}^n y_i \cdot \log(\lambda) - \sum_{i=1}^n \log(y_i!) \\ &= -n\lambda + \log(\lambda) \sum_{i=1}^n y_i - \sum_{i=1}^n \log(y_i!) \end{aligned} \quad (7)$$

The derivatives of the log-likelihood with respect to λ are

$$\begin{aligned} \frac{d\text{LL}(\lambda)}{d\lambda} &= \frac{1}{\lambda} \sum_{i=1}^n y_i - n \\ \frac{d^2\text{LL}(\lambda)}{d\lambda^2} &= -\frac{1}{\lambda^2} \sum_{i=1}^n y_i . \end{aligned} \quad (8)$$

Setting the first derivative to zero, we obtain:

$$\begin{aligned} \frac{d\text{LL}(\hat{\lambda})}{d\lambda} &= 0 \\ 0 &= \frac{1}{\hat{\lambda}} \sum_{i=1}^n y_i - n \\ \hat{\lambda} &= \frac{1}{n} \sum_{i=1}^n y_i = \bar{y} . \end{aligned} \quad (9)$$

Plugging this value into the second derivative, we confirm:

$$\begin{aligned} \frac{d^2\text{LL}(\hat{\lambda})}{d\lambda^2} &= -\frac{1}{\bar{y}^2} \sum_{i=1}^n y_i \\ &= -\frac{n \cdot \bar{y}}{\bar{y}^2} \\ &= -\frac{n}{\bar{y}} < 0 . \end{aligned} \quad (10)$$

This demonstrates that the estimate $\hat{\lambda} = \bar{y}$ maximizes the likelihood $p(y|\lambda)$.

■

3.3.3 Conjugate prior distribution

Theorem: Let there be a Poisson-distributed data (\rightarrow III/3.3.1) set $y = \{y_1, \dots, y_n\}$:

$$y_i \sim \text{Pois}(\lambda), \quad i = 1, \dots, n. \quad (1)$$

Then, the conjugate prior (\rightarrow I/5.2.5) for the model parameter λ is a gamma distribution (\rightarrow II/3.4.1):

$$p(\lambda) = \text{Gam}(\lambda; a_0, b_0). \quad (2)$$

Proof: With the probability mass function of the Poisson distribution (\rightarrow II/1.5.2), the likelihood function (\rightarrow I/5.1.2) for each observation implied by (1) is given by

$$p(y_i|\lambda) = \text{Pois}(y_i; \lambda) = \frac{\lambda^{y_i} \cdot \exp[-\lambda]}{y_i!} \quad (3)$$

and because observations are independent (\rightarrow I/1.3.6), the likelihood function for all observations is the product of the individual ones:

$$p(y|\lambda) = \prod_{i=1}^n p(y_i|\lambda) = \prod_{i=1}^n \frac{\lambda^{y_i} \cdot \exp[-\lambda]}{y_i!}. \quad (4)$$

Resolving the product in the likelihood function, we have

$$\begin{aligned} p(y|\lambda) &= \prod_{i=1}^n \frac{1}{y_i!} \cdot \prod_{i=1}^n \lambda^{y_i} \cdot \prod_{i=1}^n \exp[-\lambda] \\ &= \prod_{i=1}^n \left(\frac{1}{y_i!} \right) \cdot \lambda^{n\bar{y}} \cdot \exp[-n\lambda] \end{aligned} \quad (5)$$

where \bar{y} is the mean (\rightarrow I/1.12.2) of y :

$$\bar{y} = \frac{1}{n} \sum_{i=1}^n y_i. \quad (6)$$

In other words, the likelihood function is proportional to a power of λ times an exponential of λ :

$$p(y|\lambda) \propto \lambda^{n\bar{y}} \cdot \exp[-n\lambda]. \quad (7)$$

The same is true for a gamma distribution over λ

$$p(\lambda) = \text{Gam}(\lambda; a_0, b_0) \quad (8)$$

the probability density function of which (\rightarrow II/3.4.7)

$$p(\lambda) = \frac{b_0^{a_0}}{\Gamma(a_0)} \lambda^{a_0-1} \exp[-b_0\lambda] \quad (9)$$

exhibits the same proportionality

$$p(\lambda) \propto \lambda^{a_0-1} \cdot \exp[-b_0\lambda] \quad (10)$$

and is therefore conjugate relative to the likelihood. ■

Sources:

- Gelman A, Carlin JB, Stern HS, Dunson DB, Vehtari A, Rubin DB (2014): “Other standard single-parameter models”; in: *Bayesian Data Analysis*, 3rd edition, ch. 2.6, p. 45, eq. 2.14ff.; URL: <http://www.stat.columbia.edu/~gelman/book/>.

3.3.4 Posterior distribution

Theorem: Let there be a Poisson-distributed data (\rightarrow III/3.3.1) set $y = \{y_1, \dots, y_n\}$:

$$y_i \sim \text{Poiss}(\lambda), \quad i = 1, \dots, n. \quad (1)$$

Moreover, assume a gamma prior distribution (\rightarrow III/3.3.3) over the model parameter λ :

$$p(\lambda) = \text{Gam}(\lambda; a_0, b_0). \quad (2)$$

Then, the posterior distribution (\rightarrow I/5.1.9) is also a gamma distribution (\rightarrow II/3.4.1)

$$p(\lambda|y) = \text{Gam}(\lambda; a_n, b_n) \quad (3)$$

and the posterior hyperparameters (\rightarrow I/5.1.9) are given by

$$\begin{aligned} a_n &= a_0 + n\bar{y} \\ b_n &= b_0 + n. \end{aligned} \quad (4)$$

Proof: With the probability mass function of the Poisson distribution (\rightarrow II/1.5.2), the likelihood function (\rightarrow I/5.1.2) for each observation implied by (1) is given by

$$p(y_i|\lambda) = \text{Poiss}(y_i; \lambda) = \frac{\lambda^{y_i} \cdot \exp[-\lambda]}{y_i!} \quad (5)$$

and because observations are independent (\rightarrow I/1.3.6), the likelihood function for all observations is the product of the individual ones:

$$p(y|\lambda) = \prod_{i=1}^n p(y_i|\lambda) = \prod_{i=1}^n \frac{\lambda^{y_i} \cdot \exp[-\lambda]}{y_i!}. \quad (6)$$

Combining the likelihood function (6) with the prior distribution (2), the joint likelihood (\rightarrow I/5.1.7) of the model is given by

$$\begin{aligned} p(y, \lambda) &= p(y|\lambda) p(\lambda) \\ &= \prod_{i=1}^n \frac{\lambda^{y_i} \cdot \exp[-\lambda]}{y_i!} \cdot \frac{b_0^{a_0}}{\Gamma(a_0)} \lambda^{a_0-1} \exp[-b_0\lambda]. \end{aligned} \quad (7)$$

Resolving the product in the joint likelihood, we have

$$\begin{aligned}
 p(y, \lambda) &= \prod_{i=1}^n \frac{1}{y_i!} \prod_{i=1}^n \lambda^{y_i} \prod_{i=1}^n \exp[-\lambda] \cdot \frac{b_0^{a_0}}{\Gamma(a_0)} \lambda^{a_0-1} \exp[-b_0 \lambda] \\
 &= \prod_{i=1}^n \left(\frac{1}{y_i!} \right) \lambda^{n\bar{y}} \exp[-n\lambda] \cdot \frac{b_0^{a_0}}{\Gamma(a_0)} \lambda^{a_0-1} \exp[-b_0 \lambda] \\
 &= \prod_{i=1}^n \left(\frac{1}{y_i!} \right) \cdot \frac{b_0^{a_0}}{\Gamma(a_0)} \cdot \lambda^{a_0+n\bar{y}-1} \cdot \exp[-(b_0 + n\lambda)]
 \end{aligned} \tag{8}$$

where \bar{y} is the mean (\rightarrow I/1.12.2) of y :

$$\bar{y} = \frac{1}{n} \sum_{i=1}^n y_i . \tag{9}$$

Note that the posterior distribution is proportional to the joint likelihood (\rightarrow I/5.1.10):

$$p(\lambda|y) \propto p(y, \lambda) . \tag{10}$$

Setting $a_n = a_0 + n\bar{y}$ and $b_n = b_0 + n$, the posterior distribution is therefore proportional to

$$p(\lambda|y) \propto \lambda^{a_n-1} \cdot \exp[-b_n \lambda] \tag{11}$$

which, when normalized to one, results in the probability density function of the gamma distribution (\rightarrow II/3.4.7):

$$p(\lambda|y) = \frac{b_n^{a_n}}{\Gamma(a_n)} \lambda^{a_n-1} \exp[-b_n \lambda] = \text{Gam}(\lambda; a_n, b_n) . \tag{12}$$

■

Sources:

- Gelman A, Carlin JB, Stern HS, Dunson DB, Vehtari A, Rubin DB (2014): “Other standard single-parameter models”; in: *Bayesian Data Analysis*, 3rd edition, ch. 2.6, p. 45, eq. 2.15; URL: <http://www.stat.columbia.edu/~gelman/book/>.

3.3.5 Log model evidence

Theorem: Let there be a Poisson-distributed data (\rightarrow III/3.3.1) set $y = \{y_1, \dots, y_n\}$:

$$y_i \sim \text{Pois}(\lambda), \quad i = 1, \dots, n . \tag{1}$$

Moreover, assume a gamma prior distribution (\rightarrow III/3.3.3) over the model parameter λ :

$$p(\lambda) = \text{Gam}(\lambda; a_0, b_0) . \tag{2}$$

Then, the log model evidence (\rightarrow IV/3.1.3) for this model is

$$\log p(y|m) = - \sum_{i=1}^n \log y_i! + \log \Gamma(a_n) - \log \Gamma(a_0) + a_0 \log b_0 - a_n \log b_n . \tag{3}$$

where the posterior hyperparameters (\rightarrow I/5.1.9) are given by

$$\begin{aligned} a_n &= a_0 + n\bar{y} \\ b_n &= b_0 + n . \end{aligned} \quad (4)$$

Proof: With the probability mass function of the Poisson distribution (\rightarrow II/1.5.2), the likelihood function (\rightarrow I/5.1.2) for each observation implied by (1) is given by

$$p(y_i|\lambda) = \text{Poiss}(y_i; \lambda) = \frac{\lambda^{y_i} \cdot \exp[-\lambda]}{y_i!} \quad (5)$$

and because observations are independent (\rightarrow I/1.3.6), the likelihood function for all observations is the product of the individual ones:

$$p(y|\lambda) = \prod_{i=1}^n p(y_i|\lambda) = \prod_{i=1}^n \frac{\lambda^{y_i} \cdot \exp[-\lambda]}{y_i!} . \quad (6)$$

Combining the likelihood function (6) with the prior distribution (2), the joint likelihood (\rightarrow I/5.1.7) of the model is given by

$$\begin{aligned} p(y, \lambda) &= p(y|\lambda) p(\lambda) \\ &= \prod_{i=1}^n \frac{\lambda^{y_i} \cdot \exp[-\lambda]}{y_i!} \cdot \frac{b_0^{a_0}}{\Gamma(a_0)} \lambda^{a_0-1} \exp[-b_0\lambda] . \end{aligned} \quad (7)$$

Resolving the product in the joint likelihood, we have

$$\begin{aligned} p(y, \lambda) &= \prod_{i=1}^n \frac{1}{y_i!} \prod_{i=1}^n \lambda^{y_i} \prod_{i=1}^n \exp[-\lambda] \cdot \frac{b_0^{a_0}}{\Gamma(a_0)} \lambda^{a_0-1} \exp[-b_0\lambda] \\ &= \prod_{i=1}^n \left(\frac{1}{y_i!} \right) \lambda^{n\bar{y}} \exp[-n\lambda] \cdot \frac{b_0^{a_0}}{\Gamma(a_0)} \lambda^{a_0-1} \exp[-b_0\lambda] \\ &= \prod_{i=1}^n \left(\frac{1}{y_i!} \right) \cdot \frac{b_0^{a_0}}{\Gamma(a_0)} \cdot \lambda^{a_0+n\bar{y}-1} \cdot \exp[-(b_0 + n\lambda)] \end{aligned} \quad (8)$$

where \bar{y} is the mean (\rightarrow I/1.12.2) of y :

$$\bar{y} = \frac{1}{n} \sum_{i=1}^n y_i . \quad (9)$$

Note that the model evidence is the marginal density of the joint likelihood (\rightarrow I/5.1.15):

$$p(y) = \int p(y, \lambda) d\lambda . \quad (10)$$

Setting $a_n = a_0 + n\bar{y}$ and $b_n = b_0 + n$, the joint likelihood can also be written as

$$p(y, \lambda) = \prod_{i=1}^n \left(\frac{1}{y_i!} \right) \frac{b_0^{a_0}}{\Gamma(a_0)} \frac{\Gamma(a_n)}{b_n^{a_n}} \cdot \frac{b_n^{a_n}}{\Gamma(a_n)} \lambda^{a_n-1} \exp[-b_n\lambda] . \quad (11)$$

Using the probability density function of the gamma distribution (\rightarrow II/3.4.7), λ can now be integrated out easily

$$\begin{aligned} p(y) &= \int \prod_{i=1}^n \left(\frac{1}{y_i!} \right) \frac{b_0^{a_0}}{\Gamma(a_0)} \frac{\Gamma(a_n)}{b_n^{a_n}} \cdot \frac{b_n^{a_n}}{\Gamma(a_n)} \lambda^{a_n-1} \exp[-b_n \lambda] d\lambda \\ &= \prod_{i=1}^n \left(\frac{1}{y_i!} \right) \frac{\Gamma(a_n)}{\Gamma(a_0)} \frac{b_0^{a_0}}{b_n^{a_n}} \int \text{Gam}(\lambda; a_n, b_n) d\lambda \\ &= \prod_{i=1}^n \left(\frac{1}{y_i!} \right) \frac{\Gamma(a_n)}{\Gamma(a_0)} \frac{b_0^{a_0}}{b_n^{a_n}}, \end{aligned} \quad (12)$$

such that the log model evidence (\rightarrow IV/3.1.3) is shown to be

$$\log p(y|m) = - \sum_{i=1}^n \log y_i! + \log \Gamma(a_n) - \log \Gamma(a_0) + a_0 \log b_0 - a_n \log b_n. \quad (13)$$

■

3.4 Poisson distribution with exposure values

3.4.1 Definition

Definition: A Poisson distribution with exposure values is defined as a set of observed counts $y = \{y_1, \dots, y_n\}$, independently (\rightarrow I/1.3.6) distributed (\rightarrow I/1.5.1) according to a Poisson distribution (\rightarrow II/1.5.1) with common rate (\rightarrow I/1.5.10) λ and a set of concurrent exposures $x = \{x_1, \dots, x_n\}$:

$$y_i \sim \text{Poiss}(\lambda x_i), \quad i = 1, \dots, n. \quad (1)$$

Sources:

- Gelman A, Carlin JB, Stern HS, Dunson DB, Vehtari A, Rubin DB (2014): “Other standard single-parameter models”; in: *Bayesian Data Analysis*, 3rd edition, ch. 2.6, p. 45, eq. 2.14; URL: <http://www.stat.columbia.edu/~gelman/book/>.

3.4.2 Maximum likelihood estimation

Theorem: Consider data $y = \{y_1, \dots, y_n\}$ following a Poisson distribution with exposure values (\rightarrow III/3.4.1):

$$y_i \sim \text{Poiss}(\lambda x_i), \quad i = 1, \dots, n. \quad (1)$$

Then, the maximum likelihood estimate (\rightarrow I/4.1.3) for the rate parameter λ is given by

$$\hat{\lambda} = \frac{\bar{y}}{\bar{x}} \quad (2)$$

where \bar{y} and \bar{x} are the sample means (\rightarrow I/1.12.2)

$$\begin{aligned}\bar{y} &= \frac{1}{n} \sum_{i=1}^n y_i \\ \bar{x} &= \frac{1}{n} \sum_{i=1}^n x_i.\end{aligned}\tag{3}$$

Proof: With the probability mass function of the Poisson distribution (\rightarrow II/1.5.2), the likelihood function (\rightarrow I/5.1.2) for each observation implied by (1) is given by

$$p(y_i|\lambda) = \text{Poiss}(y_i; \lambda x_i) = \frac{(\lambda x_i)^{y_i} \cdot \exp[-\lambda x_i]}{y_i!}\tag{4}$$

and because observations are independent (\rightarrow I/1.3.6), the likelihood function for all observations is the product of the individual ones:

$$p(y|\lambda) = \prod_{i=1}^n p(y_i|\lambda) = \prod_{i=1}^n \frac{(\lambda x_i)^{y_i} \cdot \exp[-\lambda x_i]}{y_i!}.\tag{5}$$

Thus, the log-likelihood function (\rightarrow I/4.1.2) is

$$\text{LL}(\lambda) = \log p(y|\lambda) = \log \left[\prod_{i=1}^n \frac{(\lambda x_i)^{y_i} \cdot \exp[-\lambda x_i]}{y_i!} \right]\tag{6}$$

which can be developed into

$$\begin{aligned}\text{LL}(\lambda) &= \sum_{i=1}^n \log \left[\frac{(\lambda x_i)^{y_i} \cdot \exp[-\lambda x_i]}{y_i!} \right] \\ &= \sum_{i=1}^n [y_i \cdot \log(\lambda x_i) - \lambda x_i - \log(y_i!)] \\ &= -\sum_{i=1}^n \lambda x_i + \sum_{i=1}^n y_i \cdot [\log(\lambda) + \log(x_i)] - \sum_{i=1}^n \log(y_i!) \\ &= -\lambda \sum_{i=1}^n x_i + \log(\lambda) \sum_{i=1}^n y_i + \sum_{i=1}^n y_i \log(x_i) - \sum_{i=1}^n \log(y_i!) \\ &= -n\bar{x}\lambda + n\bar{y} \log(\lambda) + \sum_{i=1}^n y_i \log(x_i) - \sum_{i=1}^n \log(y_i!)\end{aligned}\tag{7}$$

where \bar{x} and \bar{y} are the sample means from equation (3).

The derivatives of the log-likelihood with respect to λ are

$$\begin{aligned}\frac{d\text{LL}(\lambda)}{d\lambda} &= -n\bar{x} + \frac{n\bar{y}}{\lambda} \\ \frac{d^2\text{LL}(\lambda)}{d\lambda^2} &= -\frac{n\bar{y}}{\lambda^2}.\end{aligned}\tag{8}$$

Setting the first derivative to zero, we obtain:

$$\begin{aligned}\frac{dLL(\hat{\lambda})}{d\lambda} &= 0 \\ 0 &= -n\bar{x} + \frac{n\bar{y}}{\hat{\lambda}} \\ \hat{\lambda} &= \frac{n\bar{y}}{n\bar{x}} = \frac{\bar{y}}{\bar{x}}.\end{aligned}\tag{9}$$

Plugging this value into the second derivative, we confirm:

$$\begin{aligned}\frac{d^2LL(\hat{\lambda})}{d\lambda^2} &= -\frac{n\bar{y}}{\hat{\lambda}^2} \\ &= -\frac{n \cdot \bar{y}}{(\bar{y}/\bar{x})^2} \\ &= -\frac{n \cdot \bar{x}^2}{\bar{y}} < 0.\end{aligned}\tag{10}$$

This demonstrates that the estimate $\hat{\lambda} = \bar{y}/\bar{x}$ maximizes the likelihood $p(y|\lambda)$. ■

3.4.3 Conjugate prior distribution

Theorem: Consider data $y = \{y_1, \dots, y_n\}$ following a Poisson distribution with exposure values (\rightarrow III/3.4.1):

$$y_i \sim \text{Poiss}(\lambda x_i), \quad i = 1, \dots, n.\tag{1}$$

Then, the conjugate prior (\rightarrow I/5.2.5) for the model parameter λ is a gamma distribution (\rightarrow II/3.4.1):

$$p(\lambda) = \text{Gam}(\lambda; a_0, b_0).\tag{2}$$

Proof: With the probability mass function of the Poisson distribution (\rightarrow II/1.5.2), the likelihood function (\rightarrow I/5.1.2) for each observation implied by (1) is given by

$$p(y_i|\lambda) = \text{Poiss}(y_i; \lambda x_i) = \frac{(\lambda x_i)^{y_i} \cdot \exp[-\lambda x_i]}{y_i!}\tag{3}$$

and because observations are independent (\rightarrow I/1.3.6), the likelihood function for all observations is the product of the individual ones:

$$p(y|\lambda) = \prod_{i=1}^n p(y_i|\lambda) = \prod_{i=1}^n \frac{(\lambda x_i)^{y_i} \cdot \exp[-\lambda x_i]}{y_i!}.\tag{4}$$

Resolving the product in the likelihood function, we have

$$\begin{aligned}
p(y|\lambda) &= \prod_{i=1}^n \frac{x_i^{y_i}}{y_i!} \cdot \prod_{i=1}^n \lambda^{y_i} \cdot \prod_{i=1}^n \exp[-\lambda x_i] \\
&= \prod_{i=1}^n \left(\frac{x_i^{y_i}}{y_i!} \right) \cdot \lambda^{\sum_{i=1}^n y_i} \cdot \exp \left[-\lambda \sum_{i=1}^n x_i \right] \\
&= \prod_{i=1}^n \left(\frac{x_i^{y_i}}{y_i!} \right) \cdot \lambda^{n\bar{y}} \cdot \exp[-n\bar{x}\lambda]
\end{aligned} \tag{5}$$

where \bar{y} and \bar{x} are the means (\rightarrow I/1.12.2) of y and x respectively:

$$\begin{aligned}
\bar{y} &= \frac{1}{n} \sum_{i=1}^n y_i \\
\bar{x} &= \frac{1}{n} \sum_{i=1}^n x_i .
\end{aligned} \tag{6}$$

In other words, the likelihood function is proportional to a power of λ times an exponential of λ :

$$p(y|\lambda) \propto \lambda^{n\bar{y}} \cdot \exp[-n\bar{x}\lambda] . \tag{7}$$

The same is true for a gamma distribution over λ

$$p(\lambda) = \text{Gam}(\lambda; a_0, b_0) \tag{8}$$

the probability density function of which (\rightarrow II/3.4.7)

$$p(\lambda) = \frac{b_0^{a_0}}{\Gamma(a_0)} \lambda^{a_0-1} \exp[-b_0\lambda] \tag{9}$$

exhibits the same proportionality

$$p(\lambda) \propto \lambda^{a_0-1} \cdot \exp[-b_0\lambda] \tag{10}$$

and is therefore conjugate relative to the likelihood. ■

Sources:

- Gelman A, Carlin JB, Stern HS, Dunson DB, Vehtari A, Rubin DB (2014): “Other standard single-parameter models”; in: *Bayesian Data Analysis*, 3rd edition, ch. 2.6, p. 45, eq. 2.14ff.; URL: <http://www.stat.columbia.edu/~gelman/book/>.

3.4.4 Posterior distribution

Theorem: Consider data $y = \{y_1, \dots, y_n\}$ following a Poisson distribution with exposure values (\rightarrow III/3.4.1):

$$y_i \sim \text{Poiss}(\lambda x_i), \quad i = 1, \dots, n . \tag{1}$$

Moreover, assume a gamma prior distribution (\rightarrow III/3.4.3) over the model parameter λ :

$$p(\lambda) = \text{Gam}(\lambda; a_0, b_0) . \quad (2)$$

Then, the posterior distribution (\rightarrow I/5.1.9) is also a gamma distribution (\rightarrow II/3.4.1)

$$p(\lambda|y) = \text{Gam}(\lambda; a_n, b_n) \quad (3)$$

and the posterior hyperparameters (\rightarrow I/5.1.9) are given by

$$\begin{aligned} a_n &= a_0 + n\bar{y} \\ b_n &= b_0 + n\bar{x} . \end{aligned} \quad (4)$$

Proof: With the probability mass function of the Poisson distribution (\rightarrow II/1.5.2), the likelihood function (\rightarrow I/5.1.2) for each observation implied by (1) is given by

$$p(y_i|\lambda) = \text{Poiss}(y_i; \lambda x_i) = \frac{(\lambda x_i)^{y_i} \cdot \exp[-\lambda x_i]}{y_i!} \quad (5)$$

and because observations are independent (\rightarrow I/1.3.6), the likelihood function for all observations is the product of the individual ones:

$$p(y|\lambda) = \prod_{i=1}^n p(y_i|\lambda) = \prod_{i=1}^n \frac{(\lambda x_i)^{y_i} \cdot \exp[-\lambda x_i]}{y_i!} . \quad (6)$$

Combining the likelihood function (6) with the prior distribution (2), the joint likelihood (\rightarrow I/5.1.7) of the model is given by

$$\begin{aligned} p(y, \lambda) &= p(y|\lambda) p(\lambda) \\ &= \prod_{i=1}^n \frac{(\lambda x_i)^{y_i} \cdot \exp[-\lambda x_i]}{y_i!} \cdot \frac{b_0^{a_0}}{\Gamma(a_0)} \lambda^{a_0-1} \exp[-b_0 \lambda] . \end{aligned} \quad (7)$$

Resolving the product in the joint likelihood, we have

$$\begin{aligned} p(y, \lambda) &= \prod_{i=1}^n \frac{x_i^{y_i}}{y_i!} \prod_{i=1}^n \lambda^{y_i} \prod_{i=1}^n \exp[-\lambda x_i] \cdot \frac{b_0^{a_0}}{\Gamma(a_0)} \lambda^{a_0-1} \exp[-b_0 \lambda] \\ &= \prod_{i=1}^n \left(\frac{x_i^{y_i}}{y_i!} \right) \lambda^{\sum_{i=1}^n y_i} \exp \left[-\lambda \sum_{i=1}^n x_i \right] \cdot \frac{b_0^{a_0}}{\Gamma(a_0)} \lambda^{a_0-1} \exp[-b_0 \lambda] \\ &= \prod_{i=1}^n \left(\frac{x_i^{y_i}}{y_i!} \right) \lambda^{n\bar{y}} \exp[-n\bar{x}\lambda] \cdot \frac{b_0^{a_0}}{\Gamma(a_0)} \lambda^{a_0-1} \exp[-b_0 \lambda] \\ &= \prod_{i=1}^n \left(\frac{x_i^{y_i}}{y_i!} \right) \cdot \frac{b_0^{a_0}}{\Gamma(a_0)} \cdot \lambda^{a_0+n\bar{y}-1} \cdot \exp[-(b_0 + n\bar{x})\lambda] \end{aligned} \quad (8)$$

where \bar{y} and \bar{x} are the means (\rightarrow I/1.12.2) of y and x respectively:

$$\begin{aligned}\bar{y} &= \frac{1}{n} \sum_{i=1}^n y_i \\ \bar{x} &= \frac{1}{n} \sum_{i=1}^n x_i .\end{aligned}\tag{9}$$

Note that the posterior distribution is proportional to the joint likelihood (\rightarrow I/5.1.10):

$$p(\lambda|y) \propto p(y, \lambda) .\tag{10}$$

Setting $a_n = a_0 + n\bar{y}$ and $b_n = b_0 + n\bar{x}$, the posterior distribution is therefore proportional to

$$p(\lambda|y) \propto \lambda^{a_n-1} \cdot \exp[-b_n \lambda]\tag{11}$$

which, when normalized to one, results in the probability density function of the gamma distribution (\rightarrow II/3.4.7):

$$p(\lambda|y) = \frac{b_n^{a_n}}{\Gamma(a_n)} \lambda^{a_n-1} \exp[-b_n \lambda] = \text{Gam}(\lambda; a_n, b_n) .\tag{12}$$

■

Sources:

- Gelman A, Carlin JB, Stern HS, Dunson DB, Vehtari A, Rubin DB (2014): “Other standard single-parameter models”; in: *Bayesian Data Analysis*, 3rd edition, ch. 2.6, p. 45, eq. 2.15; URL: <http://www.stat.columbia.edu/~gelman/book/>.

