

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 Definition I/1.2.2) out of a well-defined set of possible outcomes.

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

Together, sample space (\rightarrow Definition I/1.1.2), event space (\rightarrow Definition I/1.1.3) and probability function (\rightarrow Definition 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)).

Metadata: ID: D109 | shortcut: rexp | author: JoramSoch | date: 2020-11-19, 04:10.

1.1.2 Sample space

Definition: Given a random experiment (\rightarrow Definition 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.

Metadata: ID: D165 | shortcut: samp-spc | author: JoramSoch | date: 2021-11-26, 14:13.

1.1.3 Event space

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

Metadata: ID: D166 | shortcut: eve-spc | author: JoramSoch | date: 2021-11-26, 14:26.

1.1.4 Probability space

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

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

Metadata: ID: D167 | shortcut: prob-spc | author: JoramSoch | date: 2021-11-26, 14:30.

1.2 Random variables

1.2.1 Random event

Definition: A random event E is the outcome of a random experiment (\rightarrow Definition 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 Definition I/1.2.2) with two possible values (true and false, or 1 and 0). A random experiment (\rightarrow Definition I/1.1.1) with two possible outcomes is called a Bernoulli trial (\rightarrow Definition 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)).

Metadata: ID: D110 | shortcut: reve | author: JoramSoch | date: 2020-11-19, 04:33.

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 Definition I/1.1.1);
- formally, as a measurable function (\rightarrow Definition “meas-fct”) X defined on a probability space (\rightarrow Definition I/1.1.4) (Ω, \mathcal{E}, P) that maps from a sample space (\rightarrow Definition I/1.1.2) Ω to the real numbers \mathbb{R} using an event space (\rightarrow Definition I/1.1.3) \mathcal{E} and a probability function (\rightarrow Definition I/1.5.1) P ;
- more broadly, as any random quantity X such as a random event (\rightarrow Definition I/1.2.1), a random scalar (\rightarrow Definition I/1.2.2), a random vector (\rightarrow Definition I/1.2.3) or a random matrix (\rightarrow Definition 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.

Metadata: ID: D65 | shortcut: rvar | author: JoramSoch | date: 2020-05-27, 22:36.

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 Definition 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.

Metadata: ID: D66 | shortcut: rvec | author: JoramSoch | date: 2020-05-27, 22:44.

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 Definition I/1.2.2). Equivalently, a random matrix is an $n \times p$ matrix whose columns are n -dimensional random vectors (\rightarrow Definition 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.

Metadata: ID: D67 | shortcut: rmat | author: JoramSoch | date: 2020-05-27, 22:48.

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 Definition I/1.2.2) which is equal to its expected value (\rightarrow Definition I/1.7.1)

$$X = E(X) \tag{1}$$

or equivalently, whose variance (\rightarrow Definition I/1.8.1) is zero

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

Sources:

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

Metadata: ID: D96 | shortcut: const | author: JoramSoch | date: 2020-09-09, 01:30.

1.2.6 Discrete vs. continuous

Definition: Let X be a random variable (\rightarrow Definition 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 Definition 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 Definition I/1.6.6).

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.

Metadata: ID: D105 | shortcut: rvar-disc | author: JoramSoch | date: 2020-10-29, 04:44.

1.2.7 Univariate vs. multivariate

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

- X is called a two-valued random variable or random event (\rightarrow Definition I/1.2.1), if \mathcal{X} has exactly two elements, e.g. $\mathcal{X} = \{E, \overline{E}\}$ or $\mathcal{X} = \{\text{true}, \text{false}\}$ or $\mathcal{X} = \{1, 0\}$;
- X is called a univariate random variable or random scalar (\rightarrow Definition 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 Definition 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 Definition 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.

Metadata: ID: D106 | shortcut: rvar-uni | author: JoramSoch | date: 2020-11-06, 03:47.

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 Definition 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>.

Metadata: ID: D48 | shortcut: prob | author: JoramSoch | date: 2020-05-10, 19:41.

1.3.2 Joint probability

Definition: Let A and B be two arbitrary statements about random variables (\rightarrow Definition 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 Definition 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/>.

Metadata: ID: D49 | shortcut: prob-joint | author: JoramSoch | date: 2020-05-10, 19:49.

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

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

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/>.

Metadata: ID: D50 | shortcut: prob-marg | author: JoramSoch | date: 2020-05-10, 20:01.

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 Definition 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 Definition 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 Definition 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/>.

Metadata: ID: D51 | shortcut: prob-cond | author: JoramSoch | date: 2020-05-10, 20:06.

1.3.5 Exceedance probability

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

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

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>.

Metadata: ID: D103 | shortcut: prob-exc | author: JoramSoch | date: 2020-10-22, 04:36.

1.3.6 Statistical independence

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

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

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

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

2) A set of continuous random variables (\rightarrow Definition 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 Definition I/1.6.6) 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 Definition I/1.5.2) or marginal (\rightarrow Definition I/1.5.3) cumulative distribution functions (\rightarrow Definition I/1.6.13) and f are the respective probability density functions (\rightarrow Definition I/1.6.6).

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).

Metadata: ID: D75 | shortcut: ind | author: JoramSoch | date: 2020-06-06, 07:16.

1.3.7 Conditional independence

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

1) A set of discrete random variables (\rightarrow Definition 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 Definition I/1.3.2) of X_1, \dots, X_n given Y and $p(x_i | y)$ are the marginal (conditional) probabilities (\rightarrow Definition I/1.3.3) of X_i given Y .

2) A set of continuous random variables (\rightarrow Definition 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 Definition I/1.6.6) 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 Definition I/1.5.2) or marginal (conditional) (\rightarrow Definition I/1.5.3) cumulative distribution functions (\rightarrow Definition I/1.6.13) and f are the respective probability density functions (\rightarrow Definition I/1.6.6).

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.

Metadata: ID: D112 | shortcut: ind-cond | author: JoramSoch | date: 2020-11-19, 05:40.

1.3.8 Probability under independence

Theorem: Let A and B be two statements about random variables (\rightarrow Definition I/1.2.2). Then, if A and B are independent (\rightarrow Definition I/1.3.6), marginal (\rightarrow Definition I/1.3.3) and conditional (\rightarrow Definition 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 Definition I/1.3.6), then the joint probability (\rightarrow Definition I/1.3.2) is equal to the product of the marginal probabilities (\rightarrow Definition I/1.3.3):

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

The law of conditional probability (\rightarrow Definition 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).

Metadata: ID: P241 | shortcut: prob-ind | author: JoramSoch | date: 2021-07-23, 16:05.

1.3.9 Mutual exclusivity

Definition: Generally speaking, random events (\rightarrow Definition I/1.2.1) are mutually exclusive, if they cannot occur together, such that their intersection is equal to the empty set (\rightarrow Proof I/1.4.3).

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 Definition 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.

Metadata: ID: D156 | shortcut: exc | author: JoramSoch | date: 2021-07-23, 16:32.

1.3.10 Probability under exclusivity

Theorem: Let A and B be two statements about random variables (\rightarrow Definition I/1.2.2). Then, if A and B are mutually exclusive (\rightarrow Definition I/1.3.9), the probability (\rightarrow Definition I/1.3.1) of their disjunction is equal to the sum of the marginal probabilities (\rightarrow Definition I/1.3.3):

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

Proof: If A and B are mutually exclusive (\rightarrow Definition I/1.3.9), then their joint probability (\rightarrow Definition I/1.3.2) is zero:

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

The addition law of probability (\rightarrow Definition I/1.3.3) 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 Definition I/1.3.9) and the probability of the empty set is zero (\rightarrow Proof I/1.4.3), the joint probability (\rightarrow Definition 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.

Metadata: ID: P242 | shortcut: prob-exc | author: JoramSoch | date: 2021-07-23, 17:19.

1.4 Probability axioms

1.4.1 Axioms of probability

Definition: Let there be a sample space (\rightarrow Definition I/1.1.2) Ω , an event space (\rightarrow Definition I/1.1.3) \mathcal{E} and a probability measure (\rightarrow Definition “prob-meas”) P , such that $P(E)$ is the probability (\rightarrow Definition I/1.3.1) of some event (\rightarrow Definition 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 Definition I/1.3.9)) 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>.
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Metadata: ID: D158 | shortcut: prob-ax | author: JoramSoch | date: 2021-07-30, 11:11.

1.4.2 Monotonicity of probability

Theorem: Probability (\rightarrow Definition 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 Definition 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 Definition 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-9780470669549>.
- Wikipedia (2021): “Probability axioms”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-07-30; URL: https://en.wikipedia.org/wiki/Probability_axioms#Monotonicity.

Metadata: ID: P243 | shortcut: prob-mon | author: JoramSoch | date: 2021-07-30, 11:37.

1.4.3 Probability of the empty set

Theorem: The probability (\rightarrow Definition 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 Definition 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 Definition 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.

Metadata: ID: P244 | shortcut: prob-emp | author: JoramSoch | date: 2021-07-30, 11:58.

1.4.4 Probability of the complement

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

$$P(A^c) = 1 - P(A) \quad (1)$$

where $A^c = \Omega \setminus A$ and Ω is the sample space (\rightarrow Definition I/1.1.2).

Proof: Since A and A^c are mutually exclusive (\rightarrow Definition I/1.3.9) and $A \cup A^c = \Omega$, the third axiom of probability (\rightarrow Definition I/1.4.1) implies:

$$\begin{aligned} P(A \cup A^c) &= P(A) + P(A^c) \\ P(\Omega) &= P(A) + P(A^c) \\ P(A^c) &= P(\Omega) - P(A) . \end{aligned} \quad (2)$$

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

$$P(A^c) = 1 - P(A) . \quad (3)$$

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.

Metadata: ID: P245 | shortcut: prob-comp | author: JoramSoch | date: 2021-07-30, 12:14.

1.4.5 Range of probability

Theorem: The probability (\rightarrow Definition 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 Definition I/1.4.1), we have:

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

By combining the first axiom of probability (\rightarrow Definition I/1.4.1) and the probability of the complement (\rightarrow Proof I/1.4.4), we obtain:

$$\begin{aligned} 1 - P(E) = P(E^c) &\geq 0 \\ 1 - P(E) &\geq 0 \\ P(E) &\leq 1 . \end{aligned} \quad (3)$$

Together, (2) and (3) imply that

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

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.

Metadata: ID: P246 | shortcut: prob-range | author: JoramSoch | date: 2021-07-30, 12:25.

1.4.6 Addition law of probability

Theorem: The probability (\rightarrow Definition 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 :

$$P(A \cup B) = P(A) + P(B) - P(A \cap B) . \quad (1)$$

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 Definition I/1.4.1), we have:

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

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 Definition I/1.4.1), we obtain:

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

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

$$P(A \cup B) = P(A) + P(B) - P(A \cap B) . \quad (4)$$

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.

Metadata: ID: P247 | shortcut: prob-add | author: JoramSoch | date: 2021-07-30, 12:45.

1.4.7 Law of total probability

Theorem: Let A be a subset of sample space (\rightarrow Definition 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 Definition 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 Definition 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>.
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- 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.

Metadata: ID: P248 | shortcut: prob-tot | author: JoramSoch | date: 2021-08-08, 03:56.

1.4.8 Probability of exhaustive events

Theorem: Let B_1, \dots, B_n be mutually exclusive (\rightarrow Definition I/1.3.9) and collectively exhaustive subsets of a sample space (\rightarrow Definition I/1.1.2) Ω . Then, their total probability (\rightarrow Proof I/1.4.7) 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 Definition I/1.4.1) implies that

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

and the second axiom of probability (\rightarrow Definition 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.

Metadata: ID: P249 | shortcut: prob-exh | author: JoramSoch | date: 2021-08-08, 04:10.

1.4.9 Probability of exhaustive events

Theorem: Let B_1, \dots, B_n be mutually exclusive (\rightarrow Definition I/1.3.9) and collectively exhaustive subsets of a sample space (\rightarrow Definition I/1.1.2) Ω . Then, their total probability (\rightarrow Proof I/1.4.7) is one:

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

Proof: The addition law of probability (\rightarrow Proof I/1.4.6) states that for two events (\rightarrow Definition I/1.2.1) A and B , the probability (\rightarrow Definition 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 Proof I/1.4.3), 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 Definition 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.

Metadata: ID: P319 | shortcut: prob-exh2 | author: JoramSoch | date: 2022-03-27, 23:14.

1.5 Probability distributions

1.5.1 Probability distribution

Definition: Let X be a random variable (\rightarrow Definition 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 Definition 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.

Metadata: ID: D55 | shortcut: dist | author: JoramSoch | date: 2020-05-17, 20:23.

1.5.2 Joint distribution

Definition: Let X and Y be random variables (\rightarrow Definition 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 Definition 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 Definition I/1.2.2) is called a bivariate distribution.
- The joint distribution of a random vector (\rightarrow Definition I/1.2.3) is called a multivariate distribution.
- The joint distribution of a random matrix (\rightarrow Definition 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.

Metadata: ID: D56 | shortcut: dist-joint | author: JoramSoch | date: 2020-05-17, 20:43.

1.5.3 Marginal distribution

Definition: Let X and Y be random variables (\rightarrow Definition 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 Definition 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 Definition I/1.5.2) of X and Y using the law of marginal probability (\rightarrow Definition 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.

Metadata: ID: D57 | shortcut: dist-marg | author: JoramSoch | date: 2020-05-17, 21:02.

1.5.4 Conditional distribution

Definition: Let X and Y be random variables (\rightarrow Definition 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 Definition 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 Definition I/1.5.2) of X and Y and the marginal distribution (\rightarrow Definition I/1.5.3) of Y using the law of conditional probability (\rightarrow Definition 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.

Metadata: ID: D58 | shortcut: dist-cond | author: JoramSoch | date: 2020-05-17, 21:25.

1.5.5 Sampling distribution

Definition: Let there be a random sample (\rightarrow Definition “samp”) with finite sample size (\rightarrow Definition “samp-size”). Then, the probability distribution (\rightarrow Definition I/1.5.1) of a given statistic (\rightarrow Definition “stat”) computed from this sample, e.g. a test statistic (\rightarrow Definition 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.

Metadata: ID: D140 | shortcut: dist-samp | author: JoramSoch | date: 2021-03-31, 09:43.

1.6 Probability functions

1.6.1 Probability mass function

Definition: Let X be a discrete (\rightarrow Definition I/1.2.6) random variable (\rightarrow Definition 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.

Metadata: ID: D9 | shortcut: pmf | author: JoramSoch | date: 2020-02-13, 19:09.

1.6.2 Probability mass function of sum of independents

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

Proof: Using the definition of the probability mass function (\rightarrow Definition I/1.6.1) and the expected value (\rightarrow Definition I/1.7.1), the first equation can be derived as follows:

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

Note that the third-last transition is justified by the fact that X and Y are independent (\rightarrow Definition I/1.3.6), such that conditional probabilities are equal to marginal probabilities (\rightarrow Proof I/1.3.8). 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>.

Metadata: ID: P257 | shortcut: pmf-sumind | author: JoramSoch | date: 2021-08-30, 09:14.

1.6.3 Probability mass function of strictly increasing function

Theorem: Let X be a discrete (\rightarrow Definition I/1.2.6) random variable (\rightarrow Definition 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 Definition 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 a strictly increasing function is invertible, the probability mass function (\rightarrow Definition 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 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>.

Metadata: ID: P184 | shortcut: pmf-sifct | author: JoramSoch | date: 2020-10-29, 05:55.

1.6.4 Probability mass function of strictly decreasing function

Theorem: Let X be a discrete (\rightarrow Definition I/1.2.6) random variable (\rightarrow Definition 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 Definition 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 a strictly decreasing function is invertible, the probability mass function (\rightarrow Definition 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 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>.

Metadata: ID: P187 | shortcut: pmf-sdfct | author: JoramSoch | date: 2020-11-06, 04:21.

1.6.5 Probability mass function of invertible function

Theorem: Let X be an $n \times 1$ random vector (\rightarrow Definition I/1.2.3) of discrete random variables (\rightarrow Definition 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 Definition 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 Definition 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>.

Metadata: ID: P253 | shortcut: pmf-invft | author: JoramSoch | date: 2021-08-30, 05:13.

1.6.6 Probability density function

Definition: Let X be a continuous (\rightarrow Definition I/1.2.6) random variable (\rightarrow Definition 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.

Metadata: ID: D10 | shortcut: pdf | author: JoramSoch | date: 2020-02-13, 19:26.

1.6.7 Probability density function of sum of independents

Theorem: Let X and Y be two independent (\rightarrow Definition I/1.3.6) continuous (\rightarrow Definition I/1.2.6) random variables (\rightarrow Definition I/1.2.2) with possible values \mathcal{X} and \mathcal{Y} and let $Z = X + Y$. Then, the probability density function (\rightarrow Definition I/1.6.6) 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 Definition I/1.6.6) of X , Y and Z .

Proof: The cumulative distribution function of a sum of independent random variables (\rightarrow Proof I/1.6.14) 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 Proof I/1.6.12), 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>.

Metadata: ID: P258 | shortcut: pdf-sumind | author: JoramSoch | date: 2021-08-30, 09:31.

1.6.8 Probability density function of strictly increasing function

Theorem: Let X be a continuous (\rightarrow Definition I/1.2.6) random variable (\rightarrow Definition 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 Definition I/1.6.6) 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 Proof I/1.6.15) 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 Proof I/1.6.12)

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

the probability density function (\rightarrow Definition I/1.6.6) 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>.

Metadata: ID: P185 | shortcut: pdf-sifet | author: JoramSoch | date: 2020-10-29, 06:21.

1.6.9 Probability density function of strictly decreasing function

Theorem: Let X be a continuous (\rightarrow Definition I/1.2.6) random variable (\rightarrow Definition 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 Definition I/1.6.6) 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 Proof I/1.6.15) 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 Definition I/1.6.6) 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 Proof I/1.6.12)

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

the probability density function (\rightarrow Definition I/1.6.6) 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>.

Metadata: ID: P188 | shortcut: pdf-sdfct | author: JoramSoch | date: 2020-11-06, 05:30.

1.6.10 Probability density function of invertible function

Theorem: Let X be an $n \times 1$ random vector (\rightarrow Definition I/1.2.3) of continuous random variables (\rightarrow Definition 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 Definition I/1.6.6) 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 Definition I/1.6.13) of $Y = g(X)$. The joint CDF (\rightarrow Definition I/1.6.22) 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

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

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 Definition I/1.6.6) of $Y = g(X)$. Because the PDF is the derivative of the CDF (\rightarrow Proof I/1.6.12), 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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Metadata: ID: P254 | shortcut: pdf-invfcet | author: JoramSoch | date: 2021-08-30, 07:05.

1.6.11 Probability density function of linear transformation

Theorem: Let X be an $n \times 1$ random vector (\rightarrow Definition I/1.2.3) of continuous random variables (\rightarrow Definition 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 Definition I/1.2.5) $n \times 1$ vector μ and constant (\rightarrow Definition I/1.2.5) $n \times n$ matrix Σ . Then, the probability density function (\rightarrow Definition I/1.6.6) 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 Proof I/1.6.10) 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>.

Metadata: ID: P255 | shortcut: pdf-linfct | author: JoramSoch | date: 2021-08-30, 07:46.

1.6.12 Probability density function in terms of cumulative distribution function

Theorem: Let X be a continuous (\rightarrow Definition I/1.2.6) random variable (\rightarrow Definition I/1.2.2). Then, the probability distribution function (\rightarrow Definition I/1.6.6) of X is the first derivative of the cumulative distribution function (\rightarrow Definition I/1.6.13) 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 Proof I/1.6.18) 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.

Metadata: ID: P191 | shortcut: pdf-cdf | author: JoramSoch | date: 2020-11-12, 07:19.

1.6.13 Cumulative distribution function

Definition: The cumulative distribution function (CDF) of a random variable (\rightarrow Definition I/1.2.2) X at a given value x is defined as the probability (\rightarrow Definition 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 Definition I/1.2.6) random variable (\rightarrow Definition I/1.2.2) with possible outcomes \mathcal{X} and the probability mass function (\rightarrow Definition I/1.6.1) $f_X(x)$, then the cumulative distribution function is the function (\rightarrow Proof I/1.6.17) $F_X(x) : \mathbb{R} \rightarrow [0, 1]$ 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 Definition I/1.2.6) random variable (\rightarrow Definition I/1.2.2) with possible outcomes \mathcal{X} and the probability density function (\rightarrow Definition I/1.6.6) $f_X(x)$, then the cumulative distribution function is the function (\rightarrow Proof I/1.6.18) $F_X(x) : \mathbb{R} \rightarrow [0, 1]$ 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.

Metadata: ID: D13 | shortcut: cdf | author: JoramSoch | date: 2020-02-17, 22:07.

1.6.14 Cumulative distribution function of sum of independents

Theorem: Let X and Y be two independent (\rightarrow Definition I/1.3.6) random variables (\rightarrow Definition I/1.2.2) and let $Z = X + Y$. Then, the cumulative distribution function (\rightarrow Definition I/1.6.13) 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 Definition I/1.6.13) of X , Y and Z and $\mathbb{E}[\cdot]$ denotes the expected value (\rightarrow Definition I/1.7.1).

Proof: Using the definition of the cumulative distribution function (\rightarrow Definition I/1.6.13), 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 Definition I/1.3.6), such that conditional probabilities are equal to marginal probabilities (\rightarrow Proof I/1.3.8). 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>.

Metadata: ID: P256 | shortcut: cdf-sumind | author: JoramSoch | date: 2021-08-30, 08:53.

1.6.15 Cumulative distribution function of strictly increasing function

Theorem: Let X be a random variable (\rightarrow Definition 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 Definition I/1.6.13) 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 Definition I/1.6.13) of Y can be derived as follows:

1) If y is lower than the lowest value (\rightarrow Definition I/1.14.1) 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 Definition I/1.14.2) 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>.

Metadata: ID: P183 | shortcut: cdf-sifct | author: JoramSoch | date: 2020-10-29, 05:35.

1.6.16 Cumulative distribution function of strictly decreasing function

Theorem: Let X be a random variable (\rightarrow Definition 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 Definition I/1.6.13) 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 Definition I/1.6.13) of Y can be derived as follows:

1) If y is higher than the highest value (\rightarrow Definition I/1.14.2) 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 Definition I/1.14.1) 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>.

Metadata: ID: P186 | shortcut: cdf-sdfct | author: JoramSoch | date: 2020-11-06, 04:12.

1.6.17 Cumulative distribution function of discrete random variable

Theorem: Let X be a discrete (\rightarrow Definition I/1.2.6) random variable (\rightarrow Definition I/1.2.2) with possible values \mathcal{X} and probability mass function (\rightarrow Definition I/1.6.1) $f_X(x)$. Then, the cumulative distribution function (\rightarrow Definition I/1.6.13) 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 Definition I/1.6.13) of a random variable (\rightarrow Definition 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 Definition I/1.6.1) of a discrete (\rightarrow Definition I/1.2.6) random variable (\rightarrow Definition 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:

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

Sources:

- original work

Metadata: ID: P189 | shortcut: cdf-pmf | author: JoramSoch | date: 2020-11-12, 06:03.

1.6.18 Cumulative distribution function of continuous random variable

Theorem: Let X be a continuous (\rightarrow Definition I/1.2.6) random variable (\rightarrow Definition I/1.2.2) with possible values \mathcal{X} and probability density function (\rightarrow Definition I/1.6.6) $f_X(x)$. Then, the cumulative distribution function (\rightarrow Definition I/1.6.13) of X is

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

Proof: The cumulative distribution function (\rightarrow Definition I/1.6.13) of a random variable (\rightarrow Definition 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 Definition I/1.6.6) of a continuous (\rightarrow Definition I/1.2.6) random variable (\rightarrow Definition 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:

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

Sources:

- original work

Metadata: ID: P190 | shortcut: cdf-pdf | author: JoramSoch | date: 2020-11-12, 06:33.

1.6.19 Probability integral transform

Theorem: Let X be a continuous (\rightarrow Definition I/1.2.6) random variable (\rightarrow Definition I/1.2.2) with invertible (\rightarrow Definition I/1.6.23) cumulative distribution function (\rightarrow Definition I/1.6.13) $F_X(x)$. Then, the random variable (\rightarrow Definition I/1.2.2)

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

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

Proof: The cumulative distribution function (\rightarrow Definition I/1.6.13) 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 Proof II/3.1.4) with $a = 0$ and $b = 1$, i.e. the cumulative distribution function (\rightarrow Definition I/1.6.13) of the standard uniform distribution (\rightarrow Definition 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.

Metadata: ID: P220 | shortcut: cdf-pit | author: JoramSoch | date: 2021-04-07, 08:47.

1.6.20 Inverse transformation method

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

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

has a probability distribution (\rightarrow Definition I/1.5.1) characterized by the invertible (\rightarrow Definition I/1.6.23) cumulative distribution function (\rightarrow Definition I/1.6.13) $F_X(x)$.

Proof: The cumulative distribution function (\rightarrow Definition I/1.6.13) of the transformation $X = F_X^{-1}(U)$ can be derived as

$$\begin{aligned} \Pr(X \leq x) \\ &= \Pr(F_X^{-1}(U) \leq x) \\ &= \Pr(U \leq F_X(x)) \\ &= F_X(x) , \end{aligned} \quad (2)$$

because the cumulative distribution function (\rightarrow Definition I/1.6.13) of the standard uniform distribution (\rightarrow Definition II/3.1.2) $\mathcal{U}(0, 1)$ is

$$U \sim \mathcal{U}(0, 1) \quad \Rightarrow \quad F_U(u) = \Pr(U \leq u) = u . \quad (3)$$

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.

Metadata: ID: P221 | shortcut: cdf-itm | author: JoramSoch | date: 2021-04-07, 08:47.

1.6.21 Distributional transformation

Theorem: Let X and Y be two continuous (\rightarrow Definition I/1.2.6) random variables (\rightarrow Definition I/1.2.2) with cumulative distribution function (\rightarrow Definition I/1.6.13) $F_X(x)$ and invertible cumulative distribution function (\rightarrow Definition I/1.6.13) $F_Y(y)$. Then, the random variable (\rightarrow Definition I/1.2.2)

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

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

Proof: The cumulative distribution function (\rightarrow Definition I/1.6.13) of the transformation $\tilde{X} = F_Y^{-1}(F_X(X))$ can be derived as

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

which shows that \tilde{X} and Y have the same cumulative distribution function (\rightarrow Definition I/1.6.13) and are thus identically distributed (\rightarrow Definition 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

Metadata: ID: P222 | shortcut: cdf-dt | author: JoramSoch | date: 2021-04-07, 09:19.

1.6.22 Joint cumulative distribution function

Definition: Let $X \in \mathbb{R}^{n \times 1}$ be an $n \times 1$ random vector (\rightarrow Definition I/1.2.3). Then, the joint (\rightarrow Definition I/1.5.2) cumulative distribution function (\rightarrow Definition I/1.6.13) of X is defined as the probability (\rightarrow Definition I/1.3.1) that each entry X_i is smaller than a specific value x_i for $i = 1, \dots, n$:

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

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.

Metadata: ID: D141 | shortcut: cdf-joint | author: JoramSoch | date: 2020-04-07, 08:17.

1.6.23 Quantile function

Definition: Let X be a random variable (\rightarrow Definition I/1.2.2) with the cumulative distribution function (\rightarrow Definition I/1.6.13) (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.

Metadata: ID: D14 | shortcut: qf | author: JoramSoch | date: 2020-02-17, 22:18.

1.6.24 Quantile function in terms of cumulative distribution function

Theorem: Let X be a continuous (\rightarrow Definition I/1.2.6) random variable (\rightarrow Definition I/1.2.2) with the cumulative distribution function (\rightarrow Definition I/1.6.13) $F_X(x)$. If the cumulative distribution function is strictly monotonically increasing, then the quantile function (\rightarrow Definition I/1.6.23) is identical to the inverse of $F_X(x)$:

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

Proof: The quantile function (\rightarrow Definition I/1.6.23) $Q_X(p)$ 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

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

Sources:

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

Metadata: ID: P192 | shortcut: qf-cdf | author: JoramSoch | date: 2020-11-12, 07:48.

1.6.25 Characteristic function

Definition:

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

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

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

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

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

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

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>.

Metadata: ID: D159 | shortcut: cf | author: JoramSoch | date: 2021-09-22, 09:20.

1.6.26 Characteristic function of arbitrary function

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) with the expected value (\rightarrow Definition I/1.7.1) function $E_X[\cdot]$. Then, the characteristic function (\rightarrow Definition I/1.6.25) of $Y = g(X)$ is equal to

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

Proof: The characteristic function (\rightarrow Definition I/1.6.25) is defined as

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

Due of the law of the unconscious statistician (\rightarrow Proof I/1.7.12)

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

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

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

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>.

Metadata: ID: P259 | shortcut: cf-fct | author: JoramSoch | date: 2021-09-22, 09:12.

1.6.27 Moment-generating function

Definition:

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

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

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

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

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>.

Metadata: ID: D2 | shortcut: mgf | author: JoramSoch | date: 2020-01-22, 10:58.

1.6.28 Moment-generating function of arbitrary function

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) with the expected value (\rightarrow Definition I/1.7.1) function $\mathbb{E}_X[\cdot]$. Then, the moment-generating function (\rightarrow Definition I/1.6.27) of $Y = g(X)$ is equal to

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

Proof: The moment-generating function (\rightarrow Definition I/1.6.27) is defined as

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

Due of the law of the unconscious statistician (\rightarrow Proof I/1.7.12)

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

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

$$M_Y(t) = \mathbb{E}_X [\exp(t g(X))] . \quad (4)$$

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>.

Metadata: ID: P260 | shortcut: mgf-fct | author: JoramSoch | date: 2021-09-22, 09:00.

1.6.29 Moment-generating function of linear transformation

Theorem: Let X be an $n \times 1$ random vector (\rightarrow Definition I/1.2.3) with the moment-generating function (\rightarrow Definition I/1.6.27) $M_X(t)$. 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 Definition I/1.6.27) X is

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

and therefore the moment-generating function of the random vector (\rightarrow Definition 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.

Metadata: ID: P154 | shortcut: mgf-ltt | author: JoramSoch | date: 2020-08-19, 08:09.

1.6.30 Moment-generating function of linear combination

Theorem: Let X_1, \dots, X_n be n independent (\rightarrow Definition I/1.3.6) random variables (\rightarrow Definition I/1.2.2) with moment-generating functions (\rightarrow Definition I/1.6.27) $M_{X_i}(t)$. 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 Definition I/1.6.27) X_i is

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

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

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

Because the expected value is multiplicative for independent random variables (\rightarrow Proof I/1.7.7), we have

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

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.

Metadata: ID: P155 | shortcut: mgf-lincomb | author: JoramSoch | date: 2020-08-19, 08:36.

1.6.31 Probability-generating function

Definition:

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

$$G_X(z) = \sum_{x=0}^{\infty} p(x) z^x \tag{1}$$

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

2) If X is a discrete (\rightarrow Definition I/1.2.6) random vector (\rightarrow Definition 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

$$G_X(z) = \sum_{x_1=0}^{\infty} \cdots \sum_{x_n=0}^{\infty} p(x_1, \dots, x_n) z_1^{x_1} \cdots z_n^{x_n} \tag{2}$$

where $z \in \mathbb{C}^n$ and $p(x)$ is the probability mass function (\rightarrow Definition 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.

Metadata: ID: D69 | shortcut: pgf | author: JoramSoch | date: 2020-05-31, 23:59.

1.6.32 Probability-generating function in terms of expected value

Theorem: Let X be a discrete (\rightarrow Definition I/1.2.6) random variable (\rightarrow Definition 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 Definition I/1.6.31) of X can be expressed in terms of an expected value (\rightarrow Definition I/1.7.1) 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 Proof I/1.7.12) 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 Definition 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 Definition I/1.6.31) 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.

Metadata: ID: P360 | shortcut: pgf-mean | author: JoramSoch | date: 2022-10-11, 02:01.

1.6.33 Probability-generating function of zero

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) with probability-generating function (\rightarrow Definition I/1.6.31) $G_X(z)$ and probability mass function (\rightarrow Definition 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 Definition I/1.6.31) 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 Definition I/1.6.1) of X . Setting $z = 0$, we obtain:

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

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.

Metadata: ID: P361 | shortcut: pgf-zero | author: JoramSoch | date: 2022-10-11, 08:06.

1.6.34 Probability-generating function of one

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) with probability-generating function (\rightarrow Definition I/1.6.31) $G_X(z)$ and set of possible values \mathcal{X} . Then, the value of the probability-generating function at one is equal to one:

$$G_X(1) = 1 . \tag{1}$$

Proof: The probability-generating function (\rightarrow Definition I/1.6.31) of X is defined as

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

where $f_X(x)$ is the probability mass function (\rightarrow Definition 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 Definition 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.

Metadata: ID: P362 | shortcut: pgf-one | author: JoramSoch | date: 2022-10-11, 08:17.

1.6.35 Cumulant-generating function

Definition:

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

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

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

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

Sources:

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

Metadata: ID: D68 | shortcut: cgf | author: JoramSoch | date: 2020-05-31, 23:46.

1.7 Expected value

1.7.1 Definition

Definition:

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

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

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

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

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

where $f_X(x)$ is the probability density function (\rightarrow Definition I/1.6.6) 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.

Metadata: ID: D11 | shortcut: mean | author: JoramSoch | date: 2020-02-13, 19:38.

1.7.2 Sample mean

Definition: Let $x = \{x_1, \dots, x_n\}$ be a sample (\rightarrow Definition “samp”) from a random variable (\rightarrow Definition 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.

Metadata: ID: D142 | shortcut: mean-samp | author: JoramSoch | date: 2021-04-16, 11:53.

1.7.3 Non-negative random variable

Theorem: Let X be a non-negative random variable (\rightarrow Definition I/1.2.2). Then, the expected value (\rightarrow Definition I/1.7.1) 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 Definition I/1.6.13) of X .

Proof: Because the cumulative distribution function gives the probability of a random variable being smaller than a given value (\rightarrow Definition I/1.6.13),

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

we have

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

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 Definition I/1.6.6) of X , can be rewritten as

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

and by applying the definition of the expected value (\rightarrow Definition I/1.7.1), we see that

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

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>.

Metadata: ID: P103 | shortcut: mean-nnrvar | author: JoramSoch | date: 2020-05-18, 23:54.

1.7.4 Non-negativity

Theorem: If a random variable (\rightarrow Definition I/1.2.2) is strictly non-negative, its expected value (\rightarrow Definition I/1.7.1) is also non-negative, i.e.

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

Proof:

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

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

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 Definition I/1.6.6) is always non-negative, the integrand in

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

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.

Metadata: ID: P52 | shortcut: mean-nonneg | author: JoramSoch | date: 2020-02-13, 20:14.

1.7.5 Linearity

Theorem: The expected value (\rightarrow Definition I/1.7.1) 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 Definition I/1.2.2) X and Y and a constant (\rightarrow Definition I/1.2.5) a .

Proof:

1) If X and Y are discrete random variables (\rightarrow Definition I/1.2.6), the expected value (\rightarrow Definition I/1.7.1) is

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

and the law of marginal probability (\rightarrow Definition 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 Definition I/1.2.6), the expected value (\rightarrow Definition I/1.7.1) is

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

and the law of marginal probability (\rightarrow Definition 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 Definition I/1.7.1), for discrete (\rightarrow Definition I/1.2.6) as well as for continuous (\rightarrow Definition I/1.2.6) random variables.

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/>.

Metadata: ID: P53 | shortcut: mean-lin | author: JoramSoch | date: 2020-02-13, 21:08.

1.7.6 Monotonicity

Theorem: The expected value (\rightarrow Definition I/1.7.1) 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 Proof I/1.7.5), we have

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

With the non-negativity property of the expected value (\rightarrow Proof I/1.7.4), it also holds that

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

Together with (2), this yields

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

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.

Metadata: ID: P54 | shortcut: mean-mono | author: JoramSoch | date: 2020-02-17, 21:00.

1.7.7 (Non-)Multiplicativity

Theorem:

1) If two random variables (\rightarrow Definition I/1.2.2) X and Y are independent (\rightarrow Definition I/1.3.6), the expected value (\rightarrow Definition I/1.7.1) is multiplicative, i.e.

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

2) If two random variables (\rightarrow Definition I/1.2.2) X and Y are dependent (\rightarrow Definition I/1.3.6), the expected value (\rightarrow Definition I/1.7.1) is not necessarily multiplicative, i.e. there exist X and Y such that

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

Proof:

1) If X and Y are independent (\rightarrow Definition 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 Definition I/1.7.1), we have

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

And applying it to the expected value for continuous random variables (\rightarrow Definition I/1.7.1), 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 Definition II/1.2.1) with the following joint probability (\rightarrow Definition I/1.3.2) mass function (\rightarrow Definition 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:

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

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.

Metadata: ID: P55 | shortcut: mean-mult | author: JoramSoch | date: 2020-02-17, 21:51.

1.7.8 Expectation of a trace

Theorem: Let A be an $n \times n$ random matrix (\rightarrow Definition I/1.2.4). Then, the expectation (\rightarrow Definition I/1.7.1) of the trace of A is equal to the trace of the expectation (\rightarrow Definition I/1.7.1) of A :

$$E[\text{tr}(A)] = \text{tr}(E[A]) . \quad (1)$$

Proof: The trace of an $n \times n$ matrix A is defined as:

$$\text{tr}(A) = \sum_{i=1}^n a_{ii} . \quad (2)$$

Using this definition of the trace, the linearity of the expected value (\rightarrow Proof I/1.7.5) and the expected value of a random matrix (\rightarrow Definition I/1.7.14), we have:

$$\begin{aligned} E[\text{tr}(A)] &= E\left[\sum_{i=1}^n a_{ii}\right] \\ &= \sum_{i=1}^n E[a_{ii}] \\ &= \text{tr}\left(\begin{bmatrix} E[a_{11}] & \dots & E[a_{1n}] \\ \vdots & \ddots & \vdots \\ E[a_{n1}] & \dots & E[a_{nn}] \end{bmatrix}\right) \\ &= \text{tr}(E[A]) . \end{aligned} \quad (3)$$

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>.

Metadata: ID: P298 | shortcut: mean-tr | author: JoramSoch | date: 2021-12-07, 09:03.

1.7.9 Expectation of a quadratic form

Theorem: Let X be an $n \times 1$ random vector (\rightarrow Definition I/1.2.3) with mean (\rightarrow Definition I/1.7.1) μ and covariance (\rightarrow Definition I/1.10.1) 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 Proof I/1.7.8), 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 Proof I/1.10.11)

$$\text{Cov}(X, X) = E(X X^T) - E(X)E(X)^T , \quad (5)$$

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 and covariance of X , we have

$$\begin{aligned} E [X^T A X] &= \text{tr} (A [\Sigma + \mu \mu^T]) \\ &= \text{tr} (A \Sigma + A \mu \mu^T) \\ &= \text{tr}(A \Sigma) + \text{tr}(A \mu \mu^T) \\ &= \text{tr}(A \Sigma) + \text{tr}(\mu^T A \mu) \\ &= \mu^T A \mu + \text{tr}(A \Sigma) . \end{aligned} \quad (7)$$

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>.

Metadata: ID: P131 | shortcut: mean-qf | author: JoramSoch | date: 2020-07-13, 21:59.

1.7.10 Squared expectation of a product

Theorem: Let X and Y be two random variables (\rightarrow Definition I/1.2.2) with expected values (\rightarrow Definition I/1.7.1) $E(X)$ 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 Definition I/1.2.2) whose expected value is also non-negative (\rightarrow Proof I/1.7.4):

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

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 Proof I/1.7.5), 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 Definition I/1.2.5) with mean (\rightarrow Definition I/1.7.1) $E(Y) = 0$ and variance (\rightarrow Definition I/1.8.1) $\text{Var}(Y) = 0$, 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.

Metadata: ID: P359 | shortcut: mean-prodsqr | author: JoramSoch | date: 2022-10-11, 01:39.

1.7.11 Law of total expectation

Theorem: (law of total expectation, also called “law of iterated expectations”) Let X be a random variable (\rightarrow Definition I/1.2.2) with expected value (\rightarrow Definition I/1.7.1) $E(X)$ and let Y be any random variable (\rightarrow Definition I/1.8.1) defined on the same probability space (\rightarrow Definition I/1.1.4). Then, the expected value (\rightarrow Definition I/1.7.1) of the conditional expectation (\rightarrow Definition “mean-cond”) of X given Y is the same as the expected value (\rightarrow Definition I/1.7.1) of X :

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

Proof: Let X and Y be discrete random variables (\rightarrow Definition 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 Definition I/1.3.4), this becomes:

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

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

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

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.

Metadata: ID: P291 | shortcut: mean-tot | author: JoramSoch | date: 2021-11-26, 10:57.

1.7.12 Law of the unconscious statistician

Theorem: Let X be a random variable (\rightarrow Definition 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 Definition I/1.6.1) $f_X(x)$, the expected value (\rightarrow Definition I/1.7.1) of $g(X)$ is

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

2) If X is a continuous random variable with possible outcomes \mathcal{X} and probability density function (\rightarrow Definition I/1.6.6) $f_X(x)$, the expected value (\rightarrow Definition I/1.7.1) of $g(X)$ is

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

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

1) The expected value (\rightarrow Definition I/1.7.1) of $Y = g(X)$ is defined as

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

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

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

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

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

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

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

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

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

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

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

Considering the cumulative distribution function (\rightarrow Definition I/1.6.13) of Y , one can deduce:

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

Differentiating to get the probability density function (\rightarrow Definition I/1.6.6) of Y , the result is:

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

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>.

Metadata: ID: P138 | shortcut: mean-lotus | author: JoramSoch | date: 2020-07-22, 08:30.

1.7.13 Expected value of a random vector

Definition: Let X be an $n \times 1$ random vector (\rightarrow Definition I/1.2.3). Then, the expected value (\rightarrow Definition I/1.7.1) of X is an $n \times 1$ 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.

Metadata: ID: D154 | shortcut: mean-rvec | author: JoramSoch | date: 2021-07-08, 08:34.

1.7.14 Expected value of a random matrix

Definition: Let X be an $n \times p$ random matrix (\rightarrow Definition I/1.2.4). Then, the expected value (\rightarrow Definition I/1.7.1) of X is an $n \times p$ matrix whose entries correspond to the expected values of the entries of the random matrix:

$$E(X) = E \left(\begin{bmatrix} X_{11} & \dots & X_{1p} \\ \vdots & \ddots & \vdots \\ X_{n1} & \dots & X_{np} \end{bmatrix} \right) = \begin{bmatrix} E(X_{11}) & \dots & E(X_{1p}) \\ \vdots & \ddots & \vdots \\ E(X_{n1}) & \dots & E(X_{np}) \end{bmatrix} . \quad (1)$$

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#hid13>.

Metadata: ID: D155 | shortcut: mean-rmat | author: JoramSoch | date: 2021-07-08, 08:42.

1.8 Variance

1.8.1 Definition

Definition: The variance of a random variable (\rightarrow Definition I/1.2.2) X is defined as the expected value (\rightarrow Definition I/1.7.1) of the squared deviation from its expected value (\rightarrow Definition I/1.7.1):

$$\text{Var}(X) = \text{E} [(X - \text{E}(X))^2] . \quad (1)$$

Sources:

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

Metadata: ID: D12 | shortcut: var | author: JoramSoch | date: 2020-02-13, 19:55.

1.8.2 Sample variance

Definition: Let $x = \{x_1, \dots, x_n\}$ be a sample (\rightarrow Definition “samp”) from a random variable (\rightarrow Definition I/1.2.2) X . Then, the sample variance of x is given by

$$\hat{\sigma}^2 = \frac{1}{n} \sum_{i=1}^n (x_i - \bar{x})^2 \quad (1)$$

and the unbiased sample variance of x is given by

$$s^2 = \frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x})^2 \quad (2)$$

where \bar{x} is the sample mean (\rightarrow Definition I/1.7.2).

Sources:

- Wikipedia (2021): “Variance”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-04-16; URL: https://en.wikipedia.org/wiki/Variance#Sample_variance.

Metadata: ID: D143 | shortcut: var-samp | author: JoramSoch | date: 2021-04-16, 12:04.

1.8.3 Partition into expected values

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2). Then, the variance (\rightarrow Definition I/1.8.1) of X is equal to the mean (\rightarrow Definition I/1.7.1) of the square of X minus the square of the mean (\rightarrow Definition I/1.7.1) of X :

$$\text{Var}(X) = E(X^2) - E(X)^2 . \quad (1)$$

Proof: The variance (\rightarrow Definition I/1.8.1) 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 Proof I/1.7.5), can be rewritten as

$$\begin{aligned} \text{Var}(X) &= E [(X - E[X])^2] \\ &= E [X^2 - 2 X E(X) + E(X)^2] \\ &= E(X^2) - 2 E(X) E(X) + E(X)^2 \\ &= E(X^2) - E(X)^2 . \end{aligned} \quad (3)$$

Sources:

- Wikipedia (2020): “Variance”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-05-19; URL: <https://en.wikipedia.org/wiki/Variance#Definition>.

Metadata: ID: P104 | shortcut: var-mean | author: JoramSoch | date: 2020-05-19, 00:17.

1.8.4 Non-negativity

Theorem: The variance (\rightarrow Definition I/1.8.1) is always non-negative, i.e.

$$\text{Var}(X) \geq 0 . \quad (1)$$

Proof: The variance (\rightarrow Definition I/1.8.1) of a random variable (\rightarrow Definition I/1.2.2) is defined as

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

1) If X is a discrete random variable (\rightarrow Definition I/1.2.2), then, because squares and probabilities are strictly non-negative, all the addends in

$$\text{Var}(X) = \sum_{x \in \mathcal{X}} (x - E(X))^2 \cdot f_X(x) \quad (3)$$

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

2) If X is a continuous random variable (\rightarrow Definition I/1.2.2), then, because squares and probability densities are strictly non-negative, the integrand in

$$\text{Var}(X) = \int_{\mathcal{X}} (x - E(X))^2 \cdot f_X(x) dx \quad (4)$$

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.

Metadata: ID: P123 | shortcut: var-nonneg | author: JoramSoch | date: 2020-06-06, 07:29.

1.8.5 Variance of a constant

Theorem: The variance (\rightarrow Definition I/1.8.1) of a constant (\rightarrow Definition I/1.2.5) is zero

$$a = \text{const.} \quad \Rightarrow \quad \text{Var}(a) = 0 \quad (1)$$

and if the variance (\rightarrow Definition I/1.8.1) of X is zero, then X is a constant (\rightarrow Definition I/1.2.5)

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

Proof:

1) A constant (\rightarrow Definition I/1.2.5) is defined as a quantity that always has the same value. Thus, if understood as a random variable (\rightarrow Definition I/1.2.2), the expected value (\rightarrow Definition I/1.7.1) of a constant is equal to itself:

$$\text{E}(a) = a . \quad (3)$$

Plugged into the formula of the variance (\rightarrow Definition I/1.8.1), we have

$$\begin{aligned} \text{Var}(a) &= \text{E} [(a - \text{E}(a))^2] \\ &= \text{E} [(a - a)^2] \\ &= \text{E}(0) . \end{aligned} \quad (4)$$

Applied to the formula of the expected value (\rightarrow Definition I/1.7.1), this gives

$$\text{E}(0) = \sum_{x=0} x \cdot f_X(x) = 0 \cdot 1 = 0 . \quad (5)$$

Together, (4) and (5) imply (1).

2) The variance (\rightarrow Definition I/1.8.1) is defined as

$$\text{Var}(X) = \text{E} [(X - \text{E}(X))^2] . \quad (6)$$

Because $(X - \text{E}(X))^2$ is strictly non-negative (\rightarrow Proof I/1.7.4), the only way for the variance to become zero is, if the squared deviation is always zero:

$$(X - \text{E}(X))^2 = 0 . \quad (7)$$

This, in turn, requires that X is equal to its expected value (\rightarrow Definition I/1.7.1)

$$X = \text{E}(X) \quad (8)$$

which can only be the case, if X always has the same value (\rightarrow Definition 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.

Metadata: ID: P124 | shortcut: var-const | author: JoramSoch | date: 2020-06-27, 06:44.

1.8.6 Invariance under addition

Theorem: The variance (\rightarrow Definition I/1.8.1) is invariant under addition of a constant (\rightarrow Definition I/1.2.5):

$$\text{Var}(X + a) = \text{Var}(X) \quad (1)$$

Proof: The variance (\rightarrow Definition I/1.8.1) is defined in terms of the expected value (\rightarrow Definition I/1.7.1) as

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

Using this and the linearity of the expected value (\rightarrow Proof I/1.7.5), we can derive (1) as follows:

$$\begin{aligned} \text{Var}(X + a) &\stackrel{(2)}{=} \text{E} [((X + a) - \text{E}(X + a))^2] \\ &= \text{E} [(X + a - \text{E}(X) - a)^2] \\ &= \text{E} [(X - \text{E}(X))^2] \\ &\stackrel{(2)}{=} \text{Var}(X) . \end{aligned} \quad (3)$$

Sources:

- Wikipedia (2020): “Variance”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-07-07; URL: https://en.wikipedia.org/wiki/Variance#Basic_properties.

Metadata: ID: P126 | shortcut: var-inv | author: JoramSoch | date: 2020-07-07, 05:23.

1.8.7 Scaling upon multiplication

Theorem: The variance (\rightarrow Definition I/1.8.1) scales upon multiplication with a constant (\rightarrow Definition I/1.2.5):

$$\text{Var}(aX) = a^2 \text{Var}(X) \quad (1)$$

Proof: The variance (\rightarrow Definition I/1.8.1) is defined in terms of the expected value (\rightarrow Definition I/1.7.1) as

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

Using this and the linearity of the expected value (\rightarrow Proof I/1.7.5), we can derive (1) as follows:

$$\begin{aligned}
\text{Var}(aX) &\stackrel{(2)}{=} \mathbb{E} [((aX) - \mathbb{E}(aX))^2] \\
&= \mathbb{E} [(aX - a\mathbb{E}(X))^2] \\
&= \mathbb{E} [(a[X - \mathbb{E}(X)])^2] \\
&= \mathbb{E} [a^2(X - \mathbb{E}(X))^2] \\
&= a^2 \mathbb{E} [(X - \mathbb{E}(X))^2] \\
&\stackrel{(2)}{=} a^2 \text{Var}(X) .
\end{aligned} \tag{3}$$

Sources:

- Wikipedia (2020): “Variance”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-07-07; URL: https://en.wikipedia.org/wiki/Variance#Basic_properties.

Metadata: ID: P127 | shortcut: var-scal | author: JoramSoch | date: 2020-07-07, 05:38.