3.4.5 Log model evidence

Theorem: Consider data $y = \{y_1, \dots, y_n\}$ following a Poisson distribution with exposure values (\rightarrow III/3.4.1):

$$y_i \sim \text{Poiss}(\lambda x_i), \quad i = 1, \dots, n .\tag{1}$$

Moreover, assume a gamma prior distribution (\rightarrow III/3.4.3) over the model parameter λ :

$$p(\lambda) = \text{Gam}(\lambda; a_0, b_0) .\tag{2}$$

Then, the log model evidence (\rightarrow IV/3.1.3) for this model is

$$\begin{aligned}\log p(y|m) &= \sum_{i=1}^n y_i \log(x_i) - \sum_{i=1}^n \log y_i! + \\ &\quad \log \Gamma(a_n) - \log \Gamma(a_0) + a_0 \log b_0 - a_n \log b_n .\end{aligned}\tag{3}$$

where the posterior hyperparameters (\rightarrow I/5.1.9) are given by

$$\begin{aligned}a_n &= a_0 + n\bar{y} \\ b_n &= b_0 + n\bar{x} .\end{aligned}\tag{4}$$

Proof: With the probability mass function of the Poisson distribution (\rightarrow II/1.5.2), the likelihood function (\rightarrow I/5.1.2) for each observation implied by (1) is given by

$$p(y_i|\lambda) = \text{Poiss}(y_i; \lambda x_i) = \frac{(\lambda x_i)^{y_i} \cdot \exp[-\lambda x_i]}{y_i!} \quad (5)$$

and because observations are independent (\rightarrow I/1.3.6), the likelihood function for all observations is the product of the individual ones:

$$p(y|\lambda) = \prod_{i=1}^n p(y_i|\lambda) = \prod_{i=1}^n \frac{(\lambda x_i)^{y_i} \cdot \exp[-\lambda x_i]}{y_i!} . \quad (6)$$

Combining the likelihood function (6) with the prior distribution (2), the joint likelihood (\rightarrow I/5.1.7) of the model is given by

$$\begin{aligned} p(y, \lambda) &= p(y|\lambda) p(\lambda) \\ &= \prod_{i=1}^n \frac{(\lambda x_i)^{y_i} \cdot \exp[-\lambda x_i]}{y_i!} \cdot \frac{b_0^{a_0}}{\Gamma(a_0)} \lambda^{a_0-1} \exp[-b_0 \lambda] . \end{aligned} \quad (7)$$

Resolving the product in the joint likelihood, we have

$$\begin{aligned} p(y, \lambda) &= \prod_{i=1}^n \frac{x_i^{y_i}}{y_i!} \prod_{i=1}^n \lambda^{y_i} \prod_{i=1}^n \exp[-\lambda x_i] \cdot \frac{b_0^{a_0}}{\Gamma(a_0)} \lambda^{a_0-1} \exp[-b_0 \lambda] \\ &= \prod_{i=1}^n \left(\frac{x_i^{y_i}}{y_i!} \right) \lambda^{\sum_{i=1}^n y_i} \exp \left[-\lambda \sum_{i=1}^n x_i \right] \cdot \frac{b_0^{a_0}}{\Gamma(a_0)} \lambda^{a_0-1} \exp[-b_0 \lambda] \\ &= \prod_{i=1}^n \left(\frac{x_i^{y_i}}{y_i!} \right) \lambda^{n\bar{y}} \exp[-n\bar{x}\lambda] \cdot \frac{b_0^{a_0}}{\Gamma(a_0)} \lambda^{a_0-1} \exp[-b_0 \lambda] \\ &= \prod_{i=1}^n \left(\frac{x_i^{y_i}}{y_i!} \right) \frac{b_0^{a_0}}{\Gamma(a_0)} \cdot \lambda^{a_0+n\bar{y}-1} \cdot \exp[-(b_0 + n\bar{x})\lambda] \end{aligned} \quad (8)$$

where \bar{y} and \bar{x} are the means (\rightarrow I/1.12.2) of y and x respectively:

$$\begin{aligned} \bar{y} &= \frac{1}{n} \sum_{i=1}^n y_i \\ \bar{x} &= \frac{1}{n} \sum_{i=1}^n x_i . \end{aligned} \quad (9)$$

Note that the model evidence is the marginal density of the joint likelihood (\rightarrow I/5.1.15):

$$p(y) = \int p(y, \lambda) d\lambda . \quad (10)$$

Setting $a_n = a_0 + n\bar{y}$ and $b_n = b_0 + n\bar{x}$, the joint likelihood can also be written as

$$p(y, \lambda) = \prod_{i=1}^n \left(\frac{x_i^{y_i}}{y_i!} \right) \frac{b_0^{a_0}}{\Gamma(a_0)} \frac{\Gamma(a_n)}{b_n^{a_n}} \cdot \frac{b_n^{a_n}}{\Gamma(a_n)} \lambda^{a_n-1} \exp[-b_n \lambda] . \quad (11)$$

Using the probability density function of the gamma distribution (\rightarrow II/3.4.7), λ can now be integrated out easily

$$\begin{aligned}
 p(y) &= \int \prod_{i=1}^n \left(\frac{x_i^{y_i}}{y_i!} \right) \frac{b_0^{a_0}}{\Gamma(a_0)} \frac{\Gamma(a_n)}{b_n^{a_n}} \cdot \frac{b_n^{a_n}}{\Gamma(a_n)} \lambda^{a_n-1} \exp[-b_n \lambda] d\lambda \\
 &= \prod_{i=1}^n \left(\frac{x_i^{y_i}}{y_i!} \right) \frac{\Gamma(a_n)}{\Gamma(a_0)} \frac{b_0^{a_0}}{b_n^{a_n}} \int \text{Gam}(\lambda; a_n, b_n) d\lambda \\
 &= \prod_{i=1}^n \left(\frac{x_i^{y_i}}{y_i!} \right) \frac{\Gamma(a_n)}{\Gamma(a_0)} \frac{b_0^{a_0}}{b_n^{a_n}},
 \end{aligned} \tag{12}$$

such that the log model evidence (\rightarrow IV/3.1.3) is shown to be

$$\begin{aligned}
 \log p(y|m) &= \sum_{i=1}^n y_i \log(x_i) - \sum_{i=1}^n \log y_i! + \\
 &\quad \log \Gamma(a_n) - \log \Gamma(a_0) + a_0 \log b_0 - a_n \log b_n.
 \end{aligned} \tag{13}$$

■

4 Frequency data

4.1 Beta-distributed data

4.1.1 Definition

Definition: Beta-distributed data are defined as a set of proportions $y = \{y_1, \dots, y_n\}$ with $y_i \in [0, 1]$, $i = 1, \dots, n$, independent and identically distributed (\rightarrow I/1.2.8) according to a beta distribution (\rightarrow II/3.9.1) with shapes α and β :

$$y_i \sim \text{Bet}(\alpha, \beta), \quad i = 1, \dots, n. \quad (1)$$

4.1.2 Method of moments

Theorem: Let $y = \{y_1, \dots, y_n\}$ be a set of observed counts independent and identically distributed (\rightarrow I/1.2.8) according to a beta distribution (\rightarrow II/3.9.1) with shapes α and β :

$$y_i \sim \text{Bet}(\alpha, \beta), \quad i = 1, \dots, n. \quad (1)$$

Then, the method-of-moments estimates (\rightarrow I/4.1.8) for the shape parameters α and β are given by

$$\begin{aligned} \hat{\alpha} &= \bar{y} \left(\frac{\bar{y}(1 - \bar{y})}{\bar{v}} - 1 \right) \\ \hat{\beta} &= (1 - \bar{y}) \left(\frac{\bar{y}(1 - \bar{y})}{\bar{v}} - 1 \right) \end{aligned} \quad (2)$$

where \bar{y} is the sample mean (\rightarrow I/1.12.2) and \bar{v} is the unbiased sample variance (\rightarrow I/1.13.2):

$$\begin{aligned} \bar{y} &= \frac{1}{n} \sum_{i=1}^n y_i \\ \bar{v} &= \frac{1}{n-1} \sum_{i=1}^n (y_i - \bar{y})^2. \end{aligned} \quad (3)$$

Proof: Mean (\rightarrow II/3.9.8) and variance (\rightarrow II/3.9.11) of the beta distribution (\rightarrow II/3.9.1) in terms of the parameters α and β are given by

$$\begin{aligned} E(X) &= \frac{\alpha}{\alpha + \beta} \\ \text{Var}(X) &= \frac{\alpha\beta}{(\alpha + \beta)^2(\alpha + \beta + 1)}. \end{aligned} \quad (4)$$

Thus, matching the moments (\rightarrow I/4.1.8) requires us to solve the following equation system for α and β :

$$\begin{aligned} \bar{y} &= \frac{\alpha}{\alpha + \beta} \\ \bar{v} &= \frac{\alpha\beta}{(\alpha + \beta)^2(\alpha + \beta + 1)}. \end{aligned} \quad (5)$$

From the first equation, we can deduce:

$$\begin{aligned}
 \bar{y}(\alpha + \beta) &= \alpha \\
 \alpha\bar{y} + \beta\bar{y} &= \alpha \\
 \beta\bar{y} &= \alpha - \alpha\bar{y} \\
 \beta &= \frac{\alpha}{\bar{y}} - \alpha \\
 \beta &= \alpha \left(\frac{1}{\bar{y}} - 1 \right) .
 \end{aligned} \tag{6}$$

If we define $q = 1/\bar{y} - 1$ and plug (6) into the second equation, we have:

$$\begin{aligned}
 \bar{v} &= \frac{\alpha \cdot \alpha q}{(\alpha + \alpha q)^2 (\alpha + \alpha q + 1)} \\
 &= \frac{\alpha^2 q}{(\alpha(1 + q))^2 (\alpha(1 + q) + 1)} \\
 &= \frac{q}{(1 + q)^2 (\alpha(1 + q) + 1)} \\
 &= \frac{q}{\alpha(1 + q)^3 + (1 + q)^2} \\
 q &= \bar{v} [\alpha(1 + q)^3 + (1 + q)^2] .
 \end{aligned} \tag{7}$$

Noting that $1 + q = 1/\bar{y}$ and $q = (1 - \bar{y})/\bar{y}$, one obtains for α :

$$\begin{aligned}
 \frac{1 - \bar{y}}{\bar{y}} &= \bar{v} \left[\frac{\alpha}{\bar{y}^3} + \frac{1}{\bar{y}^2} \right] \\
 \frac{1 - \bar{y}}{\bar{y} \bar{v}} &= \frac{\alpha}{\bar{y}^3} + \frac{1}{\bar{y}^2} \\
 \frac{\bar{y}^3(1 - \bar{y})}{\bar{y} \bar{v}} &= \alpha + \bar{y} \\
 \alpha &= \frac{\bar{y}^2(1 - \bar{y})}{\bar{v}} - \bar{y} \\
 &= \bar{y} \left(\frac{\bar{y}(1 - \bar{y})}{\bar{v}} - 1 \right) .
 \end{aligned} \tag{8}$$

Plugging this into equation (6), one obtains for β :

$$\begin{aligned}
 \beta &= \bar{y} \left(\frac{\bar{y}(1 - \bar{y})}{\bar{v}} - 1 \right) \cdot \left(\frac{1 - \bar{y}}{\bar{y}} \right) \\
 &= (1 - \bar{y}) \left(\frac{\bar{y}(1 - \bar{y})}{\bar{v}} - 1 \right) .
 \end{aligned} \tag{9}$$

Together, (8) and (9) constitute the method-of-moment estimates of α and β . ■

Sources:

- Wikipedia (2020): “Beta distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-01-20; URL: https://en.wikipedia.org/wiki/Beta_distribution#Method_of_moments.

4.2 Dirichlet-distributed data

4.2.1 Definition

Definition: Dirichlet-distributed data are defined as a set of vectors of proportions $y = \{y_1, \dots, y_n\}$ where

$$\begin{aligned} y_i &= [y_{i1}, \dots, y_{ik}], \\ y_{ij} &\in [0, 1] \quad \text{and} \\ \sum_{j=1}^k y_{ij} &= 1 \end{aligned} \quad (1)$$

for all $i = 1, \dots, n$ (and $j = 1, \dots, k$) and each y_i is independent and identically distributed (\rightarrow I/1.2.8) according to a Dirichlet distribution (\rightarrow II/4.5.1) with concentration parameters $\alpha = [\alpha_1, \dots, \alpha_k]$:

$$y_i \sim \text{Dir}(\alpha), \quad i = 1, \dots, n. \quad (2)$$

4.2.2 Maximum likelihood estimation

Theorem: Let there be a Dirichlet-distributed data (\rightarrow III/4.2.1) set $y = \{y_1, \dots, y_n\}$:

$$y_i \sim \text{Dir}(\alpha), \quad i = 1, \dots, n. \quad (1)$$

Then, the maximum likelihood estimate (\rightarrow I/4.1.3) for the concentration parameters α can be obtained by iteratively computing

$$\alpha_j^{(\text{new})} = \psi^{-1} \left[\psi \left(\sum_{j=1}^k \alpha_j^{(\text{old})} \right) + \log \bar{y}_j \right] \quad (2)$$

where $\psi(x)$ is the digamma function and $\log \bar{y}_j$ is given by:

$$\log \bar{y}_j = \frac{1}{n} \sum_{i=1}^n \log y_{ij}. \quad (3)$$

Proof: The likelihood function (\rightarrow I/5.1.2) for each observation is given by the probability density function of the Dirichlet distribution (\rightarrow II/4.5.2)

$$p(y_i|\alpha) = \frac{\Gamma \left(\sum_{j=1}^k \alpha_j \right)}{\prod_{j=1}^k \Gamma(\alpha_j)} \prod_{j=1}^k y_{ij}^{\alpha_j-1} \quad (4)$$

and because observations are independent (\rightarrow I/1.3.6), the likelihood function for all observations is the product of the individual ones:

$$p(y|\alpha) = \prod_{i=1}^n p(y_i|\alpha) = \prod_{i=1}^n \left[\frac{\Gamma \left(\sum_{j=1}^k \alpha_j \right)}{\prod_{j=1}^k \Gamma(\alpha_j)} \prod_{j=1}^k y_{ij}^{\alpha_j-1} \right]. \quad (5)$$

Thus, the log-likelihood function (\rightarrow I/4.1.2) is

$$\text{LL}(\alpha) = \log p(y|\alpha) = \log \prod_{i=1}^n \left[\frac{\Gamma\left(\sum_{j=1}^k \alpha_j\right)}{\prod_{j=1}^k \Gamma(\alpha_j)} \prod_{j=1}^k y_{ij}^{\alpha_j-1} \right] \quad (6)$$

which can be developed into

$$\begin{aligned} \text{LL}(\alpha) &= \sum_{i=1}^n \log \Gamma\left(\sum_{j=1}^k \alpha_j\right) - \sum_{i=1}^n \sum_{j=1}^k \log \Gamma(\alpha_j) + \sum_{i=1}^n \sum_{j=1}^k (\alpha_j - 1) \log y_{ij} \\ &= n \log \Gamma\left(\sum_{j=1}^k \alpha_j\right) - n \sum_{j=1}^k \log \Gamma(\alpha_j) + n \sum_{j=1}^k (\alpha_j - 1) \frac{1}{n} \sum_{i=1}^n \log y_{ij} \\ &= n \log \Gamma\left(\sum_{j=1}^k \alpha_j\right) - n \sum_{j=1}^k \log \Gamma(\alpha_j) + n \sum_{j=1}^k (\alpha_j - 1) \log \bar{y}_j \end{aligned} \quad (7)$$

where we have specified

$$\log \bar{y}_j = \frac{1}{n} \sum_{i=1}^n \log y_{ij} . \quad (8)$$

The derivative of the log-likelihood with respect to a particular parameter α_j is

$$\begin{aligned} \frac{d\text{LL}(\alpha)}{d\alpha_j} &= \frac{d}{d\alpha_j} \left[n \log \Gamma\left(\sum_{j=1}^k \alpha_j\right) - n \sum_{j=1}^k \log \Gamma(\alpha_j) + n \sum_{j=1}^k (\alpha_j - 1) \log \bar{y}_j \right] \\ &= \frac{d}{d\alpha_j} \left[n \log \Gamma\left(\sum_{j=1}^k \alpha_j\right) \right] - \frac{d}{d\alpha_j} [n \log \Gamma(\alpha_j)] + \frac{d}{d\alpha_j} [n(\alpha_j - 1) \log \bar{y}_j] \\ &= n\psi\left(\sum_{j=1}^k \alpha_j\right) - n\psi(\alpha_j) + n \log \bar{y}_j \end{aligned} \quad (9)$$

where we have used the digamma function

$$\psi(x) = \frac{d \log \Gamma(x)}{dx} . \quad (10)$$

Setting this derivative to zero, we obtain:

$$\begin{aligned}
\frac{dLL(\alpha)}{d\alpha_j} &= 0 \\
0 &= n\psi\left(\sum_{j=1}^k \alpha_j\right) - n\psi(\alpha_j) + n \log \bar{y}_j \\
0 &= \psi\left(\sum_{j=1}^k \alpha_j\right) - \psi(\alpha_j) + \log \bar{y}_j \\
\psi(\alpha_j) &= \psi\left(\sum_{j=1}^k \alpha_j\right) + \log \bar{y}_j \\
\alpha_j &= \psi^{-1}\left[\psi\left(\sum_{j=1}^k \alpha_j\right) + \log \bar{y}_j\right].
\end{aligned} \tag{11}$$

In the following, we will use a fixed-point iteration to maximize $LL(\alpha)$. Given an initial guess for α , we construct a lower bound on the likelihood function (7) which is tight at α . The maximum of this bound is computed and it becomes the new guess. Because the Dirichlet distribution (\rightarrow II/4.5.1) belongs to the exponential family, the log-likelihood function is convex in α and the maximum is the only stationary point, such that the procedure is guaranteed to converge to the maximum.

In our case, we use a bound on the gamma function

$$\begin{aligned}
\Gamma(x) &\geq \Gamma(\hat{x}) \cdot \exp[(x - \hat{x})\psi(\hat{x})] \\
\log \Gamma(x) &\geq \log \Gamma(\hat{x}) + (x - \hat{x})\psi(\hat{x})
\end{aligned} \tag{12}$$

and apply it to $\Gamma\left(\sum_{j=1}^k \alpha_j\right)$ in (7) to yield

$$\begin{aligned}
\frac{1}{n}LL(\alpha) &= \log \Gamma\left(\sum_{j=1}^k \alpha_j\right) - \sum_{j=1}^k \log \Gamma(\alpha_j) + \sum_{j=1}^k (\alpha_j - 1) \log \bar{y}_j \\
\frac{1}{n}LL(\alpha) &\geq \log \Gamma\left(\sum_{j=1}^k \hat{\alpha}_j\right) + \left(\sum_{j=1}^k \alpha_j - \sum_{j=1}^k \hat{\alpha}_j\right) \psi\left(\sum_{j=1}^k \hat{\alpha}_j\right) - \sum_{j=1}^k \log \Gamma(\alpha_j) + \sum_{j=1}^k (\alpha_j - 1) \log \bar{y}_j \\
\frac{1}{n}LL(\alpha) &\geq \left(\sum_{j=1}^k \alpha_j\right) \psi\left(\sum_{j=1}^k \hat{\alpha}_j\right) - \sum_{j=1}^k \log \Gamma(\alpha_j) + \sum_{j=1}^k (\alpha_j - 1) \log \bar{y}_j + \text{const.}
\end{aligned} \tag{13}$$

which leads to the following fixed-point iteration using (11):

$$\alpha_j^{(\text{new})} = \psi^{-1}\left[\psi\left(\sum_{j=1}^k \alpha_j^{(\text{old})}\right) + \log \bar{y}_j\right]. \tag{14}$$

■

Sources:

- Minka TP (2012): “Estimating a Dirichlet distribution”; in: *Papers by Tom Minka*, retrieved on 2020-10-22; URL: <https://tminka.github.io/papers/dirichlet/minka-dirichlet.pdf>.

4.3 Beta-binomial data

4.3.1 Definition

Definition: Beta-binomial data are defined as a set of counts $y = \{y_1, \dots, y_N\}$ with $y_i \in \mathbb{N}$, $i = 1, \dots, N$, independent and identically distributed (\rightarrow I/1.2.8) according to a beta-binomial distribution (\rightarrow II/1.4.1) with number of trials n as well as shapes α and β :

$$y_i \sim \text{BetBin}(n, \alpha, \beta), \quad i = 1, \dots, N. \quad (1)$$

4.3.2 Method of moments

Theorem: Let $y = \{y_1, \dots, y_N\}$ be a set of observed counts, independent and identically distributed (\rightarrow I/1.2.8) according to a beta-binomial distribution (\rightarrow II/1.4.1) with number of trials n as well as parameters α and β :

$$y_i \sim \text{BetBin}(n, \alpha, \beta), \quad i = 1, \dots, N. \quad (1)$$

Then, the method-of-moments estimates (\rightarrow I/4.1.8) for the parameters α and β are given by

$$\begin{aligned} \hat{\alpha} &= \frac{nm_1 - m_2}{n \left(\frac{m_2}{m_1} - m_1 - 1 \right) + m_1} \\ \hat{\beta} &= \frac{(n - m_1) \left(n - \frac{m_2}{m_1} \right)}{n \left(\frac{m_2}{m_1} - m_1 - 1 \right) + m_1} \end{aligned} \quad (2)$$

where m_1 and m_2 are the first two raw sample moments (\rightarrow I/1.21.3):

$$\begin{aligned} m_1 &= \frac{1}{N} \sum_{i=1}^N y_i \\ m_2 &= \frac{1}{N} \sum_{i=1}^N y_i^2. \end{aligned} \quad (3)$$

Proof: The first two raw moments of the beta-binomial distribution in terms of the parameters α and β are given by

$$\begin{aligned} \mu_1 &= \frac{n\alpha}{\alpha + \beta} \\ \mu_2 &= \frac{n\alpha(n\alpha + \beta + n)}{(\alpha + \beta)(n\alpha + \beta + 1)} \end{aligned} \quad (4)$$

Thus, matching the moments (\rightarrow I/4.1.8) requires us to solve the following equation system for α and β :

$$\begin{aligned} m_1 &= \frac{n\alpha}{\alpha + \beta} \\ m_2 &= \frac{n\alpha(n\alpha + \beta + n)}{(\alpha + \beta)(n\alpha + \beta + 1)}. \end{aligned} \quad (5)$$

From the first equation, we can deduce:

$$\begin{aligned}
 m_1(\alpha + \beta) &= n\alpha \\
 m_1\alpha + m_1\beta &= n\alpha \\
 m_1\beta &= n\alpha - m_1\alpha \\
 \beta &= \frac{n\alpha}{m_1} - \alpha \\
 \beta &= \alpha \left(\frac{n}{m_1} - 1 \right) .
 \end{aligned} \tag{6}$$

If we define $q = n/m_1 - 1$ and plug (6) into the second equation, we have:

$$\begin{aligned}
 m_2 &= \frac{n\alpha(n\alpha + \alpha q + n)}{(\alpha + \alpha q)(\alpha + \alpha q + 1)} \\
 &= \frac{n\alpha(\alpha(n + q) + n)}{\alpha(1 + q)(\alpha(1 + q) + 1)} \\
 &= \frac{n(\alpha(n + q) + n)}{(1 + q)(\alpha(1 + q) + 1)} \\
 &= \frac{n(\alpha(n + q) + n)}{\alpha(1 + q)^2 + (1 + q)} .
 \end{aligned} \tag{7}$$

Noting that $1 + q = n/m_1$ and expanding the fraction with m_1 , one obtains:

$$\begin{aligned}
 m_2 &= \frac{n \left(\alpha \left(\frac{n}{m_1} + n - 1 \right) + n \right)}{n \left(\alpha \frac{n}{m_1^2} + \frac{1}{m_1} \right)} \\
 m_2 &= \frac{\alpha (n + nm_1 - m_1) + nm_1}{\alpha \frac{n}{m_1} + 1} \\
 m_2 \left(\frac{\alpha n}{m_1} + 1 \right) &= \alpha (n + nm_1 - m_1) + nm_1 \\
 \alpha \left(n \frac{m_2}{m_1} - (n + nm_1 - m_1) \right) &= nm_1 - m_2 \\
 \alpha \left(n \left(\frac{m_2}{m_1} - m_1 - 1 \right) + m_1 \right) &= nm_1 - m_2 \\
 \hat{\alpha} &= \frac{nm_1 - m_2}{n \left(\frac{m_2}{m_1} - m_1 - 1 \right) + m_1} .
 \end{aligned} \tag{8}$$

Plugging this into equation (6), one obtains for β :

$$\begin{aligned}
\beta &= \hat{\alpha} \left(\frac{n}{m_1} - 1 \right) \\
\beta &= \left(\frac{nm_1 - m_2}{n \left(\frac{m_2}{m_1} - m_1 - 1 \right) + m_1} \right) \left(\frac{n}{m_1} - 1 \right) \\
\beta &= \frac{n^2 - nm_1 - n \frac{m_2}{m_1} + m_2}{n \left(\frac{m_2}{m_1} - m_1 - 1 \right) + m_1} \\
\hat{\beta} &= \frac{(n - m_1) \left(n - \frac{m_2}{m_1} \right)}{n \left(\frac{m_2}{m_1} - m_1 - 1 \right) + m_1} .
\end{aligned} \tag{9}$$

Together, (8) and (9) constitute the method-of-moment estimates of α and β . ■

Sources:

- statisticsmatt (2022): “Method of Moments Estimation Beta Binomial Distribution”; in: *YouTube*, retrieved on 2022-10-07; URL: <https://www.youtube.com/watch?v=18PWnWJsPnA>.
- Wikipedia (2022): “Beta-binomial distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-10-07; URL: https://en.wikipedia.org/wiki/Beta-binomial_distribution#Method_of_moments.

5 Categorical data

5.1 Logistic regression

5.1.1 Definition

Definition: A logistic regression model is given by a set of binary observations $y_i \in \{0, 1\}$, $i = 1, \dots, n$, a set of predictors $x_j \in \mathbb{R}^n$, $j = 1, \dots, p$, a base b and the assumption that the log-odds are a linear combination of the predictors:

$$l_i = x_i \beta + \varepsilon_i, \quad i = 1, \dots, n \quad (1)$$

where l_i are the log-odds that $y_i = 1$

$$l_i = \log_b \frac{\Pr(y_i = 1)}{\Pr(y_i = 0)} \quad (2)$$

and x_i is the i -th row of the $n \times p$ matrix

$$X = [x_1, \dots, x_p] . \quad (3)$$

Within this model,

- y are called “categorical observations” or “dependent variable”;
- X is called “design matrix” or “set of independent variables”;
- β are called “regression coefficients” or “weights”;
- ε_i is called “noise” or “error term”;
- n is the number of observations;
- p is the number of predictors.

Sources:

- Wikipedia (2020): “Logistic regression”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-06-28; URL: https://en.wikipedia.org/wiki/Logistic_regression#Logistic_model.

5.1.2 Probability and log-odds

Theorem: Assume a logistic regression model (\rightarrow III/5.1.1)

$$l_i = x_i \beta + \varepsilon_i, \quad i = 1, \dots, n \quad (1)$$

where x_i are the predictors corresponding to the i -th observation y_i and l_i are the log-odds that $y_i = 1$.

Then, the log-odds in favor of $y_i = 1$ against $y_i = 0$ can also be expressed as

$$l_i = \log_b \frac{p(x_i|y_i = 1) p(y_i = 1)}{p(x_i|y_i = 0) p(y_i = 0)} \quad (2)$$

where $p(x_i|y_i)$ is a likelihood function (\rightarrow I/5.1.2) consistent with (1), $p(y_i)$ are prior probabilities (\rightarrow I/5.1.3) for $y_i = 1$ and $y_i = 0$ and where b is the base used to form the log-odds l_i .

Proof: Using Bayes’ theorem (\rightarrow I/5.3.2) and the law of marginal probability (\rightarrow I/1.3.3), the posterior probabilities (\rightarrow I/5.1.9) for $y_i = 1$ and $y_i = 0$ are given by

$$\begin{aligned}
p(y_i = 1|x_i) &= \frac{p(x_i|y_i = 1) p(y_i = 1)}{p(x_i|y_i = 1) p(y_i = 1) + p(x_i|y_i = 0) p(y_i = 0)} \\
p(y_i = 0|x_i) &= \frac{p(x_i|y_i = 0) p(y_i = 0)}{p(x_i|y_i = 1) p(y_i = 1) + p(x_i|y_i = 0) p(y_i = 0)} .
\end{aligned} \tag{3}$$

Calculating the log-odds from the posterior probabilities, we have

$$\begin{aligned}
l_i &= \log_b \frac{p(y_i = 1|x_i)}{p(y_i = 0|x_i)} \\
&= \log_b \frac{p(x_i|y_i = 1) p(y_i = 1)}{p(x_i|y_i = 0) p(y_i = 0)} .
\end{aligned} \tag{4}$$

■

Sources:

- Bishop, Christopher M. (2006): “Linear Models for Classification”; in: *Pattern Recognition for Machine Learning*, ch. 4, p. 197, eq. 4.58; URL: <http://users.isr.ist.utl.pt/~wurmd/Livros/school/Bishop%20-%20Pattern%20Recognition%20And%20Machine%20Learning%20-%20Springer%20%202006.pdf>.