1.8.8 Variance of a sum

Theorem: The variance (\rightarrow Definition I/1.8.1) of the sum of two random variables (\rightarrow Definition I/1.2.2) equals the sum of the variances of those random variables, plus two times their covariance (\rightarrow Definition I/1.10.1):

$$\text{Var}(X + Y) = \text{Var}(X) + \text{Var}(Y) + 2 \text{Cov}(X, Y) . \tag{1}$$

Proof: The variance (\rightarrow Definition I/1.8.1) is defined in terms of the expected value (\rightarrow Definition I/1.7.1) as

$$\text{Var}(X) = \mathbb{E} [(X - \mathbb{E}(X))^2] . \tag{2}$$

Using this and the linearity of the expected value (\rightarrow Proof I/1.7.5), we can derive (1) as follows:

$$\begin{aligned}
\text{Var}(X + Y) &\stackrel{(2)}{=} \mathbb{E} [((X + Y) - \mathbb{E}(X + Y))^2] \\
&= \mathbb{E} [(X - \mathbb{E}(X)) + (Y - \mathbb{E}(Y))]^2 \\
&= \mathbb{E} [(X - \mathbb{E}(X))^2 + (Y - \mathbb{E}(Y))^2 + 2(X - \mathbb{E}(X))(Y - \mathbb{E}(Y))] \\
&= \mathbb{E} [(X - \mathbb{E}(X))^2] + \mathbb{E} [(Y - \mathbb{E}(Y))^2] + \mathbb{E} [2(X - \mathbb{E}(X))(Y - \mathbb{E}(Y))] \\
&\stackrel{(2)}{=} \text{Var}(X) + \text{Var}(Y) + 2 \text{Cov}(X, Y) .
\end{aligned} \tag{3}$$

Sources:

- Wikipedia (2020): “Variance”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-07-07; URL: https://en.wikipedia.org/wiki/Variance#Basic_properties.

Metadata: ID: P128 | shortcut: var-sum | author: JoramSoch | date: 2020-07-07, 06:10.

1.8.9 Variance of linear combination

Theorem: The variance (\rightarrow Definition I/1.8.1) of the linear combination of two random variables (\rightarrow Definition I/1.2.2) is a function of the variances as well as the covariance (\rightarrow Definition I/1.10.1) 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 Definition I/1.8.1) is defined in terms of the expected value (\rightarrow Definition I/1.7.1) as

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

Using this and the linearity of the expected value (\rightarrow Proof I/1.7.5), we can derive (1) as follows:

$$\begin{aligned} \text{Var}(aX + bY) &\stackrel{(2)}{=} \text{E} [((aX + bY) - \text{E}(aX + bY))^2] \\ &= \text{E} [(a[X - \text{E}(X)] + b[Y - \text{E}(Y)])^2] \\ &= \text{E} [a^2 (X - \text{E}(X))^2 + b^2 (Y - \text{E}(Y))^2 + 2ab (X - \text{E}(X))(Y - \text{E}(Y))] \\ &= \text{E} [a^2 (X - \text{E}(X))^2] + \text{E} [b^2 (Y - \text{E}(Y))^2] + \text{E} [2ab (X - \text{E}(X))(Y - \text{E}(Y))] \\ &\stackrel{(2)}{=} a^2 \text{Var}(X) + b^2 \text{Var}(Y) + 2ab \text{Cov}(X, Y) . \end{aligned} \quad (3)$$

Sources:

- Wikipedia (2020): “Variance”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-07-07; URL: https://en.wikipedia.org/wiki/Variance#Basic_properties.

Metadata: ID: P129 | shortcut: var-lincomb | author: JoramSoch | date: 2020-07-07, 06:21.

1.8.10 Additivity under independence

Theorem: The variance (\rightarrow Definition I/1.8.1) is additive for independent (\rightarrow Definition I/1.3.6) random variables (\rightarrow Definition 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 Proof I/1.8.8) 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 Proof I/1.10.6) 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.

Metadata: ID: P130 | shortcut: var-add | author: JoramSoch | date: 2020-07-07, 06:52.

1.8.11 Law of total variance

Theorem: (law of total variance, also called “conditional variance formula”) Let X and Y be random variables (\rightarrow Definition I/1.2.2) defined on the same probability space (\rightarrow Definition I/1.1.4) and assume that the variance (\rightarrow Definition I/1.8.1) of Y is finite. Then, the sum of the expectation (\rightarrow Definition I/1.7.1) of the conditional variance and the variance (\rightarrow Definition I/1.8.1) of the conditional expectation of Y given X is equal to the variance (\rightarrow Definition I/1.8.1) 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 Proof I/1.8.3) 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 Proof I/1.7.11), 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 Proof I/1.7.11), we have:

$$\text{E}(Y^2) - \text{E}(Y)^2 = \text{E} [\text{Var}(Y|X) + \text{E}(Y|X)^2] - \text{E} [\text{E}(Y|X)^2] . \quad (6)$$

With the linearity of the expected value (\rightarrow Proof I/1.7.5), the terms can be regrouped to give:

$$\text{E}(Y^2) - \text{E}(Y)^2 = \text{E} [\text{Var}(Y|X)] + (\text{E} [\text{E}(Y|X)^2] - \text{E} [\text{E}(Y|X)]^2) . \quad (7)$$

Using the decomposition of variance into expected values (\rightarrow Proof I/1.8.3), we finally have:

$$\text{Var}(Y) = \text{E}[\text{Var}(Y|X)] + \text{Var}[\text{E}(Y|X)] . \quad (8)$$

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.

Metadata: ID: P292 | shortcut: var-tot | author: JoramSoch | date: 2021-11-26, 11:20.

1.8.12 Precision

Definition: The precision of a random variable (\rightarrow Definition I/1.2.2) X is defined as the inverse of the variance (\rightarrow Definition I/1.8.1), i.e. one divided by the expected value (\rightarrow Definition I/1.7.1) of the squared deviation from its expected value (\rightarrow Definition I/1.7.1):

$$\text{Prec}(X) = \text{Var}(X)^{-1} = \frac{1}{\mathbb{E}[(X - \mathbb{E}(X))^2]} . \quad (1)$$

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)).

Metadata: ID: D145 | shortcut: prec | author: JoramSoch | date: 2020-04-21, 07:04.

1.9 Skewness

1.9.1 Definition

Definition: Let X be a random variable (\rightarrow Definition I/1.2.2) with expected value (\rightarrow Definition I/1.7.1) μ and standard deviation (\rightarrow Definition I/1.13.1) σ . Then, the skewness of X is defined as the third standardized moment (\rightarrow Definition I/1.15.9) of X :

$$\text{Skew}(X) = \frac{\mathbb{E}[(X - \mu)^3]}{\sigma^3} . \quad (1)$$

Sources:

- Wikipedia (2023): “Skewness”; in: *Wikipedia, the free encyclopedia*, retrieved on 2023-04-20; URL: <https://en.wikipedia.org/wiki/Skewness>.

Metadata: ID: D188 | shortcut: skew | author: tomfaulkenberry | date: 2023-04-20, 12:00.

1.9.2 Partition into expected values

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) with expected value (\rightarrow Definition I/1.7.1) μ and standard deviation (\rightarrow Definition I/1.13.1) σ . Then, the skewness (\rightarrow Definition I/1.9.1) of X can be computed as:

$$\text{Skew}(X) = \frac{\mathbb{E}(X^3) - 3\mu\sigma^2 - \mu^3}{\sigma^3} . \quad (1)$$

Proof:

The skewness (\rightarrow Definition I/1.9.1) of X is defined as

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

Because the expected value is a linear operator (\rightarrow Proof I/1.7.5), we can rewrite (2) as

$$\begin{aligned}
\text{Skew}(X) &= \frac{E[(X - \mu)^3]}{\sigma^3} \\
&= \frac{E[X^3 - 3X^2\mu + 3X\mu^2 - \mu^3]}{\sigma^3} \\
&= \frac{E(X^3) - 3E(X^2)\mu + 3E(X)\mu^2 - \mu^3}{\sigma^3} \\
&= \frac{E(X^3) - 3\mu[E(X^2) - E(X)\mu] - \mu^3}{\sigma^3} \\
&= \frac{E(X^3) - 3\mu[E(X^2) - E(X)^2] - \mu^3}{\sigma^3} .
\end{aligned} \tag{3}$$

Because the variance can be written in terms of expected values (\rightarrow Proof I/1.8.3) as

$$\sigma^2 = E(X^2) - E(X)^2 , \tag{4}$$

we can rewrite (3) as

$$\text{Skew}(X) = \frac{E(X^3) - 3\mu\sigma^2 - \mu^3}{\sigma^3} . \tag{5}$$

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>.

Metadata: ID: P407 | shortcut: skew-mean | author: tomfaulkenberry | date: 2023-04-20, 12:00.

1.10 Covariance

1.10.1 Definition

Definition: The covariance of two random variables (\rightarrow Definition I/1.2.2) X and Y is defined as the expected value (\rightarrow Definition I/1.7.1) of the product of their deviations from their individual expected values (\rightarrow Definition I/1.7.1):

$$\text{Cov}(X, Y) = E[(X - E[X])(Y - E[Y])] . \tag{1}$$

Sources:

- Wikipedia (2020): “Covariance”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-02-06; URL: <https://en.wikipedia.org/wiki/Covariance#Definition>.

Metadata: ID: D70 | shortcut: cov | author: JoramSoch | date: 2020-06-02, 20:20.

1.10.2 Sample covariance

Definition: Let $x = \{x_1, \dots, x_n\}$ and $y = \{y_1, \dots, y_n\}$ be samples (\rightarrow Definition “samp”) from random variables (\rightarrow Definition 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 Definition I/1.7.2).

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.

Metadata: ID: D144 | shortcut: cov-samp | author: ciaranmci | date: 2021-04-21, 06:53.

1.10.3 Partition into expected values

Theorem: Let X and Y be random variables (\rightarrow Definition I/1.2.2). Then, the covariance (\rightarrow Definition I/1.10.1) of X and Y is equal to the mean (\rightarrow Definition I/1.7.1) of the product of X and Y minus the product of the means (\rightarrow Definition I/1.7.1) of X and Y :

$$\text{Cov}(X, Y) = E(XY) - E(X)E(Y) . \quad (1)$$

Proof: The covariance (\rightarrow Definition I/1.10.1) 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 Proof I/1.7.5), 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>.

Metadata: ID: P118 | shortcut: cov-mean | author: JoramSoch | date: 2020-06-02, 20:50.

1.10.4 Symmetry

Theorem: The covariance (\rightarrow Definition I/1.10.1) of two random variables (\rightarrow Definition I/1.2.2) is a symmetric function:

$$\text{Cov}(X, Y) = \text{Cov}(Y, X) . \quad (1)$$

Proof: The covariance (\rightarrow Definition I/1.10.1) of random variables (\rightarrow Definition I/1.2.2) X and Y is defined as:

$$\text{Cov}(X, Y) = \text{E}[(X - \text{E}[X])(Y - \text{E}[Y])] . \quad (2)$$

Switching X and Y in (2), we can easily see:

$$\begin{aligned} \text{Cov}(Y, X) &\stackrel{(2)}{=} \text{E}[(Y - \text{E}[Y])(X - \text{E}[X])] \\ &= \text{E}[(X - \text{E}[X])(Y - \text{E}[Y])] \\ &= \text{Cov}(X, Y) . \end{aligned} \quad (3)$$

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.

Metadata: ID: P353 | shortcut: cov-symm | author: JoramSoch | date: 2022-09-26, 12:14.

1.10.5 Self-covariance

Theorem: The covariance (\rightarrow Definition I/1.10.1) of a random variable (\rightarrow Definition I/1.2.2) with itself is equal to the variance (\rightarrow Definition I/1.8.1):

$$\text{Cov}(X, X) = \text{Var}(X) . \quad (1)$$

Proof: The covariance (\rightarrow Definition I/1.10.1) of random variables (\rightarrow Definition I/1.2.2) X and Y is defined as:

$$\text{Cov}(X, Y) = \text{E}[(X - \text{E}[X])(Y - \text{E}[Y])] . \quad (2)$$

Inserting X for Y in (2), the result is the variance (\rightarrow Definition I/1.8.1) of X :

$$\begin{aligned} \text{Cov}(X, X) &\stackrel{(2)}{=} \text{E}[(X - \text{E}[X])(X - \text{E}[X])] \\ &= \text{E}[(X - \text{E}[X])^2] \\ &= \text{Var}(X) . \end{aligned} \quad (3)$$

Sources:

- Wikipedia (2022): “Covariance”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-09-26; URL: https://en.wikipedia.org/wiki/Covariance#Covariance_with_itself.

Metadata: ID: P352 | shortcut: cov-var | author: JoramSoch | date: 2022-09-26, 12:08.

1.10.6 Covariance under independence

Theorem: Let X and Y be independent (\rightarrow Definition I/1.3.6) random variables (\rightarrow Definition I/1.2.2). Then, the covariance (\rightarrow Definition I/1.10.1) of X and Y is zero:

$$X, Y \text{ independent} \quad \Rightarrow \quad \text{Cov}(X, Y) = 0 . \quad (1)$$

Proof: The covariance can be expressed in terms of expected values (\rightarrow Proof I/1.10.3) as

$$\text{Cov}(X, Y) = E(XY) - E(X)E(Y) . \quad (2)$$

For independent random variables, the expected value of the product is equal to the product of the expected values (\rightarrow Proof I/1.7.7):

$$E(XY) = E(X)E(Y) . \quad (3)$$

Taking (2) and (3) together, we have

$$\begin{aligned} \text{Cov}(X, Y) &\stackrel{(2)}{=} E(XY) - E(X)E(Y) \\ &\stackrel{(3)}{=} E(X)E(Y) - E(X)E(Y) \\ &= 0 . \end{aligned} \quad (4)$$

Sources:

- Wikipedia (2020): “Covariance”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-09-03; URL: https://en.wikipedia.org/wiki/Covariance#Uncorrelatedness_and_independence.

Metadata: ID: P158 | shortcut: cov-ind | author: JoramSoch | date: 2020-09-03, 06:05.

1.10.7 Relationship to correlation

Theorem: Let X and Y be random variables (\rightarrow Definition I/1.2.2). Then, the covariance (\rightarrow Definition I/1.10.1) of X and Y is equal to the product of their correlation (\rightarrow Definition I/1.11.1) and the standard deviations (\rightarrow Definition I/1.13.1) of X and Y :

$$\text{Cov}(X, Y) = \sigma_X \text{Corr}(X, Y) \sigma_Y . \quad (1)$$

Proof: The correlation (\rightarrow Definition I/1.11.1) 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 Definition I/1.10.1) to give

$$\text{Cov}(X, Y) = \sigma_X \text{Corr}(X, Y) \sigma_Y \quad (3)$$

Sources:

- original work

Metadata: ID: P119 | shortcut: cov-corr | author: JoramSoch | date: 2020-06-02, 21:00.

1.10.8 Law of total covariance

Theorem: (law of total covariance, also called “conditional covariance formula”) Let X , Y and Z be random variables (\rightarrow Definition I/1.2.2) defined on the same probability space (\rightarrow Definition I/1.1.4) and assume that the covariance (\rightarrow Definition I/1.10.1) of X and Y is finite. Then, the sum of the expectation (\rightarrow Definition I/1.7.1) of the conditional covariance and the covariance (\rightarrow Definition I/1.10.1) of the conditional expectations of X and Y given Z is equal to the covariance (\rightarrow Definition I/1.10.1) of X and Y :

$$\text{Cov}(X, Y) = \text{E}[\text{Cov}(X, Y|Z)] + \text{Cov}[\text{E}(X|Z), \text{E}(Y|Z)] . \quad (1)$$

Proof: The covariance can be decomposed into expected values (\rightarrow Proof I/1.10.3) as follows:

$$\text{Cov}(X, Y) = \text{E}(XY) - \text{E}(X)\text{E}(Y) . \quad (2)$$

Then, conditioning on Z and applying the law of total expectation (\rightarrow Proof I/1.7.11), we have:

$$\text{Cov}(X, Y) = \text{E}[\text{E}(XY|Z)] - \text{E}[\text{E}(X|Z)] \text{E}[\text{E}(Y|Z)] . \quad (3)$$

Applying the decomposition of covariance into expected values (\rightarrow Proof I/1.10.3) to the first term gives:

$$\text{Cov}(X, Y) = \text{E}[\text{Cov}(X, Y|Z) + \text{E}(X|Z)\text{E}(Y|Z)] - \text{E}[\text{E}(X|Z)] \text{E}[\text{E}(Y|Z)] . \quad (4)$$

With the linearity of the expected value (\rightarrow Proof I/1.7.5), the terms can be regrouped to give:

$$\text{Cov}(X, Y) = \text{E}[\text{Cov}(X, Y|Z)] + (\text{E}[\text{E}(X|Z)\text{E}(Y|Z)] - \text{E}[\text{E}(X|Z)] \text{E}[\text{E}(Y|Z)]) . \quad (5)$$

Once more using the decomposition of covariance into expected values (\rightarrow Proof I/1.10.3), we finally have:

$$\text{Cov}(X, Y) = \text{E}[\text{Cov}(X, Y|Z)] + \text{Cov}[\text{E}(X|Z), \text{E}(Y|Z)] . \quad (6)$$

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.

Metadata: ID: P293 | shortcut: cov-tot | author: JoramSoch | date: 2021-11-26, 11:38.

1.10.9 Covariance matrix

Definition: Let $X = [X_1, \dots, X_n]^T$ be a random vector (\rightarrow Definition 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 Definition I/1.10.1) of X_i and X_j :

$$\Sigma_{XX} = \begin{bmatrix} \text{Cov}(X_1, X_1) & \dots & \text{Cov}(X_1, X_n) \\ \vdots & \ddots & \vdots \\ \text{Cov}(X_n, X_1) & \dots & \text{Cov}(X_n, X_n) \end{bmatrix} = \begin{bmatrix} \text{E}[(X_1 - \text{E}[X_1])(X_1 - \text{E}[X_1])] & \dots & \text{E}[(X_1 - \text{E}[X_1])(X_n - \text{E}[X_n])] \\ \vdots & \ddots & \vdots \\ \text{E}[(X_n - \text{E}[X_n])(X_1 - \text{E}[X_1])] & \dots & \text{E}[(X_n - \text{E}[X_n])(X_n - \text{E}[X_n])] \end{bmatrix} \quad (1)$$

Sources:

- Wikipedia (2020): “Covariance matrix”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-06-06; URL: https://en.wikipedia.org/wiki/Covariance_matrix#Definition.

Metadata: ID: D72 | shortcut: covmat | author: JoramSoch | date: 2020-06-06, 04:24.

1.10.10 Sample covariance matrix

Definition: Let $x = \{x_1, \dots, x_n\}$ be a sample (\rightarrow Definition “samp”) from a random vector (\rightarrow Definition 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 Definition I/1.7.2).

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.

Metadata: ID: D153 | shortcut: covmat-samp | author: JoramSoch | date: 2021-05-20, 07:46.

1.10.11 Covariance matrix and expected values

Theorem: Let X be a random vector (\rightarrow Definition I/1.2.3). Then, the covariance matrix (\rightarrow Definition I/1.10.9) of X is equal to the mean (\rightarrow Definition I/1.7.1) of the outer product of X with itself minus the outer product of the mean (\rightarrow Definition I/1.7.1) of X with itself:

$$\Sigma_{XX} = \text{E}(XX^T) - \text{E}(X)\text{E}(X)^T. \quad (1)$$

Proof: The covariance matrix (\rightarrow Definition I/1.10.9) 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 Proof I/1.7.5), 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>.

Metadata: ID: P120 | shortcut: covmat-mean | author: JoramSoch | date: 2020-06-06, 05:31.

1.10.12 Symmetry

Theorem: Each covariance matrix (\rightarrow Definition I/1.10.9) is symmetric:

$$\Sigma_{XX}^T = \Sigma_{XX}. \quad (1)$$

Proof: The covariance matrix (\rightarrow Definition I/1.10.9) of a random vector (\rightarrow Definition 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 Proof I/1.10.4), 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.

Metadata: ID: P350 | shortcut: covmat-symm | author: JoramSoch | date: 2022-09-26, 10:54.

1.10.13 Positive semi-definiteness

Theorem: Each covariance matrix (\rightarrow Definition I/1.10.9) 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 Definition I/1.10.9) of X can be expressed (\rightarrow Proof I/1.10.11) in terms of expected values (\rightarrow Definition I/1.7.1) 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 Proof I/1.7.5), 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 Definition 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 Proof I/1.7.4), 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.

Metadata: ID: P351 | shortcut: covmat-psd | author: JoramSoch | date: 2022-09-26, 11:26.

1.10.14 Invariance under addition of vector

Theorem: The covariance matrix (\rightarrow Definition I/1.10.9) Σ_{XX} of a random vector (\rightarrow Definition I/1.2.3) X is invariant under addition of a constant vector (\rightarrow Definition I/1.2.5) a :

$$\Sigma(X + a) = \Sigma(X) . \quad (1)$$

Proof: The covariance matrix (\rightarrow Definition I/1.10.9) of X can be expressed (\rightarrow Proof I/1.10.11) in terms of expected values (\rightarrow Definition I/1.7.1) 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 Proof I/1.7.5), 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.

Metadata: ID: P347 | shortcut: covmat-inv | author: JoramSoch | date: 2022-09-22, 11:29.

1.10.15 Scaling upon multiplication with matrix

Theorem: The covariance matrix (\rightarrow Definition I/1.10.9) Σ_{XX} of a random vector (\rightarrow Definition I/1.2.3) X scales upon multiplication with a constant matrix (\rightarrow Definition I/1.2.5) A :

$$\Sigma(AX) = A \Sigma(X) A^T . \quad (1)$$

Proof: The covariance matrix (\rightarrow Definition I/1.10.9) of X can be expressed (\rightarrow Proof I/1.10.11) in terms of expected values (\rightarrow Definition I/1.7.1) 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 Proof I/1.7.5), we can derive (1) as follows:

$$\begin{aligned} \Sigma(AX) &\stackrel{(2)}{=} E[(AX - E[AX])(AX - E[AX])^T] \\ &= E[(A(X - E[X]))(A(X - E[X]))^T] \\ &= E[A(X - E[X])(X - E[X])^T A^T] \\ &= A E[(X - E[X])(X - E[X])^T] A^T \\ &\stackrel{(2)}{=} A \Sigma(X) A^T . \end{aligned} \quad (3)$$

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.

Metadata: ID: P348 | shortcut: covmat-scal | author: JoramSoch | date: 2022-09-22, 11:45.

1.10.16 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 Definition 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 Definition I/1.10.1) of X_i and Y_j :

$$\Sigma_{XY} = \begin{bmatrix} \text{Cov}(X_1, Y_1) & \dots & \text{Cov}(X_1, Y_m) \\ \vdots & \ddots & \vdots \\ \text{Cov}(X_n, Y_1) & \dots & \text{Cov}(X_n, Y_m) \end{bmatrix} = \begin{bmatrix} E[(X_1 - E[X_1])(Y_1 - E[Y_1])] & \dots & E[(X_1 - E[X_1])(Y_m - E[Y_m])] \\ \vdots & \ddots & \vdots \\ E[(X_n - E[X_n])(Y_1 - E[Y_1])] & \dots & E[(X_n - E[X_n])(Y_m - E[Y_m])] \end{bmatrix} \quad (1)$$

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.

Metadata: ID: D176 | shortcut: covmat-cross | author: JoramSoch | date: 2022-09-26, 09:45.

1.10.17 Covariance matrix of a sum

Theorem: The covariance matrix (\rightarrow Definition I/1.10.9) of the sum of two random vectors (\rightarrow Definition 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 Definition I/1.10.16):

$$\Sigma(X + Y) = \Sigma_{XX} + \Sigma_{YY} + \Sigma_{XY} + \Sigma_{YX} . \quad (1)$$

Proof: The covariance matrix (\rightarrow Definition I/1.10.9) of X can be expressed (\rightarrow Proof I/1.10.11) in terms of expected values (\rightarrow Definition I/1.7.1) as follows

$$\Sigma_{XX} = \Sigma(X) = E[(X - E[X])(X - E[X])^T] \quad (2)$$

and the cross-covariance matrix (\rightarrow Definition I/1.10.16) 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 Proof I/1.7.5) as well as the definitions of covariance matrix (\rightarrow Definition I/1.10.9) and cross-covariance matrix (\rightarrow Definition I/1.10.16), we can derive (1) as follows:

$$\begin{aligned} \Sigma(X + Y) &\stackrel{(2)}{=} E[(X + Y - E[X + Y])(X + Y - E[X + Y])^T] \\ &= E[(X - E[X] + Y - E[Y])(X - E[X] + Y - E[Y])^T] \\ &= E[(X - E[X])(X - E[X])^T + (X - E[X])(Y - E[Y])^T + (Y - E[Y])(X - E[X])^T + (Y - E[Y])(Y - E[Y])^T] \\ &= E[(X - E[X])(X - E[X])^T] + E[(X - E[X])(Y - E[Y])^T] + E[(Y - E[Y])(X - E[X])^T] + E[(Y - E[Y])(Y - E[Y])^T] \\ &\stackrel{(2)}{=} \Sigma_{XX} + \Sigma_{XY} + \Sigma_{YX} + \Sigma_{YY} \\ &\stackrel{(3)}{=} \Sigma_{XX} + \Sigma_{YY} + \Sigma_{XY} + \Sigma_{YX} . \end{aligned} \quad (4)$$

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.

Metadata: ID: P349 | shortcut: covmat-sum | author: JoramSoch | date: 2022-09-26, 10:37.

1.10.18 Covariance matrix and correlation matrix

Theorem: Let X be a random vector (\rightarrow Definition I/1.2.3). Then, the covariance matrix (\rightarrow Definition I/1.10.9) Σ_{XX} of X can be expressed in terms of its correlation matrix (\rightarrow Definition I/1.11.5) C_{XX} as follows

$$\Sigma_{XX} = D_X \cdot C_{XX} \cdot D_X , \quad (1)$$

where D_X is a diagonal matrix with the standard deviations (\rightarrow Definition I/1.13.1) of X_1, \dots, X_n as entries on the diagonal:

$$D_X = \text{diag}(\sigma_{X_1}, \dots, \sigma_{X_n}) = \begin{bmatrix} \sigma_{X_1} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \sigma_{X_n} \end{bmatrix} . \quad (2)$$

Proof: Reiterating (1) and applying (2), we have:

$$\Sigma_{XX} = \begin{bmatrix} \sigma_{X_1} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \sigma_{X_n} \end{bmatrix} \cdot C_{XX} \cdot \begin{bmatrix} \sigma_{X_1} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \sigma_{X_n} \end{bmatrix}. \quad (3)$$

Together with the definition of the correlation matrix (\rightarrow Definition I/1.11.5), this gives

$$\begin{aligned} \Sigma_{XX} &= \begin{bmatrix} \sigma_{X_1} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \sigma_{X_n} \end{bmatrix} \cdot \begin{bmatrix} \frac{E[(X_1 - E[X_1])(X_1 - E[X_1])]}{\sigma_{X_1} \sigma_{X_1}} & \dots & \frac{E[(X_1 - E[X_1])(X_n - E[X_n])]}{\sigma_{X_1} \sigma_{X_n}} \\ \vdots & \ddots & \vdots \\ \frac{E[(X_n - E[X_n])(X_1 - E[X_1])]}{\sigma_{X_n} \sigma_{X_1}} & \dots & \frac{E[(X_n - E[X_n])(X_n - E[X_n])]}{\sigma_{X_n} \sigma_{X_n}} \end{bmatrix} \cdot \begin{bmatrix} \sigma_{X_1} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \sigma_{X_n} \end{bmatrix} \\ &= \begin{bmatrix} \frac{\sigma_{X_1} \cdot E[(X_1 - E[X_1])(X_1 - E[X_1])]}{\sigma_{X_1} \sigma_{X_1}} & \dots & \frac{\sigma_{X_1} \cdot E[(X_1 - E[X_1])(X_n - E[X_n])]}{\sigma_{X_1} \sigma_{X_n}} \\ \vdots & \ddots & \vdots \\ \frac{\sigma_{X_n} \cdot E[(X_n - E[X_n])(X_1 - E[X_1])]}{\sigma_{X_n} \sigma_{X_1}} & \dots & \frac{\sigma_{X_n} \cdot E[(X_n - E[X_n])(X_n - E[X_n])]}{\sigma_{X_n} \sigma_{X_n}} \end{bmatrix} \cdot \begin{bmatrix} \sigma_{X_1} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \sigma_{X_n} \end{bmatrix} \\ &= \begin{bmatrix} \frac{\sigma_{X_1} \cdot E[(X_1 - E[X_1])(X_1 - E[X_1]) \cdot \sigma_{X_1}]}{\sigma_{X_1} \sigma_{X_1}} & \dots & \frac{\sigma_{X_1} \cdot E[(X_1 - E[X_1])(X_n - E[X_n]) \cdot \sigma_{X_n}]}{\sigma_{X_1} \sigma_{X_n}} \\ \vdots & \ddots & \vdots \\ \frac{\sigma_{X_n} \cdot E[(X_n - E[X_n])(X_1 - E[X_1]) \cdot \sigma_{X_1}]}{\sigma_{X_n} \sigma_{X_1}} & \dots & \frac{\sigma_{X_n} \cdot E[(X_n - E[X_n])(X_n - E[X_n]) \cdot \sigma_{X_n}]}{\sigma_{X_n} \sigma_{X_n}} \end{bmatrix} \\ &= \begin{bmatrix} E[(X_1 - E[X_1])(X_1 - E[X_1])] & \dots & E[(X_1 - E[X_1])(X_n - E[X_n])] \\ \vdots & \ddots & \vdots \\ E[(X_n - E[X_n])(X_1 - E[X_1])] & \dots & E[(X_n - E[X_n])(X_n - E[X_n])] \end{bmatrix} \end{aligned} \quad (4)$$

which is nothing else than the definition of the covariance matrix (\rightarrow Definition I/1.10.9).

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.

Metadata: ID: P121 | shortcut: covmat-corrmat | author: JoramSoch | date: 2020-06-06, 06:02.

1.10.19 Precision matrix

Definition: Let $X = [X_1, \dots, X_n]^T$ be a random vector (\rightarrow Definition I/1.2.3). Then, the precision matrix of X is defined as the inverse of the covariance matrix (\rightarrow Definition I/1.10.9) of X :

$$\Lambda_{XX} = \Sigma_{XX}^{-1} = \begin{bmatrix} \text{Cov}(X_1, X_1) & \dots & \text{Cov}(X_1, X_n) \\ \vdots & \ddots & \vdots \\ \text{Cov}(X_n, X_1) & \dots & \text{Cov}(X_n, X_n) \end{bmatrix}^{-1}. \quad (1)$$

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)).

Metadata: ID: D74 | shortcut: precmat | author: JoramSoch | date: 2020-06-06, 05:08.

1.10.20 Precision matrix and correlation matrix

Theorem: Let X be a random vector (\rightarrow Definition I/1.2.3). Then, the precision matrix (\rightarrow Definition I/1.10.19) Λ_{XX} of X can be expressed in terms of its correlation matrix (\rightarrow Definition I/1.11.5) C_{XX} as follows

$$\Lambda_{XX} = D_X^{-1} \cdot C_{XX}^{-1} \cdot D_X^{-1}, \quad (1)$$

where D_X^{-1} is a diagonal matrix with the inverse standard deviations (\rightarrow Definition I/1.13.1) of X_1, \dots, X_n as entries on the diagonal:

$$D_X^{-1} = \text{diag}(1/\sigma_{X_1}, \dots, 1/\sigma_{X_n}) = \begin{bmatrix} \frac{1}{\sigma_{X_1}} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \frac{1}{\sigma_{X_n}} \end{bmatrix}. \quad (2)$$

Proof: The precision matrix (\rightarrow Definition I/1.10.19) is defined as the inverse of the covariance matrix (\rightarrow Definition I/1.10.9)

$$\Lambda_{XX} = \Sigma_{XX}^{-1} \quad (3)$$

and the relation between covariance matrix and correlation matrix (\rightarrow Proof I/1.10.18) 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

$$\begin{aligned}
\Lambda_{XX} &\stackrel{(3)}{=} \Sigma_{XX}^{-1} \\
&\stackrel{(4)}{=} (\mathbf{D}_X \cdot \mathbf{C}_{XX} \cdot \mathbf{D}_X)^{-1} \\
&\stackrel{(6)}{=} \mathbf{D}_X^{-1} \cdot \mathbf{C}_{XX}^{-1} \cdot \mathbf{D}_X^{-1} \\
&\stackrel{(7)}{=} \begin{bmatrix} \frac{1}{\sigma_{X_1}} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \frac{1}{\sigma_{X_n}} \end{bmatrix} \cdot \mathbf{C}_{XX}^{-1} \cdot \begin{bmatrix} \frac{1}{\sigma_{X_1}} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \frac{1}{\sigma_{X_n}} \end{bmatrix}
\end{aligned} \tag{8}$$

which conforms to equation (1).

Sources:

- original work

Metadata: ID: P122 | shortcut: precmat-corrmat | author: JoramSoch | date: 2020-06-06, 06:28.

1.11 Correlation

1.11.1 Definition

Definition: The correlation of two random variables (\rightarrow Definition I/1.2.2) X and Y , also called Pearson product-moment correlation coefficient (PPMCC), is defined as the ratio of the covariance (\rightarrow Definition I/1.10.1) of X and Y relative to the product of their standard deviations (\rightarrow Definition I/1.13.1):

$$\text{Corr}(X, Y) = \frac{\sigma_{XY}}{\sigma_X \sigma_Y} = \frac{\text{Cov}(X, Y)}{\sqrt{\text{Var}(X)} \sqrt{\text{Var}(Y)}} = \frac{\mathbb{E}[(X - \mathbb{E}[X])(Y - \mathbb{E}[Y])]}{\sqrt{\mathbb{E}[(X - \mathbb{E}[X])^2]} \sqrt{\mathbb{E}[(Y - \mathbb{E}[Y])^2]}}. \tag{1}$$

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.

Metadata: ID: D71 | shortcut: corr | author: JoramSoch | date: 2020-06-02, 20:34.

1.11.2 Range

Theorem: Let X and Y be two random variables (\rightarrow Definition I/1.2.2). Then, the correlation of X and Y is between and including -1 and $+1$:

$$-1 \leq \text{Corr}(X, Y) \leq +1. \tag{1}$$

Proof: Consider the variance (\rightarrow Definition I/1.8.1) of X plus or minus Y , each divided by their standard deviations (\rightarrow Definition I/1.13.1):

$$\text{Var} \left(\frac{X}{\sigma_X} \pm \frac{Y}{\sigma_Y} \right) . \quad (2)$$

Because the variance is non-negative (\rightarrow Proof I/1.8.4), 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 Proof I/1.8.9), 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 Proof I/1.10.7), 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>.

Metadata: ID: P300 | shortcut: corr-range | author: JoramSoch | date: 2021-12-14, 02:08.

1.11.3 Sample correlation coefficient

Definition: Let $x = \{x_1, \dots, x_n\}$ and $y = \{y_1, \dots, y_n\}$ be samples (\rightarrow Definition “samp”) from random variables (\rightarrow Definition 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 Definition I/1.7.2).

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.

Metadata: ID: D168 | shortcut: corr-samp | author: JoramSoch | date: 2021-12-14, 07:23.

1.11.4 Relationship to standard scores

Theorem: Let $x = \{x_1, \dots, x_n\}$ and $y = \{y_1, \dots, y_n\}$ be samples (\rightarrow Definition “samp”) from random variables (\rightarrow Definition I/1.2.2) X and Y . Then, the sample correlation coefficient (\rightarrow Definition I/1.11.3) r_{xy} can be expressed in terms of the standard scores (\rightarrow Definition “z”) 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 Definition I/1.7.2) and s_x and s_y are the sample variances (\rightarrow Definition I/1.8.2).

Proof: The sample correlation coefficient (\rightarrow Definition I/1.11.3) 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 Definition I/1.8.2) 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): “Peason correlation coefficient”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-12-14; URL: https://en.wikipedia.org/wiki/Pearson_correlation_coefficient#For_a_sample.

Metadata: ID: P299 | shortcut: corr-z | author: JoramSoch | date: 2021-12-14, 02:31.

1.11.5 Correlation matrix

Definition: Let $X = [X_1, \dots, X_n]^T$ be a random vector (\rightarrow Definition 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 Definition I/1.11.1) of X_i and X_j :

$$C_{XX} = \begin{bmatrix} \text{Corr}(X_1, X_1) & \dots & \text{Corr}(X_1, X_n) \\ \vdots & \ddots & \vdots \\ \text{Corr}(X_n, X_1) & \dots & \text{Corr}(X_n, X_n) \end{bmatrix} = \begin{bmatrix} \frac{E[(X_1 - E[X_1])(X_1 - E[X_1])]}{\sigma_{X_1} \sigma_{X_1}} & \dots & \frac{E[(X_1 - E[X_1])(X_n - E[X_n])]}{\sigma_{X_1} \sigma_{X_n}} \\ \vdots & \ddots & \vdots \\ \frac{E[(X_n - E[X_n])(X_1 - E[X_1])]}{\sigma_{X_n} \sigma_{X_1}} & \dots & \frac{E[(X_n - E[X_n])(X_n - E[X_n])]}{\sigma_{X_n} \sigma_{X_n}} \end{bmatrix}. \quad (1)$$

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.

Metadata: ID: D73 | shortcut: corrmatrix | author: JoramSoch | date: 2020-06-06, 04:56.

1.11.6 Sample correlation matrix

Definition: Let $x = \{x_1, \dots, x_n\}$ be a sample (\rightarrow Definition “samp”) from a random vector (\rightarrow Definition 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 Definition I/1.11.3) 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 Definition I/1.11.3) 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 Definition I/1.7.2)

$$\begin{aligned} \bar{x}^{(j)} &= \frac{1}{n} \sum_{i=1}^n x_{ij} \\ \bar{x}^{(k)} &= \frac{1}{n} \sum_{i=1}^n x_{ik} . \end{aligned} \quad (3)$$

Sources:

- original work

Metadata: ID: D169 | shortcut: corrmatrix-samp | author: JoramSoch | date: 2021-12-14, 07:45.

1.12 Measures of central tendency

1.12.1 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 Definition “samp”) from a random variable (\rightarrow Definition 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 Definition I/1.2.2) with cumulative distribution function (\rightarrow Definition I/1.6.13) $F_X(x)$. 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>.

Metadata: ID: D101 | shortcut: med | author: JoramSoch | date: 2020-10-15, 10:53.

1.12.2 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 Definition “samp”) from a random variable (\rightarrow Definition 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 Definition I/1.2.2) with probability mass function (\rightarrow Definition I/1.6.1) or probability density function (\rightarrow Definition I/1.6.6) $f_X(x)$. Then, the mode of X is the 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)).

Metadata: ID: D102 | shortcut: mode | author: JoramSoch | date: 2020-10-15, 11:10.

1.13 Measures of statistical dispersion

1.13.1 Standard deviation

Definition: The standard deviation σ of a random variable (\rightarrow Definition I/1.2.2) X with expected value (\rightarrow Definition I/1.7.1) μ is defined as the square root of the variance (\rightarrow Definition I/1.8.1), i.e.

$$\sigma(X) = \sqrt{E[(X - \mu)^2]} . \quad (1)$$

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.

Metadata: ID: D94 | shortcut: std | author: JoramSoch | date: 2020-09-03, 05:43.

1.13.2 Full width at half maximum

Definition: Let X be a continuous random variable (\rightarrow Definition I/1.2.2) with a unimodal probability density function (\rightarrow Definition I/1.6.6) $f_X(x)$ and mode (\rightarrow Definition I/1.12.2) 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.

Metadata: ID: D91 | shortcut: fwhm | author: JoramSoch | date: 2020-08-19, 05:40.

1.14 Further summary statistics

1.14.1 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 Definition “samp”) from a random variable (\rightarrow Definition I/1.2.2) X . Then, the minimum of x is

$$\min(x) = x_j, \quad \text{such that} \quad x_j \leq x_i \quad \text{for all} \quad i = 1, \dots, n, \quad i \neq j , \quad (1)$$

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 Definition I/1.2.2) with possible values \mathcal{X} . Then, the minimum of X is

$$\min(X) = \tilde{x}, \quad \text{such that} \quad \tilde{x} < x \quad \text{for all} \quad x \in \mathcal{X} \setminus \{\tilde{x}\}, \quad (2)$$

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.

Metadata: ID: D107 | shortcut: min | author: JoramSoch | date: 2020-11-12, 05:25.

1.14.2 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 Definition “samp”) from a random variable (\rightarrow Definition I/1.2.2) X . Then, the maximum of x is

$$\max(x) = x_j, \quad \text{such that} \quad x_j \geq x_i \quad \text{for all} \quad i = 1, \dots, n, i \neq j, \quad (1)$$

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 Definition I/1.2.2) with possible values \mathcal{X} . Then, the maximum of X is

$$\max(X) = \tilde{x}, \quad \text{such that} \quad \tilde{x} > x \quad \text{for all} \quad x \in \mathcal{X} \setminus \{\tilde{x}\}, \quad (2)$$

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.

Metadata: ID: D108 | shortcut: max | author: JoramSoch | date: 2020-11-12, 05:33.

1.15 Further moments

1.15.1 Moment

Definition: Let X be a random variable (\rightarrow Definition I/1.2.2), let c be a constant (\rightarrow Definition 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 Definition I/1.7.1) 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 Definition I/1.15.3) $\mu'_n = \mu_n(0)$;
- the n -th central moment (\rightarrow Definition I/1.15.6) $\mu_n = \mu_n(\mu)$;
- the n -th standardized moment (\rightarrow Definition I/1.15.9) $\mu_n^* = \mu_n/\sigma^n$.

Sources:

- Wikipedia (2020): “Moment (mathematics)”¹; 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).

Metadata: ID: D90 | shortcut: mom | author: JoramSoch | date: 2020-08-19, 05:24.

1.15.2 Moment in terms of moment-generating function

Theorem: Let X be a scalar random variable (\rightarrow Definition I/1.2.2) with the moment-generating function (\rightarrow Definition I/1.6.27) $M_X(t)$. Then, the n -th raw moment (\rightarrow Definition I/1.15.3) 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 Definition I/1.6.27), 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 Proof I/1.7.5), 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

$$\frac{d^n}{dx^n} x^m = \begin{cases} m^{\underline{n}} x^{m-n} , & \text{if } n \leq m \\ 0 , & \text{if } n > m . \end{cases} \quad (6)$$

with the falling factorial

$$m^{\underline{n}} = \prod_{i=0}^{n-1} (m - i) = \frac{m!}{(m - n)!} , \quad (7)$$

equation (5) becomes

$$\begin{aligned}
M_X^{(n)}(t) &= \sum_{m=n}^{\infty} \frac{m^n t^{m-n}}{m!} E(X^m) \\
&\stackrel{(7)}{=} \sum_{m=n}^{\infty} \frac{m! t^{m-n}}{(m-n)! m!} E(X^m) \\
&= \sum_{m=n}^{\infty} \frac{t^{m-n}}{(m-n)!} E(X^m) \\
&= \frac{t^{n-n}}{(n-n)!} E(X^n) + \sum_{m=n+1}^{\infty} \frac{t^{m-n}}{(m-n)!} E(X^m) \\
&= \frac{t^0}{0!} E(X^n) + \sum_{m=n+1}^{\infty} \frac{t^{m-n}}{(m-n)!} E(X^m) \\
&= E(X^n) + \sum_{m=n+1}^{\infty} \frac{t^{m-n}}{(m-n)!} E(X^m) .
\end{aligned} \tag{8}$$

Setting $t = 0$ in (8) yields

$$\begin{aligned}
M_X^{(n)}(0) &= E(X^n) + \sum_{m=n+1}^{\infty} \frac{0^{m-n}}{(m-n)!} E(X^m) \\
&= E(X^n)
\end{aligned} \tag{9}$$

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.

Metadata: ID: P153 | shortcut: mom-mgf | author: JoramSoch | date: 2020-08-19, 07:51.

1.15.3 Raw moment

Definition: Let X be a random variable (\rightarrow Definition 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 Definition I/1.15.1) of X about the value 0:

$$\mu'_n = \mu_n(0) = E[(X - 0)^n] = E[X^n] . \tag{1}$$

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).

Metadata: ID: D97 | shortcut: mom-raw | author: JoramSoch | date: 2020-10-08, 03:31.

1.15.4 First raw moment is mean

Theorem: The first raw moment (\rightarrow Definition I/1.15.3) equals the mean (\rightarrow Definition I/1.7.1), i.e.

$$\mu'_1 = \mu . \quad (1)$$

Proof: The first raw moment (\rightarrow Definition I/1.15.3) of a random variable (\rightarrow Definition I/1.2.2) X is defined as

$$\mu'_1 = E[(X - 0)^1] \quad (2)$$

which is equal to the expected value (\rightarrow Definition I/1.7.1) of X :

$$\mu'_1 = E[X] = \mu . \quad (3)$$

Sources:

- original work

Metadata: ID: P171 | shortcut: momraw-1st | author: JoramSoch | date: 2020-10-08, 04:19.

1.15.5 Second raw moment and variance

Theorem: The second raw moment (\rightarrow Definition I/1.15.3) can be expressed as

$$\mu'_2 = \text{Var}(X) + E(X)^2 \quad (1)$$

where $\text{Var}(X)$ is the variance (\rightarrow Definition I/1.8.1) of X and $E(X)$ is the expected value (\rightarrow Definition I/1.7.1) of X .

Proof: The second raw moment (\rightarrow Definition I/1.15.3) of a random variable (\rightarrow Definition 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 Proof I/1.8.3)

$$\text{Var}(X) = E(X^2) - E(X)^2 , \quad (3)$$

the second raw moment can be rearranged into:

$$\mu'_2 \stackrel{(2)}{=} E(X^2) \stackrel{(3)}{=} \text{Var}(X) + E(X)^2 . \quad (4)$$

Sources:

- original work

Metadata: ID: P172 | shortcut: momraw-2nd | author: JoramSoch | date: 2020-10-08, 05:05.

1.15.6 Central moment

Definition: Let X be a random variable (\rightarrow Definition I/1.2.2) with expected value (\rightarrow Definition I/1.7.1) μ and let n be a positive integer. Then, the n -th central moment of X is defined as the n -th moment (\rightarrow Definition I/1.15.1) 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).

Metadata: ID: D98 | shortcut: mom-cent | author: JoramSoch | date: 2020-10-08, 03:37.

1.15.7 First central moment is zero

Theorem: The first central moment (\rightarrow Definition I/1.15.6) is zero, i.e.

$$\mu_1 = 0 . \quad (1)$$

Proof: The first central moment (\rightarrow Definition I/1.15.6) of a random variable (\rightarrow Definition I/1.2.2) X with mean (\rightarrow Definition I/1.7.1) μ is defined as

$$\mu_1 = E[(X - \mu)^1] . \quad (2)$$

Due to the linearity of the expected value (\rightarrow Proof I/1.7.5) 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.

Metadata: ID: P167 | shortcut: momcent-1st | author: JoramSoch | date: 2020-09-09, 07:51.

1.15.8 Second central moment is variance

Theorem: The second central moment (\rightarrow Definition I/1.15.6) equals the variance (\rightarrow Definition I/1.8.1), i.e.

$$\mu_2 = \text{Var}(X) . \quad (1)$$

Proof: The second central moment (\rightarrow Definition I/1.15.6) of a random variable (\rightarrow Definition I/1.2.2) X with mean (\rightarrow Definition I/1.7.1) μ is defined as

$$\mu_2 = E[(X - \mu)^2] \quad (2)$$

which is equivalent to the definition of the variance (\rightarrow Definition I/1.8.1):

$$\mu_2 = E[(X - E(X))^2] = \text{Var}(X) . \quad (3)$$

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).

Metadata: ID: P173 | shortcut: momcent-2nd | author: JoramSoch | date: 2020-10-08, 05:13.

1.15.9 Standardized moment

Definition: Let X be a random variable (\rightarrow Definition I/1.2.2) with expected value (\rightarrow Definition I/1.7.1) μ and standard deviation (\rightarrow Definition I/1.13.1) σ and let n be a positive integer. Then, the n -th standardized moment of X is defined as the n -th moment (\rightarrow Definition I/1.15.1) 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).

Metadata: ID: D99 | shortcut: mom-stand | author: JoramSoch | date: 2020-10-08, 03:47.

2 Information theory

2.1 Shannon entropy

2.1.1 Definition

Definition: Let X be a discrete random variable (\rightarrow Definition I/1.2.2) with possible outcomes \mathcal{X} and the (observed or assumed) probability mass function (\rightarrow Definition 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.

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.

Metadata: ID: D15 | shortcut: ent | author: JoramSoch | date: 2020-02-19, 17:36.

2.1.2 Non-negativity

Theorem: The entropy of a discrete random variable (\rightarrow Definition I/1.2.2) is a non-negative number:

$$H(X) \geq 0 . \quad (1)$$

Proof: The entropy of a discrete random variable (\rightarrow Definition 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 Definition 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>.

Metadata: ID: P57 | shortcut: ent-nonneg | author: JoramSoch | date: 2020-02-19, 19:10.

2.1.3 Concavity

Theorem: The entropy (\rightarrow Definition I/2.1.1) is concave in the probability mass function (\rightarrow Definition 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 Definition I/1.2.2) with possible outcomes \mathcal{X} and let $u(x)$ be the probability mass function (\rightarrow Definition I/1.6.1) of a discrete uniform distribution (\rightarrow Definition II/1.1.1) on $X \in \mathcal{X}$. Then, the entropy (\rightarrow Definition I/2.1.1) of an arbitrary probability mass function (\rightarrow Definition I/1.6.1) $p(x)$ can be rewritten as

$$\begin{aligned} H[p] &= - \sum_{x \in \mathcal{X}} p(x) \cdot \log p(x) \\ &= - \sum_{x \in \mathcal{X}} p(x) \cdot \log \frac{p(x)}{u(x)} u(x) \\ &= - \sum_{x \in \mathcal{X}} p(x) \cdot \log \frac{p(x)}{u(x)} - \sum_{x \in \mathcal{X}} p(x) \cdot \log u(x) \\ &= -\text{KL}[p||u] - \log \frac{1}{|\mathcal{X}|} \sum_{x \in \mathcal{X}} p(x) \\ &= \log |\mathcal{X}| - \text{KL}[p||u] \\ \log |\mathcal{X}| - H[p] &= \text{KL}[p||u] \end{aligned} \quad (2)$$

where we have applied the definition of the Kullback-Leibler divergence (\rightarrow Definition I/2.5.1), the probability mass function of the discrete uniform distribution (\rightarrow Proof II/1.1.2) and the total sum over the probability mass function (\rightarrow Definition I/1.6.1).

Note that the KL divergence is convex (\rightarrow Proof I/2.5.5) in the pair of probability distributions (\rightarrow Definition 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

$$\begin{aligned}
\log |\mathcal{X}| - H[\lambda p_1 + (1 - \lambda)p_2] &\leq \lambda (\log |\mathcal{X}| - H[p_1]) + (1 - \lambda) (\log |\mathcal{X}| - H[p_2]) \\
\log |\mathcal{X}| - H[\lambda p_1 + (1 - \lambda)p_2] &\leq \log |\mathcal{X}| - \lambda H[p_1] - (1 - \lambda)H[p_2] \\
-H[\lambda p_1 + (1 - \lambda)p_2] &\leq -\lambda H[p_1] - (1 - \lambda)H[p_2] \\
H[\lambda p_1 + (1 - \lambda)p_2] &\geq \lambda H[p_1] + (1 - \lambda)H[p_2]
\end{aligned} \tag{5}$$

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>.