5.1.3 Log-odds and probability

Theorem: Assume a logistic regression model (\rightarrow III/5.1.1)

$$l_i = x_i \beta + \varepsilon_i, \quad i = 1, \dots, n \tag{1}$$

where x_i are the predictors corresponding to the i -th observation y_i and l_i are the log-odds that $y_i = 1$.

Then, the probability that $y_i = 1$ is given by

$$\Pr(y_i = 1) = \frac{1}{1 + b^{-(x_i \beta + \varepsilon_i)}} \tag{2}$$

where b is the base used to form the log-odds l_i .

Proof: Let us denote $\Pr(y_i = 1)$ as p_i . Then, the log-odds are

$$l_i = \log_b \frac{p_i}{1 - p_i} \tag{3}$$

and using (1), we have

$$\begin{aligned}
\log_b \frac{p_i}{1-p_i} &= x_i \beta + \varepsilon_i \\
\frac{p_i}{1-p_i} &= b^{x_i \beta + \varepsilon_i} \\
p_i &= (b^{x_i \beta + \varepsilon_i}) (1-p_i) \\
p_i (1 + b^{x_i \beta + \varepsilon_i}) &= b^{x_i \beta + \varepsilon_i} \\
p_i &= \frac{b^{x_i \beta + \varepsilon_i}}{1 + b^{x_i \beta + \varepsilon_i}} \\
p_i &= \frac{b^{x_i \beta + \varepsilon_i}}{b^{x_i \beta + \varepsilon_i} (1 + b^{-(x_i \beta + \varepsilon_i)})} \\
p_i &= \frac{1}{1 + b^{-(x_i \beta + \varepsilon_i)}}
\end{aligned} \tag{4}$$

which proves the identity given by (2).

■

Sources:

- Wikipedia (2020): “Logistic regression”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-03-03; URL: https://en.wikipedia.org/wiki/Logistic_regression#Logistic_model.

Chapter IV

Model Selection

1 Goodness-of-fit measures

1.1 Residual variance

1.1.1 Definition

Definition: Let there be a linear regression model (\rightarrow III/1.5.1)

$$y = X\beta + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 V) \quad (1)$$

with measured data y , known design matrix X and covariance structure V as well as unknown regression coefficients β and noise variance σ^2 .

Then, an estimate of the noise variance σ^2 is called the “residual variance” $\hat{\sigma}^2$, e.g. obtained via maximum likelihood estimation (\rightarrow I/4.1.3).

1.1.2 Maximum likelihood estimator is biased ($p = 1$)

Theorem: Let $y = \{y_1, \dots, y_n\}$ be a set of independent normally distributed (\rightarrow II/3.2.1) observations with unknown mean (\rightarrow I/1.12.1) μ and variance (\rightarrow I/1.13.1) σ^2 :

$$y_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(\mu, \sigma^2), \quad i = 1, \dots, n. \quad (1)$$

Then,

1) the maximum likelihood estimator (\rightarrow I/4.1.3) of σ^2 is

$$\hat{\sigma}^2 = \frac{1}{n} \sum_{i=1}^n (y_i - \bar{y})^2 \quad (2)$$

where

$$\bar{y} = \frac{1}{n} \sum_{i=1}^n y_i \quad (3)$$

2) and $\hat{\sigma}^2$ is a biased estimator (\rightarrow I/3.1.2) of σ^2

$$\mathbb{E} [\hat{\sigma}^2] \neq \sigma^2, \quad (4)$$

more precisely:

$$\mathbb{E} [\hat{\sigma}^2] = \frac{n-1}{n} \sigma^2. \quad (5)$$

Proof:

1) This is equivalent to the maximum likelihood estimator for the univariate Gaussian with unknown variance (\rightarrow III/1.1.2) and a special case of the maximum likelihood estimator for multiple linear regression (\rightarrow III/1.5.23) in which $X = 1_n$ and $\hat{\beta} = \bar{y}$:

$$\begin{aligned} \hat{\sigma}^2 &= \frac{1}{n} (y - X\hat{\beta})^T (y - X\hat{\beta}) \\ &= \frac{1}{n} (y - 1_n \bar{y})^T (y - 1_n \bar{y}) \\ &= \frac{1}{n} \sum_{i=1}^n (y_i - \bar{y})^2. \end{aligned} \quad (6)$$

2) The expectation (\rightarrow I/1.12.1) of the maximum likelihood estimator (\rightarrow I/4.1.3) can be developed as follows:

$$\begin{aligned}
 E[\hat{\sigma}^2] &= E\left[\frac{1}{n} \sum_{i=1}^n (y_i - \bar{y})^2\right] \\
 &= \frac{1}{n} E\left[\sum_{i=1}^n (y_i - \bar{y})^2\right] \\
 &= \frac{1}{n} E\left[\sum_{i=1}^n (y_i^2 - 2y_i\bar{y} + \bar{y}^2)\right] \\
 &= \frac{1}{n} E\left[\sum_{i=1}^n y_i^2 - 2\sum_{i=1}^n y_i\bar{y} + \sum_{i=1}^n \bar{y}^2\right] \\
 &= \frac{1}{n} E\left[\sum_{i=1}^n y_i^2 - 2n\bar{y}^2 + n\bar{y}^2\right] \\
 &= \frac{1}{n} E\left[\sum_{i=1}^n y_i^2 - n\bar{y}^2\right] \\
 &= \frac{1}{n} \left(\sum_{i=1}^n E[y_i^2] - nE[\bar{y}^2]\right) \\
 &= \frac{1}{n} \sum_{i=1}^n E[y_i^2] - E[\bar{y}^2]
 \end{aligned} \tag{7}$$

Due to the partition of variance into expected values (\rightarrow I/1.13.4)

$$\text{Var}(X) = E(X^2) - E(X)^2, \tag{8}$$

we have

$$\begin{aligned}
 \text{Var}(y_i) &= E(y_i^2) - E(y_i)^2 \\
 \text{Var}(\bar{y}) &= E(\bar{y}^2) - E(\bar{y})^2,
 \end{aligned} \tag{9}$$

such that (7) becomes

$$E[\hat{\sigma}^2] = \frac{1}{n} \sum_{i=1}^n (\text{Var}(y_i) + E(y_i)^2) - (\text{Var}(\bar{y}) + E(\bar{y})^2). \tag{10}$$

From (1), it follows that

$$E(y_i) = \mu \quad \text{and} \quad \text{Var}(y_i) = \sigma^2. \tag{11}$$

The expectation (\rightarrow I/1.12.1) of \bar{y} given by (3) is

$$\begin{aligned}
\mathbb{E}[\bar{y}] &= \mathbb{E}\left[\frac{1}{n} \sum_{i=1}^n y_i\right] = \frac{1}{n} \sum_{i=1}^n \mathbb{E}[y_i] \\
&\stackrel{(11)}{=} \frac{1}{n} \sum_{i=1}^n \mu = \frac{1}{n} \cdot n \cdot \mu \\
&= \mu .
\end{aligned} \tag{12}$$

The variance of \bar{y} given by (3) is

$$\begin{aligned}
\text{Var}[\bar{y}] &= \text{Var}\left[\frac{1}{n} \sum_{i=1}^n y_i\right] = \frac{1}{n^2} \sum_{i=1}^n \text{Var}[y_i] \\
&\stackrel{(11)}{=} \frac{1}{n^2} \sum_{i=1}^n \sigma^2 = \frac{1}{n^2} \cdot n \cdot \sigma^2 \\
&= \frac{1}{n} \sigma^2 .
\end{aligned} \tag{13}$$

Plugging (11), (12) and (13) into (10), we have

$$\begin{aligned}
\mathbb{E}[\hat{\sigma}^2] &= \frac{1}{n} \sum_{i=1}^n (\sigma^2 + \mu^2) - \left(\frac{1}{n} \sigma^2 + \mu^2\right) \\
\mathbb{E}[\hat{\sigma}^2] &= \frac{1}{n} \cdot n \cdot (\sigma^2 + \mu^2) - \left(\frac{1}{n} \sigma^2 + \mu^2\right) \\
\mathbb{E}[\hat{\sigma}^2] &= \sigma^2 + \mu^2 - \frac{1}{n} \sigma^2 - \mu^2 \\
\mathbb{E}[\hat{\sigma}^2] &= \frac{n-1}{n} \sigma^2
\end{aligned} \tag{14}$$

which proves the bias (\rightarrow I/3.1.2) given by (5). ■

Sources:

- Liang, Dawen (2020): “Maximum Likelihood Estimator for Variance is Biased: Proof”, retrieved on 2020-02-24; URL: https://dawenl.github.io/files/mle_biased.pdf.

1.1.3 Maximum likelihood estimator is biased ($p > 1$)

Theorem: Consider a linear regression model (\rightarrow III/1.5.1) with known design matrix X , known covariance structure V , unknown regression parameters β and unknown noise variance σ^2 :

$$y = X\beta + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 V) . \tag{1}$$

Then,

1) the maximum likelihood estimator (\rightarrow I/4.1.3) of σ^2 is

$$\hat{\sigma}^2 = \frac{1}{n}(y - X\hat{\beta})^T V^{-1}(y - X\hat{\beta}) \quad (2)$$

where

$$\hat{\beta} = (X^T V^{-1} X)^{-1} X^T V^{-1} y \quad (3)$$

2) and $\hat{\sigma}^2$ is a biased estimator (\rightarrow I/3.1.2) of σ^2

$$E[\hat{\sigma}^2] \neq \sigma^2, \quad (4)$$

more precisely:

$$E[\hat{\sigma}^2] = \frac{n-p}{n} \sigma^2. \quad (5)$$

Proof:

1) This follows from maximum likelihood estimation for multiple linear regression (\rightarrow III/1.5.23) and is a special case (\rightarrow III/1.5.2) of maximum likelihood estimation for the general linear model (\rightarrow III/2.2.4) in which $Y = y$, $B = \beta$ and $\Sigma = \sigma^2$:

$$\begin{aligned} \hat{\sigma}^2 &= \frac{1}{n}(Y - X\hat{B})^T V^{-1}(Y - X\hat{B}) \\ &= \frac{1}{n}(y - X\hat{\beta})^T V^{-1}(y - X\hat{\beta}). \end{aligned} \quad (6)$$

2) We know that the residual sum of squares, divided by the true noise variance, is following a chi-squared distribution (\rightarrow III/1.5.20):

$$\begin{aligned} \frac{\hat{\varepsilon}^T \hat{\varepsilon}}{\sigma^2} &\sim \chi^2(n-p) \\ \text{where } \hat{\varepsilon}^T \hat{\varepsilon} &= (y - X\hat{\beta})^T V^{-1}(y - X\hat{\beta}). \end{aligned} \quad (7)$$

Thus, combining (7) and (6), we have:

$$\frac{n\hat{\sigma}^2}{\sigma^2} \sim \chi^2(n-p). \quad (8)$$

Using the relationship between chi-squared distribution and gamma distribution (\rightarrow II/3.7.2)

$$X \sim \chi^2(k) \quad \Rightarrow \quad cX \sim \text{Gam}\left(\frac{k}{2}, \frac{1}{2c}\right), \quad (9)$$

we can deduce from (8) that

$$\hat{\sigma}^2 = \frac{\sigma^2}{n} \cdot \frac{n\hat{\sigma}^2}{\sigma^2} \sim \text{Gam}\left(\frac{n-p}{2}, \frac{n}{2\sigma^2}\right). \quad (10)$$

Using the expected value of the gamma distribution (\rightarrow II/3.4.11)

$$X \sim \text{Gam}(a, b) \quad \Rightarrow \quad E(X) = \frac{a}{b}, \quad (11)$$

we can deduce from (10) that

$$\mathbb{E} [\hat{\sigma}^2] = \frac{\frac{n-p}{2}}{\frac{n}{2\sigma^2}} = \frac{n-p}{n} \sigma^2 \quad (12)$$

which proves the relationship given by (5). ■

Sources:

- ocram (2022): “Why is RSS distributed chi square times n-p?”; in: *StackExchange Cross Validated*, retrieved on 2022-12-21; URL: <https://stats.stackexchange.com/a/20230>.

1.1.4 Construction of unbiased estimator ($p = 1$)

Theorem: Let $y = \{y_1, \dots, y_n\}$ be a set of independent normally distributed (\rightarrow II/3.2.1) observations with unknown mean (\rightarrow I/1.12.1) μ and variance (\rightarrow I/1.13.1) σ^2 :

$$y_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(\mu, \sigma^2), \quad i = 1, \dots, n. \quad (1)$$

An unbiased estimator (\rightarrow I/3.1.2) of σ^2 is given by

$$\hat{\sigma}_{\text{unb}}^2 = \frac{1}{n-1} \sum_{i=1}^n (y_i - \bar{y})^2. \quad (2)$$

Proof: It can be shown that (\rightarrow IV/1.1.2) the maximum likelihood estimator (\rightarrow I/4.1.3) of σ^2

$$\hat{\sigma}_{\text{MLE}}^2 = \frac{1}{n} \sum_{i=1}^n (y_i - \bar{y})^2 \quad (3)$$

is a biased estimator (\rightarrow I/3.1.2) in the sense that

$$\mathbb{E} [\hat{\sigma}_{\text{MLE}}^2] = \frac{n-1}{n} \sigma^2. \quad (4)$$

From (4), it follows that

$$\begin{aligned} \mathbb{E} \left[\frac{n}{n-1} \hat{\sigma}_{\text{MLE}}^2 \right] &= \frac{n}{n-1} \mathbb{E} [\hat{\sigma}_{\text{MLE}}^2] \\ &\stackrel{(4)}{=} \frac{n}{n-1} \cdot \frac{n-1}{n} \sigma^2 \\ &= \sigma^2, \end{aligned} \quad (5)$$

such that an unbiased estimator (\rightarrow I/3.1.2) can be constructed as

$$\begin{aligned} \hat{\sigma}_{\text{unb}}^2 &= \frac{n}{n-1} \hat{\sigma}_{\text{MLE}}^2 \\ &\stackrel{(3)}{=} \frac{n}{n-1} \cdot \frac{1}{n} \sum_{i=1}^n (y_i - \bar{y})^2 \\ &= \frac{1}{n-1} \sum_{i=1}^n (y_i - \bar{y})^2. \end{aligned} \quad (6)$$

**Sources:**

- Liang, Dawen (2020): “Maximum Likelihood Estimator for Variance is Biased: Proof”, retrieved on 2020-02-25; URL: https://dawenl.github.io/files/mle_biased.pdf.

1.1.5 Construction of unbiased estimator ($p > 1$)

Theorem: Consider a linear regression model (\rightarrow III/1.5.1) with known design matrix X , known covariance structure V , unknown regression parameters β and unknown noise variance σ^2 :

$$y = X\beta + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 V). \quad (1)$$

An unbiased estimator (\rightarrow I/3.1.2) of σ^2 is given by

$$\hat{\sigma}^2 = \frac{1}{n-p} (y - X\hat{\beta})^T V^{-1} (y - X\hat{\beta}) \quad (2)$$

where

$$\hat{\beta} = (X^T V^{-1} X)^{-1} X^T V^{-1} y. \quad (3)$$

Proof: It can be shown that (\rightarrow IV/1.1.3) the maximum likelihood estimator (\rightarrow I/4.1.3) of σ^2

$$\hat{\sigma}_{\text{MLE}}^2 = \frac{1}{n} (y - X\hat{\beta})^T V^{-1} (y - X\hat{\beta}) \quad (4)$$

is a biased estimator (\rightarrow I/3.1.2) in the sense that

$$\mathbb{E} [\hat{\sigma}_{\text{MLE}}^2] = \frac{n-p}{n} \sigma^2. \quad (5)$$

From (5), it follows that

$$\begin{aligned} \mathbb{E} \left[\frac{n}{n-p} \hat{\sigma}_{\text{MLE}}^2 \right] &= \frac{n}{n-p} \mathbb{E} [\hat{\sigma}_{\text{MLE}}^2] \\ &\stackrel{(5)}{=} \frac{n}{n-p} \cdot \frac{n-p}{n} \sigma^2 \\ &= \sigma^2, \end{aligned} \quad (6)$$

such that an unbiased estimator (\rightarrow I/3.1.2) can be constructed as

$$\begin{aligned} \hat{\sigma}_{\text{unb}}^2 &= \frac{n}{n-p} \hat{\sigma}_{\text{MLE}}^2 \\ &\stackrel{(4)}{=} \frac{n}{n-p} \cdot \frac{1}{n} (y - X\hat{\beta})^T V^{-1} (y - X\hat{\beta}) \\ &= \frac{1}{n-p} (y - X\hat{\beta})^T V^{-1} (y - X\hat{\beta}). \end{aligned} \quad (7)$$



1.2 R-squared

1.2.1 Definition

Definition: Let there be a linear regression model (\rightarrow III/1.5.1) with independent (\rightarrow I/1.3.6) observations

$$y = X\beta + \varepsilon, \varepsilon_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2) \quad (1)$$

with measured data y , known design matrix X as well as unknown regression coefficients β and noise variance σ^2 .

Then, the proportion of the variance of the dependent variable y (“total variance (\rightarrow III/1.5.7)”) that can be predicted from the independent variables X (“explained variance (\rightarrow III/1.5.8)”) is called “coefficient of determination”, “R-squared” or R^2 .

Sources:

- Wikipedia (2020): “Coefficient of determination”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-02-25; URL: https://en.wikipedia.org/wiki/Mean_squared_error#Proof_of_variance_and_bias_relationship.

1.2.2 Derivation of R^2 and adjusted R^2

Theorem: Given a linear regression model (\rightarrow III/1.5.1)

$$y = X\beta + \varepsilon, \varepsilon_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2) \quad (1)$$

with n independent observations and p independent variables,

1) the coefficient of determination (\rightarrow IV/1.2.1) is given by

$$R^2 = 1 - \frac{\text{RSS}}{\text{TSS}} \quad (2)$$

2) the adjusted coefficient of determination is

$$R_{\text{adj}}^2 = 1 - \frac{\text{RSS}/(n-p)}{\text{TSS}/(n-1)} \quad (3)$$

where the residual (\rightarrow III/1.5.9) and total sum of squares (\rightarrow III/1.5.7) are

$$\begin{aligned} \text{RSS} &= \sum_{i=1}^n (y_i - \hat{y}_i)^2, \quad \hat{y} = X\hat{\beta} \\ \text{TSS} &= \sum_{i=1}^n (y_i - \bar{y})^2, \quad \bar{y} = \frac{1}{n} \sum_{i=1}^n y_i \end{aligned} \quad (4)$$

where X is the $n \times p$ design matrix and $\hat{\beta}$ are the ordinary least squares (\rightarrow III/1.5.3) estimates.

Proof: The coefficient of determination (\rightarrow IV/1.2.1) R^2 is defined as the proportion of the variance explained by the independent variables, relative to the total variance in the data.

1) If we define the explained sum of squares (\rightarrow III/1.5.8) as

$$\text{ESS} = \sum_{i=1}^n (\hat{y}_i - \bar{y})^2, \quad (5)$$

then R^2 is given by

$$R^2 = \frac{\text{ESS}}{\text{TSS}}. \quad (6)$$

which is equal to

$$R^2 = \frac{\text{TSS} - \text{RSS}}{\text{TSS}} = 1 - \frac{\text{RSS}}{\text{TSS}}, \quad (7)$$

because it holds that (\rightarrow III/1.5.10)

$$\text{TSS} = \text{ESS} + \text{RSS}. \quad (8)$$

2) Using (4), the coefficient of determination can be also written as:

$$R^2 = 1 - \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2} = 1 - \frac{\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2}{\frac{1}{n} \sum_{i=1}^n (y_i - \bar{y})^2}. \quad (9)$$

If we replace the variance estimates by their unbiased estimators (\rightarrow IV/1.1.5), we obtain

$$R_{\text{adj}}^2 = 1 - \frac{\frac{1}{n-p} \sum_{i=1}^n (y_i - \hat{y}_i)^2}{\frac{1}{n-1} \sum_{i=1}^n (y_i - \bar{y})^2} = 1 - \frac{\text{RSS}/\text{df}_r}{\text{TSS}/\text{df}_t} \quad (10)$$

where $\text{df}_r = n - p$ and $\text{df}_t = n - 1$ are the residual and total degrees of freedom (\rightarrow I/1.5.12). This gives the adjusted R^2 which adjusts R^2 for the number of explanatory variables (\rightarrow III/1.5.1). ■

Sources:

- Wikipedia (2019): “Coefficient of determination”; in: *Wikipedia, the free encyclopedia*, retrieved on 2019-12-06; URL: https://en.wikipedia.org/wiki/Coefficient_of_determination#Adjusted_R2.

1.2.3 Relationship to residual variance

Theorem: Given a linear regression model with independent observations (\rightarrow III/1.5.1)

$$y = X\beta + \varepsilon, \quad \varepsilon_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2), \quad (1)$$

the coefficient of determination (\rightarrow IV/1.2.1) can be expressed in terms of residual variances (\rightarrow IV/1.1.1) as

$$R^2 = 1 - \frac{(n-p) \cdot \hat{\sigma}^2}{(n-1) \cdot s^2} \quad (2)$$

where n is the number of observations, p is the number of predictors, $\hat{\sigma}^2$ is an unbiased estimate of the noise variance (\rightarrow IV/1.1.5) σ^2 and s^2 is the unbiased sample variance (\rightarrow I/1.13.2) of y .

Proof: The coefficient of determination (\rightarrow IV/1.2.2) is given by

$$R^2 = 1 - \frac{\text{RSS}}{\text{TSS}} \quad (3)$$

where RSS is the residual sum of squares (\rightarrow III/1.5.9)

$$\text{RSS} = \sum_{i=1}^n (y_i - \hat{y}_i)^2 \quad \text{where} \quad \hat{y} = X\hat{\beta} \quad (4)$$

and TSS is the total sum of squares (\rightarrow III/1.5.7)

$$\text{TSS} = \sum_{i=1}^n (y_i - \bar{y})^2 \quad \text{where} \quad \bar{y} = \frac{1}{n} \sum_{i=1}^n y_i . \quad (5)$$

Note that the residual sum of squares can be written as:

$$\text{RSS} = \sum_{i=1}^n (y_i - \hat{y}_i)^2 = \sum_{i=1}^n (y_i - (X\hat{\beta})_i)^2 = (y - X\hat{\beta})^T (y - X\hat{\beta}) . \quad (6)$$

The unbiased estimate of the noise variance (\rightarrow IV/1.1.5) is

$$\hat{\sigma}^2 = \frac{1}{n-p} (y - X\hat{\beta})^T (y - X\hat{\beta}) \quad (7)$$

and the unbiased sample variance of the dependent variable (\rightarrow I/1.13.2) is

$$s^2 = \frac{1}{n-1} \sum_{i=1}^n (y_i - \bar{y})^2 , \quad (8)$$

Combining (3), (4) and (5), the coefficient of determination can be rewritten as follows:

$$\begin{aligned} R^2 &\stackrel{(3)}{=} 1 - \frac{\text{RSS}}{\text{TSS}} \\ &\stackrel{(5)}{=} 1 - \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2} \\ &\stackrel{(6)}{=} 1 - \frac{(y - X\hat{\beta})^T (y - X\hat{\beta})}{\sum_{i=1}^n (y_i - \bar{y})^2} \\ &= 1 - \frac{(n-p) \cdot \frac{1}{n-p} (y - X\hat{\beta})^T (y - X\hat{\beta})}{(n-1) \cdot \frac{1}{n-1} \sum_{i=1}^n (y_i - \bar{y})^2} \\ &\stackrel{(7)}{=} 1 - \frac{(n-p) \cdot \hat{\sigma}^2}{(n-1) \cdot \frac{1}{n-1} \sum_{i=1}^n (y_i - \bar{y})^2} \\ &\stackrel{(8)}{=} 1 - \frac{(n-p) \cdot \hat{\sigma}^2}{(n-1) \cdot s^2} . \end{aligned} \quad (9)$$

This completes the proof. ■

1.2.4 Relationship to maximum log-likelihood

Theorem: Given a linear regression model with independent observations (\rightarrow III/1.5.1)

$$y = X\beta + \varepsilon, \quad \varepsilon_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2) , \quad (1)$$

the coefficient of determination (\rightarrow IV/1.2.1) can be expressed in terms of the maximum log-likelihood (\rightarrow I/4.1.4) as

$$R^2 = 1 - (\exp[\Delta\text{MLL}])^{-2/n} \quad (2)$$

where n is the number of observations and ΔMLL is the difference in maximum log-likelihood between the model given by (1) and a linear regression model with only a constant regressor.

Proof: First, we express the maximum log-likelihood (\rightarrow I/4.1.4) (MLL) of a linear regression model in terms of its residual sum of squares (\rightarrow III/1.5.9) (RSS). The model in (1) implies the following log-likelihood function (\rightarrow I/4.1.2)

$$\text{LL}(\beta, \sigma^2) = \log p(y|\beta, \sigma^2) = -\frac{n}{2} \log(2\pi\sigma^2) - \frac{1}{2\sigma^2} (y - X\beta)^T (y - X\beta), \quad (3)$$

such that maximum likelihood estimates are (\rightarrow III/1.5.23)

$$\hat{\beta} = (X^T X)^{-1} X^T y \quad (4)$$

$$\hat{\sigma}^2 = \frac{1}{n} (y - X\hat{\beta})^T (y - X\hat{\beta}) \quad (5)$$

and the residual sum of squares (\rightarrow III/1.5.9) is

$$\text{RSS} = \sum_{i=1}^n \hat{\varepsilon}_i = \hat{\varepsilon}^T \hat{\varepsilon} = (y - X\hat{\beta})^T (y - X\hat{\beta}) = n \cdot \hat{\sigma}^2. \quad (6)$$

Since $\hat{\beta}$ and $\hat{\sigma}^2$ are maximum likelihood estimates (\rightarrow I/4.1.3), plugging them into the log-likelihood function gives the maximum log-likelihood:

$$\text{MLL} = \text{LL}(\hat{\beta}, \hat{\sigma}^2) = -\frac{n}{2} \log(2\pi\hat{\sigma}^2) - \frac{1}{2\hat{\sigma}^2} (y - X\hat{\beta})^T (y - X\hat{\beta}). \quad (7)$$

With (6) for the first $\hat{\sigma}^2$ and (5) for the second $\hat{\sigma}^2$, the MLL becomes

$$\text{MLL} = -\frac{n}{2} \log(\text{RSS}) - \frac{n}{2} \log\left(\frac{2\pi}{n}\right) - \frac{n}{2}. \quad (8)$$

Second, we establish the relationship between maximum log-likelihood (MLL) and coefficient of determination (R^2). Consider the two models

$$\begin{aligned} m_0 : X_0 &= 1_n \\ m_1 : X_1 &= X \end{aligned} \quad (9)$$

For m_1 , the residual sum of squares is given by (6); and for m_0 , the residual sum of squares is equal to the total sum of squares (\rightarrow III/1.5.7):

$$\text{TSS} = \sum_{i=1}^n (y_i - \bar{y})^2. \quad (10)$$

Using (8), we can therefore write

$$\Delta\text{MLL} = \text{MLL}(m_1) - \text{MLL}(m_0) = -\frac{n}{2} \log(\text{RSS}) + \frac{n}{2} \log(\text{TSS}). \quad (11)$$

Exponentiating both sides of the equation, we have:

$$\begin{aligned}
 \exp[\Delta\text{MLL}] &= \exp\left[-\frac{n}{2}\log(\text{RSS}) + \frac{n}{2}\log(\text{TSS})\right] \\
 &= (\exp[\log(\text{RSS}) - \log(\text{TSS})])^{-n/2} \\
 &= \left(\frac{\exp[\log(\text{RSS})]}{\exp[\log(\text{TSS})]}\right)^{-n/2} \\
 &= \left(\frac{\text{RSS}}{\text{TSS}}\right)^{-n/2}.
 \end{aligned} \tag{12}$$

Taking both sides to the power of $-2/n$ and subtracting from 1, we have

$$\begin{aligned}
 (\exp[\Delta\text{MLL}])^{-2/n} &= \frac{\text{RSS}}{\text{TSS}} \\
 1 - (\exp[\Delta\text{MLL}])^{-2/n} &= 1 - \frac{\text{RSS}}{\text{TSS}} = R^2
 \end{aligned} \tag{13}$$

which proves the identity given above. ■

1.2.5 Statistical significance test for R^2

Theorem: Consider a linear regression model (\rightarrow III/1.5.1) with known design matrix X , known covariance structure V , unknown regression parameters β and unknown noise variance σ^2 :

$$y = X\beta + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 V). \tag{1}$$

Further assume that X contains a constant regressor (\rightarrow III/1.5.1). Then, the coefficient of determination (\rightarrow IV/1.2.1) can be used to calculate a test statistic (\rightarrow I/4.3.5)

$$F = \frac{R^2/(p-1)}{(1-R^2)/(n-p)} \tag{2}$$

where n and p are the dimensions of the design matrix (\rightarrow III/1.5.1) X , and this test statistic follows an F-distribution (\rightarrow II/3.8.1)

$$F \sim F(p-1, n-p) \tag{3}$$

under the null hypothesis (\rightarrow I/4.3.2) that the true coefficient of determination (\rightarrow IV/1.2.1) is zero:

$$H_0 : R^2 = 0. \tag{4}$$

Proof: Consider two linear regression models (\rightarrow III/1.5.1) for the same measured data y , with design matrices $X = X_0 \in \mathbb{R}^{n \times p_0}$ and $X = [X_0, X_1] \in \mathbb{R}^{n \times p}$ as well as regression coefficients $\beta = \beta_0 \in \mathbb{R}^{p_0 \times 1}$ and $\beta = [\beta_0^T, \beta_1^T]^T \in \mathbb{R}^{p \times 1}$.

Then, under the null hypothesis that all regression coefficients (\rightarrow III/1.5.1) β_1 associated with X_1 are zero

$$H_0 : \beta_1 = 0_{p-p_0} \quad \Leftrightarrow \quad \beta_i = 0 \quad \text{for all } j = p_0 + 1, \dots, p, \tag{5}$$

the omnibus F-statistic follows an F-distribution (\rightarrow III/1.5.31)

$$F = \frac{(\text{RSS}_0 - \text{RSS})/(p - p_0)}{\text{RSS}/(n - p)} \sim F(p - p_0, n - p) \quad (6)$$

where RSS_0 and RSS are the residual sums of squares (\rightarrow III/1.5.9) of the null model with X_0 and the full model with X_0 nested in X , after regression coefficients have been estimated with weighted least squares (\rightarrow III/1.5.21) or maximum likelihood (\rightarrow III/1.5.23).

Since by the requirements of our theorem, X contains a constant regressor, we can assume the following design matrices without loss of generality:

$$X_0 = 1_n \in \mathbb{R}^{n \times 1} \quad \text{and} \quad X = [1_n, X_1] \in \mathbb{R}^{n \times p}. \quad (7)$$

Thus, since a single constant regressor estimates the mean and considering the definition of the total sum of squares (\rightarrow III/1.5.7) TSS, we in our case have:

$$\text{RSS}_0 = \text{TSS} \quad \text{and} \quad p_0 = 1. \quad (8)$$

The coefficient of determination is given by (\rightarrow IV/1.2.2)

$$R^2 = 1 - \frac{\text{RSS}}{\text{TSS}} \quad (9)$$

which can also be written as (\rightarrow III/1.5.10)

$$R^2 = \frac{\text{ESS}}{\text{TSS}}. \quad (10)$$

If all regression coefficients β_1 associated with X_1 are zero, then the true R^2 is zero, because there is no variance explained beyond the constant regressor, the explained sum of squares (\rightarrow III/1.5.8) ESS is zero and the residual sum of squares (\rightarrow III/1.5.9) RSS is equal to the total sum of squares (\rightarrow III/1.5.7) TSS.

Then, by virtue of (6), we get the following F-statistic:

$$\begin{aligned} F &\stackrel{(6)}{=} \frac{(\text{RSS}_0 - \text{RSS})/(p - p_0)}{\text{RSS}/(n - p)} \\ &\stackrel{(8)}{=} \frac{(\text{TSS} - \text{RSS})/(p - 1)}{\text{RSS}/(n - p)} \\ &= \frac{\frac{\text{TSS} - \text{RSS}}{\text{TSS}}/(p - 1)}{\frac{\text{RSS}}{\text{TSS}}/(n - p)} \\ &= \frac{\left(1 - \frac{\text{RSS}}{\text{TSS}}\right)/(p - 1)}{\left(1 - \left(1 - \frac{\text{RSS}}{\text{TSS}}\right)\right)/(n - p)} \\ &\stackrel{(9)}{=} \frac{(R^2)/(p - 1)}{(1 - R^2)/(n - p)}. \end{aligned} \quad (11)$$

This means that the null hypothesis (\rightarrow I/4.3.2) can be rejected when F as a function of R^2 is as extreme or more extreme than the critical value (\rightarrow I/4.3.9) obtained from the F-distribution (\rightarrow II/3.8.1) with $p - 1$ denominator and $n - p$ numerator degrees of freedom (\rightarrow I/1.5.12) using a significance level (\rightarrow I/4.3.8) α .



Sources:

- Alecos Papadopoulos (2014): “What is the distribution of R^2 in linear regression under the null hypothesis?”; in: *StackExchange CrossValidated*, retrieved on 2024-03-15; URL: <https://stats.stackexchange.com/a/130082>.

1.2.6 Distribution under null hypothesis

Theorem: Consider a linear regression model (\rightarrow III/1.5.1) with known design matrix X , known covariance structure V , unknown regression parameters β and unknown noise variance σ^2 :

$$y = X\beta + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 V) . \quad (1)$$

Further assume that X contains a constant regressor (\rightarrow III/1.5.1), i.e. it is of the following form:

$$X = [1_n, X_1] \in \mathbb{R}^{n \times p} . \quad (2)$$

Then, the coefficient of determination (\rightarrow IV/1.2.1) follows a beta distribution (\rightarrow II/3.9.1)

$$R^2 \sim \text{Bet} \left(\frac{p-1}{2}, \frac{n-p}{2} \right) \quad (3)$$

under the null hypothesis (\rightarrow I/4.3.2) that the true coefficient of determination (\rightarrow IV/1.2.1) is zero:

$$H_0 : R^2 = 0 . \quad (4)$$

Proof: We know that the F-statistic is related to R-squared as (\rightarrow IV/1.3.2)

$$F = \frac{R^2/(p-1)}{(1-R^2)/(n-p)} \quad (5)$$

and that the F-statistic follows an F-distribution (\rightarrow IV/1.2.5) under H_0 :

$$F \sim F(p-1, n-p), \quad \text{if } R^2 = 0 . \quad (6)$$

Rearranging equation (5) gives R-squared as a function of the F-statistic (\rightarrow IV/1.3.2)

$$R^2 = \frac{F \cdot \frac{p-1}{n-p}}{1 + F \cdot \frac{p-1}{n-p}} \quad (7)$$

which, when expanding with $(n-p)$, can also be written as:

$$R^2 = \frac{(p-1)F}{(n-p) + (p-1)F} . \quad (8)$$

Using the relationship between F-distribution and beta distribution (\rightarrow II/3.9.4)

$$X \sim F(d_1, d_2) \quad \Rightarrow \quad Y = \frac{d_1 X}{d_2 + d_1 X} \sim \text{Bet} \left(\frac{d_1}{2}, \frac{d_2}{2} \right) , \quad (9)$$

i.e. combining (6) and (8), it follows that

$$R^2 \sim \text{Bet} \left(\frac{p-1}{2}, \frac{n-p}{2} \right) \quad (10)$$

under the null hypothesis that $R^2 = 0$.

■

Sources:

- Alecos Papadopoulos (2014): “What is the distribution of R^2 in linear regression under the null hypothesis?”; in: *StackExchange CrossValidated*, retrieved on 2024-03-15; URL: <https://stats.stackexchange.com/a/130082>.

1.2.7 Mean/mode/median under null hypothesis

Theorem: Consider a linear regression model (\rightarrow III/1.5.1) with known design matrix $X = [1_n, X_1] \in \mathbb{R}^{n \times p}$, known covariance structure V , unknown regression parameters β and unknown noise variance σ^2 :

$$y = X\beta + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 V) . \quad (1)$$

Then, under the null hypothesis (\rightarrow I/4.3.2) that the true coefficient of determination (\rightarrow IV/1.2.1) is zero, i.e. $H_0 : R^2 = 0$, the expected value (\rightarrow I/1.12.1), the median (\rightarrow I/1.18.1) and the mode (\rightarrow I/1.18.3) of R^2 are

$$\begin{aligned} E(R^2) &= \frac{p-1}{n-1} \\ \text{median}(R^2) &= I^{-1}\left(\frac{1}{2}; \frac{p-1}{2}, \frac{n-p}{2}\right) \\ \text{mode}(R^2) &= \frac{p-3}{n-5} \end{aligned} \quad (2)$$

where $I^{-1}(p; a, b)$ is the inverse function of the regularized incomplete beta function (\rightarrow II/3.9.7).

Proof: We know that R-squared follows a beta distribution (\rightarrow IV/1.2.6) under H_0 :

$$R^2 \sim \text{Bet}\left(\frac{p-1}{2}, \frac{n-p}{2}\right) . \quad (3)$$

Using mean (\rightarrow II/3.9.8), median (\rightarrow II/3.9.9) and mode (\rightarrow II/3.9.10) of the beta distribution (\rightarrow II/3.9.1)

$$\begin{aligned} X &\sim \text{Bet}(\alpha, \beta) \\ \Rightarrow E(X) &= \frac{\alpha}{\alpha + \beta} \\ \text{median}(X) &= I^{-1}(1/2; \alpha, \beta) \\ \text{mode}(X) &= \frac{\alpha - 1}{\alpha + \beta - 2} , \end{aligned} \quad (4)$$

we have:

$$\begin{aligned}
E(R^2) &= \frac{(p-1)/2}{(p-1)/2 + (n-p)/2} \\
&= \frac{p-1}{n-1} \\
\text{median}(R^2) &= I^{-1}(1/2; (p-1)/2, (n-p)/2) \\
&= I^{-1}\left(\frac{1}{2}, \frac{p-1}{2}, \frac{n-p}{2}\right) \\
\text{mode}(R^2) &= \frac{(p-1)/2 - 1}{(p-1)/2 + (n-p)/2 - 2} \\
&= \frac{p-3}{n-5}.
\end{aligned} \tag{5}$$

This completes the proof. ■

1.2.8 Variance under null hypothesis

Theorem: Consider a linear regression model (\rightarrow III/1.5.1) with known design matrix $X = [1_n, X_1] \in \mathbb{R}^{n \times p}$, known covariance structure V , unknown regression parameters β and unknown noise variance σ^2 :

$$y = X\beta + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 V). \tag{1}$$

Then, under the null hypothesis (\rightarrow I/4.3.2) that the true coefficient of determination (\rightarrow IV/1.2.1) is zero, i.e. $H_0 : R^2 = 0$, the variance (\rightarrow I/1.13.1) of the coefficient of determination is

$$\text{Var}(R^2) = 2 \cdot \frac{(p-1) \cdot (n-p)}{(n+1) \cdot (n-1)^2}. \tag{2}$$

Proof: We know that R-squared follows a beta distribution (\rightarrow IV/1.2.6) under H_0 :

$$R^2 \sim \text{Bet}\left(\frac{p-1}{2}, \frac{n-p}{2}\right). \tag{3}$$

Using the variance of the beta distribution (\rightarrow II/3.9.11)

$$X \sim \text{Bet}(\alpha, \beta) \quad \Rightarrow \quad \text{Var}(X) = \frac{\alpha\beta}{(\alpha + \beta + 1) \cdot (\alpha + \beta)^2}, \tag{4}$$

we have:

$$\begin{aligned}
\text{Var}(R^2) &= \frac{\frac{p-1}{2} \cdot \frac{n-p}{2}}{\left(\frac{p-1}{2} + \frac{n-p}{2} + 1\right) \cdot \left(\frac{p-1}{2} + \frac{n-p}{2}\right)^2} \\
&= \frac{\frac{(p-1) \cdot (n-p)}{4}}{\frac{1}{2} \cdot (n+1) \cdot \frac{(n-1)^2}{4}} \\
&= 2 \cdot \frac{(p-1) \cdot (n-p)}{(n+1) \cdot (n-1)^2}.
\end{aligned} \tag{5}$$

This completes the proof.



1.3 F-statistic

1.3.1 Definition

Definition: Consider two linear regression models (\rightarrow III/1.5.1) with independent (\rightarrow I/1.3.6) observations

$$\begin{aligned} m_1 : y &= X\beta + \varepsilon, \varepsilon_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2) \\ m_0 : y &= X_0\beta_0 + \varepsilon_0, \varepsilon_{0i} \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma_0^2) \end{aligned} \quad (1)$$

operating on identical measured data y , but with different design matrices $X \in \mathbb{R}^{n \times p}$ and $X_0 \in \mathbb{R}^{n \times p_0}$ and thus different regression coefficients $\beta \in \mathbb{R}^{p \times 1}$ and $\beta_0 \in \mathbb{R}^{p_0 \times 1}$. Furthermore, let the design matrix of the null model be fully contained in the design matrix of the full model:

$$X = \begin{bmatrix} X_0 & X_1 \end{bmatrix}. \quad (2)$$

Then, the F-statistic for model comparison is defined as the ratio of the difference in residual sum of squares (\rightarrow III/1.5.9) between the two models, divided by the difference in number of parameters (\rightarrow III/1.5.1), to the residual sum of squares (\rightarrow III/1.5.9) of the full model, divided by the number of degrees of freedom (\rightarrow I/1.5.12):

$$F = \frac{(\text{RSS}_0 - \text{RSS})/(p - p_0)}{\text{RSS}/(n - p)}. \quad (3)$$

Sources:

- Wikipedia (2024): “F-test”; in: *Wikipedia, the free encyclopedia*, retrieved on 2024-03-15; URL: https://en.wikipedia.org/wiki/F-test#Regression_problems.

1.3.2 Relationship to coefficient of determination

Theorem: Let there be a linear regression model (\rightarrow III/1.5.1) with independent (\rightarrow I/1.3.6) observations

$$y = X\beta + \varepsilon, \varepsilon_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2). \quad (1)$$

Then, the F-statistic (\rightarrow IV/1.3.1) for comparing this model against a null model containing only a constant regressor (\rightarrow III/1.5.1) $x_0 = 1_n$ can be expressed in terms of the coefficient of determination (\rightarrow IV/1.2.1)

$$F = \frac{R^2/(p - 1)}{(1 - R^2)/(n - p)} \quad (2)$$

and vice versa

$$R^2 = 1 - \frac{1}{F \cdot \frac{p-1}{n-p} + 1} \quad (3)$$

where n and p are the dimensions of the design matrix $X \in \mathbb{R}^{n \times p}$.

Proof: Consider two linear regression models (\rightarrow III/1.5.1) for the same measured data y , one using design matrix X from (1) and the other with design matrix $X_0 = \mathbf{1}_n \in \mathbb{R}^{n \times 1}$. Then, RSS is the residual sum of squares (\rightarrow III/1.5.9) of the model in (1) and the residual sum of squares for the model using X_0 is equal to the total sum of squares (\rightarrow III/1.5.7).

1) Thus, the F-statistic (\rightarrow IV/1.3.1)

$$F = \frac{(\text{RSS}_0 - \text{RSS})/(p - p_0)}{\text{RSS}/(n - p)} \quad (4)$$

becomes

$$F = \frac{(\text{TSS} - \text{RSS})/(p - 1)}{\text{RSS}/(n - p)} . \quad (5)$$

From this, we can derive F in terms of R^2 :

$$\begin{aligned} F &= \frac{(\text{TSS} - \text{RSS})/(p - 1)}{\text{RSS}/(n - p)} \\ &= \frac{\frac{\text{TSS} - \text{RSS}}{\text{TSS}}/(p - 1)}{\frac{\text{RSS}}{\text{TSS}}/(n - p)} \\ &= \frac{\left(1 - \frac{\text{RSS}}{\text{TSS}}\right)/(p - 1)}{\left(1 - \left(1 - \frac{\text{RSS}}{\text{TSS}}\right)\right)/(n - p)} \\ &= \frac{(R^2)/(p - 1)}{(1 - R^2)/(n - p)} . \end{aligned} \quad (6)$$

2) Rearranging this equation, we can derive R^2 in terms of F :

$$\begin{aligned}
F &= \frac{(R^2)/(p-1)}{(1-R^2)/(n-p)} \\
F \cdot \frac{p-1}{n-p} &= \frac{R^2}{(1-R^2)} \\
F \cdot \frac{p-1}{n-p} \cdot (1-R^2) &= R^2 \\
F \cdot \frac{p-1}{n-p} - F \cdot \frac{p-1}{n-p} \cdot R^2 &= R^2 \\
F \cdot \frac{p-1}{n-p} \cdot R^2 + R^2 &= F \cdot \frac{p-1}{n-p} \\
R^2 \left(F \cdot \frac{p-1}{n-p} + 1 \right) &= F \cdot \frac{p-1}{n-p} \\
R^2 &= \frac{F \cdot \frac{p-1}{n-p}}{F \cdot \frac{p-1}{n-p} + 1} \\
R^2 &= \frac{F \cdot \frac{p-1}{n-p} + 1 - 1}{F \cdot \frac{p-1}{n-p} + 1} \\
R^2 &= \frac{F \cdot \frac{p-1}{n-p} + 1}{F \cdot \frac{p-1}{n-p} + 1} - \frac{1}{F \cdot \frac{p-1}{n-p} + 1} \\
R^2 &= 1 - \frac{1}{F \cdot \frac{p-1}{n-p} + 1}
\end{aligned} \tag{7}$$

This completes the proof. ■

Sources:

- Alecos Papadopoulos (2014): “What is the distribution of R^2 in linear regression under the null hypothesis?”; in: *StackExchange CrossValidated*, retrieved on 2024-03-15; URL: <https://stats.stackexchange.com/a/130082>.

1.3.3 Relationship to maximum log-likelihood

Theorem: Consider two linear regression models (\rightarrow III/1.5.1) with independent (\rightarrow I/1.3.6) observations

$$\begin{aligned}
m_1 : y &= X\beta + \varepsilon, \quad \varepsilon_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2) \\
m_0 : y &= X_0\beta_0 + \varepsilon_0, \quad \varepsilon_{0i} \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma_0^2) .
\end{aligned} \tag{1}$$

Then, the F-statistic (\rightarrow IV/1.3.1) can be expressed in terms of the maximum log-likelihood (\rightarrow I/4.1.4) as

$$F = \left[(\exp[\Delta \text{MLL}])^{2/n} - 1 \right] \cdot \frac{n-p}{p-p_0} \tag{2}$$

where n , p and p_0 are the dimensions of the design matrices $X = [X_0, X_1] \in \mathbb{R}^{n \times p}$ and $X_0 \in \mathbb{R}^{n \times p_0}$ and ΔMLL is the difference in maximum log-likelihood between the two models given by (1)

Proof: Under the conditions mentioned in the theorem, the F-statistic is defined in terms of the residual sum of squares (\rightarrow IV/1.3.1) as

$$F = \frac{(\text{RSS}_0 - \text{RSS})/(p - p_0)}{\text{RSS}/(n - p)} . \quad (3)$$

We also know that the maximum log-likelihood can be expressed in terms of residual sum of squares (\rightarrow III/1.5.24):

$$\text{MLL}(m) = -\frac{n}{2} \log \left(\frac{\text{RSS}}{n} \right) - \frac{n}{2} [1 + \log(2\pi)] . \quad (4)$$

Based on this, we see that the difference of the maximum log-likelihoods develops into

$$\begin{aligned} \Delta\text{MLL} &= \text{MLL}(m_1) - \text{MLL}(m_0) \\ &= \left(-\frac{n}{2} \log \left(\frac{\text{RSS}}{n} \right) - \frac{n}{2} [1 + \log(2\pi)] \right) \\ &\quad - \left(-\frac{n}{2} \log \left(\frac{\text{RSS}_0}{n} \right) - \frac{n}{2} [1 + \log(2\pi)] \right) \\ &= -\frac{n}{2} \log \left(\frac{\text{RSS}}{n} \right) + \frac{n}{2} \log \left(\frac{\text{RSS}_0}{n} \right) . \end{aligned} \quad (5)$$

Finally, we simply perform algebraic operations on both sides (\rightarrow IV/1.2.4) until we reach the F-statistic on the right side. We start by exponentiating the MLL difference:

$$\begin{aligned}
\exp[\Delta\text{MLL}] &= \exp\left[-\frac{n}{2}\log(\text{RSS}/n) + \frac{n}{2}\log(\text{RSS}_0/n)\right] \\
\exp[\Delta\text{MLL}] &= (\exp[\log(\text{RSS}/n) - \log(\text{RSS}_0/n)])^{-n/2} \\
\exp[\Delta\text{MLL}] &= \left(\frac{\exp[\log(\text{RSS}/n)]}{\exp[\log(\text{RSS}_0/n)]}\right)^{-n/2} \\
\exp[\Delta\text{MLL}] &= \left(\frac{\text{RSS}/n}{\text{RSS}_0/n}\right)^{-n/2} \\
\exp[\Delta\text{MLL}] &= \left(\frac{\text{RSS}_0}{\text{RSS}}\right)^{n/2} \\
(\exp[\Delta\text{MLL}])^{2/n} &= \frac{\text{RSS}_0}{\text{RSS}} \\
(\exp[\Delta\text{MLL}])^{2/n} - 1 &= \frac{\text{RSS}_0}{\text{RSS}} - 1 \\
(\exp[\Delta\text{MLL}])^{2/n} - 1 &= \frac{\text{RSS}_0}{\text{RSS}} - \frac{\text{RSS}}{\text{RSS}} \\
\left[(\exp[\Delta\text{MLL}])^{2/n} - 1\right] \cdot \frac{n-p}{p-p_0} &= \left[\frac{\text{RSS}_0 - \text{RSS}}{\text{RSS}}\right] \cdot \frac{n-p}{p-p_0} \\
\left[(\exp[\Delta\text{MLL}])^{2/n} - 1\right] \cdot \frac{n-p}{p-p_0} &= \frac{(\text{RSS}_0 - \text{RSS})/(p-p_0)}{\text{RSS}/(n-p)} \\
\left[(\exp[\Delta\text{MLL}])^{2/n} - 1\right] \cdot \frac{n-p}{p-p_0} &= F .
\end{aligned} \tag{6}$$

This completes the proof. ■

1.4 Signal-to-noise ratio

1.4.1 Definition

Definition: Let there be a linear regression model (\rightarrow III/1.5.1) with independent (\rightarrow I/1.3.6) observations

$$y = X\beta + \varepsilon, \quad \varepsilon_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2) \tag{1}$$

with measured data y , known design matrix X as well as unknown regression coefficients β and noise variance σ^2 .

Given estimated regression coefficients (\rightarrow III/1.5.23) $\hat{\beta}$ and residual variance (\rightarrow IV/1.1.1) $\hat{\sigma}^2$, the signal-to-noise ratio (SNR) is defined as the ratio of estimated signal variance to estimated noise variance:

$$\text{SNR} = \frac{\text{Var}(X\hat{\beta})}{\hat{\sigma}^2} . \tag{2}$$

Sources:

- Soch J, Allefeld C (2018): “MACS – a new SPM toolbox for model assessment, comparison and selection”; in: *Journal of Neuroscience Methods*, vol. 306, pp. 19-31, eq. 6; URL: <https://www.sciencedirect.com/science/article/pii/S0165027018301468>; DOI: 10.1016/j.jneumeth.2018.05.017.

1.4.2 Relationship to coefficient of determination

Theorem: Let there be a linear regression model (\rightarrow III/1.5.1) with independent (\rightarrow I/1.3.6) observations

$$y = X\beta + \varepsilon, \varepsilon_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2) \quad (1)$$

and parameter estimates (\rightarrow I/3.1.1) obtained with ordinary least squares (\rightarrow III/1.5.3)

$$\hat{\beta} = (X^T X)^{-1} X^T y. \quad (2)$$

Then, the signal-to noise ratio (\rightarrow IV/1.4.1) can be expressed in terms of the coefficient of determination (\rightarrow IV/1.2.1)

$$\text{SNR} = \frac{R^2}{1 - R^2} \quad (3)$$

and vice versa

$$R^2 = \frac{\text{SNR}}{1 + \text{SNR}}, \quad (4)$$

if the predicted signal mean is equal to the actual signal mean.

Proof: The signal-to-noise ratio (\rightarrow IV/1.4.1) (SNR) is defined as

$$\text{SNR} = \frac{\text{Var}(X\hat{\beta})}{\hat{\sigma}^2} = \frac{\text{Var}(\hat{y})}{\hat{\sigma}^2}. \quad (5)$$

Writing out the sample variances (\rightarrow I/1.13.2), we have

$$\text{SNR} = \frac{\frac{1}{n} \sum_{i=1}^n (\hat{y}_i - \bar{\hat{y}})^2}{\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2} = \frac{\sum_{i=1}^n (\hat{y}_i - \bar{\hat{y}})^2}{\sum_{i=1}^n (y_i - \hat{y}_i)^2}. \quad (6)$$

Note that it is irrelevant whether we use the biased estimator of the variance (\rightarrow IV/1.1.2) (dividing by n) or the unbiased estimator for the variance (\rightarrow IV/1.1.4) (dividing by $n - 1$), because the relevant terms cancel out.

If the predicted signal mean is equal to the actual signal mean – which is the case when variable regressors in X have mean zero, such that they are orthogonal to a constant regressor in X –, this means that $\bar{\hat{y}} = \bar{y}$, such that

$$\text{SNR} = \frac{\sum_{i=1}^n (\hat{y}_i - \bar{y})^2}{\sum_{i=1}^n (y_i - \hat{y}_i)^2}. \quad (7)$$

Then, the SNR can be written in terms of the explained (\rightarrow III/1.5.8), residual (\rightarrow III/1.5.9) and total sum of squares (\rightarrow III/1.5.7):

$$\text{SNR} = \frac{\text{ESS}}{\text{RSS}} = \frac{\text{ESS/TSS}}{\text{RSS/TSS}}. \quad (8)$$

With the derivation of the coefficient of determination (\rightarrow IV/1.2.2), this becomes

$$\text{SNR} = \frac{R^2}{1 - R^2} . \quad (9)$$

Rearranging this equation for the coefficient of determination (\rightarrow IV/1.2.1), we have

$$R^2 = \frac{\text{SNR}}{1 + \text{SNR}} . \quad (10)$$

■

1.4.3 Relationship to maximum log-likelihood

Theorem: Given a linear regression model (\rightarrow III/1.5.1) with independent (\rightarrow I/1.3.6) observations

$$y = X\beta + \varepsilon, \quad \varepsilon_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2) ; \quad (1)$$

the signal-to-noise ratio (\rightarrow IV/1.4.1) can be expressed in terms of the maximum log-likelihood (\rightarrow I/4.1.4) as

$$\text{SNR} = (\exp[\Delta\text{MLL}])^{2/n} - 1 , \quad (2)$$

where n is the number of observations and ΔMLL is the difference in maximum log-likelihood between the model given by (1) and a linear regression model with only a constant regressor.

This holds, if the predicted signal mean is equal to the actual signal mean

$$\bar{\hat{y}} = \frac{1}{n} \sum_{i=1}^n (X\hat{\beta})_i = \frac{1}{n} \sum_{i=1}^n y_i = \bar{y} \quad (3)$$

where X is the $n \times p$ design matrix and $\hat{\beta}$ are the ordinary least squares (\rightarrow III/1.5.3) estimates.