Metadata: ID: P149 | shortcut: ent-conc | author: JoramSoch | date: 2020-08-11, 08:29.

2.1.4 Conditional entropy

Definition: Let X and Y be discrete random variables (\rightarrow Definition I/1.2.2) with possible outcomes \mathcal{X} and \mathcal{Y} and probability mass functions (\rightarrow Definition 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

$$H(Y|X) = \sum_{x \in \mathcal{X}} p(x) \cdot H(Y|X = x) \tag{1}$$

where $H(Y|X = x)$ is the (marginal) entropy (\rightarrow Definition 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>.

Metadata: ID: D17 | shortcut: ent-cond | author: JoramSoch | date: 2020-02-19, 18:08.

2.1.5 Joint entropy

Definition: Let X and Y be discrete random variables (\rightarrow Definition I/1.2.2) with possible outcomes \mathcal{X} and \mathcal{Y} and joint probability (\rightarrow Definition I/1.3.2) mass function (\rightarrow Definition I/1.6.1) $p(x, y)$. Then, the joint entropy of X and Y is defined as

$$H(X, Y) = - \sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} p(x, y) \cdot \log_b p(x, y) \tag{1}$$

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>.

Metadata: ID: D18 | shortcut: ent-joint | author: JoramSoch | date: 2020-02-19, 18:18.

2.1.6 Cross-entropy

Definition: Let X be a discrete random variable (\rightarrow Definition I/1.2.2) with possible outcomes \mathcal{X} and let P and Q be two probability distributions (\rightarrow Definition I/1.5.1) on X with the probability mass functions (\rightarrow Definition 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.

Metadata: ID: D85 | shortcut: ent-cross | author: JoramSoch | date: 2020-07-28, 02:51.

2.1.7 Convexity of cross-entropy

Theorem: The cross-entropy (\rightarrow Definition I/2.1.6) is convex in the probability distribution (\rightarrow Definition I/1.5.1) q , 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 distributions and $0 \leq \lambda \leq 1$.

Proof: The relationship between Kullback-Leibler divergence, entropy and cross-entropy (\rightarrow Proof I/2.5.8) is:

$$\text{KL}[P||Q] = H(P, Q) - H(P) . \quad (2)$$

Note that the KL divergence is convex (\rightarrow Proof I/2.5.5) in the pair of probability distributions (\rightarrow Definition 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>.

Metadata: ID: P150 | shortcut: entcross-conv | author: JoramSoch | date: 2020-08-11, 09:16.

2.1.8 Gibbs’ inequality

Theorem: Let X be a discrete random variable (\rightarrow Definition I/1.2.2) and consider two probability distributions (\rightarrow Definition I/1.5.1) with probability mass functions (\rightarrow Definition I/1.6.1) $p(x)$ and $q(x)$. Then, Gibbs’ inequality states that the entropy (\rightarrow Definition I/2.1.1) of X according to P is smaller than or equal to the cross-entropy (\rightarrow Definition 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 Definition I/1.6.1), we have

$$\begin{aligned}
0 \leq p(x) \leq 1, \quad \sum_{x \in I} p(x) &= 1 \quad \text{and} \\
0 \leq q(x) \leq 1, \quad \sum_{x \in I} q(x) &\leq 1,
\end{aligned} \tag{5}$$

such that it follows from (4) that

$$\begin{aligned}
\sum_{x \in I} p(x) \ln \frac{p(x)}{q(x)} &\geq \sum_{x \in I} p(x) - \sum_{x \in I} q(x) \\
&= 1 - \sum_{x \in I} q(x) \geq 0.
\end{aligned} \tag{6}$$

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.

Metadata: ID: P164 | shortcut: gibbs-ineq | author: JoramSoch | date: 2020-09-09, 02:18.

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

$$\sum_{i=1}^n a_i \log_c \frac{a_i}{b_i} \geq a \log_c \frac{a}{b}. \tag{1}$$

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:

$$\log_c a = \frac{\ln a}{\ln c}. \tag{2}$$

Let $f(x) = x \ln x$. Then, the left-hand side of (1) can be rewritten as

$$\begin{aligned}
\sum_{i=1}^n a_i \ln \frac{a_i}{b_i} &= \sum_{i=1}^n b_i f\left(\frac{a_i}{b_i}\right) \\
&= b \sum_{i=1}^n \frac{b_i}{b} f\left(\frac{a_i}{b_i}\right).
\end{aligned} \tag{3}$$

Because $f(x)$ is a convex function and

$$\begin{aligned}
\frac{b_i}{b} &\geq 0 \\
\sum_{i=1}^n \frac{b_i}{b} &= 1,
\end{aligned} \tag{4}$$

applying Jensen's inequality yields

$$\begin{aligned}
 b \sum_{i=1}^n \frac{b_i}{b} f\left(\frac{a_i}{b_i}\right) &\geq b f\left(\sum_{i=1}^n \frac{b_i}{b} \frac{a_i}{b_i}\right) \\
 &= b f\left(\frac{1}{b} \sum_{i=1}^n a_i\right) \\
 &= b f\left(\frac{a}{b}\right) \\
 &= a \ln \frac{a}{b}.
 \end{aligned} \tag{5}$$

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.
- Wikipedia (2020): “Jensen's inequality”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-09-09; URL: https://en.wikipedia.org/wiki/Jensen%27s_inequality#Statements.

Metadata: ID: P165 | shortcut: logsum-ineq | author: JoramSoch | date: 2020-09-09, 02:46.

2.2 Differential entropy

2.2.1 Definition

Definition: Let X be a continuous random variable (\rightarrow Definition I/1.2.2) with possible outcomes \mathcal{X} and the (estimated or assumed) probability density function (\rightarrow Definition I/1.6.6) $p(x) = f_X(x)$. Then, the differential entropy (also referred to as “continuous entropy”) of X is defined as

$$h(X) = - \int_{\mathcal{X}} p(x) \log_b p(x) dx \tag{1}$$

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>.

Metadata: ID: D16 | shortcut: dent | author: JoramSoch | date: 2020-02-19, 17:53.

2.2.2 Negativity

Theorem: Unlike its discrete analogue (\rightarrow Proof I/2.1.2), the differential entropy (\rightarrow Definition I/2.2.1) can become negative.

Proof: Let X be a random variable (\rightarrow Definition I/1.2.2) following a continuous uniform distribution (\rightarrow Definition 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 Proof 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 Definition 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.

Metadata: ID: P68 | shortcut: dent-neg | author: JoramSoch | date: 2020-03-02, 20:32.

2.2.3 Invariance under addition

Theorem: Let X be a continuous (\rightarrow Definition I/1.2.6) random variable (\rightarrow Definition I/1.2.2). Then, the differential entropy (\rightarrow Definition 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 Definition 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 Definition I/1.6.6) 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 Proof I/1.6.8) 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.

Metadata: ID: P199 | shortcut: dent-inv | author: JoramSoch | date: 2020-12-02, 16:11.

2.2.4 Addition upon multiplication

Theorem: Let X be a continuous (\rightarrow Definition I/1.2.6) random variable (\rightarrow Definition I/1.2.2). Then, the differential entropy (\rightarrow Definition 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 Definition 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 Definition I/1.6.6) 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 Proof I/1.6.8) 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 Proof I/1.6.9) 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.

Metadata: ID: P200 | shortcut: dent-add | author: JoramSoch | date: 2020-12-02, 16:39.

2.2.5 Addition upon matrix multiplication

Theorem: Let X be a continuous (\rightarrow Definition I/1.2.6) random vector (\rightarrow Definition I/1.2.3). Then, the differential entropy (\rightarrow Definition 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 Definition 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 Definition I/1.6.6) 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 Proof I/1.6.11) $Y = g(X) = \Sigma X + \mu$ 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 Definition I/1.6.6) 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 Definition 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 Definition I/1.6.6) that $\int_{\mathcal{X}} f_X(x) \, dx = 1$, we can derive the differential entropy (\rightarrow Definition 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:

- 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.

Metadata: ID: P261 | shortcut: dent-addvec | author: JoramSoch | date: 2021-10-07, 09:10.

2.2.6 Non-invariance and transformation

Theorem: The differential entropy (\rightarrow Definition 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 $g : X \rightarrow Y$ 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} is the set of possible values of X .

Proof: By definition, the differential entropy (\rightarrow Definition 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 Definition I/1.6.6) of X .

The probability density function of an invertible function of a continuous random vector (\rightarrow Proof I/1.6.10) $Y = g(X)$ 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 Definition 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

$$\begin{aligned}
h(Y) &= - \int_{\mathcal{X}} [f_X(g^{-1}(g(x))) \mid J_{g^{-1}}(y)] \log [f_X(g^{-1}(g(x))) \mid J_{g^{-1}}(y)] \, d[g(x)] \\
&= - \int_{\mathcal{X}} [f_X(x) \mid J_g^{-1}(x)] \log [f_X(x) \mid J_g^{-1}(x)] \, d[g(x)] .
\end{aligned} \tag{7}$$

Using the relations $y = f(x) \Rightarrow dy = |J_f(x)| dx$ and $|A||B| = |AB|$, this becomes

$$\begin{aligned}
h(Y) &= - \int_{\mathcal{X}} [f_X(x) \mid J_g^{-1}(x) \mid |J_g(x)|] \log [f_X(x) \mid J_g^{-1}(x)] \, dx \\
&= - \int_{\mathcal{X}} f_X(x) \log f_X(x) \, dx - \int_{\mathcal{X}} f_X(x) \log |J_g^{-1}(x)| \, dx .
\end{aligned} \tag{8}$$

Finally, employing the fact (\rightarrow Definition I/1.6.6) that $\int_{\mathcal{X}} f_X(x) \, dx = 1$ and the determinant property $|A^{-1}| = 1/|A|$, we can derive the differential entropy (\rightarrow Definition I/2.2.1) of Y as

$$\begin{aligned}
h(Y) &= - \int_{\mathcal{X}} f_X(x) \log f_X(x) \, dx - \int_{\mathcal{X}} f_X(x) \log \frac{1}{|J_g(x)|} \, dx \\
&\stackrel{(3)}{=} h(X) + \int_{\mathcal{X}} f_X(x) \log |J_g(x)| \, dx .
\end{aligned} \tag{9}$$

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.

Metadata: ID: P262 | shortcut: dent-noninv | author: JoramSoch | date: 2021-10-07, 10:39.

2.2.7 Conditional differential entropy

Definition: Let X and Y be continuous random variables (\rightarrow Definition I/1.2.2) with possible outcomes \mathcal{X} and \mathcal{Y} and probability density functions (\rightarrow Definition I/1.6.6) $p(x)$ 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 Definition I/2.2.1) of Y , evaluated at x .

Sources:

- original work

Metadata: ID: D34 | shortcut: dent-cond | author: JoramSoch | date: 2020-03-21, 12:27.

2.2.8 Joint differential entropy

Definition: Let X and Y be continuous random variables (\rightarrow Definition I/1.2.2) with possible outcomes \mathcal{X} and \mathcal{Y} and joint probability (\rightarrow Definition I/1.3.2) density function (\rightarrow Definition I/1.6.6) $p(x, y)$. 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.

Sources:

- original work

Metadata: ID: D35 | shortcut: dent-joint | author: JoramSoch | date: 2020-03-21, 12:37.

2.2.9 Differential cross-entropy

Definition: Let X be a continuous random variable (\rightarrow Definition I/1.2.2) with possible outcomes \mathcal{X} and let P and Q be two probability distributions (\rightarrow Definition I/1.5.1) on X with the probability density functions (\rightarrow Definition I/1.6.6) $p(x)$ 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.

Metadata: ID: D86 | shortcut: dent-cross | author: JoramSoch | date: 2020-07-28, 03:03.

2.3 Discrete mutual information

2.3.1 Definition

Definition:

1) The mutual information of two discrete random variables (\rightarrow Definition 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 Definition I/1.6.1) of X and Y and $p(x, y)$ is the joint probability (\rightarrow Definition I/1.3.2) mass function of X and Y .

2) The mutual information of two continuous random variables (\rightarrow Definition 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 Definition I/1.6.1) of X and Y and $p(x, y)$ is the joint probability (\rightarrow Definition 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>.

Metadata: ID: D19 | shortcut: mi | author: JoramSoch | date: 2020-02-19, 18:35.

2.3.2 Relation to marginal and conditional entropy

Theorem: Let X and Y be discrete random variables (\rightarrow Definition I/1.2.2) with the joint probability (\rightarrow Definition I/1.3.2) $p(x, y)$ for $x \in \mathcal{X}$ and $y \in \mathcal{Y}$. Then, the mutual information (\rightarrow Definition 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 Definition I/2.1.1) of X and Y and $H(X|Y)$ and $H(Y|X)$ are the conditional entropies (\rightarrow Definition I/2.1.4).

Proof: The mutual information (\rightarrow Definition 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 Definition 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 Definition 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 Definition I/2.1.1) and conditional (\rightarrow Definition 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.

Metadata: ID: P19 | shortcut: dmi-mce | author: JoramSoch | date: 2020-01-13, 18:20.

2.3.3 Relation to marginal and joint entropy

Theorem: Let X and Y be discrete random variables (\rightarrow Definition I/1.2.2) with the joint probability (\rightarrow Definition I/1.3.2) $p(x, y)$ for $x \in \mathcal{X}$ and $y \in \mathcal{Y}$. Then, the mutual information (\rightarrow Definition 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 Definition I/2.1.1) of X and Y and $H(X, Y)$ is the joint entropy (\rightarrow Definition I/2.1.5).

Proof: The mutual information (\rightarrow Definition 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 Definition 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 Definition I/2.1.1) and joint (\rightarrow Definition 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.

Metadata: ID: P20 | shortcut: dmi-mje | author: JoramSoch | date: 2020-01-13, 21:53.

2.3.4 Relation to joint and conditional entropy

Theorem: Let X and Y be discrete random variables (\rightarrow Definition I/1.2.2) with the joint probability (\rightarrow Definition I/1.3.2) $p(x, y)$ for $x \in \mathcal{X}$ and $y \in \mathcal{Y}$. Then, the mutual information (\rightarrow Definition 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 Definition I/2.1.5) of X and Y and $H(X|Y)$ and $H(Y|X)$ are the conditional entropies (\rightarrow Definition I/2.1.4).

Proof: The existence of the joint probability mass function (\rightarrow Definition I/1.6.1) ensures that the mutual information (\rightarrow Definition 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 Proof 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 Proof 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.

Metadata: ID: P21 | shortcut: dmi-jce | author: JoramSoch | date: 2020-01-13, 22:17.

2.4 Continuous mutual information

2.4.1 Definition

Definition:

1) The mutual information of two discrete random variables (\rightarrow Definition 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 Definition I/1.6.1) of X and Y and $p(x, y)$ is the joint probability (\rightarrow Definition I/1.3.2) mass function of X and Y .

2) The mutual information of two continuous random variables (\rightarrow Definition 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 Definition I/1.6.1) of X and Y and $p(x, y)$ is the joint probability (\rightarrow Definition 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>.

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2.4.2 Relation to marginal and conditional differential entropy

Theorem: Let X and Y be continuous random variables (\rightarrow Definition I/1.2.2) with the joint probability (\rightarrow Definition I/1.3.2) $p(x, y)$ for $x \in \mathcal{X}$ and $y \in \mathcal{Y}$. Then, the mutual information (\rightarrow Definition 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 Definition I/2.2.1) of X and Y and $h(X|Y)$ and $h(Y|X)$ are the conditional differential entropies (\rightarrow Definition I/2.2.7).

Proof: The mutual information (\rightarrow Definition 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 Definition 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 Definition 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 Definition I/2.2.1) and conditional (\rightarrow Definition 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.

Metadata: ID: P58 | shortcut: cmi-mcde | author: JoramSoch | date: 2020-02-21, 16:53.

2.4.3 Relation to marginal and joint differential entropy

Theorem: Let X and Y be continuous random variables (\rightarrow Definition I/1.2.2) with the joint probability (\rightarrow Definition I/1.3.2) $p(x, y)$ for $x \in \mathcal{X}$ and $y \in \mathcal{Y}$. Then, the mutual information (\rightarrow Definition 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 Definition I/2.2.1) of X and Y and $h(X, Y)$ is the joint differential entropy (\rightarrow Definition I/2.2.8).

Proof: The mutual information (\rightarrow Definition 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 Definition 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 Definition I/2.2.1) and joint (\rightarrow Definition 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.

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2.4.4 Relation to joint and conditional differential entropy

Theorem: Let X and Y be continuous random variables (\rightarrow Definition I/1.2.2) with the joint probability (\rightarrow Definition I/1.3.2) $p(x, y)$ for $x \in \mathcal{X}$ and $y \in \mathcal{Y}$. Then, the mutual information (\rightarrow Definition 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 Definition I/2.2.8) of X and Y and $h(X|Y)$ and $h(Y|X)$ are the conditional differential entropies (\rightarrow Definition I/2.2.7).

Proof: The existence of the joint probability density function (\rightarrow Definition I/1.6.6) ensures that the mutual information (\rightarrow Definition 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 Proof 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 Proof 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.

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2.5 Kullback-Leibler divergence

2.5.1 Definition

Definition: Let X be a random variable (\rightarrow Definition I/1.2.2) with possible outcomes \mathcal{X} and let P and Q be two probability distributions (\rightarrow Definition 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 Definition 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 Definition I/1.6.6) of 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>.

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2.5.2 Non-negativity

Theorem: The Kullback-Leibler divergence (\rightarrow Definition 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 Definition 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 Proof I/2.1.8) states that the entropy (\rightarrow Definition I/2.1.1) of a probability distribution is always less than or equal to the cross-entropy (\rightarrow Definition 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.

Metadata: ID: P117 | shortcut: kl-nonneg | author: JoramSoch | date: 2020-05-31, 23:43.

2.5.3 Non-negativity

Theorem: The Kullback-Leibler divergence (\rightarrow Definition 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 Definition 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 Proof 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 be non-negative real numbers and $a = \sum_{i=1}^n a_i$ and $b = \sum_{i=1}^n b_i$. Because $p(x)$ and $q(x)$ are probability mass functions (\rightarrow Definition I/1.6.1), such that

$$\begin{aligned} p(x) &\geq 0, & \sum_{x \in \mathcal{X}} p(x) &= 1 \quad \text{and} \\ q(x) &\geq 0, & \sum_{x \in \mathcal{X}} q(x) &= 1 , \end{aligned} \quad (4)$$

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.

Metadata: ID: P166 | shortcut: kl-nonneg2 | author: JoramSoch | date: 2020-09-09, 07:02.

2.5.4 Non-symmetry

Theorem: The Kullback-Leibler divergence (\rightarrow Definition 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 Definition I/1.5.1) P and Q .

Proof: Let $X \in \mathcal{X} = \{0, 1, 2\}$ be a discrete random variable (\rightarrow Definition I/1.2.2) and consider the two probability distributions (\rightarrow Definition 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 Definition II/1.3.1) and $\mathcal{U}(a, b)$ indicates a discrete uniform distribution (\rightarrow Definition II/1.1.1).

Then, the probability mass function of the binomial distribution (\rightarrow Proof II/1.3.2) 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 Proof II/1.1.2) entails that

$$q(x) = \frac{1}{3}, \quad (4)$$

such that the Kullback-Leibler divergence (\rightarrow Definition 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 Definition I/2.5.1) of Q from P is

$$\begin{aligned} \text{KL}[Q||P] &= \sum_{x \in \mathcal{X}} q(x) \cdot \log \frac{q(x)}{p(x)} \\ &= \frac{1}{3} \log \frac{4}{3} + \frac{1}{3} \log \frac{2}{3} + \frac{1}{3} \log \frac{4}{3} \\ &= \frac{1}{3} \left(\log \frac{4}{3} + \log \frac{2}{3} + \log \frac{4}{3} \right) \\ &= \frac{1}{3} \log \left(\frac{4}{3} \cdot \frac{2}{3} \cdot \frac{4}{3} \right) \\ &= \frac{1}{3} \log \frac{32}{27} = 0.0566 \end{aligned} \quad (6)$$

which provides an example for

$$\text{KL}[P||Q] \neq \text{KL}[Q||P] \quad (7)$$

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.

Metadata: ID: P147 | shortcut: kl-nonsymm | author: JoramSoch | date: 2020-08-11, 06:57.

2.5.5 Convexity

Theorem: The Kullback-Leibler divergence (\rightarrow Definition I/2.5.1) is convex in the pair of probability distributions (\rightarrow Definition I/1.5.1) (p, q) , i.e.

$$\text{KL}[\lambda p_1 + (1 - \lambda)p_2 || \lambda q_1 + (1 - \lambda)q_2] \leq \lambda \text{KL}[p_1 || q_1] + (1 - \lambda) \text{KL}[p_2 || q_2] \quad (1)$$

where (p_1, q_1) and (p_2, q_2) are two pairs of probability distributions and $0 \leq \lambda \leq 1$.

Proof: The Kullback-Leibler divergence (\rightarrow Definition I/2.5.1) of P from Q is defined as

$$\text{KL}[P || Q] = \sum_{x \in \mathcal{X}} p(x) \cdot \log \frac{p(x)}{q(x)} \quad (2)$$

and the log sum inequality (\rightarrow Proof I/2.1.9) states that

$$\sum_{i=1}^n a_i \log \frac{a_i}{b_i} \geq \left(\sum_{i=1}^n a_i \right) \log \frac{\sum_{i=1}^n a_i}{\sum_{i=1}^n b_i} \quad (3)$$

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

$$\begin{aligned} & \text{KL}[\lambda p_1 + (1 - \lambda)p_2 || \lambda q_1 + (1 - \lambda)q_2] \\ & \stackrel{(2)}{=} \sum_{x \in \mathcal{X}} \left[[\lambda p_1(x) + (1 - \lambda)p_2(x)] \cdot \log \frac{\lambda p_1(x) + (1 - \lambda)p_2(x)}{\lambda q_1(x) + (1 - \lambda)q_2(x)} \right] \\ & \stackrel{(3)}{\leq} \sum_{x \in \mathcal{X}} \left[\lambda p_1(x) \cdot \log \frac{\lambda p_1(x)}{\lambda q_1(x)} + (1 - \lambda)p_2(x) \cdot \log \frac{(1 - \lambda)p_2(x)}{(1 - \lambda)q_2(x)} \right] \\ & = \lambda \sum_{x \in \mathcal{X}} p_1(x) \cdot \log \frac{p_1(x)}{q_1(x)} + (1 - \lambda) \sum_{x \in \mathcal{X}} p_2(x) \cdot \log \frac{p_2(x)}{q_2(x)} \\ & \stackrel{(2)}{=} \lambda \text{KL}[p_1 || q_1] + (1 - \lambda) \text{KL}[p_2 || q_2] \end{aligned} \quad (4)$$

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>.

Metadata: ID: P148 | shortcut: kl-conv | author: JoramSoch | date: 2020-08-11, 07:30.

2.5.6 Additivity for independent distributions

Theorem: The Kullback-Leibler divergence (\rightarrow Definition I/2.5.1) is additive for independent distributions, i.e.

$$\text{KL}[P || Q] = \text{KL}[P_1 || Q_1] + \text{KL}[P_2 || Q_2] \quad (1)$$

where P_1 and P_2 are independent (\rightarrow Definition I/1.3.6) distributions (\rightarrow Definition I/1.5.1) with the joint distribution (\rightarrow Definition 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 Definition I/2.5.1) is defined as

$$\text{KL}[P||Q] = \int_{\mathcal{X}} p(x) \cdot \log \frac{p(x)}{q(x)} dx \quad (2)$$

which, applied to the joint distributions P and Q , yields

$$\text{KL}[P||Q] = \int_{\mathcal{X}} \int_{\mathcal{Y}} p(x, y) \cdot \log \frac{p(x, y)}{q(x, y)} dy dx . \quad (3)$$

Applying $p(x, y) = p_1(x) p_2(y)$ and $q(x, y) = q_1(x) q_2(y)$, we have

$$\text{KL}[P||Q] = \int_{\mathcal{X}} \int_{\mathcal{Y}} p_1(x) p_2(y) \cdot \log \frac{p_1(x) p_2(y)}{q_1(x) q_2(y)} dy dx . \quad (4)$$

Now we can separate the logarithm and evaluate the integrals:

$$\begin{aligned} \text{KL}[P||Q] &= \int_{\mathcal{X}} \int_{\mathcal{Y}} p_1(x) p_2(y) \cdot \left(\log \frac{p_1(x)}{q_1(x)} + \log \frac{p_2(y)}{q_2(y)} \right) dy dx \\ &= \int_{\mathcal{X}} \int_{\mathcal{Y}} p_1(x) p_2(y) \cdot \log \frac{p_1(x)}{q_1(x)} dy dx + \int_{\mathcal{X}} \int_{\mathcal{Y}} p_1(x) p_2(y) \cdot \log \frac{p_2(y)}{q_2(y)} dy dx \\ &= \int_{\mathcal{X}} p_1(x) \cdot \log \frac{p_1(x)}{q_1(x)} \int_{\mathcal{Y}} p_2(y) dy dx + \int_{\mathcal{Y}} p_2(y) \cdot \log \frac{p_2(y)}{q_2(y)} \int_{\mathcal{X}} p_1(x) dx dy \\ &= \int_{\mathcal{X}} p_1(x) \cdot \log \frac{p_1(x)}{q_1(x)} dx + \int_{\mathcal{Y}} p_2(y) \cdot \log \frac{p_2(y)}{q_2(y)} dy \\ &\stackrel{(2)}{=} \text{KL}[P_1||Q_1] + \text{KL}[P_2||Q_2] . \end{aligned} \quad (5)$$

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.

Metadata: ID: P116 | shortcut: kl-add | author: JoramSoch | date: 2020-05-31, 23:26.

2.5.7 Invariance under parameter transformation

Theorem: The Kullback-Leibler divergence (\rightarrow Definition I/2.5.1) is invariant under parameter transformation, i.e.

$$\text{KL}[p(x)||q(x)] = \text{KL}[p(y)||q(y)] \quad (1)$$

where $y(x) = mx + n$ is an affine transformation of x and $p(x)$ and $q(x)$ are the probability density functions (\rightarrow Definition I/1.6.6) of the probability distributions (\rightarrow Definition I/1.5.1) P and Q on the continuous random variable (\rightarrow Definition I/1.2.2) X .

Proof: The continuous Kullback-Leibler divergence (\rightarrow Definition I/2.5.1) (KL divergence) is defined as

$$\text{KL}[p(x)||q(x)] = \int_a^b p(x) \cdot \log \frac{p(x)}{q(x)} dx \quad (2)$$

where $a = \min(\mathcal{X})$ and $b = \max(\mathcal{X})$ are the lower and upper bound of the possible outcomes \mathcal{X} of X .

Due to the identity of the differentials

$$\begin{aligned} p(x) dx &= p(y) dy \\ q(x) dx &= q(y) dy \end{aligned} \quad (3)$$

which can be rearranged into

$$\begin{aligned} p(x) &= p(y) \frac{dy}{dx} \\ q(x) &= q(y) \frac{dy}{dx} , \end{aligned} \quad (4)$$

the KL divergence can be evaluated as follows:

$$\begin{aligned} \text{KL}[p(x)||q(x)] &= \int_a^b p(x) \cdot \log \frac{p(x)}{q(x)} dx \\ &= \int_{y(a)}^{y(b)} p(y) \frac{dy}{dx} \cdot \log \left(\frac{p(y) \frac{dy}{dx}}{q(y) \frac{dy}{dx}} \right) dx \\ &= \int_{y(a)}^{y(b)} p(y) \cdot \log \frac{p(y)}{q(y)} dy \\ &= \text{KL}[p(y)||q(y)] . \end{aligned} \quad (5)$$

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#Properties.
- shimao (2018): “KL divergence invariant to affine transformation?”; in: *StackExchange Cross Validated*, retrieved on 2020-05-28; URL: <https://stats.stackexchange.com/questions/341922/kl-divergence-invariant-to-affine-transformation>.

Metadata: ID: P115 | shortcut: kl-inv | author: JoramSoch | date: 2020-05-28, 00:18.

2.5.8 Relation to discrete entropy

Theorem: Let X be a discrete random variable (\rightarrow Definition I/1.2.2) with possible outcomes \mathcal{X} and let P and Q be two probability distributions (\rightarrow Definition I/1.5.1) on X . Then, the Kullback-Leibler divergence (\rightarrow Definition 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 cross-entropy (\rightarrow Definition I/2.1.6) of P and Q and $H(P)$ is the marginal entropy (\rightarrow Definition I/2.1.1) of P .

Proof: The discrete Kullback-Leibler divergence (\rightarrow Definition I/2.5.1) is defined as

$$\text{KL}[P||Q] = \sum_{x \in \mathcal{X}} p(x) \cdot \log \frac{p(x)}{q(x)} \quad (2)$$

where $p(x)$ and $q(x)$ are the probability mass functions (\rightarrow Definition I/1.6.1) of P and Q . Separating the logarithm, we have:

$$\text{KL}[P||Q] = - \sum_{x \in \mathcal{X}} p(x) \log q(x) + \sum_{x \in \mathcal{X}} p(x) \log p(x) . \quad (3)$$

Now considering the definitions of marginal entropy (\rightarrow Definition I/2.1.1) and cross-entropy (\rightarrow Definition I/2.1.6)

$$\begin{aligned} H(P) &= - \sum_{x \in \mathcal{X}} p(x) \log p(x) \\ H(P, Q) &= - \sum_{x \in \mathcal{X}} p(x) \log q(x) , \end{aligned} \quad (4)$$

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.

Metadata: ID: P113 | shortcut: kl-ent | author: JoramSoch | date: 2020-05-27, 23:20.

2.5.9 Relation to differential entropy

Theorem: Let X be a continuous random variable (\rightarrow Definition I/1.2.2) with possible outcomes \mathcal{X} and let P and Q be two probability distributions (\rightarrow Definition I/1.5.1) on X . Then, the Kullback-Leibler divergence (\rightarrow Definition 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 Definition I/2.2.9) of P and Q and $h(P)$ is the marginal differential entropy (\rightarrow Definition I/2.2.1) of P .

Proof: The continuous Kullback-Leibler divergence (\rightarrow Definition 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 Definition I/1.6.6) 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 Definition I/2.2.1) and differential cross-entropy (\rightarrow Definition 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.

Metadata: ID: P114 | shortcut: kl-dent | author: JoramSoch | date: 2020-05-27, 23:32.

3 Estimation theory

3.1 Point estimates

3.1.1 Mean squared error

Definition: Let $\hat{\theta}$ be an estimator (\rightarrow Definition “est”) of an unknown parameter (\rightarrow Definition “para”) θ based on measured data (\rightarrow Definition “data”) y . Then, the mean squared error is defined as the expected value (\rightarrow Definition I/1.7.1) 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 Definition “samp”) 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.

Metadata: ID: D173 | shortcut: mse | author: JoramSoch | date: 2022-03-27, 23:41.

3.1.2 Partition of the mean squared error into bias and variance

Theorem: The mean squared error (\rightarrow Definition I/3.1.1) 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 Definition I/1.8.1) 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 (\rightarrow Definition “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 Definition I/3.1.1) (MSE) is defined as the expected value (\rightarrow Definition I/1.7.1) 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:

$$\begin{aligned}
\text{MSE}(\hat{\theta}) &= E_{\hat{\theta}} \left[\left(\hat{\theta} - \theta \right)^2 \right] \\
&= E_{\hat{\theta}} \left[\left(\hat{\theta} - E_{\hat{\theta}}(\hat{\theta}) + E_{\hat{\theta}}(\hat{\theta}) - \theta \right)^2 \right] \\
&= E_{\hat{\theta}} \left[\left(\hat{\theta} - E_{\hat{\theta}}(\hat{\theta}) \right)^2 + 2 \left(\hat{\theta} - E_{\hat{\theta}}(\hat{\theta}) \right) \left(E_{\hat{\theta}}(\hat{\theta}) - \theta \right) + \left(E_{\hat{\theta}}(\hat{\theta}) - \theta \right)^2 \right] \\
&= E_{\hat{\theta}} \left[\left(\hat{\theta} - E_{\hat{\theta}}(\hat{\theta}) \right)^2 \right] + E_{\hat{\theta}} \left[2 \left(\hat{\theta} - E_{\hat{\theta}}(\hat{\theta}) \right) \left(E_{\hat{\theta}}(\hat{\theta}) - \theta \right) \right] + E_{\hat{\theta}} \left[\left(E_{\hat{\theta}}(\hat{\theta}) - \theta \right)^2 \right].
\end{aligned} \tag{5}$$

Because $E_{\hat{\theta}}(\hat{\theta}) - \theta$ is constant as a function of $\hat{\theta}$, we have:

$$\begin{aligned}
\text{MSE}(\hat{\theta}) &= E_{\hat{\theta}} \left[\left(\hat{\theta} - E_{\hat{\theta}}(\hat{\theta}) \right)^2 \right] + 2 \left(E_{\hat{\theta}}(\hat{\theta}) - \theta \right) E_{\hat{\theta}} \left[\hat{\theta} - E_{\hat{\theta}}(\hat{\theta}) \right] + \left(E_{\hat{\theta}}(\hat{\theta}) - \theta \right)^2 \\
&= E_{\hat{\theta}} \left[\left(\hat{\theta} - E_{\hat{\theta}}(\hat{\theta}) \right)^2 \right] + 2 \left(E_{\hat{\theta}}(\hat{\theta}) - \theta \right) \left(E_{\hat{\theta}}(\hat{\theta}) - E_{\hat{\theta}}(\hat{\theta}) \right) + \left(E_{\hat{\theta}}(\hat{\theta}) - \theta \right)^2 \\
&= E_{\hat{\theta}} \left[\left(\hat{\theta} - E_{\hat{\theta}}(\hat{\theta}) \right)^2 \right] + \left(E_{\hat{\theta}}(\hat{\theta}) - \theta \right)^2.
\end{aligned} \tag{6}$$

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.

Metadata: ID: P5 | shortcut: mse-bnv | author: JoramSoch | date: 2019-11-27, 14:26.

3.2 Interval estimates

3.2.1 Confidence interval

Definition: Let y be a random sample (\rightarrow Definition “samp”) from a probability distributions (\rightarrow Definition I/1.5.1) governed by a parameter (\rightarrow Definition “para”) 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 Definition I/1.2.2) $u(y)$ and $v(y)$ with the property

$$\Pr(u(y) < \theta < v(y) \mid \theta, \varphi) = \gamma \quad \text{for all } (\theta, \varphi). \tag{1}$$

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.

Metadata: ID: D174 | shortcut: ci | author: JoramSoch | date: 2022-03-27, 23:56.

3.2.2 Construction of confidence intervals using Wilks' theorem

Theorem: Let m be a generative model (\rightarrow Definition I/5.1.1) for measured data y with model parameters θ , consisting of a parameter of interest ϕ and nuisance parameters λ :

$$m : p(y|\theta) = \mathcal{D}(y; \theta), \quad \theta = \{\phi, \lambda\} . \quad (1)$$

Further, let $\hat{\theta}$ be an estimate of θ , obtained using maximum-likelihood-estimation (\rightarrow Definition I/4.1.3):

$$\hat{\theta} = \arg \max_{\theta} \log p(y|\theta), \quad \hat{\theta} = \{\hat{\phi}, \hat{\lambda}\} . \quad (2)$$

Then, an asymptotic confidence interval (\rightarrow Definition I/3.2.1) for θ is given by

$$\text{CI}_{1-\alpha}(\hat{\phi}) = \left\{ \phi \mid \log p(y|\phi, \hat{\lambda}) \geq \log p(y|\hat{\phi}, \hat{\lambda}) - \frac{1}{2} \chi_{1,1-\alpha}^2 \right\} \quad (3)$$

where $1 - \alpha$ is the confidence level and $\chi_{1,1-\alpha}^2$ is the $(1 - \alpha)$ -quantile of the chi-squared distribution (\rightarrow Definition II/3.7.1) with 1 degree of freedom (\rightarrow Definition “dof”).

Proof: The confidence interval (\rightarrow Definition I/3.2.1) is defined as the interval that, under infinitely repeated random experiments (\rightarrow Definition I/1.1.1), contains the true parameter value with a certain probability.

Let us define the likelihood ratio (\rightarrow Definition “lr”)

$$\Lambda(\phi) = \frac{p(y|\phi, \hat{\lambda})}{p(y|\hat{\phi}, \hat{\lambda})} \quad (4)$$

and compute the log-likelihood ratio (\rightarrow Definition “llr”)

$$\log \Lambda(\phi) = \log p(y|\phi, \hat{\lambda}) - \log p(y|\hat{\phi}, \hat{\lambda}) . \quad (5)$$

Wilks' theorem (\rightarrow Proof “llr-wilks”) states that, when comparing two statistical models with parameter spaces Θ_1 and $\Theta_0 \subset \Theta_1$, as the sample size approaches infinity, the quantity calculated as -2 times the log-ratio of maximum likelihoods follows a chi-squared distribution (\rightarrow Definition II/3.7.1), if the null hypothesis is true:

$$H_0 : \theta \in \Theta_0 \quad \Rightarrow \quad -2 \log \frac{\max_{\theta \in \Theta_0} p(y|\theta)}{\max_{\theta \in \Theta_1} p(y|\theta)} \sim \chi_{\Delta k}^2 \quad (6)$$

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 Definition I/1.6.23) $\chi_{k,p}^2$ of the chi-squared distribution (\rightarrow Definition 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

$$\begin{aligned}
-2 \left[\log p(y|\phi, \hat{\lambda}) - \log p(y|\hat{\phi}, \hat{\lambda}) \right] &\leq \chi_{1,1-\alpha}^2 \\
\log p(y|\phi, \hat{\lambda}) - \log p(y|\hat{\phi}, \hat{\lambda}) &\geq -\frac{1}{2} \chi_{1,1-\alpha}^2 \\
\log p(y|\phi, \hat{\lambda}) &\geq \log p(y|\hat{\phi}, \hat{\lambda}) - \frac{1}{2} \chi_{1,1-\alpha}^2
\end{aligned} \tag{9}$$

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.

Metadata: ID: P56 | shortcut: ci-wilks | author: JoramSoch | date: 2020-02-19, 17:15.

4 Frequentist statistics

4.1 Likelihood theory

4.1.1 Likelihood function

Definition: Let there be a generative model (\rightarrow Definition I/5.1.1) m describing measured data y using model parameters θ . Then, the probability density function (\rightarrow Definition I/1.6.6) of the distribution of y given θ is called the likelihood function of m :

$$\mathcal{L}_m(\theta) = p(y|\theta, m) = \mathcal{D}(y; \theta) . \quad (1)$$

Sources:

- original work

Metadata: ID: D28 | shortcut: lf | author: JoramSoch | date: 2020-03-03, 15:50.

4.1.2 Log-likelihood function

Definition: Let there be a generative model (\rightarrow Definition I/5.1.1) m describing measured data y using model parameters θ . Then, the logarithm of the probability density function (\rightarrow Definition I/1.6.6) of the distribution of y given θ is called the log-likelihood function (\rightarrow Definition I/5.1.2) of m :

$$\text{LL}_m(\theta) = \log p(y|\theta, m) = \log \mathcal{D}(y; \theta) . \quad (1)$$

Sources:

- original work

Metadata: ID: D59 | shortcut: llf | author: JoramSoch | date: 2020-05-17, 22:52.

4.1.3 Maximum likelihood estimation

Definition: Let there be a generative model (\rightarrow Definition I/5.1.1) m describing measured data y using model parameters θ . Then, the parameter values maximizing the likelihood function (\rightarrow Definition I/5.1.2) or log-likelihood function (\rightarrow Definition 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”.

Sources:

- original work

Metadata: ID: D60 | shortcut: mle | author: JoramSoch | date: 2020-05-15, 23:05.

4.1.4 MLE can be biased

Theorem: Maximum likelihood estimation (\rightarrow Definition I/4.1.3) can result in biased estimates (\rightarrow Definition “est-unb”) of model parameters, i.e. estimates whose long-term expected value is unequal to the quantities they estimate:

$$\mathbb{E} \left[\hat{\theta}_{\text{MLE}} \right] = \mathbb{E} \left[\arg \max_{\theta} \text{LL}_m(\theta) \right] \neq \theta . \quad (1)$$

Proof: Consider a set of independent and identical (\rightarrow Definition “iid”) normally distributed (\rightarrow Definition II/3.2.1) observations $x = \{x_1, \dots, x_n\}$ with unknown mean (\rightarrow Definition I/1.7.1) μ and variance (\rightarrow Definition I/1.8.1) 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 (\rightarrow Definition I/4.1.3) for the variance (\rightarrow Definition I/1.8.1) σ^2 is underestimating the true variance of the data distribution (\rightarrow Proof IV/1.1.2):

$$\mathbb{E} \left[\hat{\sigma}_{\text{MLE}}^2 \right] = \frac{n-1}{n} \sigma^2 \neq \sigma^2 . \quad (3)$$

This proves the existence of cases such as those stated by the theorem.

Sources:

- original work

Metadata: ID: P317 | shortcut: mle-bias | author: JoramSoch | date: 2022-03-18, 17:26.

4.1.5 Maximum log-likelihood

Definition: Let there be a generative model (\rightarrow Definition 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 Definition 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 Definition I/4.1.3) into the log-likelihood function (\rightarrow Definition I/4.1.2).

Sources:

- original work

Metadata: ID: D61 | shortcut: mll | author: JoramSoch | date: 2020-05-15, 23:13.

4.1.6 Method of moments

Definition: Let measured data y follow a probability distribution (\rightarrow Definition I/1.5.1) with probability mass (\rightarrow Definition I/1.6.1) or probability density (\rightarrow Definition I/1.6.6) $p(y|\theta)$ 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 Definition I/1.15.1) 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 Definition I/1.15.1) 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).

Metadata: ID: D151 | shortcut: mome | author: JoramSoch | date: 2021-04-29, 07:51.

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 Definition “data”).

More precisely, let m be a generative model (\rightarrow Definition 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.

Metadata: ID: D127 | shortcut: hyp | author: JoramSoch | date: 2021-03-19, 14:18.

4.2.2 Simple vs. composite

Definition: Let H be a statistical hypothesis (\rightarrow Definition 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 Definition I/1.5.5) of the test statistic (\rightarrow Definition I/4.3.5) is a function of sample size 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.

Metadata: ID: D128 | shortcut: hyp-simp | author: JoramSoch | date: 2021-03-19, 14:24.

4.2.3 Point/exact vs. set/inexact

Definition: Let H be a statistical hypothesis (\rightarrow Definition 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.

Metadata: ID: D129 | shortcut: hyp-point | author: JoramSoch | date: 2021-03-19, 14:28.

4.2.4 One-tailed vs. two-tailed

Definition: Let H_0 be a point (\rightarrow Definition I/4.2.3) null hypothesis (\rightarrow Definition I/4.3.2)

$$H_0 : \theta = \theta_0 \quad (1)$$

and consider a set (\rightarrow Definition I/4.2.3) alternative hypothesis (\rightarrow Definition 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.

Metadata: ID: D138 | shortcut: hyp-tail | author: JoramSoch | date: 2021-03-31, 09:21.

4.3 Hypothesis testing

4.3.1 Statistical test

Definition: Let y be a set of measured data (\rightarrow Definition “data”). Then, a statistical hypothesis test consists of the following:

- an assumption about the distribution (\rightarrow Definition I/1.5.1) of the data, often expressed in terms of a statistical model (\rightarrow Definition I/5.1.1) m ;
- a null hypothesis (\rightarrow Definition I/4.3.2) H_0 and an alternative hypothesis (\rightarrow Definition I/4.3.3) H_1 which make specific statements about the distribution of the data;
- a test statistic (\rightarrow Definition I/4.3.5) $T(Y)$ which is a function of the data and whose distribution under the null hypothesis (\rightarrow Definition I/4.3.2) is known;
- a significance level (\rightarrow Definition I/4.3.8) α which imposes an upper bound on the probability (\rightarrow Definition 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 Definition 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 Definition 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.

Metadata: ID: D130 | shortcut: test | author: JoramSoch | date: 2021-03-19, 14:36.

4.3.2 Null hypothesis

Definition: The statement which is tested in a statistical hypothesis test (\rightarrow Definition 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 Definition 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 Definition 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.

Metadata: ID: D125 | shortcut: h0 | author: JoramSoch | date: 2021-03-12, 10:25.

4.3.3 Alternative hypothesis

Definition: Let H_0 be a null hypothesis (\rightarrow Definition I/4.3.2) of a statistical hypothesis test (\rightarrow Definition 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 Definition I/5.1.1) describing measured data y using model parameters $\theta \in \Theta$. Then, null and alternative hypothesis are formally specified as

$$\begin{aligned} H_0 : \theta \in \Theta_0 \quad \text{where} \quad \Theta_0 \subset \Theta \\ H_1 : \theta \in \Theta_1 \quad \text{where} \quad \Theta_1 = \Theta \setminus \Theta_0 . \end{aligned} \quad (1)$$

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.

Metadata: ID: D126 | shortcut: h1 | author: JoramSoch | date: 2021-03-12, 10:36.

4.3.4 One-tailed vs. two-tailed

Definition: Let there be a statistical test (\rightarrow Definition I/4.3.1) of an alternative hypothesis (\rightarrow Definition I/4.3.3) H_1 against a null hypothesis (\rightarrow Definition I/4.3.2) H_0 . Then,

- the test is called a one-tailed test, if H_1 is a one-tailed hypothesis (\rightarrow Definition I/4.2.4);
- the test is called a two-tailed test, if H_1 is a two-tailed hypothesis (\rightarrow Definition I/4.2.4).

The fact whether a test (\rightarrow Definition I/4.3.1) is one-tailed or two-tailed has consequences for the computation of critical value (\rightarrow Definition I/4.3.9) and p-value (\rightarrow Definition 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.

Metadata: ID: D139 | shortcut: test-tail | author: JoramSoch | date: 2021-03-31, 09:32.

4.3.5 Test statistic

Definition: In a statistical hypothesis test (\rightarrow Definition I/4.3.1), the test statistic $T(Y)$ is a scalar function of the measured data (\rightarrow Definition “data”) y whose distribution under the null hypothesis (\rightarrow Definition I/4.3.2) H_0 can be established. Together with a significance level (\rightarrow Definition I/4.3.8) α , this distribution implies a critical value (\rightarrow Definition 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.

Metadata: ID: D131 | shortcut: tstat | author: JoramSoch | date: 2021-03-19, 14:40.

4.3.6 Size of a test

Definition: Let there be a statistical hypothesis test (\rightarrow Definition I/4.3.1) with null hypothesis (\rightarrow Definition 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 Definition I/1.3.1) of rejecting the null hypothesis (\rightarrow Definition I/4.3.2) H_0 , given that H_0 is actually true.

For a simple null hypothesis (\rightarrow Definition I/4.2.2), the size is determined by the following conditional probability (\rightarrow Definition I/1.3.4):

$$\Pr(\text{test rejects } H_0 | H_0) . \quad (1)$$

For a composite null hypothesis (\rightarrow Definition I/4.2.2), the size is the supremum over all possible realizations of the null hypothesis (\rightarrow Definition 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)).

Metadata: ID: D132 | shortcut: size | author: JoramSoch | date: 2021-03-19, 14:46.

4.3.7 Power of a test

Definition: Let there be a statistical hypothesis test (\rightarrow Definition I/4.3.1) with null hypothesis (\rightarrow Definition I/4.3.2) H_0 and alternative hypothesis (\rightarrow Definition 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 Definition I/1.3.1) of rejecting H_0 , given that H_1 is actually true.

For given null (\rightarrow Definition I/4.3.2) and alternative (\rightarrow Definition I/4.3.3) hypothesis (\rightarrow Definition I/4.2.1), the size is determined by the following conditional probability (\rightarrow Definition 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.

Metadata: ID: D137 | shortcut: power | author: JoramSoch | date: 2021-03-31, 09:01.

4.3.8 Significance level

Definition: Let the size (\rightarrow Definition I/4.3.6) of a statistical hypothesis test (\rightarrow Definition I/4.3.1) be the probability of a false-positive result or making a type I error, i.e. the probability (\rightarrow Definition I/1.3.1) of rejecting the null hypothesis (\rightarrow Definition 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.

Metadata: ID: D133 | shortcut: alpha | author: JoramSoch | date: 2021-03-19, 14:50.

4.3.9 Critical value

Definition: In a statistical hypothesis test (\rightarrow Definition I/4.3.1), the critical value (\rightarrow Definition I/4.3.9) t_{crit} is that value of the test statistic (\rightarrow Definition 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 Definition I/4.3.8) α . Put differently, if the observed test statistic $t_{\text{obs}} = T(y)$ computed from actually measured data (\rightarrow Definition “data”) y is as extreme or more extreme than the critical value, the test rejects the null hypothesis (\rightarrow Definition I/4.3.2) H_0 in favor of the alternative hypothesis (\rightarrow Definition 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.

Metadata: ID: D134 | shortcut: cval | author: JoramSoch | date: 2021-03-19, 14:54.

4.3.10 p-value

Definition: Let there be a statistical test (\rightarrow Definition I/4.3.1) of the null hypothesis (\rightarrow Definition I/4.3.2) H_0 and the alternative hypothesis (\rightarrow Definition I/4.3.3) H_1 using the test statistic (\rightarrow Definition I/4.3.5) $T(Y)$. Let y be the measured data (\rightarrow Definition “data”) 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 Definition I/1.6.13) (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 Definition I/4.2.4);
- $p = 1 - F_T(t_{\text{obs}})$, if H_1 is a right-sided one-tailed hypothesis (\rightarrow Definition 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 Definition 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.

Metadata: ID: D135 | shortcut: pval | author: JoramSoch | date: 2021-03-19, 14:58.

4.3.11 Distribution of p-value under null hypothesis

Theorem: Under the null hypothesis (\rightarrow Definition I/4.3.2), the p-value (\rightarrow Definition I/4.3.10) in a statistical test (\rightarrow Definition I/4.3.1) follows a continuous uniform distribution (\rightarrow Definition 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 Definition I/4.2.4). Then, the p-value is a function of the test statistic (\rightarrow Definition I/4.3.10)

$$\begin{aligned} P &= F_T(T) \\ p &= F_T(t_{\text{obs}}) \end{aligned} \quad (2)$$

where t_{obs} is the observed test statistic (\rightarrow Definition I/4.3.5) and $F_T(t)$ is the cumulative distribution function (\rightarrow Definition I/1.6.13) of the test statistic (\rightarrow Definition I/4.3.5) under the null hypothesis (\rightarrow Definition I/4.3.2).

Then, we can obtain the cumulative distribution function (\rightarrow Definition I/1.6.13) of the p-value (\rightarrow Definition 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 Proof II/3.1.4) over the interval $[0, 1]$:

$$F_X(x) = \int_{-\infty}^x \mathcal{U}(z; 0, 1) \, dz = x \quad \text{where } 0 \leq x \leq 1. \tag{4}$$

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>.

Metadata: ID: P318 | shortcut: pval-h0 | author: JoramSoch | date: 2022-03-18, 22:37.

5 Bayesian statistics

5.1 Probabilistic modeling

5.1.1 Generative model

Definition: Consider measured data (\rightarrow Definition “data”) y and some unknown latent parameters (\rightarrow Definition “para”) θ . A statement about the distribution (\rightarrow Definition 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 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.neuroimage.2007.06.026

Metadata: ID: D27 | shortcut: gm | author: JoramSoch | date: 2020-03-03, 15:50.

5.1.2 Likelihood function

Definition: Let there be a generative model (\rightarrow Definition I/5.1.1) m describing measured data y using model parameters θ . Then, the probability density function (\rightarrow Definition I/1.6.6) of the distribution of y given θ is called the likelihood function of m :

$$\mathcal{L}_m(\theta) = p(y|\theta, m) = \mathcal{D}(y; \theta) . \quad (1)$$

Sources:

- original work

Metadata: ID: D28 | shortcut: lf | author: JoramSoch | date: 2020-03-03, 15:50.

5.1.3 Prior distribution

Definition: Consider measured data y and some unknown latent parameters θ . A distribution 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 Definition I/1.6.6) is called the prior density:

$$p(\theta|m) = \mathcal{D}(\theta; \lambda) . \quad (2)$$

Sources:

- original work

Metadata: ID: D29 | shortcut: prior | author: JoramSoch | date: 2020-03-03, 16:09.

5.1.4 Full probability model

Definition: Consider measured data y and some unknown latent parameters θ . The combination of a generative model (\rightarrow Definition I/5.1.1) for y and a prior distribution (\rightarrow Definition I/5.1.3) on θ is called a full probability model m :

$$m : y \sim \mathcal{D}(\theta), \theta \sim \mathcal{D}(\lambda) . \quad (1)$$

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/>.

Metadata: ID: D30 | shortcut: fpm | author: JoramSoch | date: 2020-03-03, 16:16.

5.1.5 Joint likelihood

Definition: Let there be a generative model (\rightarrow Definition I/5.1.1) m describing measured data y using model parameters θ and a prior distribution (\rightarrow Definition I/5.1.3) on θ . Then, the joint probability (\rightarrow Definition I/1.3.2) density function (\rightarrow Definition I/1.6.6) of y and θ is called the joint likelihood:

$$p(y, \theta|m) = p(y|\theta, m) p(\theta|m) . \quad (1)$$

Sources:

- original work

Metadata: ID: D31 | shortcut: jl | author: JoramSoch | date: 2020-03-03, 16:36.

5.1.6 Joint likelihood is product of likelihood and prior

Theorem: Let there be a generative model (\rightarrow Definition I/5.1.1) m describing measured data y using model parameters θ and a prior distribution (\rightarrow Definition I/5.1.3) on θ . Then, the joint likelihood (\rightarrow Definition I/5.1.5) is equal to the product of likelihood function (\rightarrow Definition I/5.1.2) and prior density (\rightarrow Definition I/5.1.3):

$$p(y, \theta|m) = p(y|\theta, m) p(\theta|m) . \quad (1)$$

Proof: The joint likelihood (\rightarrow Definition I/5.1.5) is defined as the joint probability (\rightarrow Definition I/1.3.2) density function (\rightarrow Definition I/1.6.6) of data y and parameters θ :

$$p(y, \theta|m) . \quad (2)$$

Applying the law of conditional probability (\rightarrow Definition I/1.3.4), we have:

$$\begin{aligned}
p(y|\theta, m) &= \frac{p(y, \theta|m)}{p(\theta|m)} \\
&\Leftrightarrow \\
p(y, \theta|m) &= p(y|\theta, m) p(\theta|m) .
\end{aligned} \tag{3}$$

Sources:

- original work

Metadata: ID: P89 | shortcut: jl-lfnprior | author: JoramSoch | date: 2020-05-05, 04:21.

5.1.7 Posterior distribution

Definition: Consider measured data y and some unknown latent parameters θ . The distribution of θ conditional on y is called the posterior distribution:

$$\theta|y \sim \mathcal{D}(\phi) . \tag{1}$$

The parameters ϕ of this distribution are called the posterior hyperparameters and the probability density function (\rightarrow Definition I/1.6.6) is called the posterior density:

$$p(\theta|y, m) = \mathcal{D}(\theta; \phi) . \tag{2}$$

Sources:

- original work

Metadata: ID: D32 | shortcut: post | author: JoramSoch | date: 2020-03-03, 16:43.

5.1.8 Posterior density is proportional to joint likelihood

Theorem: In a full probability model (\rightarrow Definition I/5.1.4) m describing measured data y using model parameters θ , the posterior density (\rightarrow Definition I/5.1.7) over the model parameters is proportional to the joint likelihood (\rightarrow Definition I/5.1.5):

$$p(\theta|y, m) \propto p(y, \theta|m) . \tag{1}$$

Proof: In a full probability model (\rightarrow Definition I/5.1.4), the posterior distribution (\rightarrow Definition I/5.1.7) can be expressed using Bayes' theorem (\rightarrow Proof I/5.3.1):

$$p(\theta|y, m) = \frac{p(y|\theta, m) p(\theta|m)}{p(y|m)} . \tag{2}$$

Applying the law of conditional probability (\rightarrow Definition I/1.3.4) to the numerator, we have:

$$p(\theta|y, m) = \frac{p(y, \theta|m)}{p(y|m)} . \tag{3}$$

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:

$$p(\theta|y, m) \propto p(y, \theta|m) . \quad (4)$$

Sources:

- original work

Metadata: ID: P90 | shortcut: post-jl | author: JoramSoch | date: 2020-05-05, 04:46.

5.1.9 Marginal likelihood

Definition: Let there be a generative model (\rightarrow Definition I/5.1.1) m describing measured data y using model parameters θ and a prior distribution (\rightarrow Definition I/5.1.3) on θ . Then, the marginal probability (\rightarrow Definition I/1.3.3) density function (\rightarrow Definition I/1.6.6) of y across the parameter space Θ is called the marginal likelihood:

$$p(y|m) = \int_{\Theta} p(y, \theta|m) d\theta . \quad (1)$$

Sources:

- original work

Metadata: ID: D33 | shortcut: ml | author: JoramSoch | date: 2020-03-03, 16:49.

5.1.10 Marginal likelihood is integral of joint likelihood

Theorem: In a full probability model (\rightarrow Definition I/5.1.4) m describing measured data y using model parameters θ , the marginal likelihood (\rightarrow Definition I/5.1.9) is the integral of the joint likelihood (\rightarrow Definition I/5.1.5) across the parameter space Θ

$$p(y|m) = \int_{\Theta} p(y, \theta|m) d\theta \quad (1)$$

and related to likelihood function (\rightarrow Definition I/5.1.2) and prior distribution (\rightarrow Definition I/5.1.7) 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 Definition I/5.1.4), the marginal likelihood (\rightarrow Definition I/5.1.9) is defined as the marginal probability (\rightarrow Definition I/1.3.3) of the data y , given only the model m :

$$p(y|m) . \quad (3)$$

Using the law of marginal probability (\rightarrow Definition I/1.3.3), this can be obtained by integrating the joint likelihood (\rightarrow Definition I/5.1.5) 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 Definition I/1.3.4), the integrand can also be written as the product of likelihood function (\rightarrow Definition I/5.1.2) and prior density (\rightarrow Definition I/5.1.3):

$$p(y|m) = \int_{\Theta} p(y|\theta, m) p(\theta|m) d\theta . \quad (5)$$

Sources:

- original work

Metadata: ID: P91 | shortcut: ml-jl | author: JoramSoch | date: 2020-05-05, 04:59.

5.2 Prior distributions

5.2.1 Flat vs. hard vs. soft

Definition: Let $p(\theta|m)$ be a prior distribution (\rightarrow Definition I/5.1.3) for the parameter θ of a generative model (\rightarrow Definition I/5.1.1) m . Then,

- the distribution is called a “flat prior”, if its precision (\rightarrow Definition I/1.8.12) is zero or variance (\rightarrow Definition I/1.8.1) is infinite;
- the distribution is called a “hard prior”, if its precision (\rightarrow Definition I/1.8.12) is infinite or variance (\rightarrow Definition I/1.8.1) is zero;
- the distribution is called a “soft prior”, if its precision (\rightarrow Definition I/1.8.12) and variance (\rightarrow Definition I/1.8.1) 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.

Metadata: ID: D116 | shortcut: prior-flat | author: JoramSoch | date: 2020-12-02, 17:04.

5.2.2 Uniform vs. non-uniform

Definition: Let $p(\theta|m)$ be a prior distribution (\rightarrow Definition I/5.1.3) for the parameter θ of a generative model (\rightarrow Definition 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 Definition I/1.6.6) or mass (\rightarrow Definition I/1.6.1) is constant over Θ ;
- the distribution is called a “non-uniform prior”, if its density (\rightarrow Definition I/1.6.6) or mass (\rightarrow Definition 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.

Metadata: ID: D117 | shortcut: prior-uni | author: JoramSoch | date: 2020-12-02, 17:21.

5.2.3 Informative vs. non-informative

Definition: Let $p(\theta|m)$ be a prior distribution (\rightarrow Definition I/5.1.3) for the parameter θ of a generative model (\rightarrow Definition 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 Proof I/5.1.8);
- the distribution is called a “non-informative prior”, if it does not influence (\rightarrow Proof I/5.1.8) the posterior hyperparameters (\rightarrow Definition I/5.1.7).

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.

Metadata: ID: D118 | shortcut: prior-inf | author: JoramSoch | date: 2020-12-02, 17:28.

5.2.4 Empirical vs. non-empirical

Definition: Let $p(\theta|m)$ be a prior distribution (\rightarrow Definition I/5.1.3) for the parameter θ of a generative model (\rightarrow Definition I/5.1.1) m . Then,

- the distribution is called an “empirical prior”, if it has been derived from empirical data (\rightarrow Proof I/5.1.8);
- 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.

Metadata: ID: D119 | shortcut: prior-emp | author: JoramSoch | date: 2020-12-02, 17:37.

5.2.5 Conjugate vs. non-conjugate

Definition: Let m be a generative model (\rightarrow Definition I/5.1.1) with likelihood function (\rightarrow Definition I/5.1.2) $p(y|\theta, m)$ and prior distribution (\rightarrow Definition I/5.1.3) $p(\theta|m)$. Then,

- the prior distribution (\rightarrow Definition I/5.1.3) is called “conjugate”, if it, when combined with the likelihood function (\rightarrow Definition I/5.1.2), leads to a posterior distribution (\rightarrow Definition I/5.1.7) that belongs to the same family of probability distributions (\rightarrow Definition 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.

Metadata: ID: D120 | shortcut: prior-conj | author: JoramSoch | date: 2020-12-02, 17:55.

5.2.6 Maximum entropy priors

Definition: Let m be a generative model (\rightarrow Definition I/5.1.1) with likelihood function (\rightarrow Definition I/5.1.2) $p(y|\theta, m)$ and prior distribution (\rightarrow Definition I/5.1.3) $p(\theta|\lambda, m)$ using prior hyperparameters (\rightarrow Definition 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 Definition I/1.2.6), it maximizes the entropy (\rightarrow Definition I/2.1.1) of the prior probability mass function (\rightarrow Definition 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 Definition I/1.2.6), it maximizes the differential entropy (\rightarrow Definition I/2.2.1) of the prior probability density function (\rightarrow Definition I/1.6.6):

$$\lambda_{\text{maxent}} = \arg \max_{\lambda} h[p(\theta|\lambda, m)] . \quad (2)$$

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.

Metadata: ID: D121 | shortcut: prior-maxent | author: JoramSoch | date: 2020-12-02, 18:13.

5.2.7 Empirical Bayes priors

Definition: Let m be a generative model (\rightarrow Definition I/5.1.1) with likelihood function (\rightarrow Definition I/5.1.2) $p(y|\theta, m)$ and prior distribution (\rightarrow Definition I/5.1.3) $p(\theta|\lambda, m)$ using prior hyperparameters (\rightarrow Definition I/5.1.3) λ . Let $p(y|\lambda, m)$ be the marginal likelihood (\rightarrow Definition I/5.1.9) when integrating the parameters out of the joint likelihood (\rightarrow Proof I/5.1.10). Then, the prior distribution is called an “Empirical Bayes (\rightarrow Definition I/5.3.3) 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.

Metadata: ID: D122 | shortcut: prior-eb | author: JoramSoch | date: 2020-12-02, 18:19.

5.2.8 Reference priors

Definition: Let m be a generative model (\rightarrow Definition I/5.1.1) with likelihood function (\rightarrow Definition I/5.1.2) $p(y|\theta, m)$ and prior distribution (\rightarrow Definition I/5.1.3) $p(\theta|\lambda, m)$ using prior hyperparameters (\rightarrow Definition I/5.1.3) λ . Let $p(\theta|y, \lambda, m)$ be the posterior distribution (\rightarrow Definition I/5.1.7) that is proportional to the joint likelihood (\rightarrow Proof I/5.1.8). Then, the prior distribution is called a “reference prior”, if it maximizes the expected (\rightarrow Definition I/1.7.1) Kullback-Leibler divergence (\rightarrow Definition 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.

Metadata: ID: D123 | shortcut: prior-ref | author: JoramSoch | date: 2020-12-02, 18:26.

5.3 Bayesian inference

5.3.1 Bayes’ theorem

Theorem: Let A and B be two arbitrary statements about random variables (\rightarrow Definition 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 Definition I/1.3.4) is defined as the ratio of joint probability (\rightarrow Definition I/1.3.2), i.e. the probability of both statements being true, and marginal probability (\rightarrow Definition 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.

Metadata: ID: P4 | shortcut: bayes-th | author: JoramSoch | date: 2019-09-27, 16:24.

5.3.2 Bayes’ rule

Theorem: Let A_1 , A_2 and B be arbitrary statements about random variables (\rightarrow Definition I/1.2.2) where A_1 and A_2 are mutually exclusive. Then, Bayes’ rule states that the posterior odds (\rightarrow Definition “post-odd”) are equal to the Bayes factor (\rightarrow Definition IV/3.3.1) times the prior odds (\rightarrow Definition “prior-odd”), 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 Proof I/5.3.1), the conditional probabilities (\rightarrow Definition 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.

Metadata: ID: P12 | shortcut: bayes-rule | author: JoramSoch | date: 2020-01-06, 20:55.

5.3.3 Empirical Bayes

Definition: Let m be a generative model (\rightarrow Definition I/5.1.1) with model parameters θ and hyper-parameters λ implying the likelihood function (\rightarrow Definition I/5.1.2) $p(y|\theta, \lambda, m)$ and prior distribution (\rightarrow Definition I/5.1.3) $p(\theta|\lambda, m)$. Then, an Empirical Bayes treatment of m , also referred to as “type II maximum likelihood (\rightarrow Definition I/4.1.3)” or “evidence (\rightarrow Definition IV/3.1.3) approximation”, consists in

1) evaluating the marginal likelihood (\rightarrow Definition I/5.1.9) 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 Definition 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 Definition I/5.1.3) at this maximum

$$p(\theta|m) = p(\theta|\hat{\lambda}, m) \quad (3)$$

for Bayesian inference (\rightarrow Proof I/5.3.1), i.e. obtaining the posterior distribution (\rightarrow Proof I/5.1.8) and computing the marginal likelihood (\rightarrow Proof I/5.1.10).

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>.

Metadata: ID: D149 | shortcut: eb | author: JoramSoch | date: 2021-04-29, 06:46.

5.3.4 Variational Bayes

Definition: Let m be a generative model (\rightarrow Definition I/5.1.1) with model parameters θ implying the likelihood function (\rightarrow Definition I/5.1.2) $p(y|\theta, m)$ and prior distribution (\rightarrow Definition 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 Definition I/5.1.7)

$$q(\theta) \approx p(\theta|y, m) , \quad (1)$$

2) evaluating the variational free energy (\rightarrow Definition IV/3.1.10)

$$F_q(m) = \int q(\theta) \log p(y|\theta, m) d\theta - \int q(\theta) \frac{q(\theta)}{p(\theta|m)} d\theta \quad (2)$$

3) and maximizing this function with respect to $q(\theta)$

$$\hat{q}(\theta) = \arg \max_q F_q(m) . \quad (3)$$

for Bayesian inference, i.e. obtaining the posterior distribution (from eq. (3)) and approximating the marginal likelihood (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.
- 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.

Metadata: ID: D150 | shortcut: vb | author: JoramSoch | date: 2021-04-29, 07:15.

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 Definition 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.

Metadata: ID: D88 | shortcut: duni | author: JoramSoch | date: 2020-07-28, 04:05.

1.1.2 Probability mass function

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a discrete uniform distribution (\rightarrow Definition II/1.1.1):

$$X \sim \mathcal{U}(a, b) . \quad (1)$$

Then, the probability mass function (\rightarrow Definition 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 Definition 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 Definition I/1.6.1) is

$$\sum_{x=a}^b f_X(x) = 1 , \quad (4)$$

we have

$$f_X(x) = \frac{1}{n} = \frac{1}{b - a + 1} . \quad (5)$$

Sources:

- original work

Metadata: ID: P140 | shortcut: duni-pmf | author: JoramSoch | date: 2020-07-28, 04:57.

1.1.3 Cumulative distribution function

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a discrete uniform distribution (\rightarrow Definition II/1.1.1):

$$X \sim \mathcal{U}(a, b) . \quad (1)$$

Then, the cumulative distribution function (\rightarrow Definition I/1.6.13) 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 Proof 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 Definition I/1.6.13) 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.

Sources:

- original work

Metadata: ID: P141 | shortcut: duni-cdf | author: JoramSoch | date: 2020-07-28, 05:34.

1.1.4 Quantile function

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a discrete uniform distribution (\rightarrow Definition II/1.1.1):

$$X \sim \mathcal{U}(a, b) . \quad (1)$$

Then, the quantile function (\rightarrow Definition I/1.6.23) 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 Proof 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 Definition I/1.6.23) $Q_X(p)$ 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 Proof II/1.1.3) multiples of $1/n$ with $n = b - a + 1$, the quantile function (\rightarrow Definition I/1.6.23) 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 Proof 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:

$$\begin{aligned} Q_X(p) &= a + p \cdot (b - a + 1) - 1 \\ &= a + pb - pa + p - 1 \\ &= a(1-p) + (b+1)p - 1 . \end{aligned} \quad (7)$$

Sources:

- original work

Metadata: ID: P142 | shortcut: duni-qf | author: JoramSoch | date: 2020-07-28, 06:17.

1.1.5 Shannon entropy

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a discrete uniform distribution (\rightarrow Definition II/1.1.1):

$$X \sim \mathcal{U}(a, b) . \quad (1)$$

Then, the (Shannon) entropy (\rightarrow Definition I/2.1.1) of X in nats is

$$H(X) = \ln(b - a + 1) . \quad (2)$$

Proof: The entropy (\rightarrow Definition 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 Proof II/1.1.2), we have:

$$\begin{aligned} H(X) &= - \sum_{x \in \mathcal{X}} p(x) \cdot \log_e p(x) \\ &= - \sum_{x=a}^b p(x) \cdot \ln p(x) \\ &= - \sum_{x=a}^b \frac{1}{b-a+1} \cdot \ln \frac{1}{b-a+1} \\ &= -(b-a+1) \cdot \frac{1}{b-a+1} \cdot \ln \frac{1}{b-a+1} \\ &= - \ln \frac{1}{b-a+1} \\ &= \ln(b-a+1) . \end{aligned} \quad (4)$$

Sources:

- original work

Metadata: ID: P410 | shortcut: duni-ent | author: JoramSoch | date: 2023-08-11, 13:13.

1.2 Bernoulli distribution

1.2.1 Definition

Definition: Let X be a random variable (\rightarrow Definition 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 Definition I/1.3.1) p and $X = 0$ with probability (\rightarrow Definition 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.

Metadata: ID: D44 | shortcut: bern | author: JoramSoch | date: 2020-03-22, 17:40.

1.2.2 Probability mass function

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a Bernoulli distribution (\rightarrow Definition II/1.2.1):

$$X \sim \text{Bern}(p) . \quad (1)$$

Then, the probability mass function (\rightarrow Definition 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 Definition II/1.2.1).

Sources:

- original work

Metadata: ID: P96 | shortcut: bern-pmf | author: JoramSoch | date: 2020-05-11, 22:10.

1.2.3 Mean

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a Bernoulli distribution (\rightarrow Definition II/1.2.1):

$$X \sim \text{Bern}(p) . \quad (1)$$

Then, the mean or expected value (\rightarrow Definition I/1.7.1) of X is

$$\mathbb{E}(X) = p . \quad (2)$$

Proof: The expected value (\rightarrow Definition I/1.7.1) is the probability-weighted average of all possible values:

$$\mathbb{E}(X) = \sum_{x \in \mathcal{X}} x \cdot \Pr(X = x) . \quad (3)$$

Since there are only two possible outcomes for a Bernoulli random variable (\rightarrow Proof II/1.2.2), we have:

$$\begin{aligned} E(X) &= 0 \cdot \Pr(X = 0) + 1 \cdot \Pr(X = 1) \\ &= 0 \cdot (1 - p) + 1 \cdot p \\ &= p . \end{aligned} \tag{4}$$

Sources:

- Wikipedia (2020): “Bernoulli distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-01-16; URL: https://en.wikipedia.org/wiki/Bernoulli_distribution#Mean.

Metadata: ID: P22 | shortcut: bern-mean | author: JoramSoch | date: 2020-01-16, 10:58.

1.2.4 Variance

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a Bernoulli distribution (\rightarrow Definition II/1.2.1):

$$X \sim \text{Bern}(p) . \tag{1}$$

Then, the variance (\rightarrow Definition I/1.7.1) of X is

$$\text{Var}(X) = p(1 - p) . \tag{2}$$

Proof: The variance (\rightarrow Definition I/1.8.1) is the probability-weighted average of the squared deviation from the expected value (\rightarrow Definition I/1.7.1) across all possible values

$$\text{Var}(X) = \sum_{x \in \mathcal{X}} (x - E(X))^2 \cdot \Pr(X = x) \tag{3}$$

and can also be written in terms of the expected values (\rightarrow Proof I/1.8.3):

$$\text{Var}(X) = E(X^2) - E(X)^2 . \tag{4}$$

The mean of a Bernoulli random variable (\rightarrow Proof II/1.2.3) is

$$X \sim \text{Bern}(p) \quad \Rightarrow \quad E(X) = p \tag{5}$$

and the mean of a squared Bernoulli random variable is

$$E(X^2) = 0^2 \cdot \Pr(X = 0) + 1^2 \cdot \Pr(X = 1) = 0 \cdot (1 - p) + 1 \cdot p = p . \tag{6}$$

Combining (4), (5) and (6), we have:

$$\text{Var}(X) = p - p^2 = p(1 - p) . \tag{7}$$

Sources:

- Wikipedia (2022): “Bernoulli distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-01-20; URL: https://en.wikipedia.org/wiki/Bernoulli_distribution#Variance.

Metadata: ID: P301 | shortcut: bern-var | author: JoramSoch | date: 2022-01-20, 15:06.

1.2.5 Range of variance

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a Bernoulli distribution (\rightarrow Definition II/1.2.1):

$$X \sim \text{Bern}(p) . \quad (1)$$

Then, the variance (\rightarrow Definition I/1.8.1) 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 Proof II/1.2.4) 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 Definition 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 Proof I/1.8.4), 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.

Metadata: ID: P303 | shortcut: bern-varrange | author: JoramSoch | date: 2022-01-27, 09:03.

1.2.6 Shannon entropy

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a Bernoulli distribution (\rightarrow Definition II/1.2.1):

$$X \sim \text{Bern}(p) . \quad (1)$$

Then, the (Shannon) entropy (\rightarrow Definition 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 Definition 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 Proof II/1.2.2), 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.

Metadata: ID: P334 | shortcut: bern-ent | author: JoramSoch | date: 2022-09-02, 12:21.

1.3 Binomial distribution

1.3.1 Definition

Definition: Let X be a random variable (\rightarrow Definition I/1.2.2). Then, X is said to follow a binomial distribution with number of trials n and success probability p

$$X \sim \text{Bin}(n, p) , \quad (1)$$

if X is the number of successes observed in n independent (\rightarrow Definition I/1.3.6) trials, where each trial has two possible outcomes (\rightarrow Definition 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.

Metadata: ID: D45 | shortcut: bin | author: JoramSoch | date: 2020-03-22, 17:52.

1.3.2 Probability mass function

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a binomial distribution (\rightarrow Definition II/1.3.1):

$$X \sim \text{Bin}(n, p) . \quad (1)$$

Then, the probability mass function (\rightarrow Definition 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 Definition II/1.3.1) is defined as the number of successes observed in n independent (\rightarrow Definition I/1.3.6) trials, where each trial has two possible outcomes (\rightarrow Definition II/1.2.1) (success/failure) and the probability (\rightarrow Definition 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.

Sources:

- original work

Metadata: ID: P97 | shortcut: bin-pmf | author: JoramSoch | date: 2020-05-11, 22:35.

1.3.3 Probability-generating function

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a binomial distribution (\rightarrow Definition II/1.3.1):

$$X \sim \text{Bin}(n, p) . \quad (1)$$

Then, the probability-generating function (\rightarrow Definition I/1.6.31) of X is

$$G_X(z) = (q + pz)^n \quad (2)$$

where $q = 1 - p$.

Proof: The probability-generating function (\rightarrow Definition I/1.6.31) of X is defined as

$$G_X(z) = \sum_{x=0}^{\infty} f_X(x) z^x \quad (3)$$

With the probability mass function of the binomial distribution (\rightarrow Proof II/1.3.2)

$$f_X(x) = \binom{n}{x} p^x (1 - p)^{n-x} , \quad (4)$$

we obtain:

$$\begin{aligned} G_X(z) &= \sum_{x=0}^n \binom{n}{x} p^x (1 - p)^{n-x} z^x \\ &= \sum_{x=0}^n \binom{n}{x} (pz)^x (1 - p)^{n-x} . \end{aligned} \quad (5)$$

According to the binomial theorem

$$(x + y)^n = \sum_{k=0}^n \binom{n}{k} x^{n-k} y^k , \quad (6)$$

the sum in equation (5) equals

$$G_X(z) = ((1 - p) + (pz))^n \quad (7)$$

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.

Metadata: ID: P363 | shortcut: bin-pgf | author: JoramSoch | date: 2022-10-11, 09:25.

1.3.4 Mean

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a binomial distribution (\rightarrow Definition II/1.3.1):

$$X \sim \text{Bin}(n, p) . \quad (1)$$

Then, the mean or expected value (\rightarrow Definition I/1.7.1) of X is

$$E(X) = np . \quad (2)$$

Proof: By definition, a binomial random variable (\rightarrow Definition II/1.3.1) is the sum of n independent and identical (\rightarrow Definition “iid”) Bernoulli trials (\rightarrow Definition 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 Proof I/1.7.5), 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 Proof II/1.2.3), 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.

Metadata: ID: P23 | shortcut: bin-mean | author: JoramSoch | date: 2020-01-16, 11:06.

1.3.5 Variance

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a binomial distribution (\rightarrow Definition II/1.3.1):

$$X \sim \text{Bin}(n, p) . \quad (1)$$

Then, the variance (\rightarrow Definition I/1.8.1) of X is

$$\text{Var}(X) = np(1 - p) . \quad (2)$$

Proof: By definition, a binomial random variable (\rightarrow Definition II/1.3.1) is the sum of n independent and identical (\rightarrow Definition “iid”) Bernoulli trials (\rightarrow Definition 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 Proof I/1.8.10), 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 Proof II/1.2.4), 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.

Metadata: ID: P302 | shortcut: bin-var | author: JoramSoch | date: 2022-01-20, 15:19.

1.3.6 Range of variance

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a binomial distribution (\rightarrow Definition II/1.3.1):

$$X \sim \text{Bin}(n, p) . \quad (1)$$

Then, the variance (\rightarrow Definition I/1.8.1) 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 Definition II/1.3.1) is the sum of n independent and identical (\rightarrow Definition “iid”) Bernoulli trials (\rightarrow Definition 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 Proof I/1.8.10), 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 Proof II/1.2.5)

$$0 \leq \text{Var}(X_i) \leq \frac{1}{4} \quad \text{for all } i = 1, \dots, n , \quad (5)$$

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:

$$\text{Var}(X) \in \left[0, \frac{n}{4}\right] . \quad (8)$$

Sources:

- original work

Metadata: ID: P304 | shortcut: bin-varrange | author: JoramSoch | date: 2022-01-27, 09:20.

1.3.7 Shannon entropy

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a binomial distribution (\rightarrow Definition II/1.3.1):

$$X \sim \text{Bin}(n, p) . \quad (1)$$

Then, the (Shannon) entropy (\rightarrow Definition 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 Proof II/1.2.6) 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 Definition I/1.7.1) of the logarithmized binomial coefficient (\rightarrow Proof II/1.3.2) with superset size n

$$E_{\text{lbc}}(n, p) = E \left[\log_2 \binom{n}{X} \right] \quad \text{where} \quad X \sim \text{Bin}(n, p) . \quad (4)$$

Proof: The entropy (\rightarrow Definition 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 Proof II/1.3.2), we have:

$$\begin{aligned}
H(X) &= - \sum_{x \in \mathcal{X}} f_X(x) \cdot \log_2 f_X(x) \\
&= - \sum_{x=0}^n \binom{n}{x} p^x (1-p)^{n-x} \cdot \log_2 \left[\binom{n}{x} p^x (1-p)^{n-x} \right] \\
&= - \sum_{x=0}^n \binom{n}{x} p^x (1-p)^{n-x} \cdot \left[\log_2 \binom{n}{x} + x \cdot \log_2 p + (n-x) \cdot \log_2(1-p) \right] \\
&= - \sum_{x=0}^n \binom{n}{x} p^x (1-p)^{n-x} \cdot \left[\log_2 \binom{n}{x} + x \cdot \log_2 p + n \cdot \log_2(1-p) - x \cdot \log_2(1-p) \right] .
\end{aligned} \tag{6}$$

Since the first factor in the sum corresponds to the probability mass (\rightarrow Definition I/1.6.1) of $X = x$, we can rewrite this as the sum of the expected values (\rightarrow Definition I/1.7.1) of the functions (\rightarrow Proof I/1.7.12) of the discrete random variable (\rightarrow Definition I/1.2.6) x in the square bracket:

$$\begin{aligned}
H(X) &= - \left\langle \log_2 \binom{n}{x} \right\rangle_{p(x)} - \langle x \cdot \log_2 p \rangle_{p(x)} - \langle n \cdot \log_2(1-p) \rangle_{p(x)} + \langle x \cdot \log_2(1-p) \rangle_{p(x)} \\
&= - \left\langle \log_2 \binom{n}{x} \right\rangle_{p(x)} - \log_2 p \cdot \langle x \rangle_{p(x)} - n \cdot \log_2(1-p) + \log_2(1-p) \cdot \langle x \rangle_{p(x)} .
\end{aligned} \tag{7}$$

Using the expected value of the binomial distribution (\rightarrow Proof II/1.3.4), i.e. $X \sim \text{Bin}(n, p) \Rightarrow \langle x \rangle = np$, this gives:

$$\begin{aligned}
H(X) &= - \left\langle \log_2 \binom{n}{x} \right\rangle_{p(x)} - np \cdot \log_2 p - n \cdot \log_2(1-p) + np \cdot \log_2(1-p) \\
&= - \left\langle \log_2 \binom{n}{x} \right\rangle_{p(x)} + n [-p \cdot \log_2 p - (1-p) \log_2(1-p)] .
\end{aligned} \tag{8}$$

Finally, we note that the first term is the negative expected value (\rightarrow Definition I/1.7.1) of the logarithm of a binomial coefficient (\rightarrow Proof II/1.3.2) and that the term in square brackets is the entropy of the Bernoulli distribution (\rightarrow Proof II/1.3.7), such that we finally get:

$$H(X) = n \cdot H_{\text{bern}}(p) - E_{\text{lbc}}(n, p) . \tag{9}$$

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 Proof I/2.1.2), it must hold that $n \geq E_{\text{lbc}}(n, p) \geq 0$.

Sources:

- original work

Metadata: ID: P335 | shortcut: bin-ent | author: JoramSoch | date: 2022-09-02, 13:52.

1.3.8 Conditional binomial

Theorem: Let X and Y be two random variables (\rightarrow Definition I/1.2.2) where Y is binomially distributed (\rightarrow Definition II/1.3.1) conditional on (\rightarrow Definition I/1.5.4) X

$$Y|X \sim \text{Bin}(X, q) \quad (1)$$

and X also follows a binomial distribution (\rightarrow Definition II/1.3.1), but with different success frequency (\rightarrow Definition II/1.3.1):

$$X \sim \text{Bin}(n, p) . \quad (2)$$

Then, the marginal distribution (\rightarrow Definition I/1.5.3) of Y unconditional on X is again a binomial distribution (\rightarrow Definition 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 Definition I/1.3.3) or the law of total probability (\rightarrow Proof I/1.4.7), 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 Proof II/1.3.2) 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 Proof II/1.3.2) 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.

Metadata: ID: P358 | shortcut: bin-margcond | author: JoramSoch | date: 2022-10-07, 21:03.

1.4 Beta-binomial distribution

1.4.1 Definition

Definition: Let p be a random variable (\rightarrow Definition I/1.2.2) following a beta distribution (\rightarrow Definition II/3.9.1)

$$p \sim \text{Bet}(\alpha, \beta) \quad (1)$$

and let X be a random variable (\rightarrow Definition I/1.2.2) following a binomial distribution (\rightarrow Definition II/1.3.1) conditional on p

$$X \mid p \sim \text{Bin}(n, p). \quad (2)$$

Then, the marginal distribution (\rightarrow Definition 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 Definition II/1.3.1) n and shape parameters (\rightarrow Definition 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.

Metadata: ID: D177 | shortcut: betabin | author: JoramSoch | date: 2022-10-20, 08:09.

1.4.2 Probability mass function

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a beta-binomial distribution (\rightarrow Definition II/1.4.1):

$$X \sim \text{BetBin}(n, \alpha, \beta) . \quad (1)$$

Then, the probability mass function (\rightarrow Definition 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 Definition II/1.4.1) is defined as a binomial variate (\rightarrow Definition II/1.3.1) for which the success probability is following a beta distribution (\rightarrow Definition 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 Definition I/1.3.3) and the law of conditional probability (\rightarrow Definition I/1.3.4) to derive the probability (\rightarrow Definition I/1.3.1) of X as

$$\begin{aligned} p(x) &= \int_{\mathcal{P}} p(x, p) \, dp \\ &= \int_{\mathcal{P}} p(x|p) p(p) \, dp . \end{aligned} \quad (4)$$

Now, we can plug in the probability mass function of the binomial distribution (\rightarrow Proof II/1.3.2) and the probability density function of the beta distribution (\rightarrow Proof II/3.9.3) 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 Proof II/3.9.3) and because probability density integrates to one (\rightarrow Definition I/1.6.6), 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.

Metadata: ID: P364 | shortcut: betabin-pmf | author: JoramSoch | date: 2022-10-20, 08:56.

1.4.3 Probability mass function in terms of gamma function

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a beta-binomial distribution (\rightarrow Definition II/1.4.1):

$$X \sim \text{BetBin}(n, \alpha, \beta) . \quad (1)$$

Then, the probability mass function (\rightarrow Definition 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 Proof 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.

Metadata: ID: P365 | shortcut: betabin-pmfitogf | author: JoramSoch | date: 2022-10-20, 08:56.

1.4.4 Cumulative distribution function

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a beta-binomial distribution (\rightarrow Definition II/1.4.1):

$$X \sim \text{BetBin}(n, \alpha, \beta) . \quad (1)$$

Then, the cumulative distribution function (\rightarrow Definition I/1.6.13) 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 Definition I/1.6.13) is defined as

$$F_X(x) = \Pr(X \leq x) \quad (3)$$

which, for a discrete random variable (\rightarrow Definition 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 Proof 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:

$$\begin{aligned}
F_X(x) &\stackrel{(6)}{=} \frac{1}{B(\alpha, \beta)} \cdot \sum_{i=0}^x \frac{n!}{i!(n-i)!} \cdot B(\alpha + i, \beta + n - i) \\
&\stackrel{(8)}{=} \frac{1}{B(\alpha, \beta)} \cdot \sum_{i=0}^x \frac{n!}{i!(n-i)!} \cdot \frac{\Gamma(\alpha + i) \cdot \Gamma(\beta + n - i)}{\Gamma(\alpha + \beta + n)} \\
&= \frac{1}{B(\alpha, \beta)} \cdot \frac{n!}{\Gamma(\alpha + \beta + n)} \cdot \sum_{i=0}^x \frac{\Gamma(\alpha + i) \cdot \Gamma(\beta + n - i)}{i!(n-i)!} \\
&\stackrel{(7)}{=} \frac{1}{B(\alpha, \beta)} \cdot \frac{\Gamma(n+1)}{\Gamma(\alpha + \beta + n)} \cdot \sum_{i=0}^x \frac{\Gamma(\alpha + i) \cdot \Gamma(\beta + n - i)}{\Gamma(i+1) \cdot \Gamma(n-i+1)} .
\end{aligned} \tag{9}$$

This completes the proof.

Sources:

- original work

Metadata: ID: P366 | shortcut: betabin-cdf | author: JoramSoch | date: 2022-10-22, 05:28.

1.5 Poisson distribution

1.5.1 Definition

Definition: Let X be a random variable (\rightarrow Definition I/1.2.2). Then, X is said to follow a Poisson distribution with rate λ

$$X \sim \text{Poiss}(\lambda) , \tag{1}$$

if and only if its probability mass function (\rightarrow Definition I/1.6.1) is given by

$$\text{Poiss}(x; \lambda) = \frac{\lambda^x e^{-\lambda}}{x!} \tag{2}$$

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.

Metadata: ID: D62 | shortcut: poiss | author: JoramSoch | date: 2020-05-25, 23:34.

1.5.2 Probability mass function

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a Poisson distribution (\rightarrow Definition II/1.5.1):

$$X \sim \text{Poiss}(\lambda) . \tag{1}$$

Then, the probability mass function (\rightarrow Definition 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 Definition II/1.5.1).

Sources:

- original work

Metadata: ID: P102 | shortcut: poiss-pmf | author: JoramSoch | date: 2020-05-14, 20:39.

1.5.3 Mean

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a Poisson distribution (\rightarrow Definition II/1.5.1):

$$X \sim \text{Pois}(\lambda). \quad (1)$$

Then, the mean or expected value (\rightarrow Definition I/1.7.1) of X is

$$\mathbb{E}(X) = \lambda. \quad (2)$$

Proof: The expected value of a discrete random variable (\rightarrow Definition I/1.7.1) 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 Proof II/1.5.2), we have:

$$\begin{aligned} \mathbb{E}(X) &= \sum_{x=0}^{\infty} x \cdot \frac{\lambda^x e^{-\lambda}}{x!} \\ &= \sum_{x=1}^{\infty} x \cdot \frac{\lambda^x e^{-\lambda}}{x!} \\ &= e^{-\lambda} \cdot \sum_{x=1}^{\infty} \frac{x}{x!} \lambda^x \\ &= \lambda e^{-\lambda} \cdot \sum_{x=1}^{\infty} \frac{\lambda^{x-1}}{(x-1)!}. \end{aligned} \quad (4)$$

Substituting $z = x - 1$, such that $x = z + 1$, we get:

$$\mathbb{E}(X) = \lambda e^{-\lambda} \cdot \sum_{z=0}^{\infty} \frac{\lambda^z}{z!}. \quad (5)$$

Using the power series expansion of the exponential function

$$e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!}, \quad (6)$$

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.

Metadata: ID: P151 | shortcut: poiss-mean | author: JoramSoch | date: 2020-08-19, 06:09.

1.5.4 Variance

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a Poisson distribution (\rightarrow Definition II/1.5.1):

$$X \sim \text{Poiss}(\lambda) . \tag{1}$$

Then, the variance (\rightarrow Definition I/1.8.1) of X is

$$\text{Var}(X) = \lambda . \tag{2}$$

Proof: The variance (\rightarrow Definition I/1.8.1) can be expressed in terms of expected values (\rightarrow Proof I/1.8.3) as

$$\text{Var}(X) = E(X^2) - E(X)^2 . \tag{3}$$

The expected value of a Poisson random variable (\rightarrow Proof II/1.5.3) is

$$E(X) = \lambda . \tag{4}$$

Let us now consider the expectation (\rightarrow Definition I/1.7.1) of $X(X-1)$ which is defined as

$$E[X(X-1)] = \sum_{x \in \mathcal{X}} x(x-1) \cdot f_X(x) , \tag{5}$$

such that, with the probability mass function of the Poisson distribution (\rightarrow Proof II/1.5.2), we have:

$$\begin{aligned} E[X(X-1)] &= \sum_{x=0}^{\infty} x(x-1) \cdot \frac{\lambda^x e^{-\lambda}}{x!} \\ &= \sum_{x=2}^{\infty} x(x-1) \cdot \frac{\lambda^x e^{-\lambda}}{x!} \\ &= e^{-\lambda} \cdot \sum_{x=2}^{\infty} x(x-1) \cdot \frac{\lambda^x}{x \cdot (x-1) \cdot (x-2)!} \\ &= \lambda^2 \cdot e^{-\lambda} \cdot \sum_{x=2}^{\infty} \frac{\lambda^{x-2}}{(x-2)!} . \end{aligned} \tag{6}$$

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.

Metadata: ID: P230 | shortcut: poiss-var | author: JoramSoch | date: 2021-04-29, 09:59.

2 Multivariate discrete distributions

2.1 Categorical distribution

2.1.1 Definition

Definition: Let X be a random vector (\rightarrow Definition I/1.2.3). Then, X is said to follow a categorical distribution with success probability p_1, \dots, p_k

$$X \sim \text{Cat}([p_1, \dots, p_k]) , \quad (1)$$

if $X = e_i$ with probability (\rightarrow Definition 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.

Metadata: ID: D46 | shortcut: cat | author: JoramSoch | date: 2020-03-22, 18:09.

2.1.2 Probability mass function

Theorem: Let X be a random vector (\rightarrow Definition I/1.2.3) following a categorical distribution (\rightarrow Definition II/2.1.1):

$$X \sim \text{Cat}([p_1, \dots, p_k]) . \quad (1)$$

Then, the probability mass function (\rightarrow Definition 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 Definition II/2.1.1).

Sources:

- original work

Metadata: ID: P98 | shortcut: cat-pmf | author: JoramSoch | date: 2020-05-11, 22:58.

2.1.3 Mean

Theorem: Let X be a random vector (\rightarrow Definition I/1.2.3) following a categorical distribution (\rightarrow Definition II/2.1.1):

$$X \sim \text{Cat}([p_1, \dots, p_k]) . \quad (1)$$

Then, the mean or expected value (\rightarrow Definition I/1.7.1) of X is

$$E(X) = [p_1, \dots, p_k] . \quad (2)$$

Proof: If we conceive the outcome of a categorical distribution (\rightarrow Definition 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 Definition I/1.7.1) is

$$\begin{aligned} E(X) &= \sum_{x \in \mathcal{X}} x \cdot \Pr(X = x) \\ &= \sum_{i=1}^k e_i \cdot \Pr(X = e_i) \\ &= \sum_{i=1}^k e_i \cdot p_i \\ &= [p_1, \dots, p_k] . \end{aligned} \quad (3)$$

Sources:

- original work

Metadata: ID: P24 | shortcut: cat-mean | author: JoramSoch | date: 2020-01-16, 11:17.

2.1.4 Covariance

Theorem: Let X be a random vector (\rightarrow Definition I/1.2.3) following a categorical distribution (\rightarrow Definition II/2.1.1):

$$X \sim \text{Cat}(n, p) . \quad (1)$$

Then, the covariance matrix (\rightarrow Definition I/1.10.9) of X is

$$\text{Cov}(X) = \text{diag}(p) - pp^T . \quad (2)$$

Proof: The categorical distribution (\rightarrow Definition II/2.1.1) is a special case of the multinomial distribution (\rightarrow Definition II/2.2.1) in which $n = 1$:

$$X \sim \text{Mult}(n, p) \quad \text{and} \quad n = 1 \quad \Rightarrow \quad X \sim \text{Cat}(p) . \quad (3)$$

The covariance matrix of the multinomial distribution (\rightarrow Proof II/2.2.4) is

$$\text{Cov}(X) = n (\text{diag}(p) - pp^T) , \quad (4)$$

thus the covariance matrix of the categorical distribution is

$$\text{Cov}(X) = \text{diag}(p) - pp^T . \quad (5)$$

Sources:

- original work

Metadata: ID: P338 | shortcut: cat-cov | author: JoramSoch | date: 2022-09-09, 16:57.

2.1.5 Shannon entropy

Theorem: Let X be a random vector (\rightarrow Definition I/1.2.3) following a categorical distribution (\rightarrow Definition II/2.1.1):

$$X \sim \text{Cat}(p) . \quad (1)$$

Then, the (Shannon) entropy (\rightarrow Definition I/2.1.1) of X is

$$H(X) = - \sum_{i=1}^k p_i \cdot \log p_i . \quad (2)$$

Proof: The entropy (\rightarrow Definition 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 Definition II/2.1.1) with probabilities given by the entries (\rightarrow Proof II/2.1.2) of the $1 \times k$ vector p , we have:

$$\begin{aligned} H(X) &= -\Pr(X = e_1) \cdot \log \Pr(X = e_1) - \dots - \Pr(X = e_k) \cdot \log \Pr(X = e_k) \\ H(X) &= - \sum_{i=1}^k \Pr(X = e_i) \cdot \log \Pr(X = e_i) \\ H(X) &= - \sum_{i=1}^k p_i \cdot \log p_i . \end{aligned} \quad (4)$$

Sources:

- original work

Metadata: ID: P336 | shortcut: cat-ent | author: JoramSoch | date: 2022-09-09, 15:41.

2.2 Multinomial distribution

2.2.1 Definition

Definition: Let X be a random vector (\rightarrow Definition 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 Definition I/1.3.6) trials, where each trial has k possible outcomes (\rightarrow Definition 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.

Metadata: ID: D47 | shortcut: mult | author: JoramSoch | date: 2020-03-22, 17:52.

2.2.2 Probability mass function

Theorem: Let X be a random vector (\rightarrow Definition I/1.2.3) following a multinomial distribution (\rightarrow Definition II/2.2.1):

$$X \sim \text{Mult}(n, [p_1, \dots, p_k]) . \quad (1)$$

Then, the probability mass function (\rightarrow Definition 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 Definition II/2.2.1) is defined as a vector of the numbers of observations belonging to k distinct categories in n independent (\rightarrow Definition I/1.3.6) trials, where each trial has k possible outcomes (\rightarrow Definition II/2.1.1) and the category probabilities (\rightarrow Definition I/1.3.1) are identical across trials.

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_k observations for category k . This number is equal to the number of possibilities in which x_1 category 1 objects, ..., x_k category k objects 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_k observations for category k , 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.

Sources:

- original work

Metadata: ID: P99 | shortcut: mult-pmf | author: JoramSoch | date: 2020-05-11, 23:30.

2.2.3 Mean

Theorem: Let X be a random vector (\rightarrow Definition I/1.2.3) following a multinomial distribution (\rightarrow Definition II/2.2.1):

$$X \sim \text{Mult}(n, [p_1, \dots, p_k]) . \quad (1)$$

Then, the mean or expected value (\rightarrow Definition I/1.7.1) of X is

$$\mathbb{E}(X) = [np_1, \dots, np_k] . \quad (2)$$

Proof: By definition, a multinomial random variable (\rightarrow Definition II/2.2.1) is the sum of n independent and identical categorical trials (\rightarrow Definition 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 Proof I/1.7.5), this is equal to

$$\begin{aligned} \mathbb{E}(X) &= \mathbb{E}(X_1) + \dots + \mathbb{E}(X_n) \\ &= \sum_{i=1}^n \mathbb{E}(X_i) . \end{aligned} \quad (4)$$

With the expected value of the categorical distribution (\rightarrow Proof II/2.1.3), we have:

$$\mathbb{E}(X) = \sum_{i=1}^n [p_1, \dots, p_k] = n \cdot [p_1, \dots, p_k] = [np_1, \dots, np_k] . \quad (5)$$

Sources:

- original work

Metadata: ID: P25 | shortcut: mult-mean | author: JoramSoch | date: 2020-01-16, 11:26.

2.2.4 Covariance

Theorem: Let X be a random vector (\rightarrow Definition I/1.2.3) following a multinomial distribution (\rightarrow Definition 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 Definition I/1.10.9) of X is

$$\text{Cov}(X) = n \left(\text{diag}(p) - pp^T \right) . \quad (2)$$

Proof: We first observe that the sample space (\rightarrow Definition 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 Definition 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 Proof II/1.3.5) $\text{Var}(X_i) = np_i(1 - p_i) = n(p_i - p_i^2)$, 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 Definition II/1.2.1) random variable with the expected value (\rightarrow Proof II/1.2.3) p_i . Then, we have

$$\begin{aligned} \text{Cov}(X_i, X_j) &= \text{Cov} \left(\sum_{k=1}^n \mathbb{I}_i(k), \sum_{l=1}^n \mathbb{I}_j(l) \right) \\ &= \sum_{k=1}^n \sum_{l=1}^n \text{Cov}(\mathbb{I}_i(k), \mathbb{I}_j(l)) \\ &= \sum_{k=1}^n \left[\text{Cov}(\mathbb{I}_i(k), \mathbb{I}_j(k)) + \underbrace{\sum_{\substack{l=1 \\ l \neq k}}^n \text{Cov}(\mathbb{I}_i(k), \mathbb{I}_j(l))}_{=0} \right] \\ &\stackrel{i \neq j}{=} \sum_{k=1}^n \left(\underbrace{\mathbb{E}(\mathbb{I}_i(k) \mathbb{I}_j(k))}_{=0} - \mathbb{E}(\mathbb{I}_i(k)) \mathbb{E}(\mathbb{I}_j(k)) \right) \\ &= - \sum_{k=1}^n \mathbb{E}(\mathbb{I}_i(k)) \mathbb{E}(\mathbb{I}_j(k)) \\ &= -np_i p_j, \end{aligned} \quad (5)$$

as desired.

Sources:

- Tutz (2012): “Regression for Categorical Data”, pp. 209ff..

Metadata: ID: P322 | shortcut: mult-cov | author: adkipnis | date: 2022-05-11, 16:40.