Proof: Under the conditions mentioned in the theorem, the signal-to-noise ratio can be expressed in terms of the coefficient of determination (\rightarrow IV/1.4.2) as

$$\text{SNR} = \frac{R^2}{1 - R^2} \quad (4)$$

and R-squared can be expressed in terms of maximum likelihood (\rightarrow IV/1.2.4) as

$$R^2 = 1 - (\exp[\Delta\text{MLL}])^{-2/n} . \quad (5)$$

Plugging (5) into (4), we obtain:

$$\begin{aligned} \text{SNR} &= \frac{1 - (\exp[\Delta\text{MLL}])^{-2/n}}{(\exp[\Delta\text{MLL}])^{-2/n}} \\ &= \frac{1}{(\exp[\Delta\text{MLL}])^{-2/n}} - \frac{(\exp[\Delta\text{MLL}])^{-2/n}}{(\exp[\Delta\text{MLL}])^{-2/n}} \\ &= (\exp[\Delta\text{MLL}])^{2/n} - 1 . \end{aligned} \quad (6)$$

■

2 Classical information criteria

2.1 Akaike information criterion

2.1.1 Definition

Definition: Let m be a generative model (\rightarrow I/5.1.1) with likelihood function (\rightarrow I/5.1.2) $p(y|\theta, m)$ and maximum likelihood estimates (\rightarrow I/4.1.3)

$$\hat{\theta} = \arg \max_{\theta} \log p(y|\theta, m) . \quad (1)$$

Then, the Akaike information criterion (AIC) of this model is defined as

$$\text{AIC}(m) = -2 \log p(y|\hat{\theta}, m) + 2k \quad (2)$$

where k is the number of free parameters estimated via (1).

Sources:

- Akaike H (1974): “A New Look at the Statistical Model Identification”; in: *IEEE Transactions on Automatic Control*, vol. AC-19, no. 6, pp. 716-723; URL: <https://ieeexplore.ieee.org/document/1100705>; DOI: 10.1109/TAC.1974.1100705.

2.1.2 Corrected AIC

Definition: Let m be a generative model (\rightarrow I/5.1.1) with likelihood function (\rightarrow I/5.1.2) $p(y|\theta, m)$ and maximum likelihood estimates (\rightarrow I/4.1.3)

$$\hat{\theta} = \arg \max_{\theta} \log p(y|\theta, m) . \quad (1)$$

Then, the corrected Akaike information criterion (\rightarrow IV/2.1.2) (AIC_c) of this model is defined as

$$\text{AIC}_c(m) = \text{AIC}(m) + \frac{2k^2 + 2k}{n - k - 1} \quad (2)$$

where $\text{AIC}(m)$ is the Akaike information criterion (\rightarrow IV/2.1.1) and k is the number of free parameters estimated via (1).

Sources:

- Hurvich CM, Tsai CL (1989): “Regression and time series model selection in small samples”; in: *Biometrika*, vol. 76, no. 2, pp. 297-307; URL: <https://academic.oup.com/biomet/article-abstract/76/2/297/265326>; DOI: 10.1093/biomet/76.2.297.

2.1.3 Corrected AIC and uncorrected AIC

Theorem: In the infinite data limit, the corrected Akaike information criterion (\rightarrow IV/2.1.2) converges to the uncorrected Akaike information criterion (\rightarrow IV/2.1.1)

$$\lim_{n \rightarrow \infty} \text{AIC}_c(m) = \text{AIC}(m) . \quad (1)$$

Proof: The corrected Akaike information criterion (\rightarrow IV/2.1.2) is defined as

$$\text{AIC}_c(m) = \text{AIC}(m) + \frac{2k^2 + 2k}{n - k - 1} . \quad (2)$$

Note that the number of free model parameters k is finite. Thus, we have:

$$\begin{aligned} \lim_{n \rightarrow \infty} \text{AIC}_c(m) &= \lim_{n \rightarrow \infty} \left[\text{AIC}(m) + \frac{2k^2 + 2k}{n - k - 1} \right] \\ &= \lim_{n \rightarrow \infty} \text{AIC}(m) + \lim_{n \rightarrow \infty} \frac{2k^2 + 2k}{n - k - 1} \\ &= \text{AIC}(m) + 0 \\ &= \text{AIC}(m) . \end{aligned} \quad (3)$$

■

Sources:

- Wikipedia (2022): “Akaike information criterion”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-03-18; URL: https://en.wikipedia.org/wiki/Akaike_information_criterion#Modification_for_small_sample_size.

2.1.4 Corrected AIC and maximum log-likelihood

Theorem: The corrected Akaike information criterion (\rightarrow IV/2.1.2) of a generative model (\rightarrow I/5.1.1) with likelihood function (\rightarrow I/5.1.2) $p(y|\theta, m)$ is equal to

$$\text{AIC}_c(m) = -2 \log p(y|\hat{\theta}, m) + \frac{2nk}{n - k - 1} \quad (1)$$

where $\log p(y|\hat{\theta}, m)$ is the maximum log-likelihood (\rightarrow I/4.1.4), k is the number of free parameters and n is the number of observations.

Proof: The Akaike information criterion (\rightarrow IV/2.1.1) (AIC) is defined as

$$\text{AIC}(m) = -2 \log p(y|\hat{\theta}, m) + 2k \quad (2)$$

and the corrected Akaike information criterion (\rightarrow IV/2.1.2) is defined as

$$\text{AIC}_c(m) = \text{AIC}(m) + \frac{2k^2 + 2k}{n - k - 1} . \quad (3)$$

Plugging (2) into (3), we obtain:

$$\begin{aligned} \text{AIC}_c(m) &= -2 \log p(y|\hat{\theta}, m) + 2k + \frac{2k^2 + 2k}{n - k - 1} \\ &= -2 \log p(y|\hat{\theta}, m) + \frac{2k(n - k - 1)}{n - k - 1} + \frac{2k^2 + 2k}{n - k - 1} \\ &= -2 \log p(y|\hat{\theta}, m) + \frac{2nk - 2k^2 - 2k}{n - k - 1} + \frac{2k^2 + 2k}{n - k - 1} \\ &= -2 \log p(y|\hat{\theta}, m) + \frac{2nk}{n - k - 1} . \end{aligned} \quad (4)$$

**Sources:**

- Wikipedia (2022): “Akaike information criterion”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-03-11; URL: https://en.wikipedia.org/wiki/Akaike_information_criterion#Modification_for_small_sample_size.

2.2 Bayesian information criterion**2.2.1 Definition**

Definition: Let m be a generative model (\rightarrow I/5.1.1) with likelihood function (\rightarrow I/5.1.2) $p(y|\theta, m)$ and maximum likelihood estimates (\rightarrow I/4.1.3)

$$\hat{\theta} = \arg \max_{\theta} \log p(y|\theta, m) . \quad (1)$$

Then, the Bayesian information criterion (BIC) of this model is defined as

$$\text{BIC}(m) = -2 \log p(y|\hat{\theta}, m) + k \log n \quad (2)$$

where n is the number of data points and k is the number of free parameters estimated via (1).

Sources:

- Schwarz G (1978): “Estimating the Dimension of a Model”; in: *The Annals of Statistics*, vol. 6, no. 2, pp. 461-464; URL: <https://www.jstor.org/stable/2958889>.

2.2.2 Derivation

Theorem: Let $p(y|\theta, m)$ be the likelihood function (\rightarrow I/5.1.2) of a generative model (\rightarrow I/5.1.1) $m \in \mathcal{M}$ with model parameters (\rightarrow I/1.5.7) $\theta \in \Theta$ describing measured data (\rightarrow I/1.1.5) $y \in \mathbb{R}^n$. Let $p(\theta|m)$ be a prior distribution (\rightarrow I/5.1.3) on the model parameters. Assume that likelihood function and prior density are twice differentiable.

Then, as the number of data points (\rightarrow I/1.1.7) goes to infinity, an approximation to the log-marginal likelihood (\rightarrow I/5.1.15) $\log p(y|m)$, up to constant terms not depending on the model, is given by the Bayesian information criterion (\rightarrow IV/2.2.1) (BIC) as

$$-2 \log p(y|m) \approx \text{BIC}(m) = -2 \log p(y|\hat{\theta}, m) + p \log n \quad (1)$$

where $\hat{\theta}$ is the maximum likelihood estimator (\rightarrow I/4.1.3) (MLE) of θ , n is the number of data points and p is the number of model parameters.

Proof: Let $\text{LL}(\theta)$ be the log-likelihood function (\rightarrow I/4.1.2)

$$\text{LL}(\theta) = \log p(y|\theta, m) \quad (2)$$

and define the functions g and h as follows:

$$\begin{aligned} g(\theta) &= p(\theta|m) \\ h(\theta) &= \frac{1}{n} \text{LL}(\theta) . \end{aligned} \quad (3)$$

Then, the marginal likelihood (\rightarrow I/5.1.15) can be written as follows:

$$\begin{aligned} p(y|m) &= \int_{\Theta} p(y|\theta, m) p(\theta|m) d\theta \\ &= \int_{\Theta} \exp[n h(\theta)] g(\theta) d\theta . \end{aligned} \quad (4)$$

This is an integral suitable for Laplace approximation which states that

$$\int_{\Theta} \exp[n h(\theta)] g(\theta) d\theta = \left(\sqrt{\frac{2\pi}{n}} \right)^p \exp[n h(\theta_0)] \left(g(\theta_0) |J(\theta_0)|^{-1/2} + O(1/n) \right) \quad (5)$$

where θ_0 is the value that maximizes $h(\theta)$ and $J(\theta_0)$ is the Hessian matrix evaluated at θ_0 . In our case, we have $h(\theta) = 1/n \text{LL}(\theta)$ such that θ_0 is the maximum likelihood estimator $\hat{\theta}$:

$$\hat{\theta} = \arg \max_{\theta} \text{LL}(\theta) . \quad (6)$$

With this, (5) can be applied to (4) using (3) to give:

$$p(y|m) \approx \left(\sqrt{\frac{2\pi}{n}} \right)^p p(y|\hat{\theta}, m) p(\hat{\theta}|m) |J(\hat{\theta})|^{-1/2} . \quad (7)$$

Logarithmizing and multiplying with -2 , we have:

$$-2 \log p(y|m) \approx -2 \text{LL}(\hat{\theta}) + p \log n - p \log(2\pi) - 2 \log p(\hat{\theta}|m) + \log |J(\hat{\theta})| . \quad (8)$$

As $n \rightarrow \infty$, the last three terms are $O_p(1)$ and can therefore be ignored when comparing between models $\mathcal{M} = \{m_1, \dots, m_M\}$ and using $p(y|m_j)$ to compute posterior model probabilities (\rightarrow IV/3.4.1) $p(m_j|y)$. With that, the BIC is given as

$$\text{BIC}(m) = -2 \log p(y|\hat{\theta}, m) + p \log n . \quad (9)$$

■

Sources:

- Claeskens G, Hjort NL (2008): “The Bayesian information criterion”; in: *Model Selection and Model Averaging*, ch. 3.2, pp. 78-81; URL: <https://www.cambridge.org/core/books/model-selection-and-model-averaging>; E6F1EC77279D1223423BB64FC3A12C37; DOI: 10.1017/CBO9780511790485.

2.3 Deviance information criterion

2.3.1 Definition

Definition: Let m be a full probability model (\rightarrow I/5.1.6) with likelihood function (\rightarrow I/5.1.2) $p(y|\theta, m)$ and prior distribution (\rightarrow I/5.1.3) $p(\theta|m)$. Together, likelihood function and prior distribution imply a posterior distribution (\rightarrow I/5.1.10) $p(\theta|y, m)$. Consider the deviance (\rightarrow IV/2.3.2) which is minus two times the log-likelihood function (\rightarrow I/4.1.2):

$$D(\theta) = -2 \log p(y|\theta, m) . \quad (1)$$

Then, the deviance information criterion (DIC) of the model m is defined as

$$\text{DIC}(m) = -2 \log p(y | \langle \theta \rangle, m) + 2 p_D \quad (2)$$

where $\log p(y | \langle \theta \rangle, m)$ is the log-likelihood function (\rightarrow I/4.1.2) at the posterior (\rightarrow I/5.1.9) expectation (\rightarrow I/1.12.1) and the “effective number of parameters” p_D is the difference between the expectation of the deviance and the deviance at the expectation (\rightarrow IV/2.3.1):

$$p_D = \langle D(\theta) \rangle - D(\langle \theta \rangle) . \quad (3)$$

In these equations, $\langle \cdot \rangle$ denotes expected values (\rightarrow I/1.12.1) across the posterior distribution (\rightarrow I/5.1.9).

Sources:

- Spiegelhalter DJ, Best NG, Carlin BP, Van Der Linde A (2002): “Bayesian measures of model complexity and fit”; in: *Journal of the Royal Statistical Society, Series B: Statistical Methodology*, vol. 64, iss. 4, pp. 583-639; URL: <https://rss.onlinelibrary.wiley.com/doi/10.1111/1467-9868.00353>; DOI: 10.1111/1467-9868.00353.
- Soch J, Allefeld C (2018): “MACS – a new SPM toolbox for model assessment, comparison and selection”; in: *Journal of Neuroscience Methods*, vol. 306, pp. 19-31, eqs. 10-12; URL: <https://www.sciencedirect.com/science/article/pii/S0165027018301468>; DOI: 10.1016/j.jneumeth.2018.05.017.

2.3.2 Deviance

Definition: Let there be a generative model (\rightarrow I/5.1.1) m describing measured data y using model parameters θ . Then, the deviance of m is a function of θ which multiplies the log-likelihood function (\rightarrow I/4.1.2) with -2 :

$$D(\theta) = -2 \log p(y | \theta, m) . \quad (1)$$

The deviance function serves the definition of the deviance information criterion (\rightarrow IV/2.3.1).

Sources:

- Spiegelhalter DJ, Best NG, Carlin BP, Van Der Linde A (2002): “Bayesian measures of model complexity and fit”; in: *Journal of the Royal Statistical Society, Series B: Statistical Methodology*, vol. 64, iss. 4, pp. 583-639; URL: <https://rss.onlinelibrary.wiley.com/doi/10.1111/1467-9868.00353>; DOI: 10.1111/1467-9868.00353.
- Soch J, Allefeld C (2018): “MACS – a new SPM toolbox for model assessment, comparison and selection”; in: *Journal of Neuroscience Methods*, vol. 306, pp. 19-31, eqs. 10-12; URL: <https://www.sciencedirect.com/science/article/pii/S0165027018301468>; DOI: 10.1016/j.jneumeth.2018.05.017.
- Wikipedia (2022): “Deviance information criterion”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-03-01; URL: https://en.wikipedia.org/wiki/Deviance_information_criterion#Definition.

3 Bayesian model selection

3.1 Model evidence

3.1.1 Definition

Definition: Let m be a generative model (\rightarrow I/5.1.1) with likelihood function (\rightarrow I/5.1.2) $p(y|\theta, m)$ and prior distribution (\rightarrow I/5.1.3) $p(\theta|m)$. Then, the model evidence (ME) of m is defined as the marginal likelihood (\rightarrow I/5.1.15) of this model:

$$\text{ME}(m) = p(y|m) . \quad (1)$$

Sources:

- Penny WD (2012): “Comparing Dynamic Causal Models using AIC, BIC and Free Energy”; in: *NeuroImage*, vol. 59, iss. 2, pp. 319-330, eq. 15; URL: <https://www.sciencedirect.com/science/article/pii/S1053811911008160>; DOI: 10.1016/j.neuroimage.2011.07.039.

3.1.2 Derivation

Theorem: Let $p(y|\theta, m)$ be a likelihood function (\rightarrow I/5.1.2) of a generative model (\rightarrow I/5.1.1) m for making inferences on model parameters θ given measured data y . Moreover, let $p(\theta|m)$ be a prior distribution (\rightarrow I/5.1.3) on model parameters θ in the parameter space Θ . Then, the model evidence (\rightarrow IV/3.1.1) (ME) can be expressed in terms of likelihood (\rightarrow I/5.1.2) and prior (\rightarrow I/5.1.3) as

$$\text{ME}(m) = \int_{\Theta} p(y|\theta, m) p(\theta|m) d\theta . \quad (1)$$

Proof: This is a consequence of the law of marginal probability (\rightarrow I/1.3.3) for continuous variables (\rightarrow I/1.2.6)

$$p(y|m) = \int_{\Theta} p(y, \theta|m) d\theta \quad (2)$$

and the law of conditional probability (\rightarrow I/1.3.4) according to which

$$p(y, \theta|m) = p(y|\theta, m) p(\theta|m) . \quad (3)$$

Plugging (3) into (2), we obtain:

$$\text{ME}(m) = p(y|m) = \int_{\Theta} p(y|\theta, m) p(\theta|m) d\theta . \quad (4)$$

■

3.1.3 Log model evidence

Definition: Let m be a full probability model (\rightarrow I/5.1.6) with likelihood function (\rightarrow I/5.1.2) $p(y|\theta, m)$ and prior distribution (\rightarrow I/5.1.3) $p(\theta|m)$. Then, the log model evidence (LME) of m is defined as the logarithm of the marginal likelihood (\rightarrow I/5.1.15) of this model:

$$\text{LME}(m) = \log p(y|m) . \quad (1)$$

Sources:

- Soch J, Allefeld C (2018): “MACS – a new SPM toolbox for model assessment, comparison and selection”; in: *Journal of Neuroscience Methods*, vol. 306, pp. 19-31, eq. 13; URL: <https://www.sciencedirect.com/science/article/pii/S0165027018301468>; DOI: 10.1016/j.jneumeth.2018.05.017.

3.1.4 Derivation of the log model evidence

Theorem: Let $p(y|\theta, m)$ be a likelihood function (\rightarrow I/5.1.2) of a generative model (\rightarrow I/5.1.1) m for making inferences on model parameters θ given measured data y . Moreover, let $p(\theta|m)$ be a prior distribution (\rightarrow I/5.1.3) on model parameters θ . Then, the log model evidence (\rightarrow IV/3.1.3) (LME), also called marginal log-likelihood,

$$\text{LME}(m) = \log p(y|m) , \quad (1)$$

can be expressed in terms of likelihood (\rightarrow I/5.1.2) and prior (\rightarrow I/5.1.3) as

$$\text{LME}(m) = \log \int p(y|\theta, m) p(\theta|m) d\theta . \quad (2)$$

Proof: This is a consequence of the law of marginal probability (\rightarrow I/1.3.3) for continuous variables (\rightarrow I/1.2.6)

$$p(y|m) = \int p(y, \theta|m) d\theta \quad (3)$$

and the law of conditional probability (\rightarrow I/1.3.4) according to which

$$p(y, \theta|m) = p(y|\theta, m) p(\theta|m) . \quad (4)$$

Combining (3) with (4) and logarithmizing, we have:

$$\text{LME}(m) = \log p(y|m) = \log \int p(y|\theta, m) p(\theta|m) d\theta . \quad (5)$$

■

3.1.5 Expression using prior and posterior

Theorem: Let $p(y|\theta, m)$ be a likelihood function (\rightarrow I/5.1.2) of a generative model (\rightarrow I/5.1.1) m for making inferences on model parameters θ given measured data y . Moreover, let $p(\theta|m)$ be a prior distribution (\rightarrow I/5.1.3) on model parameters θ . Then, the log model evidence (\rightarrow IV/3.1.3) (LME), also called marginal log-likelihood,

$$\text{LME}(m) = \log p(y|m) , \quad (1)$$

can be expressed in terms of prior (\rightarrow I/5.1.3) and posterior (\rightarrow I/5.1.9) as

$$\text{LME}(m) = \log p(y|\theta, m) + \log p(\theta|m) - \log p(\theta|y, m) . \quad (2)$$

Proof: For a full probability model (\rightarrow I/5.1.6), Bayes' theorem (\rightarrow I/5.3.2) makes a statement about the posterior distribution (\rightarrow I/5.1.9):

$$p(\theta|y, m) = \frac{p(y|\theta, m) p(\theta|m)}{p(y|m)} . \quad (3)$$

Rearranging for $p(y|m)$ and logarithmizing, we have:

$$\begin{aligned} \text{LME}(m) = \log p(y|m) &= \log \frac{p(y|\theta, m) p(\theta|m)}{p(\theta|y, m)} \\ &= \log p(y|\theta, m) + \log p(\theta|m) - \log p(\theta|y, m) . \end{aligned} \quad (4)$$

■

3.1.6 Partition into accuracy and complexity

Theorem: The log model evidence (\rightarrow IV/3.1.3) can be partitioned into accuracy and complexity

$$\text{LME}(m) = \text{Acc}(m) - \text{Com}(m) \quad (1)$$

where the accuracy term is the posterior (\rightarrow I/5.1.9) expectation (\rightarrow I/1.12.9) of the log-likelihood function (\rightarrow I/4.1.2)

$$\text{Acc}(m) = \langle \log p(y|\theta, m) \rangle_{p(\theta|y, m)} \quad (2)$$

and the complexity penalty is the Kullback-Leibler divergence (\rightarrow I/2.5.1) of posterior (\rightarrow I/5.1.9) from prior (\rightarrow I/5.1.3)

$$\text{Com}(m) = \text{KL} [p(\theta|y, m) || p(\theta|m)] . \quad (3)$$

Proof: We consider Bayesian inference on data (\rightarrow I/1.1.5) y using model (\rightarrow I/5.1.1) m with parameters θ . Then, Bayes' theorem (\rightarrow I/5.3.2) makes a statement about the posterior distribution (\rightarrow I/5.1.9), i.e. the probability of parameters, given the data and the model:

$$p(\theta|y, m) = \frac{p(y|\theta, m) p(\theta|m)}{p(y|m)} . \quad (4)$$

Rearranging this for the model evidence (\rightarrow IV/3.1.5), we have:

$$p(y|m) = \frac{p(y|\theta, m) p(\theta|m)}{p(\theta|y, m)} . \quad (5)$$

Logarithmizing both sides of the equation, we obtain:

$$\log p(y|m) = \log p(y|\theta, m) - \log \frac{p(\theta|y, m)}{p(\theta|m)} . \quad (6)$$

Now taking the expectation over the posterior distribution yields:

$$\log p(y|m) = \int p(\theta|y, m) \log p(y|\theta, m) d\theta - \int p(\theta|y, m) \log \frac{p(\theta|y, m)}{p(\theta|m)} d\theta . \quad (7)$$

By definition, the left-hand side is the log model evidence and the terms on the right-hand side correspond to the posterior expectation of the log-likelihood function and the Kullback-Leibler divergence of posterior from prior

$$\text{LME}(m) = \langle \log p(y|\theta, m) \rangle_{p(\theta|y, m)} - \text{KL} [p(\theta|y, m) || p(\theta|m)] \quad (8)$$

which proofs the partition given by (1). ■

Sources:

- Beal & Ghahramani (2003): “The variational Bayesian EM algorithm for incomplete data: with application to scoring graphical model structures”; in: *Bayesian Statistics*, vol. 7; URL: <https://mlg.eng.cam.ac.uk/zoubin/papers/valencia02.pdf>.
- Penny et al. (2007): “Bayesian Comparison of Spatially Regularised General Linear Models”; in: *Human Brain Mapping*, vol. 28, pp. 275–293; URL: <https://onlinelibrary.wiley.com/doi/full/10.1002/hbm.20327>; DOI: 10.1002/hbm.20327.
- Ostwald et al. (2014): “A tutorial on variational Bayes for latent linear stochastic time-series models”; in: *Journal of Mathematical Psychology*, vol. 60, pp. 1-19; URL: <https://www.sciencedirect.com/science/article/abs/pii/S0022249614000352>; DOI: 10.1016/j.jmp.2014.04.003.
- Soch et al. (2016): “How to avoid mismodelling in GLM-based fMRI data analysis: cross-validated Bayesian model selection”; in: *NeuroImage*, vol. 141, pp. 469–489; URL: <https://www.sciencedirect.com/science/article/pii/S1053811916303615>; DOI: 10.1016/j.neuroimage.2016.07.047.

3.1.7 Subtraction of mean from LMEs

Theorem: Subtracting the arithmetic mean from a set of log model evidences (\rightarrow IV/3.1.3) is equivalent to dividing the corresponding model evidences (\rightarrow IV/3.1.1) by their geometric mean.

Proof: Consider a model space $\mathcal{M} = \{m_1, \dots, m_M\}$ consisting of M models (\rightarrow I/5.1.1). Then, the normalized log model evidence (\rightarrow IV/3.1.3) of any model m_i , denoted as $\text{LME}^*(m_i)$, may be calculated by subtracting the mean across model space:

$$\text{LME}^*(m_i) = \log p(y|m_i) - \frac{1}{M} \sum_{j=1}^M \log p(y|m_j) . \quad (1)$$

To prove the theorem, we will now rewrite the right-hand side until we arrive at an expression for the normalized model evidence (\rightarrow IV/3.1.3). First, applying $c \log_b a = \log_b a^c$, we obtain

$$\text{LME}^*(m_i) = \log p(y|m_i) - \sum_{j=1}^M \left[\log p(y|m_j)^{1/M} \right] . \quad (2)$$

Then, exponentiating both sides, we have:

$$\begin{aligned}
\exp [\text{LME}^*(m_i)] &= \frac{\exp [\log p(y|m_i)]}{\exp \left[\sum_{j=1}^M [\log p(y|m_j)^{1/M}] \right]} \\
&= \frac{p(y|m_i)}{\prod_{j=1}^M \exp [\log p(y|m_j)^{1/M}]} \\
&= \frac{p(y|m_i)}{\prod_{j=1}^M p(y|m_j)^{1/M}} \\
&= \frac{p(y|m_i)}{\left(\prod_{j=1}^M p(y|m_j) \right)^{1/M}} \\
&= \frac{p(y|m_i)}{\sqrt[M]{\prod_{j=1}^M p(y|m_j)}} .
\end{aligned} \tag{3}$$

Finally, the right-hand side is equal to ratio of m_i 's model evidence to the geometric mean of all model evidences.

■

Sources:

- Penny, Will (2015): “Bayesian model selection for group studies using Gibbs sampling”; in: *SPM12*, retrieved on 2023-09-08; URL: https://github.com/spm/spm12/blob/master/spm_BMS_gibbs.m.
- Soch, Joram (2018): “Random Effects Bayesian Model Selection using Variational Bayes”; in: *MACS – a new SPM toolbox for model assessment, comparison and selection*, retrieved on 2023-09-08; URL: https://github.com/JoramSoch/MACS/blob/master/ME_BMS_RFX_VB.m; DOI: 10.5281/zenodo.845404.

3.1.8 Uniform-prior log model evidence

Definition: Assume a generative model (\rightarrow I/5.1.1) m with likelihood function (\rightarrow I/5.1.2) $p(y|\theta, m)$ and a uniform (\rightarrow I/5.2.2) prior distribution (\rightarrow I/5.1.3) $p_{\text{uni}}(\theta|m)$. Then, the log model evidence (\rightarrow IV/3.1.3) of this model is called “log model evidence with uniform prior” or “uniform-prior log model evidence” (upLME):

$$\text{upLME}(m) = \log \int p(y|\theta, m) p_{\text{uni}}(\theta|m) d\theta . \tag{1}$$

Sources:

- Wikipedia (2020): “Lindley’s paradox”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-11-25; URL: https://en.wikipedia.org/wiki/Lindley%27s_paradox#Bayesian_approach.

3.1.9 Cross-validated log model evidence

Definition: Let there be a data set (\rightarrow I/1.1.5) y with mutually exclusive and collectively exhaustive subsets y_1, \dots, y_S . Assume a generative model (\rightarrow I/5.1.1) m with model parameters θ implying a

likelihood function (\rightarrow I/5.1.2) $p(y|\theta, m)$ and a non-informative (\rightarrow I/5.2.3) prior density (\rightarrow I/5.1.3) $p_{\text{ni}}(\theta|m)$.