2.2.5 Shannon entropy

Theorem: Let X be a random vector (\rightarrow Definition I/1.2.3) following a multinomial distribution (\rightarrow Definition II/2.2.1):

$$X \sim \text{Mult}(n, p). \quad (1)$$

Then, the (Shannon) entropy (\rightarrow Definition I/2.1.1) of X is

$$H(X) = n \cdot H_{\text{cat}}(p) - E_{\text{lmc}}(n, p) \quad (2)$$

where $H_{\text{cat}}(p)$ is the categorical entropy function, i.e. the (Shannon) entropy of the categorical distribution (\rightarrow Proof II/2.1.5) with category probabilities p

$$H_{\text{cat}}(p) = - \sum_{i=1}^k p_i \cdot \log p_i \quad (3)$$

and $E_{\text{lmc}}(n, p)$ is the expected value (\rightarrow Definition I/1.7.1) of the logarithmized multinomial coefficient (\rightarrow Proof II/2.2.2) with superset size n

$$E_{\text{lmc}}(n, p) = E \left[\log \binom{n}{X_1, \dots, X_k} \right] \quad \text{where } X \sim \text{Mult}(n, p) . \quad (4)$$

Proof: The entropy (\rightarrow Definition 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 Proof 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 Definition I/1.6.1) of $X = x$, we can rewrite this as the sum of the expected values (\rightarrow Definition I/1.7.1) of the functions (\rightarrow Proof I/1.7.12) of the discrete random variable (\rightarrow Definition 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 Proof II/2.2.3), i.e. $X \sim \text{Mult}(n, p) \Rightarrow \langle x_i \rangle = np_i$, this gives:

$$\begin{aligned}
H(X) &= - \left\langle \log \binom{n}{x_1, \dots, x_k} \right\rangle_{p(x)} - \sum_{i=1}^k n p_i \cdot \log p_i \\
&= - \left\langle \log \binom{n}{x_1, \dots, x_k} \right\rangle_{p(x)} - n \sum_{i=1}^k p_i \cdot \log p_i .
\end{aligned} \tag{9}$$

Finally, we note that the first term is the negative expected value (\rightarrow Definition I/1.7.1) of the logarithm of a multinomial coefficient (\rightarrow Proof II/2.2.2) and that the second term is the entropy of the categorical distribution (\rightarrow Proof II/2.1.5), such that we finally get:

$$H(X) = n \cdot H_{\text{cat}}(p) - E_{\text{lmc}}(n, p) . \tag{10}$$

Sources:

- original work

Metadata: ID: P337 | shortcut: mult-ent | author: JoramSoch | date: 2022-09-09, 16:33.

3 Univariate continuous distributions

3.1 Continuous uniform distribution

3.1.1 Definition

Definition: Let X be a continuous random variable (\rightarrow Definition 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)).

Metadata: ID: D3 | shortcut: cuni | author: JoramSoch | date: 2020-01-27, 14:05.

3.1.2 Standard uniform distribution

Definition: Let X be a random variable (\rightarrow Definition I/1.2.2). Then, X is said to be standard uniformly distributed, if X follows a continuous uniform distribution (\rightarrow Definition 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.

Metadata: ID: D157 | shortcut: suni | author: JoramSoch | date: 2021-07-23, 17:32.

3.1.3 Probability density function

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a continuous uniform distribution (\rightarrow Definition II/3.1.1):

$$X \sim \mathcal{U}(a, b) . \quad (1)$$

Then, the probability density function (\rightarrow Definition I/1.6.6) 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 Definition 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 Definition I/1.6.6), 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:

$$\begin{aligned} \int_a^b 1 \, dx &= c(a, b) \\ [x]_a^b &= c(a, b) \\ c(a, b) &= b - a . \end{aligned} \quad (6)$$

Sources:

- original work

Metadata: ID: P37 | shortcut: cuni-pdf | author: JoramSoch | date: 2020-01-31, 15:41.

3.1.4 Cumulative distribution function

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a continuous uniform distribution (\rightarrow Definition II/3.1.1):

$$X \sim \mathcal{U}(a, b) . \quad (1)$$

Then, the cumulative distribution function (\rightarrow Definition I/1.6.13) 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 Proof 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 Definition I/1.6.13) 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)

$$\begin{aligned} F_X(x) &= \int_{-\infty}^a \mathcal{U}(z; a, b) \, dz + \int_a^x \mathcal{U}(z; a, b) \, dz \\ &= \int_{-\infty}^a 0 \, dz + \int_a^x \frac{1}{b-a} \, dz \\ &= 0 + \frac{1}{b-a} [z]_a^x \\ &= \frac{x-a}{b-a} . \end{aligned} \quad (6)$$

Finally, if $x > b$, we have

$$\begin{aligned} F_X(x) &= \int_{-\infty}^b \mathcal{U}(z; a, b) \, dz + \int_b^x \mathcal{U}(z; a, b) \, dz \\ &= F_X(b) + \int_b^x 0 \, dz \\ &= \frac{b-a}{b-a} + 0 \\ &= 1 . \end{aligned} \quad (7)$$

This completes the proof.

Sources:

- original work

Metadata: ID: P38 | shortcut: cuni-cdf | author: JoramSoch | date: 2020-01-02, 18:05.

3.1.5 Quantile function

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a continuous uniform distribution (\rightarrow Definition II/3.1.1):

$$X \sim \mathcal{U}(a, b) . \quad (1)$$

Then, the quantile function (\rightarrow Definition I/1.6.23) of X is

$$Q_X(p) = \begin{cases} -\infty , & \text{if } p = 0 \\ bp + a(1-p) , & \text{if } p > 0 . \end{cases} \quad (2)$$

Proof: The cumulative distribution function of the continuous uniform distribution (\rightarrow Proof II/3.1.4) is:

$$F_X(x) = \begin{cases} 0, & \text{if } x < a \\ \frac{x-a}{b-a}, & \text{if } a \leq x \leq b \\ 1, & \text{if } x > b. \end{cases} \quad (3)$$

The quantile function (\rightarrow Definition I/1.6.23) $Q_X(p)$ 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 Proof I/1.6.24)

$$Q_X(p) = F_X^{-1}(x) . \quad (5)$$

This can be derived by rearranging equation (3):

$$\begin{aligned} p &= \frac{x-a}{b-a} \\ x &= p(b-a) + a \\ x &= bp + a(1-p) . \end{aligned} \quad (6)$$

Sources:

- original work

Metadata: ID: P39 | shortcut: cuni-qf | author: JoramSoch | date: 2020-01-02, 18:27.

3.1.6 Mean

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a continuous uniform distribution (\rightarrow Definition II/3.1.1):

$$X \sim \mathcal{U}(a, b) . \quad (1)$$

Then, the mean or expected value (\rightarrow Definition I/1.7.1) of X is

$$\mathbb{E}(X) = \frac{1}{2}(a+b) . \quad (2)$$

Proof: The expected value (\rightarrow Definition I/1.7.1) 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 continuous uniform distribution (\rightarrow Proof II/3.1.3), this becomes:

$$\begin{aligned}
E(X) &= \int_a^b x \cdot \frac{1}{b-a} dx \\
&= \left[\frac{1}{2} \frac{x^2}{b-a} \right]_a^b \\
&= \frac{1}{2} \frac{b^2 - a^2}{b-a} \\
&= \frac{1}{2} \frac{(b+a)(b-a)}{b-a} \\
&= \frac{1}{2}(a+b) .
\end{aligned} \tag{4}$$

Sources:

- original work

Metadata: ID: P82 | shortcut: cuni-mean | author: JoramSoch | date: 2020-03-16, 16:12.

3.1.7 Median

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a continuous uniform distribution (\rightarrow Definition II/3.1.1):

$$X \sim \mathcal{U}(a, b) . \tag{1}$$

Then, the median (\rightarrow Definition I/1.12.1) of X is

$$\text{median}(X) = \frac{1}{2}(a+b) . \tag{2}$$

Proof: The median (\rightarrow Definition I/1.12.1) is the value at which the cumulative distribution function (\rightarrow Definition I/1.6.13) is $1/2$:

$$F_X(\text{median}(X)) = \frac{1}{2} . \tag{3}$$

The cumulative distribution function of the continuous uniform distribution (\rightarrow Proof II/3.1.4) is

$$F_X(x) = \begin{cases} 0 , & \text{if } x < a \\ \frac{x-a}{b-a} , & \text{if } a \leq x \leq b \\ 1 , & \text{if } x > b . \end{cases} \tag{4}$$

Thus, the inverse CDF (\rightarrow Proof II/3.1.5) is

$$x = bp + a(1-p) . \tag{5}$$

Setting $p = 1/2$, we obtain:

$$\text{median}(X) = b \cdot \frac{1}{2} + a \cdot \left(1 - \frac{1}{2}\right) = \frac{1}{2}(a+b) . \tag{6}$$

Sources:

- original work

Metadata: ID: P83 | shortcut: cuni-med | author: JoramSoch | date: 2020-03-16, 16:19.

3.1.8 Mode

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a continuous uniform distribution (\rightarrow Definition II/3.1.1):

$$X \sim \mathcal{U}(a, b) . \quad (1)$$

Then, the mode (\rightarrow Definition I/1.12.2) of X is

$$\text{mode}(X) \in [a, b] . \quad (2)$$

Proof: The mode (\rightarrow Definition I/1.12.2) is the value which maximizes the probability density function (\rightarrow Definition I/1.6.6):

$$\text{mode}(X) = \arg \max_x f_X(x) . \quad (3)$$

The probability density function of the continuous uniform distribution (\rightarrow Proof 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 .

Sources:

- original work

Metadata: ID: P84 | shortcut: cuni-med | author: JoramSoch | date: 2020-03-16, 16:29.

3.1.9 Variance

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a continuous uniform distribution (\rightarrow Definition II/3.1.1):

$$X \sim \mathcal{U}(a, b) . \quad (1)$$

Then, the variance (\rightarrow Definition I/1.8.1) of X is

$$\text{Var}(X) = \frac{1}{12}(b-a)^2 . \quad (2)$$

Proof: The variance (\rightarrow Definition I/1.8.1) is the probability-weighted average of the squared deviation from the mean (\rightarrow Definition I/1.7.1):

$$\text{Var}(X) = \int_{\mathbb{R}} (x - E(X))^2 \cdot f_X(x) dx . \quad (3)$$

With the expected value (\rightarrow Proof II/3.1.6) and probability density function (\rightarrow Proof II/3.1.3) of the continuous uniform distribution, this reads:

$$\begin{aligned} \text{Var}(X) &= \int_a^b \left(x - \frac{1}{2}(a+b) \right)^2 \cdot \frac{1}{b-a} dx \\ &= \frac{1}{b-a} \cdot \int_a^b \left(x - \frac{a+b}{2} \right)^2 dx \\ &= \frac{1}{b-a} \cdot \left[\frac{1}{3} \left(x - \frac{a+b}{2} \right)^3 \right]_a^b \\ &= \frac{1}{3(b-a)} \cdot \left[\left(\frac{2x - (a+b)}{2} \right)^3 \right]_a^b \\ &= \frac{1}{3(b-a)} \cdot \left[\frac{1}{8} (2x - a - b)^3 \right]_a^b \\ &= \frac{1}{24(b-a)} \cdot [(2x - a - b)^3]_a^b \\ &= \frac{1}{24(b-a)} \cdot [(2b - a - b)^3 - (2a - a - b)^3] \\ &= \frac{1}{24(b-a)} \cdot [(b-a)^3 - (a-b)^3] \\ &= \frac{1}{24(b-a)} \cdot [(b-a)^3 + (-1)^3(a-b)^3] \\ &= \frac{1}{24(b-a)} \cdot [(b-a)^3 + (b-a)^3] \\ &= \frac{2}{24(b-a)} (b-a)^3 \\ &= \frac{1}{12} (b-a)^2 . \end{aligned} \quad (4)$$

Sources:

- original work

Metadata: ID: P396 | shortcut: cuni-var | author: JoramSoch | date: 2022-12-20, 18:04.

3.1.10 Differential entropy

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a continuous uniform distribution (\rightarrow Definition II/3.1.1):

$$X \sim \mathcal{U}(a, b) . \quad (1)$$

Then, the differential entropy (\rightarrow Definition I/2.2.1) of X is

$$h(X) = \ln(b - a) . \quad (2)$$

Proof: The differential entropy (\rightarrow Definition 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

$$h(X) = - \int_{\mathcal{X}} p(x) \ln p(x) dx . \quad (4)$$

With the probability density function of the continuous uniform distribution (\rightarrow Proof II/3.1.3), the differential entropy of X is:

$$\begin{aligned} h(X) &= - \int_a^b \frac{1}{b-a} \ln \left(\frac{1}{b-a} \right) dx \\ &= \frac{1}{b-a} \cdot \int_a^b \ln(b-a) dx \\ &= \frac{1}{b-a} \cdot [x \cdot \ln(b-a)]_a^b \\ &= \frac{1}{b-a} \cdot [b \cdot \ln(b-a) - a \cdot \ln(b-a)] \\ &= \frac{1}{b-a} (b-a) \ln(b-a) \\ &= \ln(b-a) . \end{aligned} \quad (5)$$

Sources:

- original work

Metadata: ID: P397 | shortcut: cuni-dent | author: JoramSoch | date: 2022-12-20, 18:21.

3.2 Normal distribution

3.2.1 Definition

Definition: Let X be a random variable (\rightarrow Definition 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 Definition I/1.6.6) 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.

Metadata: ID: D4 | shortcut: norm | author: JoramSoch | date: 2020-01-27, 14:15.

3.2.2 Standard normal distribution

Definition: Let X be a random variable (\rightarrow Definition I/1.2.2). Then, X is said to be standard normally distributed, if X follows a normal distribution (\rightarrow Definition 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.

Metadata: ID: D63 | shortcut: snorm | author: JoramSoch | date: 2020-05-26, 23:32.

3.2.3 Relationship to standard normal distribution

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a normal distribution (\rightarrow Definition 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 Definition II/3.2.2) 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 Proof I/1.6.15) 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 Proof 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 Definition I/1.6.13) of the standard normal distribution (\rightarrow Definition II/3.2.2).

Sources:

- original work

Metadata: ID: P111 | shortcut: norm-snorm | author: JoramSoch | date: 2020-05-26, 23:01.

3.2.4 Relationship to standard normal distribution

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a normal distribution (\rightarrow Definition 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 Definition II/3.2.2) 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 Proof I/1.6.8) 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 Proof 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 Definition I/1.6.6) of the standard normal distribution (\rightarrow Definition II/3.2.2).

Sources:

- original work

Metadata: ID: P176 | shortcut: norm-snorm2 | author: JoramSoch | date: 2020-10-15, 11:42.

3.2.5 Relationship to standard normal distribution

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a normal distribution (\rightarrow Definition 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 Definition II/3.2.2) 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 Proof II/4.1.9) 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 Definition I/1.2.3) following a multivariate normal distribution (\rightarrow Definition 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:

$$Z \sim \mathcal{N}(0, 1) . \quad (6)$$

Sources:

- original work

Metadata: ID: P180 | shortcut: norm-snorm3 | author: JoramSoch | date: 2020-10-22, 06:34.

3.2.6 Relationship to chi-squared distribution

Theorem: Let X_1, \dots, X_n be independent (\rightarrow Definition I/1.3.6) random variables (\rightarrow Definition I/1.2.2) where each of them is following a normal distribution (\rightarrow Definition 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 Definition I/1.7.2)

$$\bar{X} = \frac{1}{n} \sum_{i=1}^n X_i \quad (2)$$

and the unbiased sample variance (\rightarrow Definition I/1.8.2)

$$s^2 = \frac{1}{n-1} \sum_{i=1}^n (X_i - \bar{X})^2 . \quad (3)$$

Then, the sampling distribution (\rightarrow Definition I/1.5.5) of the sample variance is given by a chi-squared distribution (\rightarrow Definition 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 Definition I/1.2.2) U_i defined as

$$U_i = \frac{X_i - \mu}{\sigma} \quad (5)$$

which follows a standard normal distribution (\rightarrow Proof II/3.2.3)

$$U_i \sim \mathcal{N}(0, 1) . \quad (6)$$

Then, the sum of squared random variables U_i can be rewritten as

$$\begin{aligned} \sum_{i=1}^n U_i^2 &= \sum_{i=1}^n \left(\frac{X_i - \mu}{\sigma} \right)^2 \\ &= \sum_{i=1}^n \left(\frac{(X_i - \bar{X}) + (\bar{X} - \mu)}{\sigma} \right)^2 \\ &= \sum_{i=1}^n \frac{(X_i - \bar{X})^2}{\sigma^2} + \sum_{i=1}^n \frac{(\bar{X} - \mu)^2}{\sigma^2} + 2 \sum_{i=1}^n \frac{(X_i - \bar{X})(\bar{X} - \mu)}{\sigma^2} \\ &= \sum_{i=1}^n \left(\frac{X_i - \bar{X}}{\sigma} \right)^2 + \sum_{i=1}^n \left(\frac{\bar{X} - \mu}{\sigma} \right)^2 + \frac{(\bar{X} - \mu)}{\sigma^2} \sum_{i=1}^n (X_i - \bar{X}) . \end{aligned} \quad (7)$$

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 (\rightarrow Proof "snorm-cochran") states that, if a sum of squared standard normal (\rightarrow Definition II/3.2.2) random variables (\rightarrow Definition 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 Definition I/1.3.6) and each term Q_j follows a chi-squared distribution (\rightarrow Definition 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

$$\begin{aligned} \sum_{i=1}^n U_i^2 &= \sum_{i=1}^n \left(\frac{X_i - \bar{X}}{\sigma^2} \right)^2 + \sum_{i=1}^n \left(\frac{\bar{X} - \mu}{\sigma^2} \right)^2 \\ &= Q_1 + Q_2 = \sum_{i=1}^n \left(U_i - \frac{1}{n} \sum_{j=1}^n U_j \right)^2 + \frac{1}{n} \left(\sum_{i=1}^n U_i \right)^2 \end{aligned} \quad (12)$$

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 (\rightarrow Proof “snorm-cochran”) are met and the squared form

$$Q_1 = \sum_{i=1}^n \left(\frac{X_i - \bar{X}}{\sigma^2} \right)^2 = (n-1) \frac{1}{\sigma^2} \frac{1}{n-1} \sum_{i=1}^n (X_i - \bar{X})^2 = (n-1) \frac{s^2}{\sigma^2} \quad (14)$$

follows a chi-squared distribution (\rightarrow Definition 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.

Metadata: ID: P233 | shortcut: norm-chi2 | author: JoramSoch | date: 2021-05-20, 10:18.

3.2.7 Relationship to t-distribution

Theorem: Let X_1, \dots, X_n be independent (\rightarrow Definition I/1.3.6) random variables (\rightarrow Definition I/1.2.2) where each of them is following a normal distribution (\rightarrow Definition II/3.2.1) with mean μ and variance σ^2 :

$$X_i \sim \mathcal{N}(\mu, \sigma^2) \quad \text{for} \quad i = 1, \dots, n . \quad (1)$$

Define the sample mean (\rightarrow Definition I/1.7.2)

$$\bar{X} = \frac{1}{n} \sum_{i=1}^n X_i \quad (2)$$

and the unbiased sample variance (\rightarrow Definition I/1.8.2)

$$s^2 = \frac{1}{n-1} \sum_{i=1}^n (X_i - \bar{X})^2 . \quad (3)$$

Then, subtracting μ from the sample mean (\rightarrow Definition I/1.7.1), dividing by the sample standard deviation (\rightarrow Definition I/1.13.1) and multiplying with \sqrt{n} results in a quantity that follows a t-distribution (\rightarrow Definition 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 Proof 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 Proof II/4.1.9) 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 Proof II/3.2.6) 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 Definition II/3.2.2) and the square root of a chi-squared random variable (\rightarrow Definition 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 Definition 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.

Metadata: ID: P234 | shortcut: norm-t | author: JoramSoch | date: 2021-05-27, 08:10.

3.2.8 Special case of multivariate normal distribution

Theorem: The normal distribution (\rightarrow Definition II/3.2.1) is a special case of the multivariate normal distribution (\rightarrow Definition II/4.1.1) with number of variables $n = 1$, i.e. random vector (\rightarrow Definition 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 Proof 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 Proof 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.

Metadata: ID: P331 | shortcut: norm-mvn | author: JoramSoch | date: 2022-08-19, 19:41.

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:

$$\begin{aligned} \int_0^{\frac{\pi}{2}} \int_0^{r_1} \exp[-r^2] r dr d\theta &\leq I_P^2 \leq \int_0^{\frac{\pi}{2}} \int_0^{r_2} \exp[-r^2] r dr d\theta \\ \int_0^{\frac{\pi}{2}} \left[-\frac{1}{2} \exp[-r^2] \right]_0^{r_1} d\theta &\leq I_P^2 \leq \int_0^{\frac{\pi}{2}} \left[-\frac{1}{2} \exp[-r^2] \right]_0^{r_2} d\theta \\ -\frac{1}{2} \int_0^{\frac{\pi}{2}} (\exp[-r_1^2] - 1) d\theta &\leq I_P^2 \leq -\frac{1}{2} \int_0^{\frac{\pi}{2}} (\exp[-r_2^2] - 1) d\theta \\ -\frac{1}{2} [(\exp[-r_1^2] - 1) \theta]_0^{\frac{\pi}{2}} &\leq I_P^2 \leq -\frac{1}{2} [(\exp[-r_2^2] - 1) \theta]_0^{\frac{\pi}{2}} \\ \frac{1}{2} (1 - \exp[-r_1^2]) \frac{\pi}{2} &\leq I_P^2 \leq \frac{1}{2} (1 - \exp[-r_2^2]) \frac{\pi}{2} \\ \frac{\pi}{4} (1 - \exp[-P^2]) &\leq I_P^2 \leq \frac{\pi}{4} (1 - \exp[-2P^2]) \end{aligned} \quad (9)$$

Calculating the limit for $P \rightarrow \infty$, we obtain

$$\lim_{P \rightarrow \infty} \frac{\pi}{4} (1 - \exp[-P^2]) \leq \lim_{P \rightarrow \infty} I_P^2 \leq \lim_{P \rightarrow \infty} \frac{\pi}{4} (1 - \exp[-2P^2])$$

$$\frac{\pi}{4} \leq I^2 \leq \frac{\pi}{4}, \quad (10)$$

such that we have a preliminary result for I :

$$I^2 = \frac{\pi}{4} \quad \Rightarrow \quad I = \frac{\sqrt{\pi}}{2}. \quad (11)$$

Because the integrand in (1) is an even function, we can calculate the final result as follows:

$$\int_{-\infty}^{+\infty} \exp[-x^2] \, dx = 2 \int_0^{\infty} \exp[-x^2] \, dx$$

$$\stackrel{(11)}{=} 2 \frac{\sqrt{\pi}}{2}$$

$$= \sqrt{\pi}. \quad (12)$$

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.

Metadata: ID: P196 | shortcut: norm-gi | author: JoramSoch | date: 2020-11-25, 04:47.

3.2.10 Probability density function

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a normal distribution (\rightarrow Definition II/3.2.1):

$$X \sim \mathcal{N}(\mu, \sigma^2). \quad (1)$$

Then, the probability density function (\rightarrow Definition I/1.6.6) 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 Definition II/3.2.1).

Sources:

- original work

Metadata: ID: P33 | shortcut: norm-pdf | author: JoramSoch | date: 2020-01-27, 15:15.

3.2.11 Moment-generating function

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a normal distribution (\rightarrow Definition II/3.2.1):

$$X \sim \mathcal{N}(\mu, \sigma^2) . \quad (1)$$

Then, the moment-generating function (\rightarrow Definition I/1.6.27) 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 Proof 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 Definition I/1.6.27) is defined as

$$M_X(t) = E [e^{tX}] . \quad (4)$$

Using the expected value for continuous random variables (\rightarrow Definition I/1.7.1), 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

$$\begin{aligned} M_X(t) &= \frac{1}{\sqrt{2\pi}\sigma} \int_{(-\infty - \mu)/(\sqrt{2}\sigma)}^{(+\infty - \mu)/(\sqrt{2}\sigma)} \exp \left[t \left(\sqrt{2}\sigma u + \mu \right) - \frac{1}{2} \left(\frac{\sqrt{2}\sigma u + \mu - \mu}{\sigma} \right)^2 \right] d \left(\sqrt{2}\sigma u + \mu \right) \\ &= \frac{\sqrt{2}\sigma}{\sqrt{2\pi}\sigma} \int_{-\infty}^{+\infty} \exp \left[\left(\sqrt{2}\sigma u + \mu \right) t - u^2 \right] du \\ &= \frac{\exp(\mu t)}{\sqrt{\pi}} \int_{-\infty}^{+\infty} \exp \left[\sqrt{2}\sigma u t - u^2 \right] du \\ &= \frac{\exp(\mu t)}{\sqrt{\pi}} \int_{-\infty}^{+\infty} \exp \left[- \left(u^2 - \sqrt{2}\sigma u t \right) \right] du \\ &= \frac{\exp(\mu t)}{\sqrt{\pi}} \int_{-\infty}^{+\infty} \exp \left[- \left(u - \frac{\sqrt{2}}{2} \sigma t \right)^2 + \frac{1}{2} \sigma^2 t^2 \right] du \\ &= \frac{\exp \left[\mu t + \frac{1}{2} \sigma^2 t^2 \right]}{\sqrt{\pi}} \int_{-\infty}^{+\infty} \exp \left[- \left(u - \frac{\sqrt{2}}{2} \sigma t \right)^2 \right] du \end{aligned} \quad (6)$$

Now substituting $v = u - \sqrt{2}/2 \sigma t$, i.e. $u = v + \sqrt{2}/2 \sigma t$, we have

$$\begin{aligned} M_X(t) &= \frac{\exp \left[\mu t + \frac{1}{2} \sigma^2 t^2 \right]}{\sqrt{\pi}} \int_{-\infty - \sqrt{2}/2 \sigma t}^{+\infty - \sqrt{2}/2 \sigma t} \exp \left[-v^2 \right] d \left(v + \sqrt{2}/2 \sigma t \right) \\ &= \frac{\exp \left[\mu t + \frac{1}{2} \sigma^2 t^2 \right]}{\sqrt{\pi}} \int_{-\infty}^{+\infty} \exp \left[-v^2 \right] dv . \end{aligned} \quad (7)$$

With the Gaussian integral (\rightarrow Proof II/3.2.9)

$$\int_{-\infty}^{+\infty} \exp \left[-x^2 \right] dx = \sqrt{\pi} , \quad (8)$$

this finally becomes

$$M_X(t) = \exp \left[\mu t + \frac{1}{2} \sigma^2 t^2 \right] . \quad (9)$$

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.

Metadata: ID: P71 | shortcut: norm-mgf | author: JoramSoch | date: 2020-03-03, 11:29.

3.2.12 Cumulative distribution function

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a normal distribution (\rightarrow Definition II/3.2.1):

$$X \sim \mathcal{N}(\mu, \sigma^2) . \quad (1)$$

Then, the cumulative distribution function (\rightarrow Definition I/1.6.13) 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 Proof 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 Definition I/1.6.13) is:

$$\begin{aligned}
F_X(x) &= \int_{-\infty}^x \mathcal{N}(z; \mu, \sigma^2) dz \\
&= \int_{-\infty}^x \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp \left[-\frac{1}{2} \left(\frac{z - \mu}{\sigma} \right)^2 \right] dz \\
&= \frac{1}{\sqrt{2\pi}\sigma} \int_{-\infty}^x \exp \left[-\left(\frac{z - \mu}{\sqrt{2}\sigma} \right)^2 \right] dz .
\end{aligned} \tag{5}$$

Substituting $t = (z - \mu)/(\sqrt{2}\sigma)$, i.e. $z = \sqrt{2}\sigma t + \mu$, this becomes:

$$\begin{aligned}
F_X(x) &= \frac{1}{\sqrt{2\pi}\sigma} \int_{(-\infty - \mu)/(\sqrt{2}\sigma)}^{(x - \mu)/(\sqrt{2}\sigma)} \exp(-t^2) d(\sqrt{2}\sigma t + \mu) \\
&= \frac{\sqrt{2}\sigma}{\sqrt{2\pi}\sigma} \int_{-\infty}^{\frac{x - \mu}{\sqrt{2}\sigma}} \exp(-t^2) dt \\
&= \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\frac{x - \mu}{\sqrt{2}\sigma}} \exp(-t^2) dt \\
&= \frac{1}{\sqrt{\pi}} \int_{-\infty}^0 \exp(-t^2) dt + \frac{1}{\sqrt{\pi}} \int_0^{\frac{x - \mu}{\sqrt{2}\sigma}} \exp(-t^2) dt \\
&= \frac{1}{\sqrt{\pi}} \int_0^{\infty} \exp(-t^2) dt + \frac{1}{\sqrt{\pi}} \int_0^{\frac{x - \mu}{\sqrt{2}\sigma}} \exp(-t^2) dt .
\end{aligned} \tag{6}$$

Applying (3) to (6), we have:

$$\begin{aligned}
F_X(x) &= \frac{1}{2} \lim_{x \rightarrow \infty} \operatorname{erf}(x) + \frac{1}{2} \operatorname{erf} \left(\frac{x - \mu}{\sqrt{2}\sigma} \right) \\
&= \frac{1}{2} + \frac{1}{2} \operatorname{erf} \left(\frac{x - \mu}{\sqrt{2}\sigma} \right) \\
&= \frac{1}{2} \left[1 + \operatorname{erf} \left(\frac{x - \mu}{\sqrt{2}\sigma} \right) \right] .
\end{aligned} \tag{7}$$

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.

Metadata: ID: P85 | shortcut: norm-cdf | author: JoramSoch | date: 2020-03-20, 01:33.

3.2.13 Cumulative distribution function without error function

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a normal distribution (\rightarrow Definition II/3.2.1):

$$X \sim \mathcal{N}(\mu, \sigma^2). \quad (1)$$

Then, the cumulative distribution function (\rightarrow Definition I/1.6.13) 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 Definition I/1.6.6) of the standard normal distribution (\rightarrow Definition II/3.2.2) and $n!!$ is a double factorial.

Proof:

1) First, consider the standard normal distribution (\rightarrow Definition II/3.2.2) $\mathcal{N}(0, 1)$ which has the probability density function (\rightarrow Proof 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

$$\begin{aligned}
T(x) &= \frac{1}{\sqrt{2\pi}} \cdot \sum_{i=1}^{\infty} \left(\frac{x^{2i-1}}{(2i-1)!!} \cdot e^{-\frac{1}{2}x^2} \right) + c \\
&= \frac{1}{\sqrt{2\pi}} \cdot e^{-\frac{1}{2}x^2} \cdot \sum_{i=1}^{\infty} \frac{x^{2i-1}}{(2i-1)!!} + c \\
&\stackrel{(3)}{=} \varphi(x) \cdot \sum_{i=1}^{\infty} \frac{x^{2i-1}}{(2i-1)!!} + c.
\end{aligned} \tag{6}$$

2) Next, let $\Phi(x)$ be the cumulative distribution function (\rightarrow Definition I/1.6.13) of the standard normal distribution (\rightarrow Definition II/3.2.2):

$$\Phi(x) = \int_{-\infty}^x \varphi(x) dx. \tag{7}$$

It can be obtained by matching $T(0)$ to $\Phi(0)$ which is $1/2$, because the standard normal distribution is symmetric around zero:

$$\begin{aligned}
T(0) &= \varphi(0) \cdot \sum_{i=1}^{\infty} \frac{0^{2i-1}}{(2i-1)!!} + c = \frac{1}{2} = \Phi(0) \\
&\Leftrightarrow c = \frac{1}{2} \\
\Rightarrow \Phi(x) &= \varphi(x) \cdot \sum_{i=1}^{\infty} \frac{x^{2i-1}}{(2i-1)!!} + \frac{1}{2}.
\end{aligned} \tag{8}$$

3) Finally, the cumulative distribution functions (\rightarrow Definition I/1.6.13) of the standard normal distribution (\rightarrow Definition II/3.2.2) and the general normal distribution (\rightarrow Definition II/3.2.1) are related to each other (\rightarrow Proof II/3.2.3) as

$$\Phi_{\mu,\sigma}(x) = \Phi\left(\frac{x-\mu}{\sigma}\right). \tag{9}$$

Combining (9) with (8), we have:

$$\Phi_{\mu,\sigma}(x) = \varphi\left(\frac{x-\mu}{\sigma}\right) \cdot \sum_{i=1}^{\infty} \frac{\left(\frac{x-\mu}{\sigma}\right)^{2i-1}}{(2i-1)!!} + \frac{1}{2}. \tag{10}$$

Sources:

- Soch J (2015): “Solution for the Indefinite Integral of the Standard Normal Probability Density Function”; in: *arXiv stat.OT*, arXiv: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.

Metadata: ID: P86 | shortcut: norm-cdfwerf | author: JoramSoch | date: 2020-03-20, 04:26.

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 Definition I/1.2.2) following a normal distribution (\rightarrow Definition II/3.2.1) with mean (\rightarrow Definition I/1.7.1) μ and variance (\rightarrow Definition I/1.8.1) σ^2 . Then, about 68%, 95% and 99.7% of the values of X will fall within 1, 2 and 3 standard deviations (\rightarrow Definition I/1.13.1) from the mean (\rightarrow Definition I/1.7.1), 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 Proof 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%9395%E2%80%9399.7_rule.

Metadata: ID: P321 | shortcut: norm-probstd | author: JoramSoch | date: 2022-05-08, 18:56.

3.2.15 Quantile function

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a normal distributions (\rightarrow Definition II/3.2.1):

$$X \sim \mathcal{N}(\mu, \sigma^2) . \quad (1)$$

Then, the quantile function (\rightarrow Definition I/1.6.23) 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 Proof 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 Proof I/1.6.24):

$$Q_X(p) = F_X^{-1}(x) . \quad (4)$$

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.

Metadata: ID: P87 | shortcut: norm-qf | author: JoramSoch | date: 2020-03-20, 04:47.

3.2.16 Mean

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a normal distribution (\rightarrow Definition II/3.2.1):

$$X \sim \mathcal{N}(\mu, \sigma^2) . \quad (1)$$

Then, the mean or expected value (\rightarrow Definition I/1.7.1) of X is

$$\mathbb{E}(X) = \mu . \quad (2)$$

Proof: The expected value (\rightarrow Definition I/1.7.1) 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 normal distribution (\rightarrow Proof II/3.2.10), this reads:

$$\begin{aligned} \mathbb{E}(X) &= \int_{-\infty}^{+\infty} x \cdot \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp \left[-\frac{1}{2} \left(\frac{x-\mu}{\sigma} \right)^2 \right] \, dx \\ &= \frac{1}{\sqrt{2\pi}\sigma} \int_{-\infty}^{+\infty} x \cdot \exp \left[-\frac{1}{2} \left(\frac{x-\mu}{\sigma} \right)^2 \right] \, dx . \end{aligned} \quad (4)$$

Substituting $z = x - \mu$, we have:

$$\begin{aligned} \mathbb{E}(X) &= \frac{1}{\sqrt{2\pi}\sigma} \int_{-\infty-\mu}^{+\infty-\mu} (z + \mu) \cdot \exp \left[-\frac{1}{2} \left(\frac{z}{\sigma} \right)^2 \right] \, d(z + \mu) \\ &= \frac{1}{\sqrt{2\pi}\sigma} \int_{-\infty}^{+\infty} (z + \mu) \cdot \exp \left[-\frac{1}{2} \left(\frac{z}{\sigma} \right)^2 \right] \, dz \\ &= \frac{1}{\sqrt{2\pi}\sigma} \left(\int_{-\infty}^{+\infty} z \cdot \exp \left[-\frac{1}{2} \left(\frac{z}{\sigma} \right)^2 \right] \, dz + \mu \int_{-\infty}^{+\infty} \exp \left[-\frac{1}{2} \left(\frac{z}{\sigma} \right)^2 \right] \, dz \right) \\ &= \frac{1}{\sqrt{2\pi}\sigma} \left(\int_{-\infty}^{+\infty} z \cdot \exp \left[-\frac{1}{2\sigma^2} \cdot z^2 \right] \, dz + \mu \int_{-\infty}^{+\infty} \exp \left[-\frac{1}{2\sigma^2} \cdot z^2 \right] \, dz \right) . \end{aligned} \quad (5)$$

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:

$$\begin{aligned}
E(X) &= \frac{1}{\sqrt{2\pi}\sigma} \left(\left[-\sigma^2 \cdot \exp \left[-\frac{1}{2\sigma^2} \cdot z^2 \right] \right]_{-\infty}^{+\infty} + \mu \left[\sqrt{\frac{\pi}{2}} \sigma \cdot \operatorname{erf} \left[\frac{1}{\sqrt{2}\sigma} z \right] \right]_{-\infty}^{+\infty} \right) \\
&= \frac{1}{\sqrt{2\pi}\sigma} \left(\left[\lim_{z \rightarrow \infty} \left(-\sigma^2 \cdot \exp \left[-\frac{1}{2\sigma^2} \cdot z^2 \right] \right) - \lim_{z \rightarrow -\infty} \left(-\sigma^2 \cdot \exp \left[-\frac{1}{2\sigma^2} \cdot z^2 \right] \right) \right] \right. \\
&\quad \left. + \mu \left[\lim_{z \rightarrow \infty} \left(\sqrt{\frac{\pi}{2}} \sigma \cdot \operatorname{erf} \left[\frac{1}{\sqrt{2}\sigma} z \right] \right) - \lim_{z \rightarrow -\infty} \left(\sqrt{\frac{\pi}{2}} \sigma \cdot \operatorname{erf} \left[\frac{1}{\sqrt{2}\sigma} z \right] \right) \right] \right) \\
&= \frac{1}{\sqrt{2\pi}\sigma} \left([0 - 0] + \mu \left[\sqrt{\frac{\pi}{2}} \sigma - \left(-\sqrt{\frac{\pi}{2}} \sigma \right) \right] \right) \\
&= \frac{1}{\sqrt{2\pi}\sigma} \cdot \mu \cdot 2\sqrt{\frac{\pi}{2}} \sigma \\
&= \mu .
\end{aligned} \tag{7}$$

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>.

Metadata: ID: P15 | shortcut: norm-mean | author: JoramSoch | date: 2020-01-09, 15:04.

3.2.17 Median

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a normal distribution (\rightarrow Definition II/3.2.1):

$$X \sim \mathcal{N}(\mu, \sigma^2) . \tag{1}$$

Then, the median (\rightarrow Definition I/1.12.1) of X is

$$\operatorname{median}(X) = \mu . \tag{2}$$

Proof: The median (\rightarrow Definition I/1.12.1) is the value at which the cumulative distribution function (\rightarrow Definition I/1.6.13) is $1/2$:

$$F_X(\operatorname{median}(X)) = \frac{1}{2} . \tag{3}$$

The cumulative distribution function of the normal distribution (\rightarrow Proof II/3.2.12) is

$$F_X(x) = \frac{1}{2} \left[1 + \operatorname{erf} \left(\frac{x - \mu}{\sqrt{2}\sigma} \right) \right] \tag{4}$$

where $\operatorname{erf}(x)$ is the error function. Thus, the inverse CDF is

$$x = \sqrt{2}\sigma \cdot \operatorname{erf}^{-1}(2p - 1) + \mu \tag{5}$$

where $\operatorname{erf}^{-1}(x)$ is the inverse error function. Setting $p = 1/2$, we obtain:

$$\text{median}(X) = \sqrt{2}\sigma \cdot \text{erf}^{-1}(0) + \mu = \mu . \quad (6)$$

Sources:

- original work

Metadata: ID: P16 | shortcut: norm-med | author: JoramSoch | date: 2020-01-09, 15:33.

3.2.18 Mode

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a normal distribution (\rightarrow Definition II/3.2.1):

$$X \sim \mathcal{N}(\mu, \sigma^2) . \quad (1)$$

Then, the mode (\rightarrow Definition I/1.12.2) of X is

$$\text{mode}(X) = \mu . \quad (2)$$

Proof: The mode (\rightarrow Definition I/1.12.2) is the value which maximizes the probability density function (\rightarrow Definition I/1.6.6):

$$\text{mode}(X) = \arg \max_x f_X(x) . \quad (3)$$

The probability density function of the normal distribution (\rightarrow Proof 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),

$$\begin{aligned}
f_X''(\mu) &= -\frac{1}{\sqrt{2\pi}\sigma^3} \cdot \exp(0) + \frac{1}{\sqrt{2\pi}\sigma^5} \cdot (0)^2 \cdot \exp(0) \\
&= -\frac{1}{\sqrt{2\pi}\sigma^3} < 0,
\end{aligned} \tag{8}$$

we confirm that it is in fact a maximum which shows that

$$\text{mode}(X) = \mu. \tag{9}$$

Sources:

- original work

Metadata: ID: P17 | shortcut: norm-mode | author: JoramSoch | date: 2020-01-09, 15:58.

3.2.19 Variance

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a normal distribution (\rightarrow Definition II/3.2.1):

$$X \sim \mathcal{N}(\mu, \sigma^2). \tag{1}$$

Then, the variance (\rightarrow Definition I/1.8.1) of X is

$$\text{Var}(X) = \sigma^2. \tag{2}$$

Proof: The variance (\rightarrow Definition I/1.8.1) is the probability-weighted average of the squared deviation from the mean (\rightarrow Definition I/1.7.1):

$$\text{Var}(X) = \int_{\mathbb{R}} (x - \text{E}(X))^2 \cdot f_X(x) dx. \tag{3}$$

With the expected value (\rightarrow Proof II/3.2.16) and probability density function (\rightarrow Proof II/3.2.10) of the normal distribution, this reads:

$$\begin{aligned}
\text{Var}(X) &= \int_{-\infty}^{+\infty} (x - \mu)^2 \cdot \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp \left[-\frac{1}{2} \left(\frac{x - \mu}{\sigma} \right)^2 \right] dx \\
&= \frac{1}{\sqrt{2\pi}\sigma} \int_{-\infty}^{+\infty} (x - \mu)^2 \cdot \exp \left[-\frac{1}{2} \left(\frac{x - \mu}{\sigma} \right)^2 \right] dx.
\end{aligned} \tag{4}$$

Substituting $z = x - \mu$, we have:

$$\begin{aligned}
\text{Var}(X) &= \frac{1}{\sqrt{2\pi}\sigma} \int_{-\infty-\mu}^{+\infty-\mu} z^2 \cdot \exp \left[-\frac{1}{2} \left(\frac{z}{\sigma} \right)^2 \right] d(z + \mu) \\
&= \frac{1}{\sqrt{2\pi}\sigma} \int_{-\infty}^{+\infty} z^2 \cdot \exp \left[-\frac{1}{2} \left(\frac{z}{\sigma} \right)^2 \right] dz.
\end{aligned} \tag{5}$$

Now substituting $z = \sqrt{2}\sigma x$, we have:

$$\begin{aligned}\text{Var}(X) &= \frac{1}{\sqrt{2\pi}\sigma} \int_{-\infty}^{+\infty} (\sqrt{2}\sigma x)^2 \cdot \exp \left[-\frac{1}{2} \left(\frac{\sqrt{2}\sigma x}{\sigma} \right)^2 \right] d(\sqrt{2}\sigma x) \\ &= \frac{1}{\sqrt{2\pi}\sigma} \cdot 2\sigma^2 \cdot \sqrt{2}\sigma \int_{-\infty}^{+\infty} x^2 \cdot \exp[-x^2] dx \\ &= \frac{2\sigma^2}{\sqrt{\pi}} \int_{-\infty}^{+\infty} x^2 \cdot e^{-x^2} dx .\end{aligned}\tag{6}$$

Since the integrand is symmetric with respect to $x = 0$, we can write:

$$\text{Var}(X) = \frac{4\sigma^2}{\sqrt{\pi}} \int_0^{\infty} x^2 \cdot e^{-x^2} dx .\tag{7}$$

If we define $z = x^2$, then $x = \sqrt{z}$ and $dx = 1/2 z^{-1/2} dz$. Substituting this into the integral

$$\text{Var}(X) = \frac{4\sigma^2}{\sqrt{\pi}} \int_0^{\infty} z \cdot e^{-z} \cdot \frac{1}{2} z^{-\frac{1}{2}} dz = \frac{2\sigma^2}{\sqrt{\pi}} \int_0^{\infty} z^{\frac{3}{2}-1} \cdot e^{-z} dz\tag{8}$$

and using the definition of the gamma function

$$\Gamma(x) = \int_0^{\infty} z^{x-1} \cdot e^{-z} dz ,\tag{9}$$

we can finally show that

$$\text{Var}(X) = \frac{2\sigma^2}{\sqrt{\pi}} \cdot \Gamma\left(\frac{3}{2}\right) = \frac{2\sigma^2}{\sqrt{\pi}} \cdot \frac{\sqrt{\pi}}{2} = \sigma^2 .\tag{10}$$

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>.

Metadata: ID: P18 | shortcut: norm-var | author: JoramSoch | date: 2020-01-09, 22:47.

3.2.20 Full width at half maximum

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a normal distribution (\rightarrow Definition II/3.2.1):

$$X \sim \mathcal{N}(\mu, \sigma^2) .\tag{1}$$

Then, the full width at half maximum (\rightarrow Definition I/1.13.2) (FWHM) of X is

$$\text{FWHM}(X) = 2\sqrt{2 \ln 2} \sigma .\tag{2}$$

Proof: The probability density function of the normal distribution (\rightarrow Proof 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 Proof 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 Definition I/1.13.2)

$$f_X(x_{\text{FWHM}}) = \frac{1}{2} f_{\max} \stackrel{(5)}{=} \frac{1}{2\sqrt{2\pi}\sigma}. \quad (6)$$

Using (3), we can develop this equation as follows:

$$\begin{aligned} \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp \left[-\frac{1}{2} \left(\frac{x_{\text{FWHM}} - \mu}{\sigma} \right)^2 \right] &= \frac{1}{2\sqrt{2\pi}\sigma} \\ \exp \left[-\frac{1}{2} \left(\frac{x_{\text{FWHM}} - \mu}{\sigma} \right)^2 \right] &= \frac{1}{2} \\ -\frac{1}{2} \left(\frac{x_{\text{FWHM}} - \mu}{\sigma} \right)^2 &= \ln \frac{1}{2} \\ \left(\frac{x_{\text{FWHM}} - \mu}{\sigma} \right)^2 &= -2 \ln \frac{1}{2} \\ \frac{x_{\text{FWHM}} - \mu}{\sigma} &= \pm \sqrt{2 \ln 2} \\ x_{\text{FWHM}} - \mu &= \pm \sqrt{2 \ln 2} \sigma \\ x_{\text{FWHM}} &= \pm \sqrt{2 \ln 2} \sigma + \mu. \end{aligned} \quad (7)$$

This implies the following two solutions for x_{FWHM}

$$\begin{aligned} x_1 &= \mu - \sqrt{2 \ln 2} \sigma \\ x_2 &= \mu + \sqrt{2 \ln 2} \sigma, \end{aligned} \quad (8)$$

such that the full width at half maximum (\rightarrow Definition I/1.13.2) of X is

$$\begin{aligned} \text{FWHM}(X) &= \Delta x = x_2 - x_1 \\ &\stackrel{(8)}{=} \left(\mu + \sqrt{2 \ln 2} \sigma \right) - \left(\mu - \sqrt{2 \ln 2} \sigma \right) \\ &= 2\sqrt{2 \ln 2} \sigma. \end{aligned} \quad (9)$$

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.

Metadata: ID: P152 | shortcut: norm-fwhm | author: JoramSoch | date: 2020-08-19, 06:39.

3.2.21 Extreme points

Theorem: The probability density function (\rightarrow Definition I/1.6.6) of the normal distribution (\rightarrow Definition 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 Definition II/3.2.1) is a unimodal probability distribution (\rightarrow Definition “dist-uni”).

Proof: The probability density function of the normal distribution (\rightarrow Proof 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 two derivatives of this function (\rightarrow Proof 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 Proof 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.

Metadata: ID: P251 | shortcut: norm-extr | author: JoramSoch | date: 2020-08-25, 21:11.

3.2.22 Inflection points

Theorem: The probability density function (\rightarrow Definition I/1.6.6) of the normal distribution (\rightarrow Definition 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 Definition I/1.13.1) away from the expected value (\rightarrow Definition I/1.7.1).

Proof: The probability density function of the normal distribution (\rightarrow Proof 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:

$$f'_X(x) = \frac{df_X(x)}{dx} = \frac{1}{\sqrt{2\pi}\sigma} \cdot \left(-\frac{x-\mu}{\sigma^2} \right) \cdot \exp \left[-\frac{1}{2} \left(\frac{x-\mu}{\sigma} \right)^2 \right] \quad (2)$$

$$\begin{aligned} f''_X(x) &= \frac{d^2 f_X(x)}{dx^2} = \frac{1}{\sqrt{2\pi}\sigma} \cdot \left(-\frac{1}{\sigma^2} \right) \cdot \exp \left[-\frac{1}{2} \left(\frac{x-\mu}{\sigma} \right)^2 \right] + \frac{1}{\sqrt{2\pi}\sigma} \cdot \left(\frac{x-\mu}{\sigma^2} \right)^2 \cdot \exp \left[-\frac{1}{2} \left(\frac{x-\mu}{\sigma} \right)^2 \right] \\ &= \frac{1}{\sqrt{2\pi}\sigma} \cdot \left[\left(\frac{x-\mu}{\sigma^2} \right)^2 - \frac{1}{\sigma^2} \right] \cdot \exp \left[-\frac{1}{2} \left(\frac{x-\mu}{\sigma} \right)^2 \right] \end{aligned} \quad (3)$$

$$\begin{aligned} f'''_X(x) &= \frac{d^3 f_X(x)}{dx^3} = \frac{1}{\sqrt{2\pi}\sigma} \cdot \left[\frac{2}{\sigma^2} \left(\frac{x-\mu}{\sigma^2} \right) \right] \cdot \exp \left[-\frac{1}{2} \left(\frac{x-\mu}{\sigma} \right)^2 \right] - \frac{1}{\sqrt{2\pi}\sigma} \cdot \left[\left(\frac{x-\mu}{\sigma^2} \right)^2 - \frac{1}{\sigma^2} \right] \cdot \left(\frac{x-\mu}{\sigma^2} \right) \cdot \exp \left[-\frac{1}{2} \left(\frac{x-\mu}{\sigma} \right)^2 \right] \\ &= \frac{1}{\sqrt{2\pi}\sigma} \cdot \left[-\left(\frac{x-\mu}{\sigma^2} \right)^3 + 3 \left(\frac{x-\mu}{\sigma^4} \right) \right] \cdot \exp \left[-\frac{1}{2} \left(\frac{x-\mu}{\sigma} \right)^2 \right]. \end{aligned} \quad (4)$$

The second derivative is zero, if and only if

$$\begin{aligned} 0 &= \left[\left(\frac{x-\mu}{\sigma^2} \right)^2 - \frac{1}{\sigma^2} \right] \\ 0 &= \frac{x^2}{\sigma^4} - \frac{2\mu x}{\sigma^4} + \frac{\mu^2}{\sigma^4} - \frac{1}{\sigma^2} \\ 0 &= x^2 - 2\mu x + (\mu^2 - \sigma^2) \\ x_{1/2} &= -\frac{-2\mu}{2} \pm \sqrt{\left(\frac{-2\mu}{2} \right)^2 - (\mu^2 - \sigma^2)} \\ x_{1/2} &= \mu \pm \sqrt{\mu^2 - \mu^2 + \sigma^2} \\ x_{1/2} &= \mu \pm \sigma. \end{aligned} \quad (5)$$

Since the third derivative is non-zero at this value

$$\begin{aligned} f'''_X(\mu \pm \sigma) &= \frac{1}{\sqrt{2\pi}\sigma} \cdot \left[-\left(\frac{\pm\sigma}{\sigma^2} \right)^3 + 3 \left(\frac{\pm\sigma}{\sigma^4} \right) \right] \cdot \exp \left[-\frac{1}{2} \left(\frac{\pm\sigma}{\sigma} \right)^2 \right] \\ &= \frac{1}{\sqrt{2\pi}\sigma} \cdot \left(\pm \frac{2}{\sigma^3} \right) \cdot \exp \left(-\frac{1}{2} \right) \neq 0, \end{aligned} \quad (6)$$

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 Definition II/3.2.1), these points are exactly one standard deviation (\rightarrow Definition I/1.13.1) 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.

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3.2.23 Differential entropy

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a normal distribution (\rightarrow Definition II/3.2.1):

$$X \sim \mathcal{N}(\mu, \sigma^2) . \quad (1)$$

Then, the differential entropy (\rightarrow Definition 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 Definition 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 Definition I/1.7.1)

$$h(X) = -\mathbb{E}[\ln p(x)] . \quad (4)$$

With the probability density function of the normal distribution (\rightarrow Proof II/3.2.10), the differential entropy of X is:

$$\begin{aligned} h(X) &= -\mathbb{E} \left[\ln \left(\frac{1}{\sqrt{2\pi}\sigma} \cdot \exp \left[-\frac{1}{2} \left(\frac{x-\mu}{\sigma} \right)^2 \right] \right) \right] \\ &= -\mathbb{E} \left[-\frac{1}{2} \ln(2\pi\sigma^2) - \frac{1}{2} \left(\frac{x-\mu}{\sigma} \right)^2 \right] \\ &= \frac{1}{2} \ln(2\pi\sigma^2) + \frac{1}{2} \mathbb{E} \left[\left(\frac{x-\mu}{\sigma} \right)^2 \right] \\ &= \frac{1}{2} \ln(2\pi\sigma^2) + \frac{1}{2} \cdot \frac{1}{\sigma^2} \cdot \mathbb{E}[(x-\mu)^2] \\ &= \frac{1}{2} \ln(2\pi\sigma^2) + \frac{1}{2} \cdot \frac{1}{\sigma^2} \cdot \sigma^2 \\ &= \frac{1}{2} \ln(2\pi\sigma^2) + \frac{1}{2} \\ &= \frac{1}{2} \ln(2\pi\sigma^2 e) . \end{aligned} \quad (5)$$

Sources:

- Wang, Peng-Hua (2012): “Differential Entropy”; in: *National Taipei University*; URL: <https://web.ntpu.edu.tw/~phwang/teaching/2012s/IT/slides/chap08.pdf>.

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3.2.24 Kullback-Leibler divergence

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2). Assume two normal distributions (\rightarrow Definition 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 Definition 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 Definition 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 Definition 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 Proof 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 Definition I/1.7.1) is a linear operator (\rightarrow Proof I/1.7.5), 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 Definition I/1.8.1)

$$\langle (X - \mu)^2 \rangle = \text{E}[(X - \text{E}(X))^2] = \text{Var}(X) \quad (7)$$

and the variance of a normally distributed random variable (\rightarrow Proof 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 Proof 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

$$\begin{aligned} \text{KL}[P \parallel Q] &= \frac{1}{2} \left[-\frac{\sigma_1^2}{\sigma_1^2} + \frac{\mu_1^2 + \sigma_1^2 - 2\mu_2\mu_1 + \mu_2^2}{\sigma_2^2} - \ln \frac{\sigma_1^2}{\sigma_2^2} \right] \\ &= \frac{1}{2} \left[\frac{\mu_1^2 - 2\mu_1\mu_2 + \mu_2^2}{\sigma_2^2} + \frac{\sigma_1^2}{\sigma_2^2} - \ln \frac{\sigma_1^2}{\sigma_2^2} - 1 \right] \\ &= \frac{1}{2} \left[\frac{(\mu_1 - \mu_2)^2}{\sigma_2^2} + \frac{\sigma_1^2}{\sigma_2^2} - \ln \frac{\sigma_1^2}{\sigma_2^2} - 1 \right] \end{aligned} \quad (10)$$

which is equivalent to (2).

Sources:

- original work

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3.2.25 Maximum entropy distribution

Theorem: The normal distribution (\rightarrow Definition II/3.2.1) maximizes differential entropy (\rightarrow Definition I/2.2.1) for a random variable (\rightarrow Definition I/1.2.2) with fixed variance (\rightarrow Definition I/1.8.1).

Proof: For a random variable (\rightarrow Definition I/1.2.2) X with set of possible values \mathcal{X} and probability density function (\rightarrow Definition I/1.6.6) $f(x)$, the differential entropy (\rightarrow Definition 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 Definition I/1.6.6) of a normal distribution (\rightarrow Definition II/3.2.1) with mean (\rightarrow Definition I/1.7.1) μ and variance (\rightarrow Definition I/1.8.1) σ^2 and

let $f(x)$ be an arbitrary probability density function (\rightarrow Definition I/1.6.6) with the same variance (\rightarrow Definition I/1.8.1). Since differential entropy (\rightarrow Definition I/2.2.1) is translation-invariant (\rightarrow Proof I/2.2.3), we can assume that $f(x)$ has the same mean as $g(x)$.

Consider the Kullback-Leibler divergence (\rightarrow Definition I/2.5.1) of distribution $f(x)$ from distribution $g(x)$ which is non-negative (\rightarrow Proof 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 normal distribution (\rightarrow Proof II/3.2.10) into the second term, we obtain:

$$\begin{aligned} \int_{\mathcal{X}} f(x) \log g(x) dx &= \int_{\mathcal{X}} f(x) \log \left(\frac{1}{\sqrt{2\pi}\sigma} \cdot \exp \left[-\frac{1}{2} \left(\frac{x-\mu}{\sigma} \right)^2 \right] \right) dx \\ &= \int_{\mathcal{X}} f(x) \log \left(\frac{1}{\sqrt{2\pi}\sigma^2} \right) dx + \int_{\mathcal{X}} f(x) \log \left(\exp \left[-\frac{(x-\mu)^2}{2\sigma^2} \right] \right) dx \\ &= -\frac{1}{2} \log(2\pi\sigma^2) \int_{\mathcal{X}} f(x) dx - \frac{\log(e)}{2\sigma^2} \int_{\mathcal{X}} f(x)(x-\mu)^2 dx . \end{aligned} \quad (3)$$

Because the entire integral over a probability density function is one (\rightarrow Definition I/1.6.6) and the second central moment is equal to the variance (\rightarrow Proof I/1.15.8), we have:

$$\begin{aligned} \int_{\mathcal{X}} f(x) \log g(x) dx &= -\frac{1}{2} \log(2\pi\sigma^2) - \frac{\log(e)\sigma^2}{2\sigma^2} \\ &= -\frac{1}{2} [\log(2\pi\sigma^2) + \log(e)] \\ &= -\frac{1}{2} \log(2\pi\sigma^2 e) . \end{aligned} \quad (4)$$

This is actually the negative of the differential entropy of the normal distribution (\rightarrow Proof II/3.2.23), such that:

$$\int_{\mathcal{X}} f(x) \log g(x) dx = -h[g(x)] . \quad (5)$$

Combining (2) with (5), we can show that

$$\begin{aligned} 0 &\leq \text{KL}[f||g] \\ 0 &\leq -h[f(x)] - (-h[g(x)]) \\ h[g(x)] &\geq h[f(x)] \end{aligned} \quad (6)$$

which means that the differential entropy (\rightarrow Definition I/2.2.1) of the normal distribution (\rightarrow Definition II/3.2.1) $\mathcal{N}(\mu, \sigma^2)$ will be larger than or equal to any other distribution (\rightarrow Definition I/1.5.1) with the same variance (\rightarrow Definition I/1.8.1) 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.

Metadata: ID: P250 | shortcut: norm-maxent | author: JoramSoch | date: 2020-08-25, 08:31.

3.2.26 Linear combination

Theorem: Let X_1, \dots, X_n be independent (\rightarrow Definition I/1.3.6) normally distributed (\rightarrow Definition II/3.2.1) random variables (\rightarrow Definition I/1.2.2) with means (\rightarrow Definition I/1.7.1) μ_1, \dots, μ_n and variances (\rightarrow Definition I/1.8.1) $\sigma_1^2, \dots, \sigma_n^2$:

$$X_i \sim \mathcal{N}(\mu_i, \sigma_i^2) \quad \text{for } i = 1, \dots, n. \quad (1)$$

Then, any linear combination of those random variables

$$Y = \sum_{i=1}^n a_i X_i \quad \text{where } a_1, \dots, a_n \in \mathbb{R} \quad (2)$$

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 Proof II/4.1.12) to an $n \times 1$ random vector (\rightarrow Definition I/1.2.3) x following a multivariate normal distribution (\rightarrow Definition II/4.1.1) with a diagonal covariance matrix (\rightarrow Definition I/1.10.9). Therefore, we can write

$$X_i \sim \mathcal{N}(\mu_i, \sigma_i^2), i = 1, \dots, n \quad \Rightarrow \quad x = \begin{bmatrix} X_1 \\ \vdots \\ X_n \end{bmatrix} \sim \mathcal{N}(\mu, \Sigma) \quad (4)$$

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 Proof II/4.1.9)

$$x \sim \mathcal{N}(\mu, \Sigma) \quad \Rightarrow \quad y = Ax + b \sim \mathcal{N}(A\mu + b, A\Sigma A^T) \quad (6)$$

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 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

$$\begin{aligned} A\mu &= [a_1, \dots, a_n] \begin{bmatrix} \mu_1 \\ \vdots \\ \mu_n \end{bmatrix} = \sum_{i=1}^n a_i \mu_i \quad \text{and} \\ A\Sigma A^T &= [a_1, \dots, a_n] \begin{bmatrix} \sigma_1^2 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \sigma_n^2 \end{bmatrix} \begin{bmatrix} a_1 \\ \vdots \\ a_n \end{bmatrix} = \sum_{i=1}^n a_i^2 \sigma_i^2 . \end{aligned} \quad (9)$$

Sources:

- original work

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3.3 t-distribution

3.3.1 Definition

Definition: Let Z and V be independent (\rightarrow Definition I/1.3.6) random variables (\rightarrow Definition I/1.2.2) following a standard normal distribution (\rightarrow Definition II/3.2.2) and a chi-squared distribution (\rightarrow Definition II/3.7.1) with ν degrees of freedom (\rightarrow Definition “dof”), 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.

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3.3.2 Non-standardized t-distribution

Definition: Let X be a random variable (\rightarrow Definition I/1.2.2) following a Student's t-distribution (\rightarrow Definition II/3.3.1) with ν degrees of freedom. Then, the random variable (\rightarrow Definition I/1.2.2)

$$Y = \sigma X + \mu \quad (1)$$

is said to follow a non-standardized t-distribution with non-centrality μ , scale σ^2 and degrees of freedom ν :

$$Y \sim \text{nst}(\mu, \sigma^2, \nu) . \quad (2)$$

Sources:

- Wikipedia (2021): “Student's t-distribution”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-05-20; URL: https://en.wikipedia.org/wiki/Student%27s_t-distribution#Generalized_Student's_t-distribution.

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3.3.3 Relationship to non-standardized t-distribution

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a non-standardized t-distribution (\rightarrow Definition II/3.3.2) with mean μ , scale σ^2 and degrees of freedom ν :

$$X \sim \text{nst}(\mu, \sigma^2, \nu) . \quad (1)$$

Then, subtracting the mean and dividing by the square root of the scale results in a random variable (\rightarrow Definition I/1.2.2) following a t-distribution (\rightarrow Definition II/3.3.1) with degrees of freedom ν :

$$Y = \frac{X - \mu}{\sigma} \sim t(\nu) . \quad (2)$$

Proof: The non-standardized t-distribution is a special case (\rightarrow Proof “nst-mvt”) of the multivariate t-distribution (\rightarrow Definition II/4.2.1) in which the mean vector and scale matrix are scalars:

$$X \sim \text{nst}(\mu, \sigma^2, \nu) \quad \Rightarrow \quad X \sim t(\mu, \sigma^2, \nu) . \quad (3)$$

Therefore, we can apply the linear transformation theorem for the multivariate t-distribution (\rightarrow Proof “mvt-ltt”) for an $n \times 1$ random vector x :

$$x \sim t(\mu, \Sigma, \nu) \quad \Rightarrow \quad y = Ax + b \sim t(A\mu + b, A\Sigma A^T, \nu) . \quad (4)$$

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 Proof II/4.2.2),

$$p(x) = \sqrt{\frac{1}{(\nu\pi)^n|\Sigma|}} \frac{\Gamma([\nu+n]/2)}{\Gamma(\nu/2)} \left[1 + \frac{1}{\nu}(x - \mu)^T \Sigma^{-1}(x - \mu) \right], \quad (6)$$

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 Proof II/3.3.5) with ν degrees of freedom.

Sources:

- original work

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3.3.4 Special case of multivariate t-distribution

Theorem: The t-distribution (\rightarrow Definition II/3.3.1) is a special case of the multivariate t-distribution (\rightarrow Definition II/4.2.1) with number of variables $n = 1$, i.e. random vector (\rightarrow Definition 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 Proof II/4.2.2) 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

$$\begin{aligned} t(x; 0, 1, \nu) &= \sqrt{\frac{1}{(\nu\pi)^1|1|}} \frac{\Gamma([\nu+1]/2)}{\Gamma(\nu/2)} \left[1 + \frac{1}{\nu}(x - 0)^T 1^{-1}(x - 0) \right]^{-(\nu+1)/2} \\ &= \sqrt{\frac{1}{\nu\pi}} \frac{\Gamma([\nu+1]/2)}{\Gamma(\nu/2)} \left[1 + \frac{x^2}{\nu} \right]^{-(\nu+1)/2} \\ &= \frac{1}{\sqrt{\nu\pi}} \cdot \frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu}{2})} \cdot \left[1 + \frac{x^2}{\nu} \right]^{-\frac{\nu+1}{2}}. \end{aligned} \quad (2)$$

which is equivalent to the probability density function of the t-distribution (\rightarrow Proof 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.

Metadata: ID: P332 | shortcut: t-mvt | author: JoramSoch | date: 2022-08-25, 12:38.

3.3.5 Probability density function

Theorem: Let T be a random variable (\rightarrow Definition I/1.2.2) following a t-distribution (\rightarrow Definition II/3.3.1):

$$T \sim t(\nu) . \quad (1)$$

Then, the probability density function (\rightarrow Definition I/1.6.6) 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 Definition II/3.3.1) is defined as the ratio of a standard normal random variable (\rightarrow Definition II/3.2.2) and the square root of a chi-squared random variable (\rightarrow Definition II/3.7.1), divided by its degrees of freedom (\rightarrow Definition “dof”)

$$X \sim \mathcal{N}(0, 1), Y \sim \chi^2(\nu) \quad \Rightarrow \quad T = \frac{X}{\sqrt{Y/\nu}} \sim t(\nu) \quad (3)$$

where X and Y are independent of each other (\rightarrow Definition I/1.3.6).

The probability density function (\rightarrow Proof II/3.2.10) of the standard normal distribution (\rightarrow Definition II/3.2.2) 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 Proof II/3.7.3) 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:

$$\begin{aligned} J &= \begin{bmatrix} \frac{dX}{dT} & \frac{dX}{dW} \\ \frac{dY}{dT} & \frac{dY}{dW} \end{bmatrix} = \begin{bmatrix} \sqrt{\frac{W}{\nu}} & \frac{T}{2\sqrt{W/\nu}} \\ 0 & 1 \end{bmatrix} \\ |J| &= \sqrt{\frac{W}{\nu}} . \end{aligned} \quad (8)$$

Because X and Y are independent (\rightarrow Definition I/1.3.6), the joint density (\rightarrow Definition I/1.5.2) of X and Y is equal to the product (\rightarrow Proof I/1.3.8) of the marginal densities (\rightarrow Definition 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 Proof I/1.6.10), the joint density (\rightarrow Definition 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:

$$\begin{aligned} f_{T,W}(t, w) &= f_X \left(t \cdot \sqrt{\frac{w}{\nu}} \right) \cdot f_Y(w) \cdot |J| \\ &= \frac{1}{\sqrt{2\pi}} \cdot e^{-\frac{(t \cdot \sqrt{\frac{w}{\nu}})^2}{2}} \cdot \frac{1}{\Gamma\left(\frac{\nu}{2}\right) \cdot 2^{\nu/2}} \cdot w^{\frac{\nu}{2}-1} \cdot e^{-\frac{w}{2}} \cdot \sqrt{\frac{w}{\nu}} \\ &= \frac{1}{\sqrt{2\pi\nu} \cdot \Gamma\left(\frac{\nu}{2}\right) \cdot 2^{\nu/2}} \cdot w^{\frac{\nu+1}{2}-1} \cdot e^{-\frac{w}{2} \left(\frac{t^2}{\nu} + 1 \right)} . \end{aligned} \quad (11)$$

The marginal density (\rightarrow Definition I/1.5.3) of T can now be obtained by integrating out (\rightarrow Definition I/1.3.3) W :

$$\begin{aligned} f_T(t) &= \int_0^\infty f_{T,W}(t, w) \, dw \\ &= \frac{1}{\sqrt{2\pi\nu} \cdot \Gamma\left(\frac{\nu}{2}\right) \cdot 2^{\nu/2}} \cdot \int_0^\infty w^{\frac{\nu+1}{2}-1} \cdot \exp \left[-\frac{1}{2} \left(\frac{t^2}{\nu} + 1 \right) w \right] \, dw \\ &= \frac{1}{\sqrt{2\pi\nu} \cdot \Gamma\left(\frac{\nu}{2}\right) \cdot 2^{\nu/2}} \cdot \frac{\Gamma\left(\frac{\nu+1}{2}\right)}{\left[\frac{1}{2} \left(\frac{t^2}{\nu} + 1 \right) \right]^{(\nu+1)/2}} \cdot \int_0^\infty \frac{\left[\frac{1}{2} \left(\frac{t^2}{\nu} + 1 \right) \right]^{(\nu+1)/2}}{\Gamma\left(\frac{\nu+1}{2}\right)} \cdot w^{\frac{\nu+1}{2}-1} \cdot \exp \left[-\frac{1}{2} \left(\frac{t^2}{\nu} + 1 \right) w \right] \, dw \end{aligned} \quad (12)$$

At this point, we can recognize that the integrand is equal to the probability density function of a gamma distribution (\rightarrow Proof II/3.4.6) with

$$a = \frac{\nu+1}{2} \quad \text{and} \quad b = \frac{1}{2} \left(\frac{t^2}{\nu} + 1 \right) , \quad (13)$$

and because a probability density function integrates to one (\rightarrow Definition I/1.6.6), we finally have:

$$\begin{aligned} f_T(t) &= \frac{1}{\sqrt{2\pi\nu} \cdot \Gamma\left(\frac{\nu}{2}\right) \cdot 2^{\nu/2}} \cdot \frac{\Gamma\left(\frac{\nu+1}{2}\right)}{\left[\frac{1}{2} \left(\frac{t^2}{\nu} + 1 \right) \right]^{(\nu+1)/2}} \\ &= \frac{\Gamma\left(\frac{\nu+1}{2}\right)}{\Gamma\left(\frac{\nu}{2}\right) \cdot \sqrt{\nu\pi}} \cdot \left(\frac{t^2}{\nu} + 1 \right)^{-\frac{\nu+1}{2}} . \end{aligned} \quad (14)$$

Sources:

- Computation Empire (2021): “Student’s t Distribution: Derivation of PDF”; in: *YouTube*, retrieved on 2021-10-11; URL: <https://www.youtube.com/watch?v=6BraaGEVRY8>.

Metadata: ID: P263 | shortcut: t-pdf | author: JoramSoch | date: 2021-10-12, 08:15.

3.4 Gamma distribution

3.4.1 Definition

Definition: Let X be a random variable (\rightarrow Definition I/1.2.2). Then, X is said to follow a gamma distribution with shape a and rate b

$$X \sim \text{Gam}(a, b) , \quad (1)$$

if and only if its probability density function (\rightarrow Definition I/1.6.6) is given by

$$\text{Gam}(x; a, b) = \frac{b^a}{\Gamma(a)} x^{a-1} \exp[-bx], \quad x > 0 \quad (2)$$

where $a > 0$ and $b > 0$, 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.

Metadata: ID: D7 | shortcut: gam | author: JoramSoch | date: 2020-02-08, 23:29.

3.4.2 Standard gamma distribution

Definition: Let X be a random variable (\rightarrow Definition I/1.2.2). Then, X is said to have a standard gamma distribution, if X follows a gamma distribution (\rightarrow Definition 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

Metadata: ID: D64 | shortcut: sgam | author: JoramSoch | date: 2020-05-26, 23:36.

3.4.3 Relationship to standard gamma distribution

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a gamma distribution (\rightarrow Definition 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 Definition II/3.4.2) 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 is positive, $g(X)$ is strictly increasing and we can calculate the cumulative distribution function of a strictly increasing function (\rightarrow Proof I/1.6.15) 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 Proof II/3.4.7) 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 Definition I/1.6.13) of the standard gamma distribution (\rightarrow Definition II/3.4.2).

Sources:

- original work

Metadata: ID: P112 | shortcut: gam-sgam | author: JoramSoch | date: 2020-05-26, 23:14.

3.4.4 Relationship to standard gamma distribution

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a gamma distribution (\rightarrow Definition 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 Definition II/3.4.2) 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 is positive, $g(X)$ is strictly increasing and we can calculate the probability density function of a strictly increasing function (\rightarrow Proof I/1.6.8) 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 Proof II/3.4.6), 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 Definition I/1.6.6) of the standard gamma distribution (\rightarrow Definition II/3.4.2).

Sources:

- original work

Metadata: ID: P177 | shortcut: gam-sgam2 | author: JoramSoch | date: 2020-10-15, 12:04.

3.4.5 Special case of Wishart distribution

Theorem: The gamma distribution (\rightarrow Definition II/3.4.1) is a special case of the Wishart distribution (\rightarrow Definition II/5.2.1) where the number of columns of the random matrix (\rightarrow Definition 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 Definition II/5.2.1):

$$Y \sim \mathcal{W}(V, n) . \quad (1)$$

Then, Y is described by the probability density function (\rightarrow Proof “wish-pdf”)

$$p(Y) = \frac{1}{\Gamma_p\left(\frac{n}{2}\right)} \cdot \frac{1}{\sqrt{2^{np}|V|^n}} \cdot |X|^{(n-p-1)/2} \cdot \exp\left[-\frac{1}{2}\text{tr}(V^{-1}X)\right] \quad (2)$$

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 Definition I/1.6.6) 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 Proof II/3.4.6).

Sources:

- original work

Metadata: ID: P328 | shortcut: gam-wish | author: JoramSoch | date: 2022-07-14, 07:45.

3.4.6 Probability density function

Theorem: Let X be a positive random variable (\rightarrow Definition I/1.2.2) following a gamma distribution (\rightarrow Definition II/3.4.1):

$$X \sim \text{Gam}(a, b) . \quad (1)$$

Then, the probability density function (\rightarrow Definition I/1.6.6) 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 Definition II/3.4.1).

Sources:

- original work

Metadata: ID: P45 | shortcut: gam-pdf | author: JoramSoch | date: 2020-02-08, 23:41.

3.4.7 Cumulative distribution function

Theorem: Let X be a positive random variable (\rightarrow Definition I/1.2.2) following a gamma distribution (\rightarrow Definition II/3.4.1):

$$X \sim \text{Gam}(a, b) . \quad (1)$$

Then, the cumulative distribution function (\rightarrow Definition I/1.6.13) 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 Proof II/3.4.6) is:

$$f_X(x) = \frac{b^a}{\Gamma(a)} x^{a-1} \exp[-bx] . \quad (3)$$

Thus, the cumulative distribution function (\rightarrow Definition I/1.6.13) 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.

Metadata: ID: P178 | shortcut: gam-cdf | author: JoramSoch | date: 2020-10-15, 12:34.

3.4.8 Quantile function

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a gamma distribution (\rightarrow Definition II/3.4.1):

$$X \sim \text{Gam}(a, b) . \quad (1)$$

Then, the quantile function (\rightarrow Definition I/1.6.23) 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 Proof II/3.4.7) 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 Definition I/1.6.23) $Q_X(p)$ 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 Proof I/1.6.24)

$$Q_X(p) = F_X^{-1}(x) . \quad (5)$$

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.

Metadata: ID: P194 | shortcut: gam-qf | author: JoramSoch | date: 2020-11-19, 07:31.

3.4.9 Mean

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a gamma distribution (\rightarrow Definition II/3.4.1):

$$X \sim \text{Gam}(a, b) . \quad (1)$$

Then, the mean or expected value (\rightarrow Definition I/1.7.1) of X is

$$\mathbb{E}(X) = \frac{a}{b} . \quad (2)$$

Proof: The expected value (\rightarrow Definition I/1.7.1) 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 gamma distribution (\rightarrow Proof II/3.4.6), this reads:

$$\begin{aligned} \mathbb{E}(X) &= \int_0^\infty x \cdot \frac{b^a}{\Gamma(a)} x^{a-1} \exp[-bx] \, dx \\ &= \int_0^\infty \frac{b^a}{\Gamma(a)} x^{(a+1)-1} \exp[-bx] \, dx \\ &= \int_0^\infty \frac{1}{b} \cdot \frac{b^{a+1}}{\Gamma(a)} x^{(a+1)-1} \exp[-bx] \, dx . \end{aligned} \quad (4)$$

Employing the relation $\Gamma(x+1) = \Gamma(x) \cdot x$, we have

$$\mathbb{E}(X) = \int_0^\infty \frac{a}{b} \cdot \frac{b^{a+1}}{\Gamma(a+1)} x^{(a+1)-1} \exp[-bx] \, dx \quad (5)$$

and again using the density of the gamma distribution (\rightarrow Proof II/3.4.6), we get

$$\begin{aligned} \mathbb{E}(X) &= \frac{a}{b} \int_0^\infty \text{Gam}(x; a+1, b) \, dx \\ &= \frac{a}{b} . \end{aligned} \quad (6)$$

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>.

Metadata: ID: P108 | shortcut: gam-mean | author: JoramSoch | date: 2020-05-19, 06:54.

3.4.10 Variance

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a gamma distribution (\rightarrow Definition II/3.4.1):

$$X \sim \text{Gam}(a, b) . \quad (1)$$

Then, the variance (\rightarrow Definition I/1.8.1) of X is

$$\text{Var}(X) = \frac{a}{b^2} . \quad (2)$$

Proof: The variance (\rightarrow Definition I/1.8.1) can be expressed in terms of expected values (\rightarrow Proof I/1.8.3) as

$$\text{Var}(X) = E(X^2) - E(X)^2 . \quad (3)$$

The expected value of a gamma random variable (\rightarrow Proof II/3.4.9) is

$$E(X) = \frac{a}{b} . \quad (4)$$

With the probability density function of the gamma distribution (\rightarrow Proof II/3.4.6), 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 Proof II/3.4.6), 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>.

Metadata: ID: P109 | shortcut: gam-var | author: JoramSoch | date: 2020-05-19, 07:20.

3.4.11 Logarithmic expectation

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a gamma distribution (\rightarrow Definition II/3.4.1):

$$X \sim \text{Gam}(a, b) . \quad (1)$$

Then, the expectation (\rightarrow Definition I/1.7.1) 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 Proof II/3.4.6) 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 Proof II/3.4.3) on a gamma-distributed (\rightarrow Definition II/3.4.1) random variable (\rightarrow Definition 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>.

Metadata: ID: P110 | shortcut: gam-logmean | author: JoramSoch | date: 2020-05-25, 21:28.

3.4.12 Expectation of $x \ln x$

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a gamma distribution (\rightarrow Definition II/3.4.1):

$$X \sim \text{Gam}(a, b) . \quad (1)$$

Then, the mean or expected value (\rightarrow Definition I/1.7.1) of $(X \cdot \ln X)$ is

$$\mathbb{E}(X \ln X) = \frac{a}{b} [\psi(a) - \ln(b)] . \quad (2)$$

Proof: With the definition of the expected value (\rightarrow Definition I/1.7.1), the law of the unconscious statistician (\rightarrow Proof I/1.7.12) and the probability density function of the gamma distribution (\rightarrow Proof II/3.4.6), 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 Proof II/3.4.11) 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 Proof II/3.4.11)

$$\mathbb{E}(\ln Y) = \psi(a+1) - \ln(b) \quad (5)$$

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:

$$\mathbb{E}(X \ln X) = \frac{a}{b} [\psi(a) - \ln(b)] . \quad (7)$$

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>.

Metadata: ID: P179 | shortcut: gam-xlogx | author: JoramSoch | date: 2020-10-15, 13:02.

3.4.13 Differential entropy

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a gamma distribution (\rightarrow Definition II/3.4.1):

$$X \sim \text{Gam}(a, b) \quad (1)$$

Then, the differential entropy (\rightarrow Definition 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 Definition 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 Definition I/1.7.1)

$$h(X) = -E[\ln p(x)] . \quad (4)$$

With the probability density function of the gamma distribution (\rightarrow Proof II/3.4.6), 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 Proof II/3.4.9) and logarithmic expectation (\rightarrow Proof II/3.4.11) of the gamma distribution (\rightarrow Definition 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 Definition 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.

Metadata: ID: P239 | shortcut: gam-dent | author: JoramSoch | date: 2021-07-14, 07:37.

3.4.14 Kullback-Leibler divergence

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2). Assume two gamma distributions (\rightarrow Definition 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 Definition 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 Definition 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 Definition 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 Proof II/3.4.6), 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 Proof II/3.4.9) and the expected value of a logarithmized gamma variate (\rightarrow Proof II/3.4.11)

$$\begin{aligned} x \sim \text{Gam}(a, b) \quad \Rightarrow \quad \langle x \rangle &= \frac{a}{b} \quad \text{and} \\ \langle \ln x \rangle &= \psi(a) - \ln(b) , \end{aligned} \quad (6)$$

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>.

Metadata: ID: P93 | shortcut: gam-kl | author: JoramSoch | date: 2020-05-05, 08:41.

3.5 Exponential distribution

3.5.1 Definition

Definition: Let X be a random variable (\rightarrow Definition 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 Definition I/1.6.6) 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.

Metadata: ID: D8 | shortcut: exp | author: JoramSoch | date: 2020-02-08, 23:48.

3.5.2 Special case of gamma distribution

Theorem: The exponential distribution (\rightarrow Definition II/3.5.1) is a special case of the gamma distribution (\rightarrow Definition II/3.4.1) with shape $a = 1$ and rate $b = \lambda$.

Proof: The probability density function of the gamma distribution (\rightarrow Proof II/3.4.6) 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 Proof II/3.5.3).

Sources:

- original work

Metadata: ID: P69 | shortcut: exp-gam | author: JoramSoch | date: 2020-03-02, 20:49.

3.5.3 Probability density function

Theorem: Let X be a non-negative random variable (\rightarrow Definition I/1.2.2) following an exponential distribution (\rightarrow Definition II/3.5.1):

$$X \sim \text{Exp}(\lambda) . \quad (1)$$

Then, the probability density function (\rightarrow Definition I/1.6.6) of X is

$$f_X(x) = \lambda \exp[-\lambda x] . \quad (2)$$

Proof: This follows directly from the definition of the exponential distribution (\rightarrow Definition II/3.5.1).

Sources:

- original work

Metadata: ID: P46 | shortcut: exp-pdf | author: JoramSoch | date: 2020-02-08, 23:53.

3.5.4 Moment-generating function

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following an exponential distribution (\rightarrow Definition II/3.5.1):

$$X \sim \text{Exp}(\lambda) . \quad (1)$$

Then, the moment generating function (\rightarrow Definition I/1.6.27) 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 Definition II/3.5.1) with rate λ ; that is, $X \sim \text{Exp}(\lambda)$. Then, the probability density function (\rightarrow Proof II/3.5.3) is given by

$$f_X(x) = \lambda e^{-\lambda x} \quad (3)$$

and the moment-generating function (\rightarrow Definition I/1.6.27) is defined as

$$M_X(t) = \text{E} [e^{tX}] . \quad (4)$$

Using the definition of expected value for continuous random variables (\rightarrow Definition I/1.7.1), the moment-generating function of X is thus:

$$\begin{aligned}
M_X(t) &= \int_0^\infty e^{tx} \cdot f_X(x) dx \\
&= \int_0^\infty e^{tx} \cdot \lambda e^{-\lambda x} dx \\
&= \int_0^\infty \lambda e^{x(t-\lambda)} dx \\
&= \frac{\lambda}{t-\lambda} e^{x(t-\lambda)} \Big|_{x=0}^{x=\infty} \\
&= \lim_{x \rightarrow \infty} \left[\frac{\lambda}{t-\lambda} e^{x(t-\lambda)} - \frac{\lambda}{t-\lambda} \right] \\
&= \frac{\lambda}{t-\lambda} \left[\lim_{x \rightarrow \infty} e^{x(t-\lambda)} - 1 \right] .
\end{aligned} \tag{5}$$

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).

Sources:

- original work

Metadata: ID: P403 | shortcut: exp-mgf | author: tomfaulkenberry | date: 2023-04-19, 12:00.

3.5.5 Cumulative distribution function

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following an exponential distribution (\rightarrow Definition II/3.5.1):

$$X \sim \text{Exp}(\lambda) . \tag{1}$$

Then, the cumulative distribution function (\rightarrow Definition I/1.6.13) 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 Proof II/3.5.3) is:

$$\text{Exp}(x; \lambda) = \begin{cases} 0, & \text{if } x < 0 \\ \lambda \exp[-\lambda x], & \text{if } x \geq 0. \end{cases} \quad (3)$$

Thus, the cumulative distribution function (\rightarrow Definition I/1.6.13) is:

$$F_X(x) = \int_{-\infty}^x \text{Exp}(z; \lambda) \, dz. \quad (4)$$

If $x < 0$, we have:

$$F_X(x) = \int_{-\infty}^x 0 \, dz = 0. \quad (5)$$

If $x \geq 0$, we have using (3):

$$\begin{aligned} F_X(x) &= \int_{-\infty}^0 \text{Exp}(z; \lambda) \, dz + \int_0^x \text{Exp}(z; \lambda) \, dz \\ &= \int_{-\infty}^0 0 \, dz + \int_0^x \lambda \exp[-\lambda z] \, dz \\ &= 0 + \lambda \left[-\frac{1}{\lambda} \exp[-\lambda z] \right]_0^x \\ &= \lambda \left[\left(-\frac{1}{\lambda} \exp[-\lambda x] \right) - \left(-\frac{1}{\lambda} \exp[-\lambda \cdot 0] \right) \right] \\ &= 1 - \exp[-\lambda x]. \end{aligned} \quad (6)$$

Sources:

- original work

Metadata: ID: P48 | shortcut: exp-cdf | author: JoramSoch | date: 2020-02-11, 14:48.

3.5.6 Quantile function

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following an exponential distribution (\rightarrow Definition II/3.5.1):

$$X \sim \text{Exp}(\lambda). \quad (1)$$

Then, the quantile function (\rightarrow Definition I/1.6.23) of X is

$$Q_X(p) = \begin{cases} -\infty, & \text{if } p = 0 \\ -\frac{\ln(1-p)}{\lambda}, & \text{if } p > 0. \end{cases} \quad (2)$$

Proof: The cumulative distribution function of the exponential distribution (\rightarrow Proof II/3.5.5) is:

$$F_X(x) = \begin{cases} 0, & \text{if } x < 0 \\ 1 - \exp[-\lambda x], & \text{if } x \geq 0. \end{cases} \quad (3)$$

The quantile function (\rightarrow Definition I/1.6.23) $Q_X(p)$ 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 Proof I/1.6.24)

$$Q_X(p) = F_X^{-1}(p) . \quad (5)$$

This can be derived by rearranging equation (3):

$$\begin{aligned} p &= 1 - \exp[-\lambda x] \\ \exp[-\lambda x] &= 1 - p \\ -\lambda x &= \ln(1 - p) \\ x &= -\frac{\ln(1 - p)}{\lambda} . \end{aligned} \quad (6)$$

Sources:

- original work

Metadata: ID: P50 | shortcut: exp-qf | author: JoramSoch | date: 2020-02-12, 15:48.

3.5.7 Mean

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following an exponential distribution (\rightarrow Definition II/3.5.1):

$$X \sim \text{Exp}(\lambda) . \quad (1)$$

Then, the mean or expected value (\rightarrow Definition I/1.7.1) of X is

$$\mathbb{E}(X) = \frac{1}{\lambda} . \quad (2)$$

Proof: The expected value (\rightarrow Definition I/1.7.1) 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 exponential distribution (\rightarrow Proof II/3.5.3), this reads:

$$\begin{aligned} \mathbb{E}(X) &= \int_0^{+\infty} x \cdot \lambda \exp(-\lambda x) \, dx \\ &= \lambda \int_0^{+\infty} x \cdot \exp(-\lambda x) \, dx . \end{aligned} \quad (4)$$

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

$$\begin{aligned} E(X) &= \lambda \left[\left(-\frac{1}{\lambda}x - \frac{1}{\lambda^2}\right) \exp(-\lambda x) \right]_0^{+\infty} \\ &= \lambda \left[\lim_{x \rightarrow \infty} \left(-\frac{1}{\lambda}x - \frac{1}{\lambda^2}\right) \exp(-\lambda x) - \left(-\frac{1}{\lambda} \cdot 0 - \frac{1}{\lambda^2}\right) \exp(-\lambda \cdot 0) \right] \\ &= \lambda \left[0 + \frac{1}{\lambda^2} \right] \\ &= \frac{1}{\lambda} . \end{aligned} \quad (6)$$

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.

Metadata: ID: P47 | shortcut: exp-mean | author: JoramSoch | date: 2020-02-10, 21:57.

3.5.8 Median

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following an exponential distribution (\rightarrow Definition II/3.5.1):

$$X \sim \text{Exp}(\lambda) . \quad (1)$$

Then, the median (\rightarrow Definition I/1.12.1) of X is

$$\text{median}(X) = \frac{\ln 2}{\lambda} . \quad (2)$$

Proof: The median (\rightarrow Definition I/1.12.1) is the value at which the cumulative distribution function (\rightarrow Definition I/1.6.13) is $1/2$:

$$F_X(\text{median}(X)) = \frac{1}{2} . \quad (3)$$

The cumulative distribution function of the exponential distribution (\rightarrow Proof 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:

$$\text{median}(X) = -\frac{\ln(1 - \frac{1}{2})}{\lambda} = \frac{\ln 2}{\lambda} . \quad (6)$$

Sources:

- original work

Metadata: ID: P49 | shortcut: exp-med | author: JoramSoch | date: 2020-02-11, 15:03.

3.5.9 Mode

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following an exponential distribution (\rightarrow Definition II/3.5.1):

$$X \sim \text{Exp}(\lambda) . \quad (1)$$

Then, the mode (\rightarrow Definition I/1.12.2) of X is

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

Proof: The mode (\rightarrow Definition I/1.12.2) is the value which maximizes the probability density function (\rightarrow Definition I/1.6.6):

$$\text{mode}(X) = \arg \max_x f_X(x) . \quad (3)$$

The probability density function of the exponential distribution (\rightarrow Proof 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

$$\text{mode}(X) = 0 . \quad (7)$$

Sources:

- original work

Metadata: ID: P51 | shortcut: exp-mode | author: kantundpeterpan | date: 2020-02-12, 15:53.

3.5.10 Variance

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following an exponential distribution (\rightarrow Definition II/3.5.1):

$$X \sim \text{Exp}(\lambda). \quad (1)$$

Then, the variance (\rightarrow Definition I/1.8.1) of X is

$$\text{Var}(X) = \frac{1}{\lambda^2}. \quad (2)$$

Proof: The variance (\rightarrow Definition I/1.8.1) 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 Proof I/1.8.3), reads:

$$\text{Var}(X) = \text{E}[X^2] - \text{E}[X]^2. \quad (4)$$

The expected value of the exponential distribution (\rightarrow Proof II/3.5.7) is:

$$\text{E}[X] = \frac{1}{\lambda} \quad (5)$$

The second moment $\text{E}[X^2]$ can be derived as follows:

$$\begin{aligned} \text{E}[X^2] &= \int_{-\infty}^{+\infty} x^2 \cdot f_X(x) \, dx \\ &= \int_0^{+\infty} x^2 \cdot \lambda \exp(-\lambda x) \, dx \\ &= \lambda \int_0^{+\infty} x^2 \cdot \exp(-\lambda x) \, dx \end{aligned} \quad (6)$$

Using the following anti-derivative

$$\begin{aligned} \int x^2 \cdot \exp(-\lambda x) \, dx &= \left[-\frac{1}{\lambda} x^2 \cdot \exp(-\lambda x) \right]_0^{+\infty} - \int 2x \left(-\frac{1}{\lambda} x \cdot \exp(-\lambda x) \right) \, dx \\ &= \left[-\frac{1}{\lambda} x^2 \cdot \exp(-\lambda x) \right]_0^{+\infty} - \left(\left[\frac{1}{\lambda^2} 2x \cdot \exp(-\lambda x) \right]_0^{+\infty} - \int 2 \left(\frac{1}{\lambda^2} \cdot \exp(-\lambda x) \right) \, dx \right) \\ &= \left[-\frac{x^2}{\lambda} \cdot \exp(-\lambda x) \right]_0^{+\infty} - \left(\left[\frac{2x}{\lambda^2} \cdot \exp(-\lambda x) \right]_0^{+\infty} - \left[-\frac{2}{\lambda^3} \cdot \exp(-\lambda x) \right]_0^{+\infty} \right) \\ &= \left[\left(-\frac{x^2}{\lambda} - \frac{2x}{\lambda^2} - \frac{2}{\lambda^3} \right) \exp(-\lambda x) \right]_0^{+\infty}, \end{aligned} \quad (7)$$

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>.

Metadata: ID: P401 | shortcut: exp-var | author: majapavlo | date: 2023-01-23, 09:02.

3.5.11 Skewness

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following an exponential distribution (\rightarrow Definition II/3.5.1):

$$X \sim \text{Exp}(\lambda) . \tag{1}$$

Then the skewness (\rightarrow Definition I/1.9.1) of X is

$$\text{Skew}(X) = 2 . \tag{2}$$

Proof:

To compute the skewness of X , we partition the skewness into expected values (\rightarrow Proof I/1.9.2):

$$\text{Skew}(X) = \frac{E(X^3) - 3\mu\sigma^2 - \mu^3}{\sigma^3} , \tag{3}$$

where μ and σ are the mean and standard deviation of X , respectively. Since X follows an exponential distribution (\rightarrow Definition II/3.5.1), the mean (\rightarrow Proof II/3.5.7) of X is given by

$$\mu = E(X) = \frac{1}{\lambda} \quad (4)$$

and the standard deviation (\rightarrow Proof 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 Proof 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 Proof I/1.15.2). First, we differentiate the moment-generating function of the exponential distribution (\rightarrow Proof 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:

$$\begin{aligned} M_X''(t) &= -2 \cdot \lambda(\lambda - t)^{-3} \cdot (-1) \\ &= 2\lambda(\lambda - t)^{-3}. \end{aligned} \quad (10)$$

Finally, one more application of the chain rule gives us the third derivative:

$$\begin{aligned} M_X'''(t) &= -3 \cdot 2\lambda(\lambda - t)^{-4} \cdot (-1) \\ &= 6\lambda(\lambda - t)^{-4} \\ &= \frac{6\lambda}{(\lambda - t)^4}. \end{aligned} \quad (11)$$

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).

Sources:

- original work

Metadata: ID: P409 | shortcut: exp-skew | author: tomfaulkenberry | date: 2023-04-24, 12:00.

3.6 Log-normal distribution

3.6.1 Definition

Definition: Let $\ln X$ be a random variable (\rightarrow Definition I/1.2.2) following a normal distribution (\rightarrow Definition 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.

Metadata: ID: D170 | shortcut: lognorm | author: majapavlo | date: 2022-02-07, 22:33.

3.6.2 Probability density function

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a log-normal distribution (\rightarrow Definition II/3.6.1):

$$X \sim \ln \mathcal{N}(\mu, \sigma^2) . \quad (1)$$

Then, the probability density function (\rightarrow Definition I/1.6.6) 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 Definition II/3.6.1) is defined as the exponential function of a normal random variable (\rightarrow Definition 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 Proof 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 Proof I/1.6.8) 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 Proof II/3.2.10), we have

$$\begin{aligned} f_X(x) &= f_Y(g^{-1}(x)) \cdot \frac{dg^{-1}(x)}{dx} \\ &= \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp \left[-\frac{1}{2} \left(\frac{g^{-1}(x) - \mu}{\sigma} \right)^2 \right] \cdot \frac{dg^{-1}(x)}{dx} \\ &= \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp \left[-\frac{1}{2} \left(\frac{(\ln x) - \mu}{\sigma} \right)^2 \right] \cdot \frac{d(\ln x)}{dx} \\ &= \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp \left[-\frac{1}{2} \left(\frac{\ln x - \mu}{\sigma} \right)^2 \right] \cdot \frac{1}{x} \\ &= \frac{1}{x\sigma\sqrt{2\pi}} \cdot \exp \left[-\frac{(\ln x - \mu)^2}{2\sigma^2} \right] \end{aligned} \quad (8)$$

which is the probability density function (\rightarrow Definition I/1.6.6) of the log-normal distribution (\rightarrow Definition 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>.

Metadata: ID: P310 | shortcut: lognorm-pdf | author: majapavlo | date: 2022-02-13, 10:05.

3.6.3 Cumulative distribution function

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a log-normal distribution (\rightarrow Definition II/3.6.1):

$$X \sim \ln \mathcal{N}(\mu, \sigma^2) . \quad (1)$$

Then, the cumulative distribution function (\rightarrow Definition “lognorm-cdf”) of X is

$$F_X(x) = \frac{1}{2} \left[1 + \operatorname{erf} \left(\frac{\ln x - \mu}{\sqrt{2}\sigma} \right) \right] \quad (2)$$

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 log-normal distribution (\rightarrow Proof II/3.6.2) is:

$$f_X(x) = \frac{1}{x\sigma\sqrt{2\pi}} \cdot \exp \left[- \left(\frac{\ln x - \mu}{\sqrt{2}\sigma} \right)^2 \right] . \quad (4)$$

Thus, the cumulative distribution function (\rightarrow Definition “lognorm-cdf”) is:

$$\begin{aligned} F_X(x) &= \int_{-\infty}^x \ln \mathcal{N}(z; \mu, \sigma^2) dz \\ &= \int_{-\infty}^x \frac{1}{z\sigma\sqrt{2\pi}} \cdot \exp \left[- \left(\frac{\ln z - \mu}{\sqrt{2}\sigma} \right)^2 \right] dz \\ &= \frac{1}{\sigma\sqrt{2\pi}} \int_{-\infty}^x \frac{1}{z} \cdot \exp \left[- \left(\frac{\ln z - \mu}{\sqrt{2}\sigma} \right)^2 \right] dz . \end{aligned} \quad (5)$$

From this point forward, the proof is similar to the derivation of the cumulative distribution function for the normal distribution (\rightarrow Proof 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>.

Metadata: ID: P325 | shortcut: lognorm-cdf | author: majapavlo | date: 2022-06-29, 22:20.

3.6.4 Quantile function

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a log-normal distribution (\rightarrow Definition II/3.6.1):

$$X \sim \ln \mathcal{N}(\mu, \sigma^2) . \tag{1}$$

Then, the quantile function (\rightarrow Definition I/1.6.23) of X is

$$Q_X(p) = \exp(\mu + \sqrt{2}\sigma \cdot \operatorname{erf}^{-1}(2p - 1)) \tag{2}$$

where $\operatorname{erf}^{-1}(x)$ is the inverse error function.

Proof: The cumulative distribution function of the log-normal distribution (\rightarrow Proof II/3.6.3) is:

$$F_X(x) = \frac{1}{2} \left[1 + \operatorname{erf} \left(\frac{\ln x - \mu}{\sqrt{2}\sigma} \right) \right] . \tag{3}$$

From this point forward, the proof is similar to the derivation of the quantile function for the normal distribution (\rightarrow Proof 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 Proof I/1.6.24):

$$Q_X(p) = F_X^{-1}(x) . \quad (4)$$

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.

Metadata: ID: P326 | shortcut: lognorm-qf | author: majapavlo | date: 2022-07-09, 11:05.

3.6.5 Mean

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a log-normal distribution (\rightarrow Definition II/3.6.1):

$$X \sim \ln \mathcal{N}(\mu, \sigma^2) \quad (1)$$

Then, the mean or expected value (\rightarrow Definition I/1.7.1) of X is

$$\mathbb{E}(X) = \exp \left(\mu + \frac{1}{2}\sigma^2 \right) \quad (2)$$

Proof: The expected value (\rightarrow Definition I/1.7.1) 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 Proof II/3.6.2), this is:

$$\begin{aligned} \mathbb{E}(X) &= \int_0^{+\infty} x \cdot \frac{1}{x\sqrt{2\pi\sigma^2}} \cdot \exp \left[-\frac{1}{2} \frac{(\ln x - \mu)^2}{\sigma^2} \right] \, dx \\ &= \frac{1}{\sqrt{2\pi\sigma^2}} \int_0^{+\infty} \exp \left[-\frac{1}{2} \frac{(\ln x - \mu)^2}{\sigma^2} \right] \, dx \end{aligned} \quad (4)$$

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 $\exp(\frac{1}{2}\sigma^2)$ 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 Proof 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 Definition I/1.6.6), 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>.

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3.6.6 Median

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a log-normal distribution (\rightarrow Definition II/3.6.1):

$$X \sim \ln \mathcal{N}(\mu, \sigma^2) . \quad (1)$$

Then, the median (\rightarrow Definition I/1.12.1) of X is

$$\text{median}(X) = e^\mu . \quad (2)$$

Proof: The median (\rightarrow Definition I/1.12.1) 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 Proof 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. Thus, the inverse CDF is

$$\begin{aligned} \ln(x) &= \sigma\sqrt{2} \cdot \text{erf}^{-1}(2p - 1) + \mu \\ x &= \exp \left[\sigma\sqrt{2} \cdot \text{erf}^{-1}(2p - 1) + \mu \right] \end{aligned} \quad (5)$$

where $\text{erf}^{-1}(x)$ is the inverse error function. Setting $p = 1/2$, we obtain:

$$\begin{aligned} \ln [\text{median}(X)] &= \sigma\sqrt{2} \cdot \text{erf}^{-1}(0) + \mu \\ \text{median}(X) &= e^\mu . \end{aligned} \quad (6)$$

Sources:

- original work

Metadata: ID: P306 | shortcut: lognorm-med | author: majapavlo | date: 2022-02-07, 22:33.