Then, the cross-validated log model evidence (cvLME) of m is given by

$$\text{cvLME}(m) = \sum_{i=1}^S \log \int p(y_i|\theta, m) p(\theta|y_{-i}, m) d\theta \quad (1)$$

where $y_{-i} = \bigcup_{j \neq i} y_j$ is the union of all data subsets except y_i and $p(\theta|y_{-i}, m)$ is the posterior distribution (\rightarrow I/5.1.9) obtained from y_{-i} when using the prior distribution (\rightarrow I/5.1.3) $p_{\text{ni}}(\theta|m)$:

$$p(\theta|y_{-i}, m) = \frac{p(y_{-i}|\theta, m) p_{\text{ni}}(\theta|m)}{p(y_{-i}|m)} . \quad (2)$$

One addend of the cvLME is referred to as the out-of-sample log model evidence (oosLME) of m for the i -th data subset:

$$\text{oosLME}_i(m) = \log \int p(y_i|\theta, m) p(\theta|y_{-i}, m) d\theta . \quad (3)$$

Sources:

- Soch J, Allefeld C, Haynes JD (2016): “How to avoid mismodelling in GLM-based fMRI data analysis: cross-validated Bayesian model selection”; in: *NeuroImage*, vol. 141, pp. 469-489, eqs. 13-15; URL: <https://www.sciencedirect.com/science/article/pii/S1053811916303615>; DOI: 10.1016/j.neuroimage.2016.06.056.
- Soch J, Meyer AP, Allefeld C, Haynes JD (2017): “How to improve parameter estimates in GLM-based fMRI data analysis: cross-validated Bayesian model averaging”; in: *NeuroImage*, vol. 158, pp. 186-195, eq. 6; URL: <https://www.sciencedirect.com/science/article/pii/S105381191730527X>; DOI: 10.1016/j.neuroimage.2017.06.056.
- Soch J, Allefeld C (2018): “MACS – a new SPM toolbox for model assessment, comparison and selection”; in: *Journal of Neuroscience Methods*, vol. 306, pp. 19-31, eqs. 14-15; URL: <https://www.sciencedirect.com/science/article/pii/S0165027018301468>; DOI: 10.1016/j.jneumeth.2018.05.017.
- Soch J (2018): “cvBMS and cvBMA: filling in the gaps”; in: *arXiv stat.ME*, 1807.01585, eq. 1; URL: <https://arxiv.org/abs/1807.01585>.

3.1.10 Empirical Bayesian log model evidence

Definition: Let m be a generative model (\rightarrow I/5.1.1) with model parameters θ and hyper-parameters λ implying the likelihood function (\rightarrow I/5.1.2) $p(y|\theta, \lambda, m)$ and prior distribution (\rightarrow I/5.1.3) $p(\theta|\lambda, m)$. Then, the Empirical Bayesian (\rightarrow I/5.3.4) log model evidence (\rightarrow IV/3.1.3) is the logarithm of the marginal likelihood (\rightarrow I/5.1.15), maximized with respect to the hyper-parameters:

$$\text{ebLME}(m) = \log p(y|\hat{\lambda}, m) \quad (1)$$

where

$$p(y|\lambda, m) = \int p(y|\theta, \lambda, m) p(\theta|\lambda, m) d\theta \quad (2)$$

and (\rightarrow I/5.2.7)

$$\hat{\lambda} = \arg \max_{\lambda} \log p(y|\lambda, m) . \quad (3)$$

Sources:

- Wikipedia (2020): “Empirical Bayes method”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-11-25; URL: https://en.wikipedia.org/wiki/Empirical_Bayes_method#Introduction.
- Penny, W.D. and Ridgway, G.R. (2013): “Efficient Posterior Probability Mapping Using Savage-Dickey Ratios”; in: *PLoS ONE*, vol. 8, iss. 3, art. e59655, eqs. 7/11; URL: <https://journals.plos.org/plosone/article?id=10.1371/journal.pone.0059655>; DOI: 10.1371/journal.pone.0059655.

3.1.11 Variational Bayesian log model evidence

Definition: Let m be a generative model (\rightarrow I/5.1.1) with model parameters (\rightarrow I/1.5.7) $\theta \in \Theta$ implying the likelihood function (\rightarrow I/5.1.2) $p(y|\theta, m)$ and prior distribution (\rightarrow I/5.1.3) $p(\theta|m)$. Moreover, assume an approximate (\rightarrow I/5.3.5) posterior distribution (\rightarrow I/5.1.9) $q(\theta)$. Then, the Variational Bayesian (\rightarrow I/5.3.5) log model evidence (\rightarrow IV/3.1.3), also referred to as the “variational free energy”, is defined as the expected logarithm of the likelihood function, divided by the approximate posterior:

$$\text{vbLME}(m) = F_m[q(\theta)] = \int_{\Theta} q(\theta) \log \frac{p(\theta|y, m)}{q(\theta)} d\theta . \quad (1)$$

The variational free energy can be decomposed into the difference between log model evidence and KL divergence of approximate from true posterior (\rightarrow I/5.3.6) or, alternatively, as the difference of expected log-likelihood and KL divergence of approximate posterior from prior (\rightarrow I/5.3.6).

Sources:

- Wikipedia (2020): “Variational Bayesian methods”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-11-25; URL: https://en.wikipedia.org/wiki/Variational_Bayesian_methods#Evidence_lower_bound.
- Penny W, Flandin G, Trujillo-Barreto N (2007): “Bayesian Comparison of Spatially Regularised General Linear Models”; in: *Human Brain Mapping*, vol. 28, pp. 275–293, eqs. 2-9; URL: <https://onlinelibrary.wiley.com/doi/full/10.1002/hbm.20327>; DOI: 10.1002/hbm.20327.

3.2 Family evidence**3.2.1 Definition**

Definition: Let f be a family of M generative models (\rightarrow I/5.1.1) m_1, \dots, m_M , such that the following statement holds true:

$$f \Leftrightarrow m_1 \vee \dots \vee m_M . \quad (1)$$

Then, the family evidence (FE) of f is defined as the marginal probability (\rightarrow I/1.3.3) relative to the model evidences (\rightarrow IV/3.1.1) $p(y|m_i)$, conditional only on f :

$$\text{FE}(f) = p(y|f) . \quad (2)$$

Sources:

- Soch J, Allefeld C (2018): “MACS – a new SPM toolbox for model assessment, comparison and selection”; in: *Journal of Neuroscience Methods*, vol. 306, pp. 19-31, eq. 16; URL: <https://www.sciencedirect.com/science/article/pii/S0165027018301468>; DOI: 10.1016/j.jneumeth.2018.05.017.

3.2.2 Derivation

Theorem: Let f be a family of M generative models (\rightarrow I/5.1.1) m_1, \dots, m_M with model evidences (\rightarrow IV/3.1.1) $p(y|m_1), \dots, p(y|m_M)$. Then, the family evidence (\rightarrow IV/3.2.1) can be expressed in terms of the model evidences as

$$\text{FE}(f) = \sum_{i=1}^M p(y|m_i) p(m_i|f) \quad (1)$$

where $p(m_i|f)$ are the within-family (\rightarrow IV/3.2.3) prior (\rightarrow I/5.1.3) model (\rightarrow I/5.1.1) probabilities (\rightarrow I/1.3.1).

Proof: This is a consequence of the law of marginal probability (\rightarrow I/1.3.3) for discrete variables (\rightarrow I/1.2.6)

$$p(y|f) = \sum_{i=1}^M p(y, m_i|f) \quad (2)$$

and the law of conditional probability (\rightarrow I/1.3.4) according to which

$$p(y, m_i|f) = p(y|m_i, f) p(m_i|f) . \quad (3)$$

Since models are nested within model families (\rightarrow IV/3.2.1), such that $m_i \wedge f \leftrightarrow m_i$, we have the following equality of probabilities:

$$p(y|m_i, f) = p(y|m_i \wedge f) = p(y|m_i) . \quad (4)$$

Plugging (3) into (2) and applying (4), we obtain:

$$\text{FE}(f) = p(y|f) = \sum_{i=1}^M p(y|m_i) p(m_i|f) . \quad (5)$$

■

3.2.3 Log family evidence

Definition: Let f be a family of M generative models (\rightarrow I/5.1.1) m_1, \dots, m_M , such that the following statement holds true:

$$f \Leftrightarrow m_1 \vee \dots \vee m_M . \quad (1)$$

Then, the log family evidence is given by the logarithm of the family evidence (\rightarrow IV/3.2.1):

$$\text{LFE}(f) = \log p(y|f) = \log \sum_{i=1}^M p(y|m_i) p(m_i|f) . \quad (2)$$

Sources:

- Soch J, Allefeld C (2018): “MACS – a new SPM toolbox for model assessment, comparison and selection”; in: *Journal of Neuroscience Methods*, vol. 306, pp. 19-31, eq. 16; URL: <https://www.sciencedirect.com/science/article/pii/S0165027018301468>; DOI: 10.1016/j.jneumeth.2018.05.017.

3.2.4 Derivation of the log family evidence

Theorem: Let f be a family of M generative models (\rightarrow I/5.1.1) m_1, \dots, m_M with model evidences (\rightarrow I/5.1.15) $p(y|m_1), \dots, p(y|m_M)$. Then, the log family evidence (\rightarrow IV/3.2.3)

$$\text{LFE}(f) = \log p(y|f) \quad (1)$$

can be expressed as

$$\text{LFE}(f) = \log \sum_{i=1}^M p(y|m_i) p(m_i|f) \quad (2)$$

where $p(m_i|f)$ are the within-family (\rightarrow IV/3.2.3) prior (\rightarrow I/5.1.3) model (\rightarrow I/5.1.1) probabilities (\rightarrow I/1.3.1).

Proof: We will assume “prior additivity”

$$p(f) = \sum_{i=1}^M p(m_i) \quad (3)$$

and “posterior additivity” for family probabilities:

$$p(f|y) = \sum_{i=1}^M p(m_i|y) \quad (4)$$

Bayes’ theorem (\rightarrow I/5.3.2) for the family evidence (\rightarrow IV/3.2.3) gives

$$p(y|f) = \frac{p(f|y) p(y)}{p(f)} . \quad (5)$$

Applying (3) and (4), we have

$$p(y|f) = \frac{\sum_{i=1}^M p(m_i|y) p(y)}{\sum_{i=1}^M p(m_i)} . \quad (6)$$

Bayes’ theorem (\rightarrow I/5.3.2) for the model evidence (\rightarrow IV/3.2.3) gives

$$p(y|m_i) = \frac{p(m_i|y) p(y)}{p(m_i)} \quad (7)$$

which can be rearranged into

$$p(m_i|y) p(y) = p(y|m_i) p(m_i) . \quad (8)$$

Plugging (8) into (6), we have

$$\begin{aligned}
p(y|f) &= \frac{\sum_{i=1}^M p(y|m_i) p(m_i)}{\sum_{i=1}^M p(m_i)} \\
&= \sum_{i=1}^M p(y|m_i) \cdot \frac{p(m_i)}{\sum_{i=1}^M p(m_i)} \\
&= \sum_{i=1}^M p(y|m_i) \cdot \frac{p(m_i, f)}{p(f)} \\
&= \sum_{i=1}^M p(y|m_i) \cdot p(m_i|f) .
\end{aligned} \tag{9}$$

Equation (2) follows by logarithmizing both sides of (9). ■

3.2.5 Calculation from log model evidences

Theorem: Let m_1, \dots, m_M be M statistical models with log model evidences (\rightarrow IV/3.1.3) $\text{LME}(m_1), \dots, \text{LME}(m_M)$ and belonging to F mutually exclusive model families (\rightarrow IV/3.2.1) f_1, \dots, f_F . Then, the log family evidences (\rightarrow IV/3.2.3) are given by:

$$\text{LFE}(f_j) = \log \sum_{m_i \in f_j} [\exp[\text{LME}(m_i)] \cdot p(m_i|f_j)], \quad j = 1, \dots, F, \tag{1}$$

where $p(m_i|f_j)$ are within-family (\rightarrow IV/3.2.1) prior (\rightarrow I/5.1.3) model (\rightarrow I/5.1.1) probabilities (\rightarrow I/1.3.1).

Proof: Let us consider the (unlogarithmized) family evidence (\rightarrow IV/3.2.1) $p(y|f_j)$. According to the law of marginal probability (\rightarrow I/1.3.3), this conditional probability is given by

$$p(y|f_j) = \sum_{m_i \in f_j} [p(y|m_i, f_j) \cdot p(m_i|f_j)] . \tag{2}$$

Because model families are mutually exclusive, it holds that $p(y|m_i, f_j) = p(y|m_i)$, such that

$$p(y|f_j) = \sum_{m_i \in f_j} [p(y|m_i) \cdot p(m_i|f_j)] . \tag{3}$$

Logarithmizing transforms the family evidence $p(y|f_j)$ into the log family evidence (\rightarrow IV/3.2.3) $\text{LFE}(f_j)$:

$$\text{LFE}(f_j) = \log \sum_{m_i \in f_j} [p(y|m_i) \cdot p(m_i|f_j)] . \tag{4}$$

The definition of the log model evidence (\rightarrow IV/3.1.3)

$$\text{LME}(m) = \log p(y|m) \tag{5}$$

can be exponentiated to then read

$$\exp [\text{LME}(m)] = p(y|m) \quad (6)$$

and applying (6) to (4), we finally have:

$$\text{LFE}(f_j) = \log \sum_{m_i \in f_j} [\exp[\text{LME}(m_i)] \cdot p(m_i|f_j)] . \quad (7)$$

■

Sources:

- Soch J, Allefeld C (2018): “MACS – a new SPM toolbox for model assessment, comparison and selection”; in: *Journal of Neuroscience Methods*, vol. 306, pp. 19-31, eq. 16; URL: <https://www.sciencedirect.com/science/article/pii/S0165027018301468>; DOI: 10.1016/j.jneumeth.2018.05.017.

3.2.6 Approximation of log family evidences

Theorem: Let m_1, \dots, m_M be M statistical models with log model evidences (\rightarrow IV/3.1.3) $\text{LME}(m_1), \dots, \text{LME}(m_M)$ and belonging to F mutually exclusive (\rightarrow I/1.3.10) model families (\rightarrow IV/3.2.1) f_1, \dots, f_F .

1) Then, the log family evidences (\rightarrow IV/3.2.3) can be approximated as

$$\text{LFE}(f_j) = L^*(f_j) + \log \left[\sum_{m_i \in f_j} \exp[L'(m_i)] \cdot p(m_i|f_j) \right] \quad (1)$$

where $L^*(f_j)$ is the maximum log model evidence in family f_j , $L'(m_i)$ is the difference of each log model evidence to each family's maximum and $p(m_i|f_j)$ are within-family prior model probabilities (\rightarrow IV/3.2.2).

2) Under the condition that prior model probabilities are equal within model families, the approximation simplifies to

$$\text{LFE}(f_j) = L^*(f_j) + \log \sum_{m_i \in f_j} \exp[L'(m_i)] - \log M_j \quad (2)$$

where M_j is the number of models within family f_j .

Proof: The log family evidence is given in terms of log model evidences (\rightarrow IV/3.2.5) as

$$\text{LFE}(f_j) = \log \sum_{m_i \in f_j} [\exp[\text{LME}(m_i)] \cdot p(m_i|f_j)] . \quad (3)$$

Often, especially for complex models or many observations, log model evidences (\rightarrow IV/3.1.3) are highly negative, such that calculation of the term $\exp[\text{LME}(m_i)]$ in modern computers will give model evidences (\rightarrow IV/3.1.1) as zero, making calculation of LFEs impossible.

1) As a solution, we select the maximum LME within each family

$$L^*(f_j) = \max_{m_i \in f_j} [\text{LME}(m_i)] \quad (4)$$

and define differences between LMEs and maximum LME as

$$L'(m_i) = \text{LME}(m_i) - L^*(f_j) . \quad (5)$$

In this way, only the differences $L'(m_i)$ need to be exponentiated. If such a difference is highly negative, this model's contribution to the LFE will be zero – making this an approximation. However, the model is also much less evident that the family's best model in this case – making the approximation acceptable.

Using the relation (5), equation (3) can be reworked into

$$\begin{aligned}
 \text{LFE}(f_j) &= \log \sum_{m_i \in f_j} \exp[L'(m_i) + L^*(f_j)] \cdot p(m_i|f_j) \\
 &= \log \sum_{m_i \in f_j} \exp[L'(m_i)] \cdot \exp[L^*(f_j)] \cdot p(m_i|f_j) \\
 &= \log \left[\exp[L^*(f_j)] \cdot \sum_{m_i \in f_j} \exp[L'(m_i)] \cdot p(m_i|f_j) \right] \\
 &= L^*(f_j) + \log \left[\sum_{m_i \in f_j} \exp[L'(m_i)] \cdot p(m_i|f_j) \right].
 \end{aligned} \tag{6}$$

2) Under uniform within-family prior model probabilities (\rightarrow IV/3.2.2), we have

$$p(m_i|f_j) = \frac{1}{M_j} \quad \text{for all } m_i \in f_j, \tag{7}$$

such that the approximated log family evidences (\rightarrow IV/3.2.3) becomes

$$\begin{aligned}
 \text{LFE}(f_j) &= L^*(f_j) + \log \left[\sum_{m_i \in f_j} \exp[L'(m_i)] \cdot \frac{1}{M_j} \right] \\
 &= L^*(f_j) + \log \left[\frac{1}{M_j} \cdot \sum_{m_i \in f_j} \exp[L'(m_i)] \right] \\
 &= L^*(f_j) + \log \sum_{m_i \in f_j} \exp[L'(m_i)] - \log M_j.
 \end{aligned} \tag{8}$$

■

Sources:

- Soch J (2018): “cvBMS and cvBMA: filling in the gaps”; in: *arXiv stat.ME*, 1807.01585, sect. 2.3, eq. 32; URL: <https://arxiv.org/abs/1807.01585>.

3.3 Bayes factor

3.3.1 Definition

Definition: Consider two competing generative models (\rightarrow I/5.1.1) m_1 and m_2 for observed data y . Then the Bayes factor in favor m_1 over m_2 is the ratio of marginal likelihoods (\rightarrow I/5.1.15) of m_1 and m_2 :

$$\text{BF}_{12} = \frac{p(y \mid m_1)}{p(y \mid m_2)}. \tag{1}$$

Note that by Bayes' theorem (\rightarrow I/5.3.2), the ratio of posterior model probabilities (\rightarrow IV/3.4.1) (i.e., the posterior model odds) can be written as

$$\frac{p(m_1 | y)}{p(m_2 | y)} = \frac{p(m_1)}{p(m_2)} \cdot \frac{p(y | m_1)}{p(y | m_2)}, \quad (2)$$

or equivalently by (1),

$$\frac{p(m_1 | y)}{p(m_2 | y)} = \frac{p(m_1)}{p(m_2)} \cdot \text{BF}_{12}. \quad (3)$$

In other words, the Bayes factor can be viewed as the factor by which the prior model odds are updated (after observing data y) to posterior model odds – which is also expressed by Bayes' rule (\rightarrow I/5.3.3).

Sources:

- Kass, Robert E. and Raftery, Adrian E. (1995): “Bayes Factors”; in: *Journal of the American Statistical Association*, vol. 90, no. 430, pp. 773-795; URL: <https://dx.doi.org/10.1080/01621459.1995.10476572>; DOI: 10.1080/01621459.1995.10476572.

3.3.2 Transitivity

Theorem: Consider three competing models (\rightarrow I/5.1.1) m_1 , m_2 , and m_3 for observed data y . Then, the Bayes factor (\rightarrow IV/3.3.1) in favor of m_1 against m_3 can be written as:

$$\text{BF}_{13} = \text{BF}_{12} \cdot \text{BF}_{23}. \quad (1)$$

Proof: By definition (\rightarrow IV/3.3.1), the Bayes factor BF_{13} is the ratio of marginal likelihoods of data y under m_1 and m_3 , respectively. That is,

$$\text{BF}_{13} = \frac{p(y | m_1)}{p(y | m_3)}. \quad (2)$$

We can equivalently write

$$\begin{aligned} \text{BF}_{13} &\stackrel{(2)}{=} \frac{p(y | m_1)}{p(y | m_3)} \\ &= \frac{p(y | m_1)}{p(y | m_3)} \cdot \frac{p(y | m_2)}{p(y | m_2)} \\ &= \frac{p(y | m_1)}{p(y | m_2)} \cdot \frac{p(y | m_2)}{p(y | m_3)} \\ &\stackrel{(2)}{=} \text{BF}_{12} \cdot \text{BF}_{23}, \end{aligned} \quad (3)$$

which completes the proof of (1). ■

3.3.3 Computation using Savage-Dickey density ratio

Theorem: Consider two competing models (\rightarrow I/5.1.1) on data y containing parameters δ and φ , namely $m_0 : \delta = \delta_0, \varphi$ and $m_1 : \delta, \varphi$. In this context, we say that δ is a parameter of interest, φ is a nuisance parameter (i.e., common to both models), and m_0 is a sharp point hypothesis nested within m_1 . Suppose further that the prior for the nuisance parameter φ in m_0 is equal to the prior for φ in m_1 after conditioning on the restriction – that is, $p(\varphi | m_0) = p(\varphi | \delta = \delta_0, m_1)$. Then the Bayes factor (\rightarrow IV/3.3.1) for m_0 over m_1 can be computed as:

$$\text{BF}_{01} = \frac{p(\delta = \delta_0 | y, m_1)}{p(\delta = \delta_0 | m_1)}. \quad (1)$$

Proof: By definition (\rightarrow IV/3.3.1), the Bayes factor BF_{01} is the ratio of marginal likelihoods of data y over m_0 and m_1 , respectively. That is,

$$\text{BF}_{01} = \frac{p(y | m_0)}{p(y | m_1)}. \quad (2)$$

The key idea in the proof is that we can use a “change of variables” technique to express BF_{01} entirely in terms of the “encompassing” model m_1 . This proceeds by first unpacking the marginal likelihood (\rightarrow I/5.1.15) for m_0 over the nuisance parameter φ and then using the fact that m_0 is a sharp hypothesis nested within m_1 to rewrite everything in terms of m_1 . Specifically,

$$\begin{aligned} p(y | m_0) &= \int p(y | \varphi, m_0) p(\varphi | m_0) d\varphi \\ &= \int p(y | \varphi, \delta = \delta_0, m_1) p(\varphi | \delta = \delta_0, m_1) d\varphi \\ &= p(y | \delta = \delta_0, m_1). \end{aligned} \quad (3)$$

By Bayes’ theorem (\rightarrow I/5.3.2), we can rewrite this last line as

$$p(y | \delta = \delta_0, m_1) = \frac{p(\delta = \delta_0 | y, m_1) p(y | m_1)}{p(\delta = \delta_0 | m_1)}. \quad (4)$$

Thus we have

$$\begin{aligned} \text{BF}_{01} &\stackrel{(2)}{=} \frac{p(y | m_0)}{p(y | m_1)} \\ &= p(y | m_0) \cdot \frac{1}{p(y | m_1)} \\ &\stackrel{(3)}{=} p(y | \delta = \delta_0, m_1) \cdot \frac{1}{p(y | m_1)} \\ &\stackrel{(4)}{=} \frac{p(\delta = \delta_0 | y, m_1) p(y | m_1)}{p(\delta = \delta_0 | m_1)} \cdot \frac{1}{p(y | m_1)} \\ &= \frac{p(\delta = \delta_0 | y, m_1)}{p(\delta = \delta_0 | m_1)}, \end{aligned} \quad (5)$$

which completes the proof of (1).

**Sources:**

- Faulkenberry, Thomas J. (2019): “A tutorial on generalizing the default Bayesian t-test via posterior sampling and encompassing priors”; in: *Communications for Statistical Applications and Methods*, vol. 26, no. 2, pp. 217-238; URL: <https://dx.doi.org/10.29220/CSAM.2019.26.2.217>; DOI: 10.29220/CSAM.2019.26.2.217.
- Penny, W.D. and Ridgway, G.R. (2013): “Efficient Posterior Probability Mapping Using Savage-Dickey Ratios”; in: *PLoS ONE*, vol. 8, iss. 3, art. e59655, eq. 16; URL: <https://journals.plos.org/plosone/article?id=10.1371/journal.pone.0059655>; DOI: 10.1371/journal.pone.0059655.

3.3.4 Computation using encompassing prior method

Theorem: Consider two models m_1 and m_e , where m_1 is nested within an encompassing model (\rightarrow IV/3.3.5) m_e via an inequality constraint on some parameter θ , and θ is unconstrained under m_e . Then, the Bayes factor (\rightarrow IV/3.3.1) is

$$\text{BF}_{1e} = \frac{c}{d} = \frac{1/d}{1/c} \quad (1)$$

where $1/d$ and $1/c$ represent the proportions of the posterior and prior of the encompassing model, respectively, that are in agreement with the inequality constraint imposed by the nested model m_1 .

Proof: Consider first that for any model m_1 on data y with parameter θ , Bayes’ theorem (\rightarrow I/5.3.2) implies

$$p(\theta \mid y, m_1) = \frac{p(y \mid \theta, m_1) \cdot p(\theta \mid m_1)}{p(y \mid m_1)}. \quad (2)$$

Rearranging equation (2) allows us to write the marginal likelihood (\rightarrow I/5.1.15) for y under m_1 as

$$p(y \mid m_1) = \frac{p(y \mid \theta, m_1) \cdot p(\theta \mid m_1)}{p(\theta \mid y, m_1)}. \quad (3)$$

Taking the ratio of the marginal likelihoods for m_1 and the encompassing model (\rightarrow IV/3.3.5) m_e yields the following Bayes factor (\rightarrow IV/3.3.1):

$$\text{BF}_{1e} = \frac{p(y \mid \theta, m_1) \cdot p(\theta \mid m_1) / p(\theta \mid y, m_1)}{p(y \mid \theta, m_e) \cdot p(\theta \mid m_e) / p(\theta \mid y, m_e)}. \quad (4)$$

Now, both the constrained model m_1 and the encompassing model (\rightarrow IV/3.3.5) m_e contain the same parameter vector θ . Choose a specific value of θ , say θ' , that exists in the support of both models m_1 and m_e (we can do this, because m_1 is nested within m_e). Then, for this parameter value θ' , we have $p(y \mid \theta', m_1) = p(y \mid \theta', m_e)$, so the expression for the Bayes factor in equation (4) reduces to an expression involving only the priors and posteriors for θ' under m_1 and m_e :

$$\text{BF}_{1e} = \frac{p(\theta' \mid m_1) / p(\theta' \mid y, m_1)}{p(\theta' \mid m_e) / p(\theta' \mid y, m_e)}. \quad (5)$$

Because m_1 is nested within m_e via an inequality constraint, the prior $p(\theta' \mid m_1)$ is simply a truncation of the encompassing prior $p(\theta' \mid m_e)$. Thus, we can express $p(\theta' \mid m_1)$ in terms of the encompassing prior $p(\theta' \mid m_e)$ by multiplying the encompassing prior by an indicator function over m_1 and then normalizing the resulting product. That is,

$$\begin{aligned}
p(\theta' | m_1) &= \frac{p(\theta' | m_e) \cdot I_{\theta' \in m_1}}{\int p(\theta' | m_e) \cdot I_{\theta' \in m_1} d\theta'} \\
&= \left(\frac{I_{\theta' \in m_1}}{\int p(\theta' | m_e) \cdot I_{\theta' \in m_1} d\theta'} \right) \cdot p(\theta' | m_e),
\end{aligned} \tag{6}$$

where $I_{\theta' \in m_1}$ is an indicator function. For parameters $\theta' \in m_1$, this indicator function is identically equal to 1, so the expression in parentheses reduces to a constant, say c , allowing us to write the prior as

$$p(\theta' | m_1) = c \cdot p(\theta' | m_e). \tag{7}$$

By similar reasoning, we can write the posterior as

$$p(\theta' | y, m_1) = \left(\frac{I_{\theta' \in m_1}}{\int p(\theta' | y, m_e) \cdot I_{\theta' \in m_1} d\theta'} \right) \cdot p(\theta' | y, m_e) = d \cdot p(\theta' | y, m_e). \tag{8}$$

Plugging (7) and (8) into (5), this gives us

$$\text{BF}_{1e} = \frac{c \cdot p(\theta' | m_e) / d \cdot p(\theta' | y, m_e)}{p(\theta' | m_e) / p(\theta' | y, m_e)} = \frac{c}{d} = \frac{1/d}{1/c}, \tag{9}$$

which completes the proof. Note that by definition, $1/d$ represents the proportion of the posterior distribution for θ under the encompassing model (\rightarrow IV/3.3.5) m_e that agrees with the constraints imposed by m_1 . Similarly, $1/c$ represents the proportion of the prior distribution for θ under the encompassing model (\rightarrow IV/3.3.5) m_e that agrees with the constraints imposed by m_1 . ■

Sources:

- Klugkist, I., Kato, B., and Hoijsink, H. (2005): “Bayesian model selection using encompassing priors”; in: *Statistica Neerlandica*, vol. 59, no. 1, pp. 57-69; URL: <https://dx.doi.org/10.1111/j.1467-9574.2005.00279.x>; DOI: 10.1111/j.1467-9574.2005.00279.x.
- Faulkenberry, Thomas J. (2019): “A tutorial on generalizing the default Bayesian t-test via posterior sampling and encompassing priors”; in: *Communications for Statistical Applications and Methods*, vol. 26, no. 2, pp. 217-238; URL: <https://dx.doi.org/10.29220/CSAM.2019.26.2.217>; DOI: 10.29220/CSAM.2019.26.2.217.

3.3.5 Encompassing model

Definition: Consider a family f of generative models (\rightarrow I/5.1.1) m on data y , where each $m \in f$ is defined by placing an inequality constraint on model parameter(s) θ (e.g., $m : \theta > 0$). Then the encompassing model m_e is constructed such that each m is nested within m_e and all inequality constraints on the parameter(s) θ are removed.

Sources:

- Klugkist, I., Kato, B., and Hoijsink, H. (2005): “Bayesian model selection using encompassing priors”; in: *Statistica Neerlandica*, vol. 59, no. 1, pp. 57-69; URL: <https://dx.doi.org/10.1111/j.1467-9574.2005.00279.x>; DOI: 10.1111/j.1467-9574.2005.00279.x.

3.3.6 Log Bayes factor

Definition: Let there be two generative models (\rightarrow I/5.1.1) m_1 and m_2 which are mutually exclusive, but not necessarily collectively exhaustive:

$$\neg(m_1 \wedge m_2) \quad (1)$$

Then, the Bayes factor in favor of m_1 and against m_2 is the ratio of the model evidences (\rightarrow I/5.1.15) of m_1 and m_2 :

$$\text{BF}_{12} = \frac{p(y|m_1)}{p(y|m_2)}. \quad (2)$$

The log Bayes factor is given by the logarithm of the Bayes factor:

$$\text{LBF}_{12} = \log \text{BF}_{12} = \log \frac{p(y|m_1)}{p(y|m_2)}. \quad (3)$$

Sources:

- Soch J, Allefeld C (2018): “MACS – a new SPM toolbox for model assessment, comparison and selection”; in: *Journal of Neuroscience Methods*, vol. 306, pp. 19-31, eq. 18; URL: <https://www.sciencedirect.com/science/article/pii/S0165027018301468>; DOI: 10.1016/j.jneumeth.2018.05.017.

3.3.7 Derivation of the log Bayes factor

Theorem: Let there be two generative models (\rightarrow I/5.1.1) m_1 and m_2 with model evidences (\rightarrow I/5.1.15) $p(y|m_1)$ and $p(y|m_2)$. Then, the log Bayes factor (\rightarrow IV/3.3.6)

$$\text{LBF}_{12} = \log \text{BF}_{12} \quad (1)$$

can be expressed as

$$\text{LBF}_{12} = \log \frac{p(y|m_1)}{p(y|m_2)}. \quad (2)$$

Proof: The Bayes factor (\rightarrow IV/3.3.1) is defined as the posterior (\rightarrow I/5.1.9) odds ratio (\rightarrow I/5.3.1) when both models (\rightarrow I/5.1.1) are equally likely apriori (\rightarrow I/5.1.3):

$$\text{BF}_{12} = \frac{p(m_1|y)}{p(m_2|y)} \quad (3)$$

Plugging in the posterior odds ratio according to Bayes’ rule (\rightarrow I/5.3.3), we have

$$\text{BF}_{12} = \frac{p(y|m_1)}{p(y|m_2)} \cdot \frac{p(m_1)}{p(m_2)}. \quad (4)$$

When both models are equally likely apriori, the prior (\rightarrow I/5.1.3) odds ratio (\rightarrow I/5.3.1) is one, such that

$$\text{BF}_{12} = \frac{p(y|m_1)}{p(y|m_2)}. \quad (5)$$

Equation (2) follows by logarithmizing both sides of (5). ■

3.3.8 Calculation from log model evidences

Theorem: Let m_1 and m_2 be two statistical models with log model evidences (\rightarrow IV/3.1.3) $\text{LME}(m_1)$ and $\text{LME}(m_2)$. Then, the log Bayes factor (\rightarrow IV/3.3.6) in favor of model m_1 and against model m_2 is the difference of the log model evidences:

$$\text{LBF}_{12} = \text{LME}(m_1) - \text{LME}(m_2) . \quad (1)$$

Proof: The Bayes factor (\rightarrow IV/3.3.1) is defined as the ratio of the model evidences (\rightarrow I/5.1.15) of m_1 and m_2

$$\text{BF}_{12} = \frac{p(y|m_1)}{p(y|m_2)} \quad (2)$$

and the log Bayes factor (\rightarrow IV/3.3.6) is defined as the logarithm of the Bayes factor

$$\text{LBF}_{12} = \log \text{BF}_{12} . \quad (3)$$

Thus, the log Bayes factor can be expressed as

$$\text{LBF}_{12} = \log \frac{p(y|m_1)}{p(y|m_2)} . \quad (4)$$

and, with the definition of the log model evidence (\rightarrow IV/3.1.3)

$$\text{LME}(m) = \log p(y|m) \quad (5)$$

and resolving the logarithm, we finally have:

$$\begin{aligned} \text{LBF}_{12} &= \log p(y|m_1) - \log p(y|m_2) \\ &= \text{LME}(m_1) - \text{LME}(m_2) . \end{aligned} \quad (6)$$

■

Sources:

- Soch J, Allefeld C (2018): “MACS – a new SPM toolbox for model assessment, comparison and selection”; in: *Journal of Neuroscience Methods*, vol. 306, pp. 19-31, eq. 18; URL: <https://www.sciencedirect.com/science/article/pii/S0165027018301468>; DOI: 10.1016/j.jneumeth.2018.05.017.

3.4 Posterior model probability

3.4.1 Definition

Definition: Let m_1, \dots, m_M be M statistical models (\rightarrow I/5.1.6) with model evidences (\rightarrow I/5.1.15) $p(y|m_1), \dots, p(y|m_M)$ and prior probabilities (\rightarrow I/5.1.3) $p(m_1), \dots, p(m_M)$. Then, the conditional probability (\rightarrow I/1.3.4) of model m_i , given the data y , is called the posterior probability (\rightarrow I/5.1.9) of model m_i :

$$\text{PP}(m_i) = p(m_i|y) . \quad (1)$$

Sources:

- Soch J, Allefeld C (2018): “MACS – a new SPM toolbox for model assessment, comparison and selection”; in: *Journal of Neuroscience Methods*, vol. 306, pp. 19-31, eq. 23; URL: <https://www.sciencedirect.com/science/article/pii/S0165027018301468>; DOI: 10.1016/j.jneumeth.2018.05.017.

3.4.2 Derivation

Theorem: Let there be a set of generative models (\rightarrow I/5.1.1) m_1, \dots, m_M with model evidences (\rightarrow I/5.1.15) $p(y|m_1), \dots, p(y|m_M)$ and prior probabilities (\rightarrow I/5.1.3) $p(m_1), \dots, p(m_M)$. Then, the posterior probability (\rightarrow IV/3.4.1) of model m_i is given by

$$p(m_i|y) = \frac{p(y|m_i) p(m_i)}{\sum_{j=1}^M p(y|m_j) p(m_j)}, \quad i = 1, \dots, M. \quad (1)$$

Proof: From Bayes’ theorem (\rightarrow I/5.3.2), the posterior model probability (\rightarrow IV/3.4.1) of the i -th model can be derived as

$$p(m_i|y) = \frac{p(y|m_i) p(m_i)}{p(y)}. \quad (2)$$

Using the law of marginal probability (\rightarrow I/1.3.3), the denominator can be rewritten, such that

$$p(m_i|y) = \frac{p(y|m_i) p(m_i)}{\sum_{j=1}^M p(y, m_j)}. \quad (3)$$

Finally, using the law of conditional probability (\rightarrow I/1.3.4), we have

$$p(m_i|y) = \frac{p(y|m_i) p(m_i)}{\sum_{j=1}^M p(y|m_j) p(m_j)}. \quad (4)$$

■

3.4.3 Calculation from Bayes factors

Theorem: Let m_0, m_1, \dots, m_M be $M + 1$ statistical models (\rightarrow I/5.1.1) with model evidences (\rightarrow IV/3.1.3) $p(y|m_0), p(y|m_1), \dots, p(y|m_M)$. Then, the posterior model probabilities (\rightarrow IV/3.4.1) of the models m_1, \dots, m_M are given by

$$p(m_i|y) = \frac{\text{BF}_{i,0} \cdot \alpha_i}{\sum_{j=1}^M \text{BF}_{j,0} \cdot \alpha_j}, \quad i = 1, \dots, M, \quad (1)$$

where $\text{BF}_{i,0}$ is the Bayes factor (\rightarrow IV/3.3.1) comparing model m_i with m_0 and α_i is the prior (\rightarrow I/5.1.3) odds ratio (\rightarrow I/5.3.1) of model m_i against m_0 .

Proof: Define the Bayes factor (\rightarrow IV/3.3.1) for m_i

$$\text{BF}_{i,0} = \frac{p(y|m_i)}{p(y|m_0)} \quad (2)$$

and prior odds ratio (\rightarrow I/5.3.1) of m_i against m_0

$$\alpha_i = \frac{p(m_i)}{p(m_0)}. \quad (3)$$

The posterior model probability (\rightarrow IV/3.4.2) of m_i is given by

$$p(m_i|y) = \frac{p(y|m_i) \cdot p(m_i)}{\sum_{j=1}^M p(y|m_j) \cdot p(m_j)} . \quad (4)$$

Now applying (2) and (3) to (4), we have

$$\begin{aligned} p(m_i|y) &= \frac{\text{BF}_{i,0} p(y|m_0) \cdot \alpha_i p(m_0)}{\sum_{j=1}^M \text{BF}_{j,0} p(y|m_0) \cdot \alpha_j p(m_0)} \\ &= \frac{[p(y|m_0) p(m_0)] \text{BF}_{i,0} \cdot \alpha_i}{[p(y|m_0) p(m_0)] \sum_{j=1}^M \text{BF}_{j,0} \cdot \alpha_j} , \end{aligned} \quad (5)$$

such that

$$p(m_i|y) = \frac{\text{BF}_{i,0} \cdot \alpha_i}{\sum_{j=1}^M \text{BF}_{j,0} \cdot \alpha_j} . \quad (6)$$

■

Sources:

- Hoeting JA, Madigan D, Raftery AE, Volinsky CT (1999): “Bayesian Model Averaging: A Tutorial”; in: *Statistical Science*, vol. 14, no. 4, pp. 382–417, eq. 9; URL: <https://projecteuclid.org/euclid.ss/1009212519>; DOI: 10.1214/ss/1009212519.

3.4.4 Calculation from log Bayes factor

Theorem: Let m_1 and m_2 be two statistical models with the log Bayes factor (\rightarrow IV/3.3.6) LBF_{12} in favor of model m_1 and against model m_2 . Then, if both models are equally likely apriori (\rightarrow I/5.1.3), the posterior model probability (\rightarrow IV/3.4.1) of m_1 is

$$p(m_1|y) = \frac{\exp(\text{LBF}_{12})}{\exp(\text{LBF}_{12}) + 1} . \quad (1)$$

Proof: From Bayes’ rule (\rightarrow I/5.3.3), the posterior odds ratio (\rightarrow I/5.3.1) is

$$\frac{p(m_1|y)}{p(m_2|y)} = \frac{p(y|m_1)}{p(y|m_2)} \cdot \frac{p(m_1)}{p(m_2)} . \quad (2)$$

When both models are equally likely apriori (\rightarrow I/5.1.3), the prior odds ratio (\rightarrow I/5.3.1) is one, such that

$$\frac{p(m_1|y)}{p(m_2|y)} = \frac{p(y|m_1)}{p(y|m_2)} . \quad (3)$$

Now the right-hand side corresponds to the Bayes factor (\rightarrow IV/3.3.1), therefore

$$\frac{p(m_1|y)}{p(m_2|y)} = \text{BF}_{12} . \quad (4)$$

Because the two posterior model probabilities (\rightarrow IV/3.4.1) add up to 1, we have

$$\frac{p(m_1|y)}{1 - p(m_1|y)} = \text{BF}_{12} . \quad (5)$$

Now rearranging for the posterior probability (\rightarrow IV/3.4.1), this gives

$$p(m_1|y) = \frac{\text{BF}_{12}}{\text{BF}_{12} + 1} . \quad (6)$$

Because the log Bayes factor is the logarithm of the Bayes factor (\rightarrow IV/3.3.6), we finally have

$$p(m_1|y) = \frac{\exp(\text{LBF}_{12})}{\exp(\text{LBF}_{12}) + 1} . \quad (7)$$

■

Sources:

- Soch J, Allefeld C (2018): “MACS – a new SPM toolbox for model assessment, comparison and selection”; in: *Journal of Neuroscience Methods*, vol. 306, pp. 19-31, eq. 21; URL: <https://www.sciencedirect.com/science/article/pii/S0165027018301468>; DOI: 10.1016/j.jneumeth.2018.05.017.
- Zeidman P, Silson EH, Schwarzkopf DS, Baker CI, Penny W (2018): “Bayesian population receptive field modelling”; in: *NeuroImage*, vol. 180, pp. 173-187, eq. 11; URL: <https://www.sciencedirect.com/science/article/pii/S1053811917307462>; DOI: 10.1016/j.neuroimage.2017.09.008.
- Zeidman P, Friston K, Parr T (2023): “A primer on Variational Laplace (VL)”; in: *NeuroImage*, vol. 279, art. 120310, eq. 56; URL: <https://www.sciencedirect.com/science/article/pii/S1053811923004615>; DOI: 10.1016/j.neuroimage.2023.120310.

3.4.5 Calculation from log model evidences

Theorem: Let m_1, \dots, m_M be M statistical models with log model evidences (\rightarrow IV/3.1.3) $\text{LME}(m_1), \dots, \text{LME}(m_M)$. Then, the posterior model probabilities (\rightarrow IV/3.4.1) are given by:

$$p(m_i|y) = \frac{\exp[\text{LME}(m_i)] p(m_i)}{\sum_{j=1}^M \exp[\text{LME}(m_j)] p(m_j)}, \quad i = 1, \dots, M , \quad (1)$$

where $p(m_i)$ are prior (\rightarrow I/5.1.3) model probabilities.

Proof: The posterior model probability (\rightarrow IV/3.4.2) can be derived as

$$p(m_i|y) = \frac{p(y|m_i) p(m_i)}{\sum_{j=1}^M p(y|m_j) p(m_j)} . \quad (2)$$

The definition of the log model evidence (\rightarrow IV/3.1.3)

$$\text{LME}(m) = \log p(y|m) \quad (3)$$

can be exponentiated to then read

$$\exp [\text{LME}(m)] = p(y|m) \quad (4)$$

and applying (4) to (2), we finally have:

$$p(m_i|y) = \frac{\exp[\text{LME}(m_i)] p(m_i)}{\sum_{j=1}^M \exp[\text{LME}(m_j)] p(m_j)} . \quad (5)$$

Sources:

- Soch J, Allefeld C (2018): “MACS – a new SPM toolbox for model assessment, comparison and selection”; in: *Journal of Neuroscience Methods*, vol. 306, pp. 19-31, eq. 23; URL: <https://www.sciencedirect.com/science/article/pii/S0165027018301468>; DOI: 10.1016/j.jneumeth.2018.05.017.

3.5 Bayesian model averaging**3.5.1 Definition**

Definition: Let m_1, \dots, m_M be M statistical models (\rightarrow I/5.1.6) with posterior model probabilities (\rightarrow IV/3.4.1) $p(m_1|y), \dots, p(m_M|y)$ and posterior distributions (\rightarrow I/5.1.9) $p(\theta|y, m_1), \dots, p(\theta|y, m_M)$. Then, Bayesian model averaging (BMA) consists in finding the marginal (\rightarrow I/1.5.3) posterior (\rightarrow I/5.1.9) density (\rightarrow I/1.7.1), conditional (\rightarrow I/1.3.4) on the measured data y , but unconditional (\rightarrow I/1.3.3) on the modelling approach m :

$$p(\theta|y) = \sum_{i=1}^M p(\theta|y, m_i) \cdot p(m_i|y) . \quad (1)$$

Sources:

- Hoeting JA, Madigan D, Raftery AE, Volinsky CT (1999): “Bayesian Model Averaging: A Tutorial”; in: *Statistical Science*, vol. 14, no. 4, pp. 382–417, eq. 1; URL: <https://projecteuclid.org/euclid.ss/1009212519>; DOI: 10.1214/ss/1009212519.

3.5.2 Derivation

Theorem: Let m_1, \dots, m_M be M statistical models (\rightarrow I/5.1.6) with posterior model probabilities (\rightarrow IV/3.4.1) $p(m_1|y), \dots, p(m_M|y)$ and posterior distributions (\rightarrow I/5.1.9) $p(\theta|y, m_1), \dots, p(\theta|y, m_M)$. Then, the marginal (\rightarrow I/1.5.3) posterior (\rightarrow I/5.1.9) density (\rightarrow I/1.7.1), conditional (\rightarrow I/1.3.4) on the measured data y , but unconditional (\rightarrow I/1.3.3) on the modelling approach m , is given by:

$$p(\theta|y) = \sum_{i=1}^M p(\theta|y, m_i) \cdot p(m_i|y) . \quad (1)$$

Proof: Using the law of marginal probability (\rightarrow I/1.3.3), the probability distribution of the shared parameters θ conditional (\rightarrow I/1.3.4) on the measured data y can be obtained by marginalizing (\rightarrow I/1.3.3) over the discrete random variable (\rightarrow I/1.2.2) model m :

$$p(\theta|y) = \sum_{i=1}^M p(\theta, m_i|y) . \quad (2)$$

Using the law of the conditional probability (\rightarrow I/1.3.4), the summand can be expanded to give

$$p(\theta|y) = \sum_{i=1}^M p(\theta|y, m_i) \cdot p(m_i|y) \quad (3)$$

where $p(\theta|y, m_i)$ is the posterior distribution (\rightarrow I/5.1.9) of the i -th model and $p(m_i|y)$ happens to be the posterior probability (\rightarrow IV/3.4.1) of the i -th model.

■

3.5.3 Calculation from log model evidences

Theorem: Let m_1, \dots, m_M be M statistical models (\rightarrow I/5.1.6) describing the same measured data y with log model evidences (\rightarrow IV/3.1.3) $\text{LME}(m_1), \dots, \text{LME}(m_M)$ and shared model parameters θ . Then, Bayesian model averaging (\rightarrow IV/3.5.1) determines the following posterior distribution over θ :

$$p(\theta|y) = \sum_{i=1}^M p(\theta|m_i, y) \cdot \frac{\exp[\text{LME}(m_i)] p(m_i)}{\sum_{j=1}^M \exp[\text{LME}(m_j)] p(m_j)} , \quad (1)$$

where $p(\theta|m_i, y)$ is the posterior distributions over θ obtained using m_i .

Proof: According to the law of marginal probability (\rightarrow I/1.3.3), the probability of the shared parameters θ conditional on the measured data y can be obtained (\rightarrow IV/3.5.2) by marginalizing over the discrete variable model m :

$$p(\theta|y) = \sum_{i=1}^M p(\theta|m_i, y) \cdot p(m_i|y) , \quad (2)$$

where $p(m_i|y)$ is the posterior probability (\rightarrow IV/3.4.1) of the i -th model. One can express posterior model probabilities in terms of log model evidences (\rightarrow IV/3.4.5) as

$$p(m_i|y) = \frac{\exp[\text{LME}(m_i)] p(m_i)}{\sum_{j=1}^M \exp[\text{LME}(m_j)] p(m_j)} \quad (3)$$

and by plugging (3) into (2), one arrives at (1).

■

Sources:

- Soch J, Allefeld C (2018): “MACS – a new SPM toolbox for model assessment, comparison and selection”; in: *Journal of Neuroscience Methods*, vol. 306, pp. 19-31, eq. 25; URL: <https://www.sciencedirect.com/science/article/pii/S0165027018301468>; DOI: 10.1016/j.jneumeth.2018.05.017.

Chapter V

Appendix

1 Proof by Number

ID	Shortcut	Theorem	Author	Date	Page
P1	mvn-ltt	Linear transformation theorem for the multivariate normal distribution	JoramSoch	2019-08-27	348
P2	mlr-ols	Ordinary least squares for multiple linear regression	JoramSoch	2019-09-27	524
P3	lme-anc	Partition of the log model evidence into accuracy and complexity	JoramSoch	2019-09-27	711
P4	bayes-th	Bayes' theorem	JoramSoch	2019-09-27	156
P5	mse-bnv	Partition of the mean squared error into bias and variance	JoramSoch	2019-11-27	134
P6	ng-kl	Kullback-Leibler divergence for the normal-gamma distribution	JoramSoch	2019-12-06	374
P7	glm-mle	Maximum likelihood estimation for the general linear model	JoramSoch	2019-12-06	603
P8	rsq-der	Derivation of R^2 and adjusted R^2	JoramSoch	2019-12-06	688
P9	blr-prior	Conjugate prior distribution for Bayesian linear regression	JoramSoch	2020-01-03	564
P10	blr-post	Posterior distribution for Bayesian linear regression	JoramSoch	2020-01-03	565
P11	blr-lme	Log model evidence for Bayesian linear regression	JoramSoch	2020-01-03	567
P12	bayes-rule	Bayes' rule	JoramSoch	2020-01-06	157
P13	lme-der	Derivation of the log model evidence	JoramSoch	2020-01-06	710
P14	rsq-mll	Relationship between R^2 and maximum log-likelihood	JoramSoch	2020-01-08	690
P15	norm-mean	Mean of the normal distribution	JoramSoch	2020-01-09	235
P16	norm-med	Median of the normal distribution	JoramSoch	2020-01-09	237
P17	norm-mode	Mode of the normal distribution	JoramSoch	2020-01-09	237
P18	norm-var	Variance of the normal distribution	JoramSoch	2020-01-09	238
P19	dmi-mce	Relation of mutual information to marginal and conditional entropy	JoramSoch	2020-01-13	117

P20	dmi-mje	Relation of mutual information to marginal and joint entropy	JoramSoch	2020-01-13	118
P21	dmi-jce	Relation of mutual information to joint and conditional entropy	JoramSoch	2020-01-13	119
P22	bern-mean	Mean of the Bernoulli distribution	JoramSoch	2020-01-16	179
P23	bin-mean	Mean of the binomial distribution	JoramSoch	2020-01-16	186
P24	cat-mean	Mean of the categorical distribution	JoramSoch	2020-01-16	201
P25	mult-mean	Mean of the multinomial distribution	JoramSoch	2020-01-16	205
P26	matn-mvn	Equivalence of matrix-normal distribution and multivariate normal distribution	JoramSoch	2020-01-20	386
P27	poiss-mle	Maximum likelihood estimation for Poisson-distributed data	JoramSoch	2020-01-20	655
P28	beta-mome	Method of moments for beta-distributed data	JoramSoch	2020-01-22	669
P29	bin-prior	Conjugate prior distribution for binomial observations	JoramSoch	2020-01-23	632
P30	bin-post	Posterior distribution for binomial observations	JoramSoch	2020-01-24	633
P31	bin-lme	Log model evidence for binomial observations	JoramSoch	2020-01-24	634
P32	bic-der	Derivation of the Bayesian information criterion	JoramSoch	2020-01-26	706
P33	norm-pdf	Probability density function of the normal distribution	JoramSoch	2020-01-27	228
P34	mvn-pdf	Probability density function of the multivariate normal distribution	JoramSoch	2020-01-27	337
P35	mvn-marg	Marginal distributions of the multivariate normal distribution	JoramSoch	2020-01-29	349
P36	ng-marg	Marginal distributions of the normal-gamma distribution	JoramSoch	2020-01-29	376
P37	cuni-pdf	Probability density function of the continuous uniform distribution	JoramSoch	2020-01-31	210
P38	cuni-cdf	Cumulative distribution function of the continuous uniform distribution	JoramSoch	2020-01-02	211

P39	cuni-qf	Quantile function of the continuous uniform distribution	JoramSoch	2020-01-02	212
P40	mlr-ols2	Ordinary least squares for multiple linear regression	JoramSoch	2020-02-03	524
P41	poissexp-prior	Conjugate prior distribution for the Poisson distribution with exposure values	JoramSoch	2020-02-04	663
P42	poissexp-post	Posterior distribution for the Poisson distribution with exposure values	JoramSoch	2020-02-04	664
P43	poissexp-lme	Log model evidence for the Poisson distribution with exposure values	JoramSoch	2020-02-04	666
P44	ng-pdf	Probability density function of the normal-gamma distribution	JoramSoch	2020-02-07	369
P45	gam-pdf	Probability density function of the gamma distribution	JoramSoch	2020-02-08	260
P46	exp-pdf	Probability density function of the exponential distribution	JoramSoch	2020-02-08	274
P47	exp-mean	Mean of the exponential distribution	JoramSoch	2020-02-10	277
P48	exp-cdf	Cumulative distribution function of the exponential distribution	JoramSoch	2020-02-11	275
P49	exp-med	Median of the exponential distribution	JoramSoch	2020-02-11	278
P50	exp-qf	Quantile function of the exponential distribution	JoramSoch	2020-02-12	276
P51	exp-mode	Mode of the exponential distribution	kantundpeterpan	2020-02-12	278
P52	mean-nonneg	Non-negativity of the expected value	JoramSoch	2020-02-13	52
P53	mean-lin	Linearity of the expected value	JoramSoch	2020-02-13	53
P54	mean-mono	Monotonicity of the expected value	JoramSoch	2020-02-17	54
P55	mean-mult	(Non-)Multiplicativity of the expected value	JoramSoch	2020-02-17	55
P56	ci-wilks	Construction of confidence intervals using Wilks' theorem	JoramSoch	2020-02-19	135
P57	ent-nonneg	Non-negativity of the Shannon entropy	JoramSoch	2020-02-19	104

P58	cmi-mcde	Relation of continuous mutual information to marginal and conditional differential entropy	JoramSoch	2020-02-21	121
P59	cmi-mjde	Relation of continuous mutual information to marginal and joint differential entropy	JoramSoch	2020-02-21	122
P60	cmi-jcde	Relation of continuous mutual information to joint and conditional differential entropy	JoramSoch	2020-02-21	123
P61	resvar-bias	Maximum likelihood estimator of variance is biased	JoramSoch	2020-02-24	682
P62	resvar-unb	Construction of unbiased estimator for variance	JoramSoch	2020-02-25	686
P63	snr-rsq	Relationship between signal-to-noise ratio and R^2	JoramSoch	2020-02-26	702
P64	lbf-lme	Log Bayes factor in terms of log model evidences	JoramSoch	2020-02-27	726
P65	lfe-lme	Log family evidences in terms of log model evidences	JoramSoch	2020-02-27	718
P66	pmp-lme	Posterior model probabilities in terms of log model evidences	JoramSoch	2020-02-27	729
P67	bma-lme	Bayesian model averaging in terms of log model evidences	JoramSoch	2020-02-27	731
P68	dent-neg	Differential entropy can be negative	JoramSoch	2020-03-02	110
P69	exp-gam	Exponential distribution is a special case of gamma distribution	JoramSoch	2020-03-02	273
P70	matn-pdf	Probability density function of the matrix-normal distribution	JoramSoch	2020-03-02	387
P71	norm-mgf	Moment-generating function of the normal distribution	JoramSoch	2020-03-03	229
P72	logreg-lonp	Log-odds and probability in logistic regression	JoramSoch	2020-03-03	678
P73	pmp-lbf	Posterior model probability in terms of log Bayes factor	JoramSoch	2020-03-03	728
P74	pmp-bf	Posterior model probabilities in terms of Bayes factors	JoramSoch	2020-03-03	727