3.6.7 Mode

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a log-normal distribution (\rightarrow Definition II/3.6.1):

$$X \sim \ln \mathcal{N}(\mu, \sigma^2) . \quad (1)$$

Then, the mode (\rightarrow Definition I/1.12.2) of X is

$$\text{mode}(X) = e^{(\mu - \sigma^2)} . \quad (2)$$

Proof: The mode (\rightarrow Definition I/1.12.2) is the value which maximizes the probability density function (\rightarrow Definition I/1.6.6):

$$\text{mode}(X) = \arg \max_x f_X(x) . \quad (3)$$

The probability density function of the log-normal distribution (\rightarrow Proof 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:

$$f'_X(x) = -\frac{1}{x^2\sigma\sqrt{2\pi}} \cdot \exp \left[-\frac{(\ln x - \mu)^2}{2\sigma^2} \right] \cdot \left(1 + \frac{\ln x - \mu}{\sigma^2} \right) \quad (5)$$

$$\begin{aligned} f''_X(x) &= \frac{1}{\sqrt{2\pi}\sigma^2 x^3} \exp \left[-\frac{(\ln x - \mu)^2}{2\sigma^2} \right] \cdot (\ln x - \mu) \cdot \left(1 + \frac{\ln x - \mu}{\sigma^2} \right) \\ &\quad + \frac{\sqrt{2}}{\sqrt{\pi}x^3} \exp \left[-\frac{(\ln x - \mu)^2}{2\sigma^2} \right] \cdot \left(1 + \frac{\ln x - \mu}{\sigma^2} \right) \\ &\quad - \frac{1}{\sqrt{2\pi}\sigma^2 x^3} \exp \left[-\frac{(\ln x - \mu)^2}{2\sigma^2} \right] . \end{aligned} \quad (6)$$

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),

$$\begin{aligned} f''_X(e^{(\mu - \sigma^2)}) &= \frac{1}{\sqrt{2\pi}\sigma^2(e^{(\mu - \sigma^2)})^3} \exp \left[-\frac{\sigma^2}{2} \right] \cdot (\sigma^2) \cdot (0) \\ &\quad + \frac{\sqrt{2}}{\sqrt{\pi}(e^{(\mu - \sigma^2)})^3} \exp \left[-\frac{\sigma^2}{2} \right] \cdot (0) \\ &\quad - \frac{1}{\sqrt{2\pi}\sigma^2(e^{(\mu - \sigma^2)})^3} \exp \left[-\frac{\sigma^2}{2} \right] \\ &= -\frac{1}{\sqrt{2\pi}\sigma^2(e^{(\mu - \sigma^2)})^3} \exp \left[-\frac{\sigma^2}{2} \right] < 0 , \end{aligned} \quad (8)$$

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>.

Metadata: ID: P311 | shortcut: lognorm-mode | author: majapavlo | date: 2022-02-13, 10:15.

3.6.8 Variance

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a log-normal distribution (\rightarrow Definition II/3.6.1):

$$X \sim \ln \mathcal{N}(\mu, \sigma^2). \quad (1)$$

Then, the variance (\rightarrow Definition I/1.8.1) of X is

$$\text{Var}(X) = \exp(2\mu + 2\sigma^2) - \exp(2\mu + \sigma^2). \quad (2)$$

Proof: The variance (\rightarrow Definition I/1.8.1) 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 Proof I/1.8.3), reads:

$$\text{Var}(X) = \text{E}[X^2] - \text{E}[X]^2. \quad (4)$$

The expected value of the log-normal distribution (\rightarrow Proof 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:

$$\begin{aligned} \text{E}[X^2] &= \frac{1}{\sqrt{2\pi\sigma^2}} \int_{(-\infty - \mu)/(\sigma)}^{(\ln x - \mu)/(\sigma)} \exp(\mu + \sigma z) \exp\left(-\frac{1}{2}z^2\right) d[\exp(\mu + \sigma z)] \\ &= \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{+\infty} \exp\left(-\frac{1}{2}z^2\right) \sigma \exp(2\mu + 2\sigma z) dz \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \exp\left[-\frac{1}{2}(z^2 - 4\sigma z - 4\mu)\right] dz \end{aligned} \quad (7)$$

Now multiplying by $\exp(2\sigma^2)$ and $\exp(-2\sigma^2)$, this becomes:

$$\begin{aligned} E[X^2] &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \exp\left[-\frac{1}{2}(z^2 - 4\sigma z + 4\sigma^2 - 4\sigma^2 - 4\mu)\right] dz \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \exp\left[-\frac{1}{2}(z^2 - 4\sigma z + 4\sigma^2)\right] \exp(2\sigma^2 + 2\mu) dz \\ &= \exp(2\sigma^2 + 2\mu) \int_{-\infty}^{+\infty} \frac{1}{\sqrt{2\pi}} \exp\left[-\frac{1}{2}(z - 2\sigma)^2\right] dz \end{aligned} \quad (8)$$

The probability density function of a normal distribution (\rightarrow Proof II/3.2.10) is given by

$$f_X(x) = \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp\left[-\frac{1}{2}\left(\frac{x - \mu}{\sigma}\right)^2\right] \quad (9)$$

and, with $\mu = 2\sigma$ and unit variance, this reads:

$$f_X(x) = \frac{1}{\sqrt{2\pi}} \cdot \exp\left[-\frac{1}{2}(x - 2\sigma)^2\right] . \quad (10)$$

Using the definition of the probability density function (\rightarrow Definition I/1.6.6), we get

$$\int_{-\infty}^{+\infty} \frac{1}{\sqrt{2\pi}} \cdot \exp\left[-\frac{1}{2}(x - 2\sigma)^2\right] dx = 1 \quad (11)$$

and applying (11) to (8), we have:

$$E[X]^2 = \exp(2\sigma^2 + 2\mu) . \quad (12)$$

Finally, plugging (12) and (5) into (4), we have:

$$\begin{aligned} \text{Var}(X) &= E[X^2] - E[X]^2 \\ &= \exp(2\sigma^2 + 2\mu) - \left[\exp\left(\mu + \frac{1}{2}\sigma^2\right)\right]^2 \\ &= \exp(2\sigma^2 + 2\mu) - \exp(2\mu + \sigma^2) . \end{aligned} \quad (13)$$

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>.

Metadata: ID: P355 | shortcut: lognorm-var | author: majapavlo | date: 2022-10-02, 09:02.

3.7 Chi-squared distribution

3.7.1 Definition

Definition: Let X_1, \dots, X_k be independent (\rightarrow Definition I/1.3.6) random variables (\rightarrow Definition I/1.2.2) where each of them is following a standard normal distribution (\rightarrow Definition II/3.2.2):

$$X_i \sim \mathcal{N}(0, 1) \quad \text{for } i = 1, \dots, n. \quad (1)$$

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 Proof II/3.7.3) with k degree of freedom is

$$\chi^2(x; k) = \frac{1}{2^{k/2} \Gamma(k/2)} x^{k/2-1} e^{-x/2} \quad (3)$$

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>.

Metadata: ID: D100 | shortcut: chi2 | author: kjpetrykowski | date: 2020-10-13, 01:20.

3.7.2 Special case of gamma distribution

Theorem: The chi-squared distribution (\rightarrow Definition II/3.7.1) with k degrees of freedom is a special case of the gamma distribution (\rightarrow Definition II/3.4.1) with shape $\frac{k}{2}$ and rate $\frac{1}{2}$:

$$X \sim \text{Gam}\left(\frac{k}{2}, \frac{1}{2}\right) \Rightarrow X \sim \chi^2(k). \quad (1)$$

Proof: The probability density function of the gamma distribution (\rightarrow Proof II/3.4.6) for $x > 0$, where α is the shape parameter and β is the rate parameter, is as follows:

$$\text{Gam}(x; \alpha, \beta) = \frac{\beta^\alpha}{\Gamma(\alpha)} x^{\alpha-1} e^{-\beta x} \quad (2)$$

If we let $\alpha = k/2$ and $\beta = 1/2$, we obtain

$$\text{Gam}\left(x; \frac{k}{2}, \frac{1}{2}\right) = \frac{x^{k/2-1} e^{-x/2}}{\Gamma(k/2) 2^{k/2}} = \frac{1}{2^{k/2} \Gamma(k/2)} x^{k/2-1} e^{-x/2} \quad (3)$$

which is equivalent to the probability density function of the chi-squared distribution (\rightarrow Proof II/3.7.3).

Sources:

- original work

Metadata: ID: P174 | shortcut: chi2-gam | author: kjpetrykowski | date: 2020-10-12, 22:15.

3.7.3 Probability density function

Theorem: Let Y be a random variable (\rightarrow Definition I/1.2.2) following a chi-squared distribution (\rightarrow Definition II/3.7.1):

$$Y \sim \chi^2(k) . \quad (1)$$

Then, the probability density function (\rightarrow Definition I/1.6.6) of Y is

$$f_Y(y) = \frac{1}{2^{k/2} \Gamma(k/2)} y^{k/2-1} e^{-y/2} . \quad (2)$$

Proof: A chi-square-distributed random variable (\rightarrow Definition II/3.7.1) with k degrees of freedom is defined as the sum of k squared standard normal random variables (\rightarrow Definition II/3.2.2):

$$X_1, \dots, X_k \sim \mathcal{N}(0, 1) \quad \Rightarrow \quad Y = \sum_{i=1}^k X_i^2 \sim \chi^2(k) . \quad (3)$$

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 Definition I/1.6.6) and cumulative distribution function (\rightarrow Definition I/1.6.13) of Y . Because the PDF is the first derivative of the CDF (\rightarrow Proof I/1.6.12), we can write:

$$F_Y(y) = \frac{F_Y(y)}{dy} dy = f_Y(y) dy . \quad (5)$$

Then, the cumulative distribution function (\rightarrow Definition I/1.6.13) 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 Definition I/1.6.6) of the standard normal distribution (\rightarrow Definition II/3.2.2) 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 Proof 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

$$\frac{dr}{dy} = \frac{1}{2} y^{-1/2} \quad \Leftrightarrow \quad dr = \frac{dy}{2y^{1/2}} . \tag{10}$$

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):

$$f_Y(y) = \frac{1}{2^{k/2} \Gamma(k/2)} y^{k/2-1} e^{-y/2} . \tag{12}$$

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.

Metadata: ID: P197 | shortcut: chi2-pdf | author: JoramSoch | date: 2020-11-25, 05:56.

3.7.4 Moments

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a chi-squared distribution (\rightarrow Definition II/3.7.1):

$$X \sim \chi^2(k) . \quad (1)$$

If $m > -k/2$, then $E(X^m)$ exists and is equal to:

$$E(X^m) = \frac{2^m \Gamma\left(\frac{k}{2} + m\right)}{\Gamma\left(\frac{k}{2}\right)} . \quad (2)$$

Proof: Combining the definition of the m -th raw moment (\rightarrow Definition I/1.15.3) with the probability density function of the chi-squared distribution (\rightarrow Proof II/3.7.3), we have:

$$E(X^m) = \int_0^\infty \frac{1}{\Gamma\left(\frac{k}{2}\right) 2^{k/2}} x^{(k/2)+m-1} e^{-x/2} dx . \quad (3)$$

Now define a new variable $u = x/2$. As a result, we obtain:

$$E(X^m) = \int_0^\infty \frac{1}{\Gamma\left(\frac{k}{2}\right) 2^{(k/2)-1}} 2^{(k/2)+m-1} u^{(k/2)+m-1} e^{-u} du . \quad (4)$$

This leads to the desired result when $m > -k/2$. Observe that, if m is a nonnegative integer, then $m > -k/2$ is always true. Therefore, all moments (\rightarrow Definition I/1.15.1) of a chi-squared distribution (\rightarrow Definition II/3.7.1) exist and the m -th raw moment is given by the foregoing equation.

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>.

Metadata: ID: P175 | shortcut: chi2-mom | author: kjpetrykowski | date: 2020-10-13, 01:30.

3.8 F-distribution

3.8.1 Definition

Definition: Let X_1 and X_2 be independent (\rightarrow Definition I/1.3.6) random variables (\rightarrow Definition I/1.2.2) following a chi-squared distribution (\rightarrow Definition II/3.7.1) with d_1 and d_2 degrees of freedom (\rightarrow Definition “dof”), respectively:

$$\begin{aligned} X_1 &\sim \chi^2(d_1) \\ X_2 &\sim \chi^2(d_2) . \end{aligned} \quad (1)$$

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 d_1 and denominator degrees of freedom d_2 :

$$Y = \frac{X_1/d_1}{X_2/d_2} \sim F(d_1, d_2) \quad \text{where} \quad d_1, d_2 > 0 . \quad (2)$$

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>.

Metadata: ID: D146 | shortcut: f | author: JoramSoch | date: 2020-04-21, 07:26.

3.8.2 Probability density function

Theorem: Let F be a random variable (\rightarrow Definition I/1.2.2) following an F -distribution (\rightarrow Definition II/3.8.1):

$$F \sim F(u, v) . \quad (1)$$

Then, the probability density function (\rightarrow Definition I/1.6.6) 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 Definition II/3.8.1) is defined as the ratio of two chi-squared random variables (\rightarrow Definition II/3.7.1), divided by their degrees of freedom (\rightarrow Definition “dof”)

$$X \sim \chi^2(u), Y \sim \chi^2(v) \quad \Rightarrow \quad F = \frac{X/u}{Y/v} \sim F(u, v) \quad (3)$$

where X and Y are independent of each other (\rightarrow Definition I/1.3.6).

The probability density function of the chi-squared distribution (\rightarrow Proof II/3.7.3) 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:

$$J = \begin{bmatrix} \frac{dX}{dF} & \frac{dX}{dW} \\ \frac{dY}{dF} & \frac{dY}{dW} \end{bmatrix} = \begin{bmatrix} \frac{u}{v}W & \frac{u}{v}F \\ 0 & 1 \end{bmatrix} \quad (7)$$

$$|J| = \frac{u}{v}W.$$

Because X and Y are independent (\rightarrow Definition I/1.3.6), the joint density (\rightarrow Definition I/1.5.2) of X and Y is equal to the product (\rightarrow Proof I/1.3.8) of the marginal densities (\rightarrow Definition 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 Proof I/1.6.10), the joint density (\rightarrow Definition 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 Definition I/1.5.3) of F can now be obtained by integrating out (\rightarrow Definition 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 Proof II/3.4.6) 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 Definition I/1.6.6), 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>.

Metadata: ID: P264 | shortcut: f-pdf | author: JoramSoch | date: 2021-10-12, 09:00.

3.9 Beta distribution

3.9.1 Definition

Definition: Let X be a random variable (\rightarrow Definition 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 Definition I/1.6.6) is given by

$$\text{Bet}(x; \alpha, \beta) = \frac{1}{\text{B}(\alpha, \beta)} x^{\alpha-1} (1-x)^{\beta-1} \quad (2)$$

where $\alpha > 0$ and $\beta > 0$, 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.

Metadata: ID: D53 | shortcut: beta | author: JoramSoch | date: 2020-05-10, 20:29.

3.9.2 Relationship to chi-squared distribution

Theorem: Let X and Y be independent (\rightarrow Definition I/1.3.6) random variables (\rightarrow Definition I/1.2.2) following chi-squared distributions (\rightarrow Definition 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 Definition 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 Proof II/3.7.3) 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 Definition I/1.3.6), the joint density (\rightarrow Definition I/1.5.2) of X and Y is equal to the product (\rightarrow Proof I/1.3.8) of the marginal densities (\rightarrow Definition 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 Proof I/1.6.10), the joint density (\rightarrow Definition 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 Definition I/1.5.3) of Z can now be obtained by integrating out (\rightarrow Definition I/1.5.3) 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 Proof II/3.4.6) 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 Definition I/1.6.6), we have:

$$\begin{aligned} f_Z(z) &= \frac{1}{\Gamma\left(\frac{m}{2}\right) \Gamma\left(\frac{n}{2}\right) \cdot 2^{(m+n)/2}} \cdot z^{\frac{m}{2}-1} \cdot (1-z)^{-\frac{m}{2}-1} \cdot \frac{\Gamma\left(\frac{m+n}{2}\right)}{\left(\frac{1}{2(1-z)}\right)^{\frac{m+n}{2}}} \\ &= \frac{\Gamma\left(\frac{m+n}{2}\right) \cdot 2^{(m+n)/2}}{\Gamma\left(\frac{m}{2}\right) \Gamma\left(\frac{n}{2}\right) \cdot 2^{(m+n)/2}} \cdot z^{\frac{m}{2}-1} \cdot (1-z)^{-\frac{m}{2}+\frac{m+n}{2}-1} \\ &= \frac{\Gamma\left(\frac{m+n}{2}\right)}{\Gamma\left(\frac{m}{2}\right) \Gamma\left(\frac{n}{2}\right)} \cdot z^{\frac{m}{2}-1} \cdot (1-z)^{\frac{n}{2}-1}. \end{aligned} \quad (12)$$

With the definition of the beta function (\rightarrow Proof II/3.9.6), this becomes

$$f_Z(z) = \frac{1}{B\left(\frac{m}{2}, \frac{n}{2}\right)} \cdot z^{\frac{m}{2}-1} \cdot (1-z)^{\frac{n}{2}-1} \quad (13)$$

which is the probability density function of the beta distribution (\rightarrow Proof II/3.9.3) with parameters

$$\alpha = \frac{m}{2} \quad \text{and} \quad \beta = \frac{n}{2}, \quad (14)$$

such that

$$Z \sim \text{Bet}\left(\frac{m}{2}, \frac{n}{2}\right). \quad (15)$$

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>.

Metadata: ID: P356 | shortcut: beta-chi2 | author: JoramSoch | date: 2022-10-07, 13:20.

3.9.3 Probability density function

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a beta distribution (\rightarrow Definition II/3.9.1):

$$X \sim \text{Bet}(\alpha, \beta). \quad (1)$$

Then, the probability density function (\rightarrow Definition I/1.6.6) of X is

$$f_X(x) = \frac{1}{B(\alpha, \beta)} x^{\alpha-1} (1-x)^{\beta-1}. \quad (2)$$

Proof: This follows directly from the definition of the beta distribution (\rightarrow Definition II/3.9.1).

Sources:

- original work

Metadata: ID: P94 | shortcut: beta-pdf | author: JoramSoch | date: 2020-05-05, 21:03.

3.9.4 Moment-generating function

Theorem: Let X be a positive random variable (\rightarrow Definition I/1.2.2) following a beta distribution (\rightarrow Definition II/3.4.1):

$$X \sim \text{Bet}(\alpha, \beta) . \quad (1)$$

Then, the moment-generating function (\rightarrow Definition I/1.6.27) 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 Proof II/3.9.3) 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 Definition I/1.6.27) is defined as

$$M_X(t) = \text{E} [e^{tX}] . \quad (4)$$

Using the expected value for continuous random variables (\rightarrow Definition I/1.7.1), 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.

Metadata: ID: P198 | shortcut: beta-mgf | author: JoramSoch | date: 2020-11-25, 06:55.

3.9.5 Cumulative distribution function

Theorem: Let X be a positive random variable (\rightarrow Definition I/1.2.2) following a beta distribution (\rightarrow Definition II/3.4.1):

$$X \sim \text{Bet}(\alpha, \beta) . \quad (1)$$

Then, the cumulative distribution function (\rightarrow Definition I/1.6.13) 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 Proof II/3.9.3) is:

$$f_X(x) = \frac{1}{B(\alpha, \beta)} x^{\alpha-1} (1-x)^{\beta-1} . \quad (3)$$

Thus, the cumulative distribution function (\rightarrow Definition I/1.6.13) is:

$$\begin{aligned}
F_X(x) &= \int_0^x \text{Bet}(z; \alpha, \beta) \, dz \\
&= \int_0^x \frac{1}{B(\alpha, \beta)} z^{\alpha-1} (1-z)^{\beta-1} \, dz \\
&= \frac{1}{B(\alpha, \beta)} \int_0^x z^{\alpha-1} (1-z)^{\beta-1} \, dz .
\end{aligned} \tag{4}$$

With the definition of the incomplete beta function

$$B(x; a, b) = \int_0^x t^{a-1} (1-t)^{b-1} \, dt , \tag{5}$$

we arrive at the final result given by equation (2):

$$F_X(x) = \frac{B(x; \alpha, \beta)}{B(\alpha, \beta)} . \tag{6}$$

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.

Metadata: ID: P195 | shortcut: beta-cdf | author: JoramSoch | date: 2020-11-19, 08:01.

3.9.6 Mean

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a beta distribution (\rightarrow Definition II/3.9.1):

$$X \sim \text{Bet}(\alpha, \beta) . \tag{1}$$

Then, the mean or expected value (\rightarrow Definition I/1.7.1) of X is

$$E(X) = \frac{\alpha}{\alpha + \beta} . \tag{2}$$

Proof: The expected value (\rightarrow Definition I/1.7.1) is the probability-weighted average over all possible values:

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

The probability density function of the beta distribution (\rightarrow Proof II/3.9.3) is

$$f_X(x) = \frac{1}{B(\alpha, \beta)} x^{\alpha-1} (1-x)^{\beta-1}, \quad 0 \leq x \leq 1 \tag{4}$$

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:

$$\begin{aligned} E(X) &= \int_0^1 x \cdot \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha) \cdot \Gamma(\beta)} x^{\alpha-1} (1-x)^{\beta-1} dx \\ &= \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)} \cdot \frac{\Gamma(\alpha + 1)}{\Gamma(\alpha + 1 + \beta)} \int_0^1 \frac{\Gamma(\alpha + 1 + \beta)}{\Gamma(\alpha + 1) \cdot \Gamma(\beta)} x^{(\alpha+1)-1} (1-x)^{\beta-1} dx . \end{aligned} \quad (6)$$

Employing the relation $\Gamma(x + 1) = \Gamma(x) \cdot x$, we have

$$\begin{aligned} E(X) &= \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)} \cdot \frac{\alpha \cdot \Gamma(\alpha)}{(\alpha + \beta) \cdot \Gamma(\alpha + \beta)} \int_0^1 \frac{\Gamma(\alpha + 1 + \beta)}{\Gamma(\alpha + 1) \cdot \Gamma(\beta)} x^{(\alpha+1)-1} (1-x)^{\beta-1} dx \\ &= \frac{\alpha}{\alpha + \beta} \int_0^1 \frac{\Gamma(\alpha + 1 + \beta)}{\Gamma(\alpha + 1) \cdot \Gamma(\beta)} x^{(\alpha+1)-1} (1-x)^{\beta-1} dx \end{aligned} \quad (7)$$

and again using the density of the beta distribution (\rightarrow Proof II/3.9.3), we get

$$\begin{aligned} E(X) &= \frac{\alpha}{\alpha + \beta} \int_0^1 \text{Bet}(x; \alpha + 1, \beta) dx \\ &= \frac{\alpha}{\alpha + \beta} . \end{aligned} \quad (8)$$

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>.

Metadata: ID: P228 | shortcut: beta-mean | author: JoramSoch | date: 2021-04-29, 09:12.

3.9.7 Variance

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following a beta distribution (\rightarrow Definition II/3.9.1):

$$X \sim \text{Bet}(\alpha, \beta) . \quad (1)$$

Then, the variance (\rightarrow Definition I/1.8.1) of X is

$$\text{Var}(X) = \frac{\alpha\beta}{(\alpha + \beta + 1) \cdot (\alpha + \beta)^2} . \quad (2)$$

Proof: The variance (\rightarrow Definition I/1.8.1) can be expressed in terms of expected values (\rightarrow Proof I/1.8.3) as

$$\text{Var}(X) = E(X^2) - E(X)^2 . \quad (3)$$

The expected value of a beta random variable (\rightarrow Proof II/3.9.6) is

$$E(X) = \frac{\alpha}{\alpha + \beta} . \quad (4)$$

The probability density function of the beta distribution (\rightarrow Proof II/3.9.3) is

$$f_X(x) = \frac{1}{B(\alpha, \beta)} x^{\alpha-1} (1-x)^{\beta-1}, \quad 0 \leq x \leq 1 \quad (5)$$

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 Proof II/3.9.3), 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>.

Metadata: ID: P229 | shortcut: beta-var | author: JoramSoch | date: 2021-04-29, 09:31.

3.10 Wald distribution

3.10.1 Definition

Definition: Let X be a random variable (\rightarrow Definition 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 Definition I/1.6.6) 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.

Metadata: ID: D95 | shortcut: wald | author: tomfaulkenberry | date: 2020-09-04, 12:00.

3.10.2 Probability density function

Theorem: Let X be a positive random variable (\rightarrow Definition I/1.2.2) following a Wald distribution (\rightarrow Definition II/3.10.1):

$$X \sim \text{Wald}(\gamma, \alpha) . \quad (1)$$

Then, the probability density function (\rightarrow Definition I/1.6.6) 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 Definition II/3.10.1).

Sources:

- original work

Metadata: ID: P162 | shortcut: wald-pdf | author: tomfaulkenberry | date: 2020-09-04, 12:00.

3.10.3 Moment-generating function

Theorem: Let X be a positive random variable (\rightarrow Definition I/1.2.2) following a Wald distribution (\rightarrow Definition II/3.10.1):

$$X \sim \text{Wald}(\gamma, \alpha) . \quad (1)$$

Then, the moment-generating function (\rightarrow Definition I/1.6.27) 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 Proof 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 Definition I/1.6.27) is defined as

$$M_X(t) = \mathbb{E} [e^{tX}] . \quad (4)$$

Using the definition of expected value for continuous random variables (\rightarrow Definition I/1.7.1), 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:

¹<https://dlmf.nist.gov/10.25>

²<https://dlmf.nist.gov/10.39.2>

³<https://dlmf.nist.gov/10.32.10>

$$\begin{aligned}
M_X(t) &= \frac{\alpha}{\sqrt{2\pi}} \int_0^\infty x^{-3/2} \cdot \exp \left[tx - \frac{\alpha^2}{2x} + \alpha\gamma - \frac{\gamma^2 x}{2} \right] dx \\
&= \frac{\alpha}{\sqrt{2\pi}} \cdot e^{\alpha\gamma} \int_0^\infty x^{-3/2} \cdot \exp \left[\left(t - \frac{\gamma^2}{2} \right) x - \frac{\alpha^2}{2x} \right] dx \\
&= \frac{\alpha}{\sqrt{2\pi}} \cdot e^{\alpha\gamma} \int_0^\infty x^{-3/2} \cdot \exp \left[-\frac{1}{2} (\gamma^2 - 2t) x - \frac{1}{2} \cdot \frac{\alpha^2}{x} \right] dx .
\end{aligned} \tag{9}$$

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 $K_{-1/2}$:

$$M_X(t) = \frac{\alpha}{\sqrt{2\pi}} \cdot e^{\alpha\gamma} \cdot 2 \left(\frac{\gamma^2 - 2t}{\alpha^2} \right)^{1/4} \cdot K_{-1/2} \left(\sqrt{\alpha^2(\gamma^2 - 2t)} \right) . \tag{10}$$

Combining with (7) and simplifying gives

$$\begin{aligned}
M_X(t) &= \frac{\alpha}{\sqrt{2\pi}} \cdot e^{\alpha\gamma} \cdot 2 \left(\frac{\gamma^2 - 2t}{\alpha^2} \right)^{1/4} \cdot \sqrt{\frac{\pi}{2\sqrt{\alpha^2(\gamma^2 - 2t)}}} \cdot \exp \left[-\sqrt{\alpha^2(\gamma^2 - 2t)} \right] \\
&= \frac{\alpha}{\sqrt{2} \cdot \sqrt{\pi}} \cdot e^{\alpha\gamma} \cdot 2 \cdot \frac{(\gamma^2 - 2t)^{1/4}}{\sqrt{\alpha}} \cdot \frac{\sqrt{\pi}}{\sqrt{2} \cdot \sqrt{\alpha} \cdot (\gamma^2 - 2t)^{1/4}} \cdot \exp \left[-\sqrt{\alpha^2(\gamma^2 - 2t)} \right] \\
&= e^{\alpha\gamma} \cdot \exp \left[-\sqrt{\alpha^2(\gamma^2 - 2t)} \right] \\
&= \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)} \right] .
\end{aligned} \tag{11}$$

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>.

Metadata: ID: P168 | shortcut: wald-mgf | author: tomfaulkenberry | date: 2020-09-13, 12:00.

3.10.4 Mean

Theorem: Let X be a positive random variable (\rightarrow Definition I/1.2.2) following a Wald distribution (\rightarrow Definition II/3.10.1):

$$X \sim \text{Wald}(\gamma, \alpha) . \tag{1}$$

Then, the mean or expected value (\rightarrow Definition I/1.7.1) of X is

$$E(X) = \frac{\alpha}{\gamma} . \tag{2}$$

Proof: The mean or expected value $E(X)$ is the first moment (\rightarrow Definition I/1.15.1) of X , so we can use (\rightarrow Proof I/1.15.2) the moment-generating function of the Wald distribution (\rightarrow Proof 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:

$$\begin{aligned} M'_X(0) &= \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2(0))} \right] \cdot \frac{\alpha^2}{\sqrt{\alpha^2(\gamma^2 - 2(0))}} \\ &= \exp \left[\alpha\gamma - \sqrt{\alpha^2 \cdot \gamma^2} \right] \cdot \frac{\alpha^2}{\sqrt{\alpha^2 \cdot \gamma^2}} \\ &= \exp[0] \cdot \frac{\alpha^2}{\alpha\gamma} \\ &= \frac{\alpha}{\gamma} . \end{aligned} \quad (6)$$

Sources:

- original work

Metadata: ID: P169 | shortcut: wald-mean | author: tomfaulkenberry | date: 2020-09-13, 12:00.

3.10.5 Variance

Theorem: Let X be a positive random variable (\rightarrow Definition I/1.2.2) following a Wald distribution (\rightarrow Definition II/3.10.1):

$$X \sim \text{Wald}(\gamma, \alpha) . \quad (1)$$

Then, the variance (\rightarrow Definition I/1.8.1) of X is

$$\text{Var}(X) = \frac{\alpha}{\gamma^3} . \quad (2)$$

Proof: To compute the variance of X , we partition the variance into expected values (\rightarrow Proof I/1.8.3):

$$\text{Var}(X) = E(X^2) - E(X)^2. \quad (3)$$

We then use the moment-generating function of the Wald distribution (\rightarrow Proof II/3.10.3) to calculate

$$E(X^2) = M_X''(0). \quad (4)$$

First we differentiate

$$M_X(t) = \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)} \right] \quad (5)$$

with respect to t . Using the chain rule gives

$$\begin{aligned} M_X'(t) &= \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)} \right] \cdot -\frac{1}{2} (\alpha^2(\gamma^2 - 2t))^{-1/2} \cdot -2\alpha^2 \\ &= \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)} \right] \cdot \frac{\alpha^2}{\sqrt{\alpha^2(\gamma^2 - 2t)}} \\ &= \alpha \cdot \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)} \right] \cdot (\gamma^2 - 2t)^{-1/2}. \end{aligned} \quad (6)$$

Now we use the product rule to obtain the second derivative:

$$\begin{aligned} M_X''(t) &= \alpha \cdot \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)} \right] \cdot (\gamma^2 - 2t)^{-1/2} \cdot -\frac{1}{2} (\alpha^2(\gamma^2 - 2t))^{-1/2} \cdot -2\alpha^2 \\ &\quad + \alpha \cdot \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)} \right] \cdot -\frac{1}{2} (\gamma^2 - 2t)^{-3/2} \cdot -2 \\ &= \alpha^2 \cdot \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)} \right] \cdot (\gamma^2 - 2t)^{-1} \\ &\quad + \alpha \cdot \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)} \right] \cdot (\gamma^2 - 2t)^{-3/2} \\ &= \alpha \cdot \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2t)} \right] \left[\frac{\alpha}{\gamma^2 - 2t} + \frac{1}{\sqrt{(\gamma^2 - 2t)^3}} \right]. \end{aligned} \quad (7)$$

Applying (4) yields

$$\begin{aligned} E(X^2) &= M_X''(0) \\ &= \alpha \cdot \exp \left[\alpha\gamma - \sqrt{\alpha^2(\gamma^2 - 2(0))} \right] \left[\frac{\alpha}{\gamma^2 - 2(0)} + \frac{1}{\sqrt{(\gamma^2 - 2(0))^3}} \right] \\ &= \alpha \cdot \exp [\alpha\gamma - \alpha\gamma] \cdot \left[\frac{\alpha}{\gamma^2} + \frac{1}{\gamma^3} \right] \\ &= \frac{\alpha^2}{\gamma^2} + \frac{\alpha}{\gamma^3}. \end{aligned} \quad (8)$$

Since the mean of a Wald distribution (\rightarrow Proof 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).

Sources:

- original work

Metadata: ID: P170 | shortcut: wald-var | author: tomfaulkenberry | date: 2020-09-13, 12:00.

3.11 ex-Gaussian distribution

3.11.1 Definition

Definition: Let A be a random variable (\rightarrow Definition I/1.2.2) that is normally distributed (\rightarrow Definition II/3.2.1) with mean μ and variance σ^2 , and let B be a random variable that is exponentially distributed (\rightarrow Definition II/3.5.1) with rate λ . Suppose further that A and B are independent (\rightarrow Definition 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,

$$X \sim \text{ex-Gaussian}(\mu, \sigma, \lambda), \tag{1}$$

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>.

Metadata: ID: D187 | shortcut: exg | author: tomfaulkenberry | date: 2023-04-18, 12:00.

3.11.2 Probability density function

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following an ex-Gaussian distribution (\rightarrow Definition II/3.11.1):

$$X \sim \text{ex-Gaussian}(\mu, \sigma, \lambda). \tag{1}$$

Then the probability density function (\rightarrow Definition I/1.6.6) of X is

$$f_X(t) = \frac{\lambda}{\sqrt{2\pi}} \exp\left[\frac{\lambda^2 \sigma^2}{2} - \lambda(t - \mu)\right] \cdot \int_{-\infty}^{\frac{t-\mu}{\sigma} - \lambda\sigma} \exp\left[-\frac{1}{2}y^2\right] dy. \tag{2}$$

Proof: Suppose X follows an ex-Gaussian distribution (\rightarrow Definition II/3.11.1). Then $X = A + B$, where A and B are independent (\rightarrow Definition I/1.3.6), A is normally distributed (\rightarrow Definition

II/3.2.1) with mean (\rightarrow Proof II/3.2.16) μ and variance (\rightarrow Proof II/3.2.19) σ^2 , and B is exponentially distributed (\rightarrow Definition II/3.5.1) with rate λ . Then, the probability density function (\rightarrow Proof 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 Proof 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 Proof I/1.6.7) $X = A + B$ is given by taking the convolution of f_A and f_B :

$$\begin{aligned} f_X(t) &= \int_{-\infty}^{\infty} f_A(x) f_B(t-x) dx \\ &= \int_{-\infty}^t f_A(x) f_B(t-x) dx + \int_t^{\infty} f_A(x) f_B(t-x) dx \\ &= \int_{-\infty}^t f_A(x) f_B(t-x) dx, \end{aligned} \quad (5)$$

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):

$$\begin{aligned} f_X(t) &= \int_{-\infty}^t \frac{1}{\sigma\sqrt{2\pi}} \exp \left[-\frac{1}{2} \left(\frac{x-\mu}{\sigma} \right)^2 \right] \cdot \lambda \exp[-\lambda(t-x)] dx \\ &= \frac{\lambda}{\sigma\sqrt{2\pi}} \int_{-\infty}^t \exp \left[-\frac{1}{2} \left(\frac{x-\mu}{\sigma} \right)^2 \right] \cdot \exp[-\lambda t + \lambda x] dx \\ &= \frac{\lambda}{\sigma\sqrt{2\pi}} \int_{-\infty}^t \exp \left[-\frac{1}{2} \left(\frac{x-\mu}{\sigma} \right)^2 \right] \cdot \exp[-\lambda t] \cdot \exp[\lambda x] dx \\ &= \frac{\lambda \exp[-\lambda t]}{\sigma\sqrt{2\pi}} \int_{-\infty}^t \exp \left[-\frac{1}{2} \left(\frac{x-\mu}{\sigma} \right)^2 + \lambda x \right] dx. \end{aligned} \quad (6)$$

We can further simplify the integrand with a substitution; to this end, let

$$y = g(x) = \frac{x-\mu}{\sigma} - \lambda\sigma \quad (7)$$

This gives the following three identities:

$$\frac{dy}{dx} = \frac{1}{\sigma}, \quad \text{or equivalently, } dx = \sigma dy, \quad (8)$$

$$\frac{x-\mu}{\sigma} = y + \lambda\sigma, \quad \text{and} \quad (9)$$

$$x = y\sigma + \lambda\sigma^2 + \mu . \quad (10)$$

Substituting these identities into (6) gives

$$\begin{aligned}
f_X(t) &= \frac{\lambda \exp[-\lambda t]}{\sigma \sqrt{2\pi}} \int_{-\infty}^{g(t)} \exp \left[-\frac{1}{2}(y + \lambda\sigma)^2 + \lambda(y\sigma + \lambda\sigma^2 + \mu) \right] \sigma dy \\
&= \frac{\lambda \sigma \exp[-\lambda t]}{\sigma \sqrt{2\pi}} \int_{-\infty}^{\frac{x-\mu}{\sigma} + \lambda\sigma} \exp \left[-\frac{1}{2}(y^2 + 2y\lambda\sigma + \lambda^2\sigma^2) + \lambda y\sigma + \lambda^2\sigma^2 + \lambda\mu \right] dy \\
&= \frac{\lambda \exp[-\lambda t]}{\sqrt{2\pi}} \int_{-\infty}^{\frac{x-\mu}{\sigma} + \lambda\sigma} \exp \left[-\frac{1}{2}y^2 - y\lambda\sigma - \frac{\lambda^2\sigma^2}{2} + \lambda y\sigma + \lambda^2\sigma^2 + \lambda\mu \right] dy \\
&= \frac{\lambda \exp[-\lambda t]}{\sqrt{2\pi}} \int_{-\infty}^{\frac{x-\mu}{\sigma} + \lambda\sigma} \exp \left[-\frac{1}{2}y^2 \right] \cdot \exp \left[\frac{\lambda^2\sigma^2}{2} + \lambda\mu \right] dy \\
&= \frac{\lambda \exp[-\lambda t]}{\sqrt{2\pi}} \cdot \exp \left[\frac{\lambda^2\sigma^2}{2} + \lambda\mu \right] \int_{-\infty}^{\frac{x-\mu}{\sigma} + \lambda\sigma} \exp \left[-\frac{1}{2}y^2 \right] \cdot dy \\
&= \frac{\lambda}{\sqrt{2\pi}} \cdot \exp \left[-\lambda t + \frac{\lambda^2\sigma^2}{2} + \lambda\mu \right] \int_{-\infty}^{\frac{x-\mu}{\sigma} + \lambda\sigma} \exp \left[-\frac{1}{2}y^2 \right] \cdot dy \\
&= \frac{\lambda}{\sqrt{2\pi}} \cdot \exp \left[\frac{\lambda^2\sigma^2}{2} - \lambda(t - \mu) \right] \int_{-\infty}^{\frac{x-\mu}{\sigma} + \lambda\sigma} \exp \left[-\frac{1}{2}y^2 \right] \cdot dy .
\end{aligned} \quad (11)$$

This finishes the proof of (2).

Sources:

- original work

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3.11.3 Moment-generating function

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following an ex-Gaussian distribution (\rightarrow Definition II/3.11.1):

$$X \sim \text{ex-Gaussian}(\mu, \sigma, \lambda) . \quad (1)$$

Then, the moment generating function (\rightarrow Definition I/1.6.27) of X is

$$M_X(t) = \left(\frac{\lambda}{\lambda - t} \right) \exp \left[\mu t + \frac{1}{2} \sigma^2 t^2 \right] . \quad (2)$$

Proof: Suppose X follows an ex-Gaussian distribution (\rightarrow Definition II/3.11.1). Then, $X = A + B$ where A and B are independent (\rightarrow Definition I/1.3.6), A is normally distributed (\rightarrow Definition II/3.2.1) with mean (\rightarrow Proof II/3.2.16) μ and variance (\rightarrow Proof II/3.2.19) σ^2 , and B is exponentially distributed (\rightarrow Definition II/3.5.1) with rate λ . Then the moment generating function (\rightarrow Proof II/3.2.11) for A is given by

$$M_A(t) = \exp \left[\mu t + \frac{1}{2} \sigma^2 t^2 \right] \quad (3)$$

and the moment generating function (\rightarrow Proof II/3.5.4) for B is given by

$$M_B(t) = \frac{\lambda}{\lambda - t} . \quad (4)$$

By definition, X is a linear combination of independent random variables A and B , so the moment generating function (\rightarrow Proof I/1.6.30) of X is the product of $M_A(t)$ and $M_B(t)$. That is,

$$\begin{aligned} M_X(t) &= M_A(t) \cdot M_B(t) \\ &= \exp \left[\mu t + \frac{1}{2} \sigma^2 t^2 \right] \cdot \left(\frac{\lambda}{\lambda - t} \right) \\ &= \left(\frac{\lambda}{\lambda - t} \right) \exp \left[\mu t + \frac{1}{2} \sigma^2 t^2 \right] . \end{aligned} \quad (5)$$

This finishes the proof of (2).

Sources:

- original work

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3.11.4 Mean

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following an ex-Gaussian distribution (\rightarrow Definition II/3.11.1):

$$X \sim \text{ex-Gaussian}(\mu, \sigma, \lambda) . \quad (1)$$

Then, the mean or expected value (\rightarrow Definition I/1.7.1) of X is

$$E(X) = \mu + \frac{1}{\lambda} . \quad (2)$$

Proof: The mean or expected value $E(X)$ is the first raw moment (\rightarrow Definition I/1.15.1) of X , so we can use (\rightarrow Proof I/1.15.2) the moment-generating function of the ex-Gaussian distribution (\rightarrow Proof II/3.11.3) to calculate

$$E(X) = M'_X(0) . \quad (3)$$

First, we differentiate

$$M_X(t) = \left(\frac{\lambda}{\lambda - t} \right) \exp \left[\mu t + \frac{1}{2} \sigma^2 t^2 \right] \quad (4)$$

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:

$$\begin{aligned}
M'_X(0) &= \left(\frac{\lambda}{\lambda - 0} \right) \cdot \exp \left[\mu \cdot 0 + \frac{1}{2} \sigma^2 \cdot 0^2 \right] \cdot \left[\frac{1}{\lambda - 0} + \mu + \sigma^2 \cdot 0 \right] \\
&= 1 \cdot 1 \cdot \left[\frac{1}{\lambda} + \mu \right] \\
&= \mu + \frac{1}{\lambda} .
\end{aligned} \tag{6}$$

Sources:

- original work

Metadata: ID: P405 | shortcut: exg-mean | author: tomfaulkenberry | date: 2023-04-19, 12:00.

3.11.5 Variance

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following an ex-Gaussian distribution (\rightarrow Definition II/3.11.1):

$$X \sim \text{ex-Gaussian}(\mu, \sigma, \lambda) . \tag{1}$$

Then, the variance (\rightarrow Definition I/1.8.1) of X is

$$\text{Var}(X) = \sigma^2 + \frac{1}{\lambda^2} . \tag{2}$$

Proof: To compute the variance of X , we partition the variance into expected values (\rightarrow Proof I/1.8.3):

$$\text{Var}(X) = \text{E}(X^2) - \text{E}(X)^2 . \tag{3}$$

We then use the moment-generating function of the ex-Gaussian distribution (\rightarrow Proof II/3.11.3) to calculate

$$\text{E}(X^2) = M''_X(0) \tag{4}$$

based on the relationship between raw moment and moment-generating function (\rightarrow Proof I/1.15.2). First, we differentiate

$$M_X(t) = \left(\frac{\lambda}{\lambda - t} \right) \exp \left[\mu t + \frac{1}{2} \sigma^2 t^2 \right] \tag{5}$$

with respect to t . Using the product rule and chain rule gives:

$$\begin{aligned}
M'_X(t) &= \frac{\lambda}{(\lambda-t)^2} \exp \left[\mu t + \frac{1}{2} \sigma^2 t^2 \right] + \left(\frac{\lambda}{\lambda-t} \right) \exp \left[\mu t + \frac{1}{2} \sigma^2 t^2 \right] (\mu + \sigma^2 t) \\
&= \left(\frac{\lambda}{\lambda-t} \right) \cdot \exp \left[\mu t + \frac{1}{2} \sigma^2 t^2 \right] \cdot \left[\frac{1}{\lambda-t} + \mu + \sigma^2 t \right] \\
&= M_X(t) \cdot \left[\frac{1}{\lambda-t} + \mu + \sigma^2 t \right].
\end{aligned} \tag{6}$$

We now use the product rule to obtain the second derivative:

$$\begin{aligned}
M''_X(t) &= M'_X(t) \cdot \left[\frac{1}{\lambda-t} + \mu + \sigma^2 t \right] + M_X(t) \cdot \left[\frac{1}{(\lambda-t)^2} + \sigma^2 \right] \\
&\stackrel{(6)}{=} M_X(t) \cdot \left[\frac{1}{\lambda-t} + \mu + \sigma^2 t \right]^2 + M_X(t) \cdot \left[\frac{1}{(\lambda-t)^2} + \sigma^2 \right] \\
&= M_X(t) \cdot \left[\left(\frac{1}{\lambda-t} + \mu + \sigma^2 t \right)^2 + \frac{1}{(\lambda-t)^2} + \sigma^2 \right] \\
&= \left(\frac{\lambda}{\lambda-t} \right) \cdot \exp \left[\mu t + \frac{1}{2} \sigma^2 t^2 \right] \cdot \left[\left(\frac{1}{\lambda-t} + \mu + \sigma^2 t \right)^2 + \frac{1}{(\lambda-t)^2} + \sigma^2 \right]
\end{aligned} \tag{7}$$

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 Proof 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).

Sources:

- original work

Metadata: ID: P406 | shortcut: exg-var | author: tomfaulkenberry | date: 2023-04-19, 12:00.

3.11.6 Skewness

Theorem: Let X be a random variable (\rightarrow Definition I/1.2.2) following an ex-Gaussian distribution (\rightarrow Definition II/3.11.1):

$$X \sim \text{ex-Gaussian}(\mu, \sigma, \lambda) . \quad (1)$$

Then the skewness (\rightarrow Definition I/1.9.1) of X is

$$\text{Skew}(X) = \frac{2}{\lambda^3 \left(\sigma^2 + \frac{1}{\lambda^2} \right)^{\frac{3}{2}}} . \quad (2)$$

Proof:

To compute the skewness of X , we partition the skewness into expected values (\rightarrow Proof I/1.9.2):

$$\text{Skew}(X) = \frac{\text{E}(X^3) - 3\mu\sigma^2 - \mu^3}{\sigma^3} , \quad (3)$$

where μ and σ are the mean and standard deviation of X , respectively. 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

$$\text{Skew}(X) = \frac{\text{E}(X^3) - 3 \cdot \text{E}(X) \cdot \text{Var}(X) - \text{E}(X)^3}{\text{Var}(X)^{\frac{3}{2}}} . \quad (4)$$

Since X follows an ex-Gaussian distribution (\rightarrow Definition II/3.11.1), the mean (\rightarrow Proof II/3.11.4) of X is given by

$$\text{E}(X) = \mu + \frac{1}{\lambda} \quad (5)$$

and the variance (\rightarrow Proof 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 $\text{E}(X^3)$. To do this, we use the moment-generating function of the ex-Gaussian distribution (\rightarrow Proof II/3.11.3) to calculate

$$\text{E}(X^3) = M_X'''(0) \quad (7)$$

based on the relationship between raw moment and moment-generating function (\rightarrow Proof I/1.15.2). First, we differentiate the moment-generating function of the ex-Gaussian distribution (\rightarrow Proof 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:

$$\begin{aligned} E(X^3) &= M'''_X(0) \\ &= M'_X(0) \left[\left(\frac{1}{\lambda} + \mu \right)^2 + \frac{1}{\lambda^2} + \sigma^2 \right] + M_X(0) \left[2 \left(\frac{1}{\lambda} + \mu \right) \left(\frac{1}{\lambda^2} + \sigma^2 \right) + \frac{2}{\lambda^3} \right] \\ &= \left(\mu + \frac{1}{\lambda} \right) \left(\frac{1}{\lambda^2} + \frac{2\mu}{\lambda} + \mu^2 + \frac{1}{\lambda^2} + \sigma^2 \right) + \left(\frac{2}{\lambda^3} + \frac{2\sigma^2}{\lambda} + \frac{2\mu}{\lambda^2} + 2\mu\sigma^2 + \frac{2}{\lambda^3} \right) \\ &= \left(\mu + \frac{1}{\lambda} \right) \left(\frac{2}{\lambda^2} + \frac{2\mu}{\lambda} + \mu^2 + \sigma^2 \right) + \left(\frac{4}{\lambda^3} + \frac{2\sigma^2}{\lambda} + \frac{2\mu}{\lambda^2} + 2\mu\sigma^2 \right) \\ &= \frac{2\mu}{\lambda^2} + \frac{2\mu^2}{\lambda} + \mu^3 + \mu\sigma^2 + \frac{2}{\lambda^3} + \frac{2\mu}{\lambda^2} + \frac{\mu^2}{\lambda} + \frac{\sigma^2}{\lambda} + \frac{4}{\lambda^3} + \frac{2\sigma^2}{\lambda} + \frac{2\mu}{\lambda^2} + 2\mu\sigma^2 \\ &= \frac{6\mu}{\lambda^2} + \frac{6}{\lambda^3} + \frac{3\mu^2 + 3\sigma^2}{\lambda} + 3\mu\sigma^2 + \mu^3. \end{aligned} \quad (12)$$

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).

Sources:

- original work

Metadata: ID: P408 | shortcut: exg-skew | author: tomfaulkenberry | date: 2023-04-21, 12:00.

4 Multivariate continuous distributions

4.1 Multivariate normal distribution

4.1.1 Definition

Definition: Let X be an $n \times 1$ random vector (\rightarrow Definition 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 Definition I/1.6.6) 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 $n \times 1$ 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.

Metadata: ID: D1 | shortcut: mvn | author: JoramSoch | date: 2020-01-22, 05:20.