P75	mlr-mat	Transformation matrices for ordinary least squares	JoramSoch	2020-03-09	531
P76	mlr-pss	Partition of sums of squares for multiple linear regression	JoramSoch	2020-03-09	529
P77	mlr-wls	Weighted least squares for multiple linear regression	JoramSoch	2020-03-11	541
P78	mlr-mle	Maximum likelihood estimation for multiple linear regression	JoramSoch	2020-03-11	543
P79	mult-prior	Conjugate prior distribution for multinomial observations	JoramSoch	2020-03-11	645
P80	mult-post	Posterior distribution for multinomial observations	JoramSoch	2020-03-11	646
P81	mult-lme	Log model evidence for multinomial observations	JoramSoch	2020-03-11	647
P82	cuni-mean	Mean of the continuous uniform distribution	JoramSoch	2020-03-16	213
P83	cuni-med	Median of the continuous uniform distribution	JoramSoch	2020-03-16	214
P84	cuni-mode	Mode of the continuous uniform distribution	JoramSoch	2020-03-16	214
P85	norm-cdf	Cumulative distribution function of the normal distribution	JoramSoch	2020-03-20	230
P86	norm-cdfwerf	Expression of the cumulative distribution function of the normal distribution without the error function	JoramSoch	2020-03-20	232
P87	norm-qf	Quantile function of the normal distribution	JoramSoch	2020-03-20	235
P88	mvn-cond	Conditional distributions of the multivariate normal distribution	JoramSoch	2020-03-20	350
P89	jl-lfnprior	Joint likelihood is the product of likelihood function and prior density	JoramSoch	2020-05-05	149
P90	post-jl	Posterior density is proportional to joint likelihood	JoramSoch	2020-05-05	149
P91	ml-jl	Marginal likelihood is a definite integral of the joint likelihood	JoramSoch	2020-05-05	152
P92	mvn-kl	Kullback-Leibler divergence for the multivariate normal distribution	JoramSoch	2020-05-05	345

P93	gam-kl	Kullback-Leibler divergence for the gamma distribution	JoramSoch	2020-05-05	272
P94	beta-pdf	Probability density function of the beta distribution	JoramSoch	2020-05-05	306
P95	dir-pdf	Probability density function of the Dirichlet distribution	JoramSoch	2020-05-05	381
P96	bern-pmf	Probability mass function of the Bernoulli distribution	JoramSoch	2020-05-11	178
P97	bin-pmf	Probability mass function of the binomial distribution	JoramSoch	2020-05-11	183
P98	cat-pmf	Probability mass function of the categorical distribution	JoramSoch	2020-05-11	201
P99	mult-pmf	Probability mass function of the multinomial distribution	JoramSoch	2020-05-11	203
P100	mvn-dent	Differential entropy of the multivariate normal distribution	JoramSoch	2020-05-14	343
P101	norm-dent	Differential entropy of the normal distribution	JoramSoch	2020-05-14	243
P102	poiss-pmf	Probability mass function of the Poisson distribution	JoramSoch	2020-05-14	196
P103	mean-nnrvar	Expected value of a non-negative random variable	JoramSoch	2020-05-18	51
P104	var-mean	Partition of variance into expected values	JoramSoch	2020-05-19	70
P105	logreg-pnlo	Probability and log-odds in logistic regression	JoramSoch	2020-05-19	677
P106	glm-ols	Ordinary least squares for the general linear model	JoramSoch	2020-05-19	602
P107	glm-wls	Weighted least squares for the general linear model	JoramSoch	2020-05-19	602
P108	gam-mean	Mean of the gamma distribution	JoramSoch	2020-05-19	263
P109	gam-var	Variance of the gamma distribution	JoramSoch	2020-05-19	266
P110	gam-logmean	Logarithmic expectation of the gamma distribution	JoramSoch	2020-05-25	268
P111	norm-snorm	Relationship between normal distribution and standard normal distribution	JoramSoch	2020-05-26	220

P112	gam-sgam	Relationship between gamma distribution and standard gamma distribution	JoramSoch	2020-05-26	258
P113	kl-ent	Relation of discrete Kullback-Leibler divergence to Shannon entropy	JoramSoch	2020-05-27	131
P114	kl-dent	Relation of continuous Kullback-Leibler divergence to differential entropy	JoramSoch	2020-05-27	132
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P348	covmat-scal	Scaling of the covariance matrix upon multiplication with constant matrix	JoramSoch	2022-09-22	85
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P353	cov-symm	Symmetry of the covariance	JoramSoch	2022-09-26	79
P354	lognorm-mean	Mean of the log-normal distribution	majapavlo	2022-10-02	286
P355	lognorm-var	Variance of the log-normal distribution	majapavlo	2022-10-02	290

P356	beta-chi2	Relationship between chi-squared distribution and beta distribution	JoramSoch	2022-10-07	302
P357	betabin-mome	Method of moments for beta-binomial data	JoramSoch	2022-10-07	674
P358	bin-margcond	Marginal distribution of a conditional binomial distribution	JoramSoch	2022-10-07	190
P359	mean-prodsqr	Square of expectation of product is less than or equal to product of expectation of squares	JoramSoch	2022-10-11	59
P360	pgf-mean	Probability-generating function is expectation of function of random variable	JoramSoch	2022-10-11	46
P361	pgf-zero	Value of the probability-generating function for argument zero	JoramSoch	2022-10-11	47
P362	pgf-one	Value of the probability-generating function for argument one	JoramSoch	2022-10-11	47
P363	bin-pgf	Probability-generating function of the binomial distribution	JoramSoch	2022-10-11	185
P364	betabin-pmf	Probability mass function of the beta-binomial distribution	JoramSoch	2022-10-20	193
P365	betabin-pmfitogf	Expression of the probability mass function of the beta-binomial distribution using only the gamma function	JoramSoch	2022-10-20	194
P366	betabin-cdf	Cumulative distribution function of the beta-binomial distribution	JoramSoch	2022-10-22	194
P367	me-der	Derivation of the model evidence	JoramSoch	2022-10-20	709
P368	fe-der	Derivation of the family evidence	JoramSoch	2022-10-20	716
P369	anova1-ols	Ordinary least squares for one-way analysis of variance	JoramSoch	2022-11-06	451
P370	anova1-f	F-test for main effect in one-way analysis of variance	JoramSoch	2022-11-06	453
P371	anova2-ols	Ordinary least squares for two-way analysis of variance	JoramSoch	2022-11-06	462
P372	anova2-fme	F-test for main effect in two-way analysis of variance	JoramSoch	2022-11-10	474

P373	anova2-fia	F-test for interaction in two-way analysis of variance	JoramSoch	2022-11-11	477
P374	anova2-fgm	F-test for grand mean in two-way analysis of variance	JoramSoch	2022-11-11	478
P375	anova1-repara	Reparametrization for one-way analysis of variance	JoramSoch	2022-11-15	458
P376	anova1-pss	Partition of sums of squares in one-way analysis of variance	JoramSoch	2022-11-15	452
P377	anova1-fols	F-statistic in terms of ordinary least squares estimates in one-way analysis of variance	JoramSoch	2022-11-15	457
P378	anova2-cochran	Application of Cochran's theorem to two-way analysis of variance	JoramSoch	2022-11-16	468
P379	anova2-pss	Partition of sums of squares in two-way analysis of variance	JoramSoch	2022-11-16	466
P380	anova2-fols	F-statistics in terms of ordinary least squares estimates in two-way analysis of variance	JoramSoch	2022-11-16	480
P381	bin-mle	Maximum likelihood estimation for binomial observations	JoramSoch	2022-11-23	629
P382	bin-mll	Maximum log-likelihood for binomial observations	JoramSoch	2022-11-24	630
P383	bin-lbf	Log Bayes factor for binomial observations	JoramSoch	2022-11-25	635
P384	bin-pp	Posterior probability of the alternative model for binomial observations	JoramSoch	2022-11-26	637
P385	mult-mle	Maximum likelihood estimation for multinomial observations	JoramSoch	2022-12-02	642
P386	mult-mll	Maximum log-likelihood for multinomial observations	JoramSoch	2022-12-02	642
P387	mult-lbf	Log Bayes factor for multinomial observations	JoramSoch	2022-12-02	649
P388	mult-pp	Posterior probability of the alternative model for multinomial observations	JoramSoch	2022-12-02	650

P389	mlr-wlsdist	Distributions of estimated parameters, fitted signal and residuals in multiple linear regression upon weighted least squares	JoramSoch	2022-12-13	537
P390	mlr-rssdist	Distribution of residual sum of squares in multiple linear regression with weighted least squares	JoramSoch	2022-12-13	539
P391	mlr-t	t-test for multiple linear regression using contrast-based inference	JoramSoch	2022-12-13	548
P392	mlr-f	F-test for multiple linear regression using contrast-based inference	JoramSoch	2022-12-13	551
P393	mlr-ind	Independence of estimated parameters and residuals in multiple linear regression	JoramSoch	2022-12-13	534
P394	mvn-indprod	Independence of products of multivariate normal random vector	JoramSoch	2022-12-13	355
P395	mvn-chi2	Relationship between multivariate normal distribution and chi-squared distribution	JoramSoch	2022-12-20	336
P396	cuni-var	Variance of the continuous uniform distribution	JoramSoch	2022-12-20	215
P397	cuni-dent	Differential entropy of the continuous uniform distribution	JoramSoch	2022-12-20	216
P398	resvar-biasp	Maximum likelihood estimator of variance in multiple linear regression is biased	JoramSoch	2022-12-21	684
P399	mlr-symm	Projection matrix and residual-forming matrix are symmetric	JoramSoch	2022-12-22	533
P400	mlr-olsdist	Distributions of estimated parameters, fitted signal and residuals in multiple linear regression upon ordinary least squares	JoramSoch	2022-12-23	536
P401	exp-var	Variance of the exponential distribution	majapavlo	2023-01-23	279
P402	exg-pdf	Probability density function of the ex-Gaussian distribution	tomfaulkenberry	2023-04-18	325
P403	exp-mgf	Moment-generating function of the exponential distribution	tomfaulkenberry	2023-04-19	274

P404	exg-mgf	Moment-generating function of the ex-Gaussian distribution	tomfaulkenberry	2023-04-19	327
P405	exg-mean	Mean of the ex-Gaussian distribution	tomfaulkenberry	2023-04-19	328
P406	exg-var	Variance of the ex-Gaussian distribution	tomfaulkenberry	2023-04-19	329
P407	skew-mean	Partition of skewness into expected values	tomfaulkenberry	2023-04-20	77
P408	exg-skew	Skewness of the ex-Gaussian distribution	tomfaulkenberry	2023-04-21	330
P409	exp-skew	Skewness of the exponential distribution	tomfaulkenberry	2023-04-24	280
P410	duni-ent	Entropy of the discrete uniform distribution	JoramSoch	2023-08-11	174
P411	duni-maxent	Discrete uniform distribution maximizes entropy for finite support	JoramSoch	2023-08-18	176
P412	cuni-maxent	Continuous uniform distribution maximizes differential entropy for fixed range	JoramSoch	2023-08-25	218
P413	post-ind	Combined posterior distributions in terms of individual posterior distributions obtained from conditionally independent data	JoramSoch	2023-09-01	150
P414	lme-mean	Equivalence of operations for model evidence and log model evidence	JoramSoch	2023-09-08	712
P415	lfe-approx	Approximation of log family evidences based on log model evidences	JoramSoch	2023-09-15	719
P416	bvn-pdf	Probability density function of the bivariate normal distribution	JoramSoch	2023-09-22	357
P417	bvn-pdfcorr	Probability density function of the bivariate normal distribution in terms of correlation coefficient	JoramSoch	2023-09-29	358
P418	mlr-olstr	Ordinary least squares for multiple linear regression with two regressors	JoramSoch	2023-10-06	527
P419	bern-kl	Kullback-Leibler divergence for the Bernoulli distribution	JoramSoch	2023-10-13	182
P420	bin-kl	Kullback-Leibler divergence for the binomial distribution	JoramSoch	2023-10-20	189

P421	wald-skew	Skewness of the Wald distribution	tomfaulkenberry	2023-10-24	320
P422	cuni-kl	Kullback-Leibler divergence for the continuous uniform distribution	JoramSoch	2023-10-27	217
P423	wald-mome	Method of moments for Wald-distributed data	tomfaulkenberry	2023-10-30	323
P424	exg-mome	Method of moments for ex-Gaussian-distributed data	tomfaulkenberry	2023-10-30	332
P425	duni-kl	Kullback-Leibler divergence for the discrete uniform distribution	JoramSoch	2023-11-17	175
P426	gam-scal	Scaling of a random variable following the gamma distribution	JoramSoch	2023-11-24	259
P427	bin-map	Maximum-a-posteriori estimation for binomial observations	JoramSoch	2023-12-01	631
P428	mult-map	Maximum-a-posteriori estimation for multinomial observations	JoramSoch	2023-12-08	644
P429	bin-test	Binomial test	JoramSoch	2023-12-16	628
P430	mult-test	Multinomial test	JoramSoch	2023-12-23	640
P431	blr-anc	Accuracy and complexity for Bayesian linear regression	JoramSoch	2024-01-12	569
P432	blrkc-prior	Conjugate prior distribution for Bayesian linear regression with known covariance	JoramSoch	2024-01-19	587
P433	blrkc-post	Posterior distribution for Bayesian linear regression with known covariance	JoramSoch	2024-01-19	588
P434	blrkc-lme	Log model evidence for Bayesian linear regression with known covariance	JoramSoch	2024-01-19	590
P435	blrkc-anc	Accuracy and complexity for Bayesian linear regression with known covariance	JoramSoch	2024-01-19	593
P436	mvn-mgf	Moment-generating function of the multivariate normal distribution	JoramSoch	2024-02-16	337
P437	gam-mgf	Moment-generating function of the gamma distribution	JoramSoch	2024-02-23	261
P438	lpsr-spsr	The log probability scoring rule is a strictly proper scoring rule	KarahanS	2024-02-28	163

P439	resvar-unbp	Construction of unbiased estimator for variance in multiple linear regression	JoramSoch	2024-03-08	687
P440	rsq-resvar	Expression of R^2 in terms of residual variances	JoramSoch	2024-03-08	689
P441	rsq-test	Statistical significance test for the coefficient of determination based on an omnibus F-test	JoramSoch	2024-03-08	692
P442	fstat-rsq	Relationship between F-statistic and R^2	JoramSoch	2024-03-15	697
P443	fstat-mll	Relationship between F-statistic and maximum log-likelihood	JoramSoch	2024-03-28	699
P444	snr-mll	Relationship between signal-to-noise ratio and maximum log-likelihood	JoramSoch	2024-03-28	703
P445	bsr-spsr	Brier scoring rule is strictly proper scoring rule	KarahanS	2024-03-28	167
P446	blr-posterr	Expression of the noise precision posterior for Bayesian linear regression using prediction and parameter errors	JoramSoch	2024-04-05	577
P447	blr-postind	Combined posterior distribution for Bayesian linear regression when analyzing conditionally independent data sets	JoramSoch	2024-04-12	581
P448	blr-map	Maximum-a-posteriori estimation for Bayesian linear regression	JoramSoch	2024-04-19	575
P449	blr-lbf	Log Bayes factor for Bayesian linear regression	JoramSoch	2024-04-26	585
P450	mlr-tsingle	Specific t-test for single regressor in multiple linear regression	JoramSoch	2024-05-03	553
P451	slr-tint	Statistical test for intercept parameter in simple linear regression model	JoramSoch	2024-05-10	511
P452	slr-tslo	Statistical test for slope parameter in simple linear regression model	JoramSoch	2024-05-17	513
P453	slr-fcomp	Statistical test for comparing simple linear regression models with and without slope parameter	JoramSoch	2024-05-24	515

P454	mlr-fomnibus	Omnibus F-test for multiple regressors in multiple linear regression	JoramSoch	2024-05-31	555
P455	glm-llr	Log-likelihood ratio for the general linear model	JoramSoch	2024-06-07	606
P456	glm-mll	Maximum log-likelihood for the general linear model	JoramSoch	2024-06-14	605
P457	glm-mi	Mutual information of dependent and independent variables in the general linear model	JoramSoch	2024-06-21	608
P458	glm-llrmi	Equivalence of log-likelihood ratio and mutual information for the general linear model	JoramSoch	2024-06-21	610
P459	iglm-llrs	Equivalence of log-likelihood ratios for regular and inverse general linear model	JoramSoch	2024-06-28	616
P460	ug-fev	F-test for equality of variances in two independent samples	JoramSoch	2024-07-05	412
P461	slr-pss	Partition of sums of squares for simple linear regression	JoramSoch	2024-07-12	500
P462	mlr-ols3	Ordinary least squares for multiple linear regression	JoramSoch	2024-07-18	525
P463	mlr-llr	Log-likelihood ratio for multiple linear regression	JoramSoch	2024-07-25	546
P464	prob-emp2	Probability of the empty set	JoramSoch	2024-08-08	14
P465	prob-mon2	Monotonicity of probability	JoramSoch	2024-08-08	13
P466	cdf-probexc	Exceedance probability for a random variable in terms of cumulative distribution function	JoramSoch	2024-09-06	40
P467	postpred-jl	Posterior predictive distribution is a marginal distribution of the joint likelihood	alocavodia	2024-09-11	151
P468	mean-wlln	Weak law of large numbers	JoramSoch	2024-09-13	63
P469	mean-mse	The expected value minimizes the mean squared error	salbalkus	2024-09-13	65
P470	ind-self	Self-independence of random event	JoramSoch	2024-09-20	10
P471	med-mae	The median minimizes the mean absolute error	salbalkus	2024-09-23	94

P472	corr-ind	Independent random variables are uncorrelated	JoramSoch	2024-09-27	92
P473	norm-corrind	Normally distributed and uncorrelated does not imply independent	JoramSoch	2024-10-04	249
P474	norm-margjoint	Marginally normal does not imply jointly normal	JoramSoch	2024-10-11	251
P475	bvn-lincomb	Linear combination of bivariate normal random variables	JoramSoch	2024-10-25	364
P476	bvn-mi	Mutual information of the bivariate normal distribution	JoramSoch	2024-11-01	362
P477	mvn-mi	Mutual information of the multivariate normal distribution	JoramSoch	2024-11-01	344
P478	mgf-sumind	Moment-generating function of a sum of independent random variables	JoramSoch	2024-11-08	43
P479	lognorm-prodind	The product of independent log-normal random variables is a log-normal random variable	JoramSoch	2024-11-15	292
P480	lognorm-geomind	The geometric mean of independent log-normal random variables is a log-normal random variable	JoramSoch	2024-11-22	293
P481	mark-ineq	Markov's inequality	JoramSoch	2025-01-10	62
P482	cheb-ineq	Chebyshev's inequality	JoramSoch	2025-01-10	62
P483	bool-ineq	Boole's inequality	JoramSoch	2025-01-10	17
P484	bonf-ineq	Bonferroni's inequality	JoramSoch	2025-01-10	17
P485	mult-marg	Marginal distributions of the multinomial distribution	JoramSoch	2025-02-06	209
P486	poiss-ent	Entropy of the Poisson distribution	JoramSoch	2025-02-06	199
P487	gam-mode	Mode of the gamma distribution	JoramSoch	2025-02-06	265
P488	bin-cdf	Cumulative distribution function of the binomial distribution	JoramSoch	2025-02-06	184
P489	mult-cdf	Cumulative distribution function of the multinomial distribution	JoramSoch	2025-02-06	204
P490	ug-cvlme	Cross-validated log model evidence for the univariate Gaussian	JoramSoch	2025-03-06	424

P491	ug-cvlbf	Cross-validated log Bayes factor for the univariate Gaussian	JoramSoch	2025-03-07	429
P492	bin-cvlme	Cross-validated log model evidence for binomial observations	JoramSoch	2025-03-07	638
P493	mult-cvlme	Cross-validated log model evidence for multinomial observations	JoramSoch	2025-03-07	652
P494	bern-cat	Bernoulli distribution is a special case of categorical distribution	JoramSoch	2025-04-04	178
P495	bin-mult	Binomial distribution is a special case of multinomial distribution	JoramSoch	2025-04-04	183
P496	beta-dir	Beta distribution is a special case of Dirichlet distribution	JoramSoch	2025-04-04	301
P497	beta-f	Relationship between F-distribution and beta distribution	JoramSoch	2025-04-04	304
P498	mvn-mode	Mode of the multivariate normal distribution	JoramSoch	2025-05-21	339
P499	mvn-meanqf	Expectation of a quadratic form for the multivariate normal distribution	JoramSoch	2025-05-21	342
P500	mvn-maxent	Multivariate normal distribution maximizes differential entropy for fixed covariance	JoramSoch	2025-05-21	347
P501	mvn-samp	Sampling from the multivariate normal distribution	JoramSoch	2025-05-21	356
P502	bvn-snorm	Construction of a bivariate normal distribution from univariate standard normal random variables	JoramSoch	2025-05-22	360
P503	bvn-mle	Maximum likelihood estimation for bivariate normally distributed data	JoramSoch	2025-06-20	596
P504	mvn-mle	Maximum likelihood estimation for multivariate normally distributed data	JoramSoch	2025-06-20	598
P505	matn-red	Redundancy of parameters describing the matrix-normal distribution	JoramSoch	2025-06-24	396
P506	matn-red2	Redundancy of parameters describing the matrix-normal distribution	JoramSoch	2025-06-24	397
P507	rsq-dist	Distribution of the coefficient of determination under the null hypothesis	JoramSoch	2025-07-04	694

P508	rsq-mmm	Mean, mode and median of the coefficient of determination under the null hypothesis	JoramSoch	2025-07-04	695
P509	rsq-var	Variance of the coefficient of determination under the null hypothesis	JoramSoch	2025-07-04	696
P510	priorpred-jl	Prior predictive distribution is a marginal distribution of the joint likelihood	JoramSoch	2025-07-04	148
P511	ug-ttest1power	Power analysis, minimum detectable effect and minimum required sample size for a one-sample t-test	alexanderdbolton	2025-07-23	413
P512	covmatcross-mean	Partition of a cross-covariance matrix into expected values	JoramSoch	2025-08-29	88
P513	mean-blf	Expectation of a bilinear form	JoramSoch	2025-08-29	67
P514	jens-ineq	Jensen's inequality	JoramSoch	2025-09-25	61
P515	kl-nonneg3	Non-negativity of the Kullback-Leibler divergence	JoramSoch	2025-09-25	126
P516	fren-dec	Decompositions of the variational free energy	JoramSoch	2025-09-25	159
P517	fren-lme	The variational free energy is a lower bound on the log model evidence	JoramSoch	2025-09-25	161
P518	gam-med	Median of the gamma distribution	JoramSoch	2025-10-24	264
P519	beta-med	Median of the beta distribution	JoramSoch	2025-10-24	310
P520	beta-mode	Mode of the beta distribution	JoramSoch	2025-10-24	311
P521	chi2-gam2	Chi-squared distribution is a special case of gamma distribution	natrium-256	2026-01-02	295

2 Definition by Number

ID	Shortcut	Definition	Author	Date	Page
D1	mvn	Multivariate normal distribution	JoramSoch	2020-01-22	335
D2	mgf	Moment-generating function	JoramSoch	2020-01-22	43
D3	cuni	Continuous uniform distribution	JoramSoch	2020-01-27	210
D4	norm	Normal distribution	JoramSoch	2020-01-27	219
D5	ng	Normal-gamma distribution	JoramSoch	2020-01-27	367
D6	matn	Matrix-normal distribution	JoramSoch	2020-01-27	386
D7	gam	Gamma distribution	JoramSoch	2020-02-08	256
D8	exp	Exponential distribution	JoramSoch	2020-02-08	273
D9	pmf	Probability mass function	JoramSoch	2020-02-13	25
D10	pdf	Probability density function	JoramSoch	2020-02-13	28
D11	mean	Expected value	JoramSoch	2020-02-13	50
D12	var	Variance	JoramSoch	2020-02-13	69
D13	cdf	Cumulative distribution function	JoramSoch	2020-02-17	36
D14	qf	Quantile function	JoramSoch	2020-02-17	48
D15	ent	Shannon entropy	JoramSoch	2020-02-19	104
D16	dent	Differential entropy	JoramSoch	2020-02-19	110
D17	ent-cond	Conditional entropy	JoramSoch	2020-02-19	106
D18	ent-joint	Joint entropy	JoramSoch	2020-02-19	106
D19	mi	Mutual information	JoramSoch	2020-02-19	120
D19	mi	Mutual information	JoramSoch	2020-02-19	120
D20	resvar	Residual variance	JoramSoch	2020-02-25	682
D21	rsq	Coefficient of determination	JoramSoch	2020-02-25	688
D22	snr	Signal-to-noise ratio	JoramSoch	2020-02-25	701
D23	aic	Akaike information criterion	JoramSoch	2020-02-25	704
D24	bic	Bayesian information criterion	JoramSoch	2020-02-25	706
D25	dic	Deviance information criterion	JoramSoch	2020-02-25	707
D26	lme	Log model evidence	JoramSoch	2020-02-25	709
D27	gm	Generative model	JoramSoch	2020-03-03	147

D28	lf	Likelihood function	JoramSoch	2020-03-03	147
D28	lf	Likelihood function	JoramSoch	2020-03-03	147
D29	prior	Prior distribution	JoramSoch	2020-03-03	147
D30	fpm	Full probability model	JoramSoch	2020-03-03	148
D31	jl	Joint likelihood	JoramSoch	2020-03-03	148
D32	post	Posterior distribution	JoramSoch	2020-03-03	149
D33	ml	Marginal likelihood	JoramSoch	2020-03-03	152
D34	dent-cond	Conditional differential entropy	JoramSoch	2020-03-21	116
D35	dent-joint	Joint differential entropy	JoramSoch	2020-03-21	116
D36	mlr	Multiple linear regression	JoramSoch	2020-03-21	522
D37	tss	Total sum of squares	JoramSoch	2020-03-21	528
D38	ess	Explained sum of squares	JoramSoch	2020-03-21	528
D39	rss	Residual sum of squares	JoramSoch	2020-03-21	529
D40	glm	General linear model	JoramSoch	2020-03-21	601
D41	poiss-data	Poisson-distributed data	JoramSoch	2020-03-22	655
D42	poissexp	Poisson distribution with exposure values	JoramSoch	2020-03-22	661
D43	wish	Wishart distribution	JoramSoch	2020-03-22	398
D44	bern	Bernoulli distribution	JoramSoch	2020-03-22	177
D45	bin	Binomial distribution	JoramSoch	2020-03-22	182
D46	cat	Categorical distribution	JoramSoch	2020-03-22	201
D47	mult	Multinomial distribution	JoramSoch	2020-03-22	203
D48	prob	Probability	JoramSoch	2020-05-10	6
D49	prob-joint	Joint probability	JoramSoch	2020-05-10	7
D50	prob-marg	Law of marginal probability	JoramSoch	2020-05-10	7
D51	prob-cond	Law of conditional probability	JoramSoch	2020-05-10	7
D52	kl	Kullback-Leibler divergence	JoramSoch	2020-05-10	124
D53	beta	Beta distribution	JoramSoch	2020-05-10	301
D54	dir	Dirichlet distribution	JoramSoch	2020-05-10	381
D55	dist	Probability distribution	JoramSoch	2020-05-17	21
D56	dist-joint	Joint probability distribution	JoramSoch	2020-05-17	21

D57	dist-marg	Marginal probability distribution	JoramSoch	2020-05-17	22
D58	dist-cond	Conditional probability distribution	JoramSoch	2020-05-17	22
D59	llf	Log-likelihood function	JoramSoch	2020-05-17	137
D60	mle	Maximum likelihood estimation	JoramSoch	2020-05-15	137
D61	mll	Maximum log-likelihood	JoramSoch	2020-05-15	137
D62	poiss	Poisson distribution	JoramSoch	2020-05-25	196
D63	snorm	Standard normal distribution	JoramSoch	2020-05-26	220
D64	sgam	Standard gamma distribution	JoramSoch	2020-05-26	257
D65	rvar	Random variable	JoramSoch	2020-05-27	4
D66	rvec	Random vector	JoramSoch	2020-05-27	5
D67	rmat	Random matrix	JoramSoch	2020-05-27	5
D68	cgf	Cumulant-generating function	JoramSoch	2020-05-31	50
D69	pgf	Probability-generating function	JoramSoch	2020-05-31	46
D70	cov	Covariance	JoramSoch	2020-06-02	78
D71	corr	Correlation	JoramSoch	2020-06-02	90
D72	covmat	Covariance matrix	JoramSoch	2020-06-06	82
D73	corrmat	Correlation matrix	JoramSoch	2020-06-06	93
D74	precmat	Precision matrix	JoramSoch	2020-06-06	89
D75	ind	Statistical independence	JoramSoch	2020-06-06	8
D76	logreg	Logistic regression	JoramSoch	2020-06-28	677
D77	beta-data	Beta-distributed data	JoramSoch	2020-06-28	669
D78	bin-data	Binomial observations	JoramSoch	2020-07-07	628
D79	mult-data	Multinomial observations	JoramSoch	2020-07-07	640
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