4.1.2 Relationship to chi-squared distribution

Theorem: Let x be an $n \times 1$ random vector (\rightarrow Definition I/1.2.3) following a multivariate normal distribution (\rightarrow Definition II/4.1.1) with zero mean (\rightarrow Definition I/1.7.13) and arbitrary covariance matrix (\rightarrow Proof II/4.1.6) Σ :

$$x \sim \mathcal{N}(0, \Sigma) . \quad (1)$$

Then, the quadratic form of x , weighted by Σ , follows a chi-squared distribution (\rightarrow Definition II/3.7.1) with n degrees of freedom (\rightarrow Definition “dof”):

$$y = x^T \Sigma^{-1} x \sim \chi^2(n) . \quad (2)$$

Proof: Define a new random vector (\rightarrow Definition 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 Definition I/1.10.9) and thus positive semi-definite (\rightarrow Proof I/1.10.13). Due to the linear transformation theorem (\rightarrow Proof II/4.1.9), z is distributed as

$$\begin{aligned} z &\sim \mathcal{N} \left(\Sigma^{-1/2} 0, \Sigma^{-1/2} \Sigma \Sigma^{-1/2 T} \right) \\ &\sim \mathcal{N} \left(\Sigma^{-1/2} 0, \Sigma^{-1/2} \Sigma^{1/2} \Sigma^{1/2} \Sigma^{-1/2} \right) \\ &\sim \mathcal{N}(0, I_n) , \end{aligned} \quad (4)$$

i.e. each entry of this vector follows (\rightarrow Proof II/4.1.10) a standard normal distribution (\rightarrow Definition II/3.2.2):

$$z_i \sim \mathcal{N}(0, 1) \quad \text{for all } i = 1, \dots, n. \quad (5)$$

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 Definition II/3.2.2) random variables (\rightarrow Definition 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 Definition 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.

Metadata: ID: P395 | shortcut: mvn-chi2 | author: JoramSoch | date: 2022-12-20, 16:27.

4.1.3 Special case of matrix-normal distribution

Theorem: The multivariate normal distribution (\rightarrow Definition II/4.1.1) is a special case of the matrix-normal distribution (\rightarrow Definition II/5.1.1) with number of variables $p = 1$, i.e. random matrix (\rightarrow Definition 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 Proof 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 Proof 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.

Metadata: ID: P330 | shortcut: mvn-matn | author: JoramSoch | date: 2022-07-31, 11:00.

4.1.4 Probability density function

Theorem: Let X be a random vector (\rightarrow Definition I/1.2.3) following a multivariate normal distribution (\rightarrow Definition II/4.1.1):

$$X \sim \mathcal{N}(\mu, \Sigma) . \quad (1)$$

Then, the probability density function (\rightarrow Definition I/1.6.6) 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 Definition II/4.1.1).

Sources:

- original work

Metadata: ID: P34 | shortcut: mvn-pdf | author: JoramSoch | date: 2020-01-27, 15:23.

4.1.5 Mean

Theorem: Let x follow a multivariate normal distribution (\rightarrow Definition II/4.1.1):

$$x \sim \mathcal{N}(\mu, \Sigma) . \quad (1)$$

Then, the mean or expected value (\rightarrow Definition I/1.7.1) of x is

$$\mathbb{E}(x) = \mu . \quad (2)$$

Proof:

1) First, consider a set of independent (\rightarrow Definition I/1.3.6) and standard normally (\rightarrow Definition II/3.2.2) distributed random variables (\rightarrow Definition 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 Proof II/4.1.12) distributed random vector (\rightarrow Definition I/1.2.3):

$$z \sim \mathcal{N}(0_n, I_n) . \quad (4)$$

By definition, the expected value of a random vector is equal to the vector of all expected values (\rightarrow Definition I/1.7.13):

$$\mathbb{E}(z) = \mathbb{E} \left(\begin{bmatrix} z_1 \\ \vdots \\ z_n \end{bmatrix} \right) = \begin{bmatrix} \mathbb{E}(z_1) \\ \vdots \\ \mathbb{E}(z_n) \end{bmatrix} . \quad (5)$$

Because the expected value of all its entries is zero (\rightarrow Proof 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 Definition II/4.1.1). Then, x can be represented as a linear transformation of (\rightarrow Proof II/4.1.9) z :

$$x = Az + \mu \sim \mathcal{N}(A0_n + \mu, AI_nA^T) = \mathcal{N}(\mu, \Sigma) . \quad (7)$$

Thus, the expected value (\rightarrow Definition I/1.7.1) of x can be written as:

$$\mathbb{E}(x) = \mathbb{E}(Az + \mu) . \quad (8)$$

With the linearity of the expected value (\rightarrow Proof I/1.7.5), 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>.

Metadata: ID: P339 | shortcut: mvn-mean | author: JoramSoch | date: 2022-09-15, 02:22.

4.1.6 Covariance

Theorem: Let x follow a multivariate normal distribution (\rightarrow Definition II/4.1.1):

$$x \sim \mathcal{N}(\mu, \Sigma) . \quad (1)$$

Then, the covariance matrix (\rightarrow Definition I/1.10.9) of x is

$$\text{Cov}(x) = \Sigma . \quad (2)$$

Proof:

1) First, consider a set of independent (\rightarrow Definition I/1.3.6) and standard normally (\rightarrow Definition II/3.2.2) distributed random variables (\rightarrow Definition 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 Proof II/4.1.12) distributed random vector (\rightarrow Definition I/1.2.3):

$$z \sim \mathcal{N}(0_n, I_n). \quad (4)$$

Because the covariance is zero for independent random variables (\rightarrow Proof I/1.10.6), 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 Proof 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 Definition I/1.10.9) 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 Definition II/4.1.1). Then, x can be represented as a linear transformation of (\rightarrow Proof II/4.1.9) z :

$$x = Az + \mu \sim \mathcal{N}(A0_n + \mu, AI_nA^T) = \mathcal{N}(\mu, \Sigma). \quad (8)$$

Thus, the covariance (\rightarrow Definition I/1.10.1) 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 Proof I/1.10.14)

$$\text{Cov}(x + a) = \text{Cov}(x) \quad (10)$$

and the scaling of the covariance matrix upon multiplication (\rightarrow Proof I/1.10.15)

$$\text{Cov}(Ax) = A\text{Cov}(x)A^T, \quad (11)$$

this becomes:

$$\begin{aligned} \text{Cov}(x) &= \text{Cov}(Az + \mu) \\ &\stackrel{(10)}{=} \text{Cov}(Az) \\ &\stackrel{(11)}{=} A\text{Cov}(z)A^T \\ &\stackrel{(7)}{=} AI_nA^T \\ &= AA^T \\ &= \Sigma. \end{aligned} \quad (12)$$

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>.

Metadata: ID: P340 | shortcut: mvn-cov | author: JoramSoch | date: 2022-09-15, 08:41.

4.1.7 Differential entropy

Theorem: Let x follow a multivariate normal distribution (\rightarrow Definition II/4.1.1)

$$x \sim \mathcal{N}(\mu, \Sigma) . \quad (1)$$

Then, the differential entropy (\rightarrow Definition 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 Definition 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 Definition I/1.7.1)

$$h(X) = -E [\ln p(x)] . \quad (4)$$

With the probability density function of the multivariate normal distribution (\rightarrow Proof 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:

- Kiuahnm (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>

Metadata: ID: P100 | shortcut: mvn-dent | author: JoramSoch | date: 2020-05-14, 19:49.

4.1.8 Kullback-Leibler divergence

Theorem: Let x be an $n \times 1$ random vector (\rightarrow Definition I/1.2.3). Assume two multivariate normal distributions (\rightarrow Definition II/4.1.1) P and Q specifying the probability distribution of x as

$$\begin{aligned} P : x &\sim \mathcal{N}(\mu_1, \Sigma_1) \\ Q : x &\sim \mathcal{N}(\mu_2, \Sigma_2) . \end{aligned} \quad (1)$$

Then, the Kullback-Leibler divergence (\rightarrow Definition I/2.5.1) of P from Q is given by

$$\text{KL}[P || Q] = \frac{1}{2} \left[(\mu_2 - \mu_1)^T \Sigma_2^{-1} (\mu_2 - \mu_1) + \text{tr}(\Sigma_2^{-1} \Sigma_1) - \ln \frac{|\Sigma_1|}{|\Sigma_2|} - n \right] . \quad (2)$$

Proof: The KL divergence for a continuous random variable (\rightarrow Definition I/2.5.1) is given by

$$\text{KL}[P || Q] = \int_{\mathcal{X}} p(x) \ln \frac{p(x)}{q(x)} dx \quad (3)$$

which, applied to the multivariate normal distributions (\rightarrow Definition II/4.1.1) in (1), yields

$$\begin{aligned} \text{KL}[P || Q] &= \int_{\mathbb{R}^n} \mathcal{N}(x; \mu_1, \Sigma_1) \ln \frac{\mathcal{N}(x; \mu_1, \Sigma_1)}{\mathcal{N}(x; \mu_2, \Sigma_2)} dx \\ &= \left\langle \ln \frac{\mathcal{N}(x; \mu_1, \Sigma_1)}{\mathcal{N}(x; \mu_2, \Sigma_2)} \right\rangle_{p(x)} . \end{aligned} \quad (4)$$

Using the probability density function of the multivariate normal distribution (\rightarrow Proof II/4.1.4), this becomes:

$$\begin{aligned} \text{KL}[P || Q] &= \left\langle \ln \frac{\frac{1}{\sqrt{(2\pi)^n |\Sigma_1|}} \cdot \exp \left[-\frac{1}{2} (x - \mu_1)^T \Sigma_1^{-1} (x - \mu_1) \right]}{\frac{1}{\sqrt{(2\pi)^n |\Sigma_2|}} \cdot \exp \left[-\frac{1}{2} (x - \mu_2)^T \Sigma_2^{-1} (x - \mu_2) \right]} \right\rangle_{p(x)} \\ &= \left\langle \frac{1}{2} \ln \frac{|\Sigma_2|}{|\Sigma_1|} - \frac{1}{2} (x - \mu_1)^T \Sigma_1^{-1} (x - \mu_1) + \frac{1}{2} (x - \mu_2)^T \Sigma_2^{-1} (x - \mu_2) \right\rangle_{p(x)} \\ &= \frac{1}{2} \left\langle \ln \frac{|\Sigma_2|}{|\Sigma_1|} - (x - \mu_1)^T \Sigma_1^{-1} (x - \mu_1) + (x - \mu_2)^T \Sigma_2^{-1} (x - \mu_2) \right\rangle_{p(x)} . \end{aligned} \quad (5)$$

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:

$$\begin{aligned} \text{KL}[P || Q] &= \frac{1}{2} \left\langle \ln \frac{|\Sigma_2|}{|\Sigma_1|} - \text{tr} [\Sigma_1^{-1}(x - \mu_1)(x - \mu_1)^T] + \text{tr} [\Sigma_2^{-1}(x - \mu_2)(x - \mu_2)^T] \right\rangle_{p(x)} \\ &= \frac{1}{2} \left\langle \ln \frac{|\Sigma_2|}{|\Sigma_1|} - \text{tr} [\Sigma_1^{-1}(x - \mu_1)(x - \mu_1)^T] + \text{tr} [\Sigma_2^{-1}(xx^T - 2\mu_2x^T + \mu_2\mu_2^T)] \right\rangle_{p(x)}. \end{aligned} \quad (6)$$

Because trace function and expected value are both linear operators (\rightarrow Proof I/1.7.8), the expectation can be moved inside the trace:

$$\begin{aligned} \text{KL}[P || Q] &= \frac{1}{2} \left(\ln \frac{|\Sigma_2|}{|\Sigma_1|} - \text{tr} \left[\Sigma_1^{-1} \langle (x - \mu_1)(x - \mu_1)^T \rangle_{p(x)} \right] + \text{tr} \left[\Sigma_2^{-1} \langle xx^T - 2\mu_2x^T + \mu_2\mu_2^T \rangle_{p(x)} \right] \right) \\ &= \frac{1}{2} \left(\ln \frac{|\Sigma_2|}{|\Sigma_1|} - \text{tr} \left[\Sigma_1^{-1} \langle (x - \mu_1)(x - \mu_1)^T \rangle_{p(x)} \right] + \text{tr} \left[\Sigma_2^{-1} \left(\langle xx^T \rangle_{p(x)} - \langle 2\mu_2x^T \rangle_{p(x)} + \langle \mu_2\mu_2^T \rangle_{p(x)} \right) \right] \right) \end{aligned} \quad (7)$$

Using the expectation of a linear form for the multivariate normal distribution (\rightarrow Proof II/4.1.9)

$$x \sim \mathcal{N}(\mu, \Sigma) \quad \Rightarrow \quad \langle Ax \rangle = A\mu \quad (8)$$

and the expectation of a quadratic form for the multivariate normal distribution (\rightarrow Proof I/1.7.9)

$$x \sim \mathcal{N}(\mu, \Sigma) \quad \Rightarrow \quad \langle x^T Ax \rangle = \mu^T A\mu + \text{tr}(A\Sigma), \quad (9)$$

the Kullback-Leibler divergence from (7) becomes:

$$\begin{aligned} \text{KL}[P || Q] &= \frac{1}{2} \left(\ln \frac{|\Sigma_2|}{|\Sigma_1|} - \text{tr} [\Sigma_1^{-1}\Sigma_1] + \text{tr} [\Sigma_2^{-1}(\Sigma_1 + \mu_1\mu_1^T - 2\mu_2\mu_1^T + \mu_2\mu_2^T)] \right) \\ &= \frac{1}{2} \left(\ln \frac{|\Sigma_2|}{|\Sigma_1|} - \text{tr} [I_n] + \text{tr} [\Sigma_2^{-1}\Sigma_1] + \text{tr} [\Sigma_2^{-1}(\mu_1\mu_1^T - 2\mu_2\mu_1^T + \mu_2\mu_2^T)] \right) \\ &= \frac{1}{2} \left(\ln \frac{|\Sigma_2|}{|\Sigma_1|} - n + \text{tr} [\Sigma_2^{-1}\Sigma_1] + \text{tr} [\mu_1^T \Sigma_2^{-1} \mu_1 - 2\mu_1^T \Sigma_2^{-1} \mu_2 + \mu_2^T \Sigma_2^{-1} \mu_2] \right) \\ &= \frac{1}{2} \left[\ln \frac{|\Sigma_2|}{|\Sigma_1|} - n + \text{tr} [\Sigma_2^{-1}\Sigma_1] + (\mu_2 - \mu_1)^T \Sigma_2^{-1} (\mu_2 - \mu_1) \right]. \end{aligned} \quad (10)$$

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.

Metadata: ID: P92 | shortcut: mvn-kl | author: JoramSoch | date: 2020-05-05, 06:57.

4.1.9 Linear transformation

Theorem: Let x follow a multivariate normal distribution (\rightarrow Definition 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 Definition I/1.6.27) x is

$$M_x(t) = \mathbb{E}(\exp[t^T x]) \quad (3)$$

and therefore the moment-generating function of the random vector y is given by

$$\begin{aligned} M_y(t) &\stackrel{(2)}{=} \mathbb{E}(\exp[t^T(Ax + b)]) \\ &= \mathbb{E}(\exp[t^T Ax] \cdot \exp[t^T b]) \\ &= \exp[t^T b] \cdot \mathbb{E}(\exp[t^T Ax]) \\ &\stackrel{(3)}{=} \exp[t^T b] \cdot M_x(A^T t) . \end{aligned} \quad (4)$$

The moment-generating function of the multivariate normal distribution (\rightarrow Proof “mvn-mgf”) 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>.

Metadata: ID: P1 | shortcut: mvn-lett | author: JoramSoch | date: 2019-08-27, 12:14.

4.1.10 Marginal distributions

Theorem: Let x follow a multivariate normal distribution (\rightarrow Definition II/4.1.1):

$$x \sim \mathcal{N}(\mu, \Sigma) . \quad (1)$$

Then, the marginal distribution (\rightarrow Definition 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 Proof II/4.1.9) to give

$$x_s \sim \mathcal{N}(S\mu, S\Sigma S^T) . \quad (4)$$

Finally, we see that $S\mu = \mu_s$ and $S\Sigma S^T = \Sigma_s$.

Sources:

- original work

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4.1.11 Conditional distributions

Theorem: Let x follow a multivariate normal distribution (\rightarrow Definition II/4.1.1)

$$x \sim \mathcal{N}(\mu, \Sigma) . \quad (1)$$

Then, the conditional distribution (\rightarrow Definition 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 Definition I/1.7.1) and covariance (\rightarrow Definition I/1.10.1) 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

$$\begin{aligned}\mu &= \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix} \\ \Sigma &= \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix} .\end{aligned}\tag{4}$$

Proof: Without loss of generality, we assume that, in parallel to (4),

$$x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}\tag{5}$$

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 Definition I/1.5.2) of x_1 and x_2 is:

$$x_1, x_2 \sim \mathcal{N}(\mu, \Sigma) .\tag{6}$$

Moreover, the marginal distribution (\rightarrow Definition I/1.5.3) of x_2 follows from (\rightarrow Proof II/4.1.10) (1) and (4) as

$$x_2 \sim \mathcal{N}(\mu_2, \Sigma_{22}) .\tag{7}$$

According to the law of conditional probability (\rightarrow Definition I/1.3.4), it holds that

$$p(x_1|x_2) = \frac{p(x_1, x_2)}{p(x_2)}\tag{8}$$

Applying (6) and (7) to (8), we have:

$$p(x_1|x_2) = \frac{\mathcal{N}(x; \mu, \Sigma)}{\mathcal{N}(x_2; \mu_2, \Sigma_{22})} .\tag{9}$$

Using the probability density function of the multivariate normal distribution (\rightarrow Proof II/4.1.4), this becomes:

$$\begin{aligned}p(x_1|x_2) &= \frac{1/\sqrt{(2\pi)^n |\Sigma|} \cdot \exp \left[-\frac{1}{2}(x - \mu)^T \Sigma^{-1} (x - \mu) \right]}{1/\sqrt{(2\pi)^{n_2} |\Sigma_{22}|} \cdot \exp \left[-\frac{1}{2}(x_2 - \mu_2)^T \Sigma_{22}^{-1} (x_2 - \mu_2) \right]} \\ &= \frac{1}{\sqrt{(2\pi)^{n-n_2}}} \cdot \sqrt{\frac{|\Sigma_{22}|}{|\Sigma|}} \cdot \exp \left[-\frac{1}{2}(x - \mu)^T \Sigma^{-1} (x - \mu) + \frac{1}{2}(x_2 - \mu_2)^T \Sigma_{22}^{-1} (x_2 - \mu_2) \right] .\end{aligned}\tag{10}$$

Writing the inverse of Σ as

$$\Sigma^{-1} = \begin{bmatrix} \Sigma^{11} & \Sigma^{12} \\ \Sigma^{21} & \Sigma^{22} \end{bmatrix}\tag{11}$$

and applying (4) to (10), we get:

$$\begin{aligned}
p(x_1|x_2) &= \frac{1}{\sqrt{(2\pi)^{n-n_2}}} \cdot \sqrt{\frac{|\Sigma_{22}|}{|\Sigma|}} \cdot \\
&\exp \left[-\frac{1}{2} \left(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} - \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix} \right)^T \begin{bmatrix} \Sigma^{11} & \Sigma^{12} \\ \Sigma^{21} & \Sigma^{22} \end{bmatrix} \left(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} - \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix} \right) \right. \\
&\quad \left. + \frac{1}{2} (x_2 - \mu_2)^T \Sigma_{22}^{-1} (x_2 - \mu_2) \right] .
\end{aligned} \tag{12}$$

Multiplying out within the exponent of (12), we have

$$\begin{aligned}
p(x_1|x_2) &= \frac{1}{\sqrt{(2\pi)^{n-n_2}}} \cdot \sqrt{\frac{|\Sigma_{22}|}{|\Sigma|}} \cdot \\
&\exp \left[-\frac{1}{2} \left((x_1 - \mu_1)^T \Sigma^{11} (x_1 - \mu_1) + 2(x_1 - \mu_1)^T \Sigma^{12} (x_2 - \mu_2) + (x_2 - \mu_2)^T \Sigma^{22} (x_2 - \mu_2) \right) \right. \\
&\quad \left. + \frac{1}{2} (x_2 - \mu_2)^T \Sigma_{22}^{-1} (x_2 - \mu_2) \right]
\end{aligned} \tag{13}$$

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

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix}^{-1} = \begin{bmatrix} (A - BD^{-1}C)^{-1} & -(A - BD^{-1}C)^{-1}BD^{-1} \\ -D^{-1}C(A - BD^{-1}C)^{-1} & D^{-1} + D^{-1}C(A - BD^{-1}C)^{-1}BD^{-1} \end{bmatrix}, \tag{14}$$

thus the inverse of Σ in (11) is

$$\begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix}^{-1} = \begin{bmatrix} (\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})^{-1} & -(\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})^{-1}\Sigma_{12}\Sigma_{22}^{-1} \\ -\Sigma_{22}^{-1}\Sigma_{21}(\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})^{-1} & \Sigma_{22}^{-1} + \Sigma_{22}^{-1}\Sigma_{21}(\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})^{-1}\Sigma_{12}\Sigma_{22}^{-1} \end{bmatrix}. \tag{15}$$

Plugging this into (13), we have:

$$\begin{aligned}
p(x_1|x_2) &= \frac{1}{\sqrt{(2\pi)^{n-n_2}}} \cdot \sqrt{\frac{|\Sigma_{22}|}{|\Sigma|}} \cdot \\
&\exp \left[-\frac{1}{2} \left((x_1 - \mu_1)^T (\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})^{-1} (x_1 - \mu_1) - \right. \right. \\
&\quad 2(x_1 - \mu_1)^T (\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})^{-1} \Sigma_{12} \Sigma_{22}^{-1} (x_2 - \mu_2) + \\
&\quad (x_2 - \mu_2)^T \left[\Sigma_{22}^{-1} + \Sigma_{22}^{-1} \Sigma_{21} (\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})^{-1} \Sigma_{12} \Sigma_{22}^{-1} \right] (x_2 - \mu_2) \left. \right) \\
&\quad \left. + \frac{1}{2} ((x_2 - \mu_2)^T \Sigma_{22}^{-1} (x_2 - \mu_2)) \right] .
\end{aligned} \tag{16}$$

Eliminating some terms, we have:

$$\begin{aligned}
 p(x_1|x_2) &= \frac{1}{\sqrt{(2\pi)^{n-n_2}}} \cdot \sqrt{\frac{|\Sigma_{22}|}{|\Sigma|}} \cdot \\
 &\exp \left[-\frac{1}{2} \left((x_1 - \mu_1)^T (\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})^{-1} (x_1 - \mu_1) - \right. \right. \\
 &\quad 2(x_1 - \mu_1)^T (\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})^{-1} \Sigma_{12}\Sigma_{22}^{-1} (x_2 - \mu_2) + \\
 &\quad \left. \left. (x_2 - \mu_2)^T \Sigma_{22}^{-1} \Sigma_{21} (\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})^{-1} \Sigma_{12}\Sigma_{22}^{-1} (x_2 - \mu_2) \right) \right] .
 \end{aligned} \tag{17}$$

Rearranging the terms, we have

$$\begin{aligned}
 p(x_1|x_2) &= \frac{1}{\sqrt{(2\pi)^{n-n_2}}} \cdot \sqrt{\frac{|\Sigma_{22}|}{|\Sigma|}} \cdot \exp \left[-\frac{1}{2} \cdot \right. \\
 &\quad \left. \left[(x_1 - \mu_1) - \Sigma_{12}\Sigma_{22}^{-1}(x_2 - \mu_2) \right]^T (\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})^{-1} \left[(x_1 - \mu_1) - \Sigma_{12}\Sigma_{22}^{-1}(x_2 - \mu_2) \right] \right] \\
 &= \frac{1}{\sqrt{(2\pi)^{n-n_2}}} \cdot \sqrt{\frac{|\Sigma_{22}|}{|\Sigma|}} \cdot \exp \left[-\frac{1}{2} \cdot \right. \\
 &\quad \left. \left[x_1 - (\mu_1 + \Sigma_{12}\Sigma_{22}^{-1}(x_2 - \mu_2)) \right]^T (\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})^{-1} \left[x_1 - (\mu_1 + \Sigma_{12}\Sigma_{22}^{-1}(x_2 - \mu_2)) \right] \right]
 \end{aligned} \tag{18}$$

where we have used the fact that $\Sigma_{21} = \Sigma_{12}^T$, because Σ is a covariance matrix (\rightarrow Definition I/1.10.9).

The determinant of a block matrix is

$$\begin{vmatrix} A & B \\ C & D \end{vmatrix} = |D| \cdot |A - BD^{-1}C| , \tag{19}$$

such that we have for Σ that

$$\begin{vmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{vmatrix} = |\Sigma_{22}| \cdot |\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}| . \tag{20}$$

With this and $n - n_2 = n_1$, we finally arrive at

$$\begin{aligned}
 p(x_1|x_2) &= \frac{1}{\sqrt{(2\pi)^{n_1} |\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}|}} \cdot \exp \left[-\frac{1}{2} \cdot \right. \\
 &\quad \left. \left[x_1 - (\mu_1 + \Sigma_{12}\Sigma_{22}^{-1}(x_2 - \mu_2)) \right]^T (\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})^{-1} \left[x_1 - (\mu_1 + \Sigma_{12}\Sigma_{22}^{-1}(x_2 - \mu_2)) \right] \right]
 \end{aligned} \tag{21}$$

which is the probability density function of a multivariate normal distribution (\rightarrow Proof II/4.1.4)

$$p(x_1|x_2) = \mathcal{N}(x_1; \mu_{1|2}, \Sigma_{1|2}) \tag{22}$$

with the mean (\rightarrow Definition I/1.7.1) $\mu_{1|2}$ and covariance (\rightarrow Definition I/1.10.1) $\Sigma_{1|2}$ 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.

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4.1.12 Conditions for independence

Theorem: Let x be an $n \times 1$ random vector (\rightarrow Definition I/1.2.3) following a multivariate normal distribution (\rightarrow Definition II/4.1.1):

$$x \sim \mathcal{N}(\mu, \Sigma) . \quad (1)$$

Then, the components of x are statistically independent (\rightarrow Definition I/1.3.6), if and only if the covariance matrix (\rightarrow Definition I/1.10.9) 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 Proof II/4.1.10) where mean (\rightarrow Definition I/1.7.1) and variance (\rightarrow Definition I/1.8.1) 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 Proof 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 Proof 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, we have

$$\begin{aligned}
& \frac{1}{\sqrt{(2\pi)^n |\Sigma|}} \cdot \exp \left[-\frac{1}{2} (x - \mu)^T \Sigma^{-1} (x - \mu) \right] \stackrel{(4),(5)}{=} \prod_{i=1}^n \frac{1}{\sqrt{2\pi\sigma_i^2}} \cdot \exp \left[-\frac{1}{2} \left(\frac{x_i - \mu_i}{\sigma_i} \right)^2 \right] \\
& \frac{1}{\sqrt{(2\pi)^n |\Sigma|}} \cdot \exp \left[-\frac{1}{2} (x - \mu)^T \Sigma^{-1} (x - \mu) \right] = \frac{1}{\sqrt{(2\pi)^n \prod_{i=1}^n \sigma_i^2}} \cdot \exp \left[-\frac{1}{2} \sum_{i=1}^n (x_i - \mu_i) \frac{1}{\sigma_i^2} (x_i - \mu_i) \right] \\
& -\frac{1}{2} \log |\Sigma| - \frac{1}{2} (x - \mu)^T \Sigma^{-1} (x - \mu) = -\frac{1}{2} \sum_{i=1}^n \log \sigma_i^2 - \frac{1}{2} \sum_{i=1}^n (x_i - \mu_i) \frac{1}{\sigma_i^2} (x_i - \mu_i)
\end{aligned} \tag{7}$$

which is only fulfilled by a diagonal covariance matrix

$$\Sigma = \text{diag}([\sigma_1^2, \dots, \sigma_n^2]) , \tag{8}$$

because the determinant of a diagonal matrix is a product

$$|\text{diag}([a_1, \dots, a_n])| = \prod_{i=1}^n a_i , \tag{9}$$

the inverse of a diagonal matrix is a diagonal matrix

$$\text{diag}([a_1, \dots, a_n])^{-1} = \text{diag}([1/a_1, \dots, 1/a_n]) \tag{10}$$

and the squared form with a diagonal matrix is

$$x^T \text{diag}([a_1, \dots, a_n]) x = \sum_{i=1}^n a_i x_i^2 . \tag{11}$$

2) Let

$$\Sigma = \text{diag}([\sigma_1^2, \dots, \sigma_n^2]) . \tag{12}$$

Then, we have

$$\begin{aligned}
p(x) & \stackrel{(4)}{=} \frac{1}{\sqrt{(2\pi)^n |\text{diag}([\sigma_1^2, \dots, \sigma_n^2])|}} \cdot \exp \left[-\frac{1}{2} (x - \mu)^T \text{diag}([\sigma_1^2, \dots, \sigma_n^2])^{-1} (x - \mu) \right] \\
& = \frac{1}{\sqrt{(2\pi)^n \prod_{i=1}^n \sigma_i^2}} \cdot \exp \left[-\frac{1}{2} (x - \mu)^T \text{diag}([1/\sigma_1^2, \dots, 1/\sigma_n^2]) (x - \mu) \right] \\
& = \frac{1}{\sqrt{(2\pi)^n \prod_{i=1}^n \sigma_i^2}} \cdot \exp \left[-\frac{1}{2} \sum_{i=1}^n \frac{(x_i - \mu_i)^2}{\sigma_i^2} \right] \\
& = \prod_{i=1}^n \frac{1}{\sqrt{2\pi\sigma_i^2}} \cdot \exp \left[-\frac{1}{2} \left(\frac{x_i - \mu_i}{\sigma_i} \right)^2 \right]
\end{aligned} \tag{13}$$

which implies that

$$p(x) = p(x_1) \cdot \dots \cdot p(x_n) . \tag{14}$$

Sources:

- original work

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4.1.13 Independence of products

Theorem: Let X be an $n \times 1$ random vector (\rightarrow Definition I/1.2.3) following a multivariate normal distribution (\rightarrow Definition 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 Definition I/1.3.6), if and only if the cross-matrix product, weighted with the covariance matrix (\rightarrow Proof II/4.1.6) 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 Definition 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 Proof II/4.1.9), 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 Definition I/1.10.9)

$$C\Sigma C^T = \begin{bmatrix} A\Sigma A^T & A\Sigma B^T \\ B\Sigma A^T & B\Sigma B^T \end{bmatrix}. \quad (5)$$

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 Proof II/4.1.12). Thus, AX and BX are independent (\rightarrow Definition 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>.

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4.2 Multivariate t-distribution

4.2.1 Definition

Definition: Let X be an $n \times 1$ random vector (\rightarrow Definition 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 Definition I/1.6.6) 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 $n \times 1$ 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.

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4.2.2 Probability density function

Theorem: Let X be a random vector (\rightarrow Definition I/1.2.3) following a multivariate t -distribution (\rightarrow Definition II/4.2.1):

$$X \sim t(\mu, \Sigma, \nu) . \quad (1)$$

Then, the probability density function (\rightarrow Definition I/1.6.6) 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 Definition II/4.2.1).

Sources:

- original work

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4.2.3 Relationship to F-distribution

Theorem: Let X be a $n \times 1$ random vector (\rightarrow Definition I/1.2.3) following a multivariate t -distribution (\rightarrow Definition II/4.2.1) 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 Definition 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 (\rightarrow Proof “mvt-ltt”) 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 $n \times 1$ random vector (\rightarrow Definition I/1.2.3) following a multivariate t-distribution (\rightarrow Definition II/4.2.1), 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. Y is an $n \times 1$ vector of independent and identically distributed (\rightarrow Definition “iid”) random variables (\rightarrow Definition I/1.2.2) following a univariate t-distribution (\rightarrow Definition 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 Definition II/3.3.1) an expression of X in terms of a standard normal (\rightarrow Definition II/3.2.2) random variable Z and a chi-squared (\rightarrow Definition 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 Definition 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 Definition 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.

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4.3 Normal-gamma distribution

4.3.1 Definition

Definition: Let X be an $n \times 1$ random vector (\rightarrow Definition I/1.2.3) and let Y be a positive random variable (\rightarrow Definition 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 Definition II/4.1.1) with mean vector μ and covariance matrix $(Y\Lambda)^{-1}$ and Y follows a gamma distribution (\rightarrow Definition 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 Definition I/1.10.19) 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.

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4.3.2 Special case of normal-Wishart distribution

Theorem: The normal-gamma distribution (\rightarrow Definition II/4.3.1) is a special case of the normal-Wishart distribution (\rightarrow Definition II/5.3.1) where the number of columns of the random matrices (\rightarrow Definition 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 Definition 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 Proof II/5.3.2)

$$p(X, Y) = \frac{1}{\sqrt{(2\pi)^{np}|U|^p|V|^\nu}} \cdot \frac{\sqrt{2^{-\nu p}}}{\Gamma_p\left(\frac{\nu}{2}\right)} \cdot |Y|^{(\nu+n-p-1)/2} \cdot \exp\left[-\frac{1}{2}\text{tr}\left(Y[(X-M)^T U^{-1}(X-M) + V^{-1}]\right)\right] \quad (2)$$

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, $x = X$ is a column vector and $y = Y$ is a real number. Thus, the probability density function (\rightarrow Definition I/1.6.6) of x and y can be developed as

$$\begin{aligned} p(x, y) &= \frac{1}{\sqrt{(2\pi)^n|U||V|^\nu}} \cdot \frac{\sqrt{2^{-\nu}}}{\Gamma\left(\frac{\nu}{2}\right)} \cdot y^{(\nu+n-2)/2} \cdot \exp\left[-\frac{1}{2}\text{tr}\left(y[(x-M)^T U^{-1}(x-M) + V^{-1}]\right)\right] \\ &= \sqrt{\frac{|U^{-1}|}{(2\pi)^n}} \cdot \frac{\sqrt{(2|V|)^{-\nu}}}{\Gamma\left(\frac{\nu}{2}\right)} \cdot y^{\frac{\nu}{2} + \frac{n}{2} - 1} \cdot \exp\left[-\frac{1}{2}\left(y[(x-M)^T U^{-1}(x-M) + 2(2V)^{-1}]\right)\right] \\ &= \sqrt{\frac{|U^{-1}|}{(2\pi)^n}} \cdot \frac{\left(\frac{1}{2|V|}\right)^{\frac{\nu}{2}}}{\Gamma\left(\frac{\nu}{2}\right)} \cdot y^{\frac{\nu}{2} + \frac{n}{2} - 1} \cdot \exp\left[-\frac{y}{2}\left((x-M)^T U^{-1}(x-M) + 2\left(\frac{1}{2V}\right)\right)\right] \end{aligned} \quad (3)$$

In the matrix-normal distribution (\rightarrow Definition 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

$$p(x, y) = \sqrt{\frac{|\Lambda|}{(2\pi)^n}} \frac{b^a}{\Gamma(a)} \cdot y^{a + \frac{n}{2} - 1} \exp\left[-\frac{y}{2}\left((x-\mu)^T \Lambda(x-\mu) + 2b\right)\right] \quad (4)$$

which is the probability density function of the normal-gamma distribution (\rightarrow Proof II/4.3.3).

Sources:

- original work

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4.3.3 Probability density function

Theorem: Let x and y follow a normal-gamma distribution (\rightarrow Definition II/4.3.1):

$$x, y \sim \text{NG}(\mu, \Lambda, a, b) . \quad (1)$$

Then, the joint probability (\rightarrow Definition I/1.3.2) density function (\rightarrow Definition I/1.6.6) of x and y is

$$p(x, y) = \sqrt{\frac{|\Lambda|}{(2\pi)^n}} \frac{b^a}{\Gamma(a)} \cdot y^{a+\frac{n}{2}-1} \exp \left[-\frac{y}{2} \left((x - \mu)^T \Lambda (x - \mu) + 2b \right) \right] . \quad (2)$$

Proof: The normal-gamma distribution (\rightarrow Definition II/4.3.1) is defined as X conditional on Y following a multivariate distribution (\rightarrow Definition II/4.1.1) and Y following a gamma distribution (\rightarrow Definition II/3.4.1):

$$\begin{aligned} X|Y &\sim \mathcal{N}(\mu, (Y\Lambda)^{-1}) \\ Y &\sim \text{Gam}(a, b) . \end{aligned} \quad (3)$$

Thus, using the probability density function of the multivariate normal distribution (\rightarrow Proof II/4.1.4) and the probability density function of the gamma distribution (\rightarrow Proof II/3.4.6), we have the following probabilities:

$$\begin{aligned} p(x|y) &= \mathcal{N}(x; \mu, (y\Lambda)^{-1}) \\ &= \sqrt{\frac{|y\Lambda|}{(2\pi)^n}} \exp \left[-\frac{1}{2} (x - \mu)^T (y\Lambda) (x - \mu) \right] \\ p(y) &= \text{Gam}(y; a, b) \\ &= \frac{b^a}{\Gamma(a)} y^{a-1} \exp[-by] . \end{aligned} \quad (4)$$

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

$$p(x, y) = p(x|y) p(y) , \quad (5)$$

such that the normal-Wishart density function becomes:

$$p(x, y) = \sqrt{\frac{|y\Lambda|}{(2\pi)^n}} \exp \left[-\frac{1}{2} (x - \mu)^T (y\Lambda) (x - \mu) \right] \cdot \frac{b^a}{\Gamma(a)} y^{a-1} \exp[-by] . \quad (6)$$

Using the relation $|yA| = y^n |A|$ for an $n \times n$ matrix A and rearranging the terms, we have:

$$p(x, y) = \sqrt{\frac{|\Lambda|}{(2\pi)^n}} \frac{b^a}{\Gamma(a)} \cdot y^{a+\frac{n}{2}-1} \exp \left[-\frac{y}{2} ((x - \mu)^T \Lambda (x - \mu) + 2b) \right] . \quad (7)$$

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.

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4.3.4 Mean

Theorem: Let $x \in \mathbb{R}^n$ and $y > 0$ follow a normal-gamma distribution (\rightarrow Definition II/4.3.1):

$$x, y \sim \text{NG}(\mu, \Lambda, a, b) . \quad (1)$$

Then, the expected value (\rightarrow Definition I/1.7.1) of x and y is

$$\mathbb{E}[(x, y)] = \left(\mu, \frac{a}{b} \right) . \quad (2)$$

Proof: Consider the random vector (\rightarrow Definition I/1.2.3)

$$\begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} x_1 \\ \vdots \\ x_n \\ y \end{bmatrix} . \quad (3)$$

According to the expected value of a random vector (\rightarrow Definition I/1.7.13), 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 Definition II/4.3.1) by definition x follows a multivariate normal distribution (\rightarrow Definition II/4.1.1) conditional on y and y follows a univariate gamma distribution (\rightarrow Definition II/3.4.1):

$$x, y \sim \text{NG}(\mu, \Lambda, a, b) \Leftrightarrow x|y \sim \mathcal{N}(\mu, (y\Lambda)^{-1}) \quad \wedge \quad y \sim \text{Gam}(a, b) . \quad (5)$$

Thus, with the expected value of the multivariate normal distribution (\rightarrow Proof II/4.1.5) and the law of conditional probability (\rightarrow Definition I/1.3.4), $\mathbb{E}(x)$ becomes

$$\begin{aligned}
E(x) &= \iint x \cdot p(x, y) \, dx \, dy \\
&= \iint x \cdot p(x|y) \cdot p(y) \, dx \, dy \\
&= \int p(y) \int x \cdot p(x|y) \, dx \, dy \\
&= \int p(y) \langle x \rangle_{\mathcal{N}(\mu, (y\Lambda)^{-1})} \, dy \\
&= \int p(y) \cdot \mu \, dy \\
&= \mu \int p(y) \, dy \\
&= \mu ,
\end{aligned} \tag{6}$$

and with the expected value of the gamma distribution (\rightarrow Proof II/3.4.9), $E(y)$ becomes

$$\begin{aligned}
E(y) &= \int y \cdot p(y) \, dy \\
&= \langle y \rangle_{\text{Gam}(a,b)} \\
&= \frac{a}{b} .
\end{aligned} \tag{7}$$

Thus, the expectation of the random vector in equations (3) and (4) is

$$E \left(\begin{bmatrix} x \\ y \end{bmatrix} \right) = \begin{bmatrix} \mu \\ a/b \end{bmatrix} , \tag{8}$$

as indicated by equation (2).

Sources:

- original work

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4.3.5 Covariance

Theorem: Let $x \in \mathbb{R}^n$ and $y > 0$ follow a normal-gamma distribution (\rightarrow Definition II/4.3.1):

$$x, y \sim \text{NG}(\mu, \Lambda, a, b) . \tag{1}$$

Then,

1) the covariance (\rightarrow Definition I/1.10.1) of x , conditional (\rightarrow Definition I/1.5.4) on y is

$$\text{Cov}(x|y) = \frac{1}{y} \Lambda^{-1} ; \tag{2}$$

2) the covariance (\rightarrow Definition I/1.10.1) of x , unconditional (\rightarrow Definition I/1.5.3) on y is

$$\text{Cov}(x) = \frac{b}{a-1} \Lambda^{-1} ; \quad (3)$$

3) the variance (\rightarrow Definition I/1.8.1) of y is

$$\text{Var}(y) = \frac{a}{b^2} . \quad (4)$$

Proof:

1) According to the definition of the normal-gamma distribution (\rightarrow Definition II/4.3.1), the distribution of x given y is a multivariate normal distribution (\rightarrow Definition II/4.1.1):

$$x|y \sim \mathcal{N}(\mu, (y\Lambda)^{-1}) . \quad (5)$$

The covariance of the multivariate normal distribution (\rightarrow Proof II/4.1.6) 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 Proof II/4.3.8) with respect to x is a multivariate t-distribution (\rightarrow Definition II/4.2.1):

$$x \sim t\left(\mu, \left(\frac{a}{b}\Lambda\right)^{-1}, 2a\right) . \quad (8)$$

The covariance of the multivariate t-distribution (\rightarrow Proof “mvt-cov”) 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 Proof II/4.3.8) with respect to y is a univariate gamma distribution (\rightarrow Definition II/3.4.1):

$$y \sim \text{Gam}(a, b) . \quad (11)$$

The variance of the gamma distribution (\rightarrow Proof II/3.4.10) is

$$x \sim \text{Gam}(a, b) \quad \Rightarrow \quad \text{Var}(x) = \frac{a}{b^2} , \quad (12)$$

such that we have:

$$\text{Var}(y) = \frac{a}{b^2} . \quad (13)$$

Sources:

- original work

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4.3.6 Differential entropy

Theorem: Let x be an $n \times 1$ random vector (\rightarrow Definition I/1.2.3) and let y be a positive random variable (\rightarrow Definition 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 Definition 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 Proof II/4.3.3) 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 Proof II/4.1.7) 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 Proof II/3.4.13) 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 Definition 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 Definition II/4.3.1) 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 Definition I/1.3.4), this can be evaluated as follows:

$$\begin{aligned} h(x, y) &= - \int_0^\infty \int_{\mathbb{R}^n} p(x|y) p(y) \ln p(x|y) p(y) \, dx \, dy \\ &= - \int_0^\infty \int_{\mathbb{R}^n} p(x|y) p(y) \ln p(x|y) \, dx \, dy - \int_0^\infty \int_{\mathbb{R}^n} p(x|y) p(y) \ln p(y) \, dx \, dy \\ &= \int_0^\infty p(y) \int_{\mathbb{R}^n} p(x|y) \ln p(x|y) \, dx \, dy + \int_0^\infty p(y) \ln p(y) \int_{\mathbb{R}^n} p(x|y) \, dx \, dy \\ &= \langle h(x|y) \rangle_{p(y)} + h(y) . \end{aligned} \quad (8)$$

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 Proof II/3.4.11) $y \sim \text{Gam}(a, b) \Rightarrow \langle \ln y \rangle = \psi(a) - \ln(b)$, 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).

Sources:

- original work

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4.3.7 Kullback-Leibler divergence

Theorem: Let x be an $n \times 1$ random vector (\rightarrow Definition I/1.2.3) and let y be a positive random variable (\rightarrow Definition I/1.2.2). Assume two normal-gamma distributions (\rightarrow Definition II/4.3.1) 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 Definition 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 Proof II/4.3.3) 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 Proof II/4.1.8) is

$$\text{KL}[P \parallel Q] = \frac{1}{2} \left[(\mu_2 - \mu_1)^T \Sigma_2^{-1} (\mu_2 - \mu_1) + \text{tr}(\Sigma_2^{-1} \Sigma_1) - \ln \frac{|\Sigma_1|}{|\Sigma_2|} - n \right] \quad (4)$$

and the Kullback-Leibler divergence of the univariate gamma distribution (\rightarrow Proof II/3.4.14) is

$$\text{KL}[P \parallel Q] = a_2 \ln \frac{b_1}{b_2} - \ln \frac{\Gamma(a_1)}{\Gamma(a_2)} + (a_1 - a_2) \psi(a_1) - (b_1 - b_2) \frac{a_1}{b_1} \quad (5)$$

where $\Gamma(x)$ is the gamma function and $\psi(x)$ is the digamma function.

The KL divergence for a continuous random variable (\rightarrow Definition I/2.5.1) is given by

$$\text{KL}[P \parallel Q] = \int_{\mathcal{Z}} p(z) \ln \frac{p(z)}{q(z)} dz \quad (6)$$

which, applied to the normal-gamma distribution (\rightarrow Definition II/4.3.1) over x and y , yields

$$\text{KL}[P \parallel Q] = \int_0^\infty \int_{\mathbb{R}^n} p(x, y) \ln \frac{p(x, y)}{q(x, y)} dx dy . \quad (7)$$

Using the law of conditional probability (\rightarrow Definition I/1.3.4), this can be evaluated as follows:

$$\begin{aligned} \text{KL}[P \parallel Q] &= \int_0^\infty \int_{\mathbb{R}^n} p(x|y) p(y) \ln \frac{p(x|y) p(y)}{q(x|y) q(y)} dx dy \\ &= \int_0^\infty \int_{\mathbb{R}^n} p(x|y) p(y) \ln \frac{p(x|y)}{q(x|y)} dx dy + \int_0^\infty \int_{\mathbb{R}^n} p(x|y) p(y) \ln \frac{p(y)}{q(y)} dx dy \\ &= \int_0^\infty p(y) \int_{\mathbb{R}^n} p(x|y) \ln \frac{p(x|y)}{q(x|y)} dx dy + \int_0^\infty p(y) \ln \frac{p(y)}{q(y)} \int_{\mathbb{R}^n} p(x|y) dx dy \\ &= \langle \text{KL}[p(x|y) \parallel q(x|y)] \rangle_{p(y)} + \text{KL}[p(y) \parallel q(y)] . \end{aligned} \quad (8)$$

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

$$\begin{aligned} &\langle \text{KL}[p(x|y) \parallel q(x|y)] \rangle_{p(y)} \\ &= \left\langle \frac{1}{2} \left[(\mu_2 - \mu_1)^T (y\Lambda_2) (\mu_2 - \mu_1) + \text{tr}((y\Lambda_2)(y\Lambda_1)^{-1}) - \ln \frac{|(y\Lambda_1)^{-1}|}{|(y\Lambda_2)^{-1}|} - n \right] \right\rangle_{p(y)} \\ &= \left\langle \frac{y}{2} (\mu_2 - \mu_1)^T \Lambda_2 (\mu_2 - \mu_1) + \frac{1}{2} \text{tr}(\Lambda_2 \Lambda_1^{-1}) - \frac{1}{2} \ln \frac{|\Lambda_2|}{|\Lambda_1|} - \frac{n}{2} \right\rangle_{p(y)} \end{aligned} \quad (9)$$

and using the relation (\rightarrow Proof II/3.4.9) $y \sim \text{Gam}(a, b) \Rightarrow \langle y \rangle = a/b$, we have

$$\langle \text{KL}[p(x|y) \parallel q(x|y)] \rangle_{p(y)} = \frac{1}{2} \frac{a_1}{b_1} (\mu_2 - \mu_1)^T \Lambda_2 (\mu_2 - \mu_1) + \frac{1}{2} \text{tr}(\Lambda_2 \Lambda_1^{-1}) - \frac{1}{2} \ln \frac{|\Lambda_2|}{|\Lambda_1|} - \frac{n}{2} . \quad (10)$$

By plugging (10) and (5) into (8), one arrives at the KL divergence given by (2).

Sources:

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4.3.8 Marginal distributions

Theorem: Let x and y follow a normal-gamma distribution (\rightarrow Definition II/4.3.1):

$$x, y \sim \text{NG}(\mu, \Lambda, a, b) . \quad (1)$$

Then, the marginal distribution (\rightarrow Definition I/1.5.3) of y is a gamma distribution (\rightarrow Definition II/3.4.1)

$$y \sim \text{Gam}(a, b) \quad (2)$$

and the marginal distribution (\rightarrow Definition I/1.5.3) of x is a multivariate t-distribution (\rightarrow Definition II/4.2.1)

$$x \sim t\left(\mu, \left(\frac{a}{b}\Lambda\right)^{-1}, 2a\right) . \quad (3)$$

Proof: The probability density function of the normal-gamma distribution (\rightarrow Proof II/4.3.3) 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 Definition 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 Proof II/3.4.6) with shape parameter a and rate parameter b .

Using the law of marginal probability (\rightarrow Definition 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} \tag{6}$$

which is the probability density function of a multivariate t-distribution (\rightarrow Proof II/4.2.2) with mean vector μ , shape matrix $\left(\frac{a}{b}\Lambda\right)^{-1}$ and $2a$ degrees of freedom.

Sources:

- original work

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4.3.9 Conditional distributions

Theorem: Let x and y follow a normal-gamma distribution (\rightarrow Definition II/4.3.1):

$$x, y \sim \text{NG}(\mu, \Lambda, a, b) . \quad (1)$$

Then,

1) the conditional distribution (\rightarrow Definition I/1.5.4) of x given y is a multivariate normal distribution (\rightarrow Definition II/4.1.1)

$$x|y \sim \mathcal{N}(\mu, (y\Lambda)^{-1}) ; \quad (2)$$

2) the conditional distribution (\rightarrow Definition 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 Definition 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 Definition I/1.7.1) and covariance (\rightarrow Definition I/1.10.1)

$$\begin{aligned} \mu_{1|2}(y) &= \mu_1 + \Sigma_{12}\Sigma_{22}^{-1}(x_2 - \mu_2) \\ \Sigma_{1|2}(y) &= \Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{12} \end{aligned} \quad (4)$$

where μ_1, μ_2 and $\Sigma_{11}, \Sigma_{12}, \Sigma_{22}, \Sigma_{21}$ are block-wise components (\rightarrow Proof II/4.1.11) of μ and $\Sigma(y) = (y\Lambda)^{-1}$;

3) the conditional distribution (\rightarrow Definition I/1.5.4) of y given x is a gamma distribution (\rightarrow Definition 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 Definition II/4.3.1):

$$\begin{aligned} p(x, y) &= p(x|y) \cdot p(y) \\ &= \mathcal{N}(x; \mu, (y\Lambda)^{-1}) \cdot \text{Gam}(y; a, b) . \end{aligned} \quad (6)$$

2) This follows from (2) and the conditional distributions of the multivariate normal distribution (\rightarrow Proof II/4.1.11):

$$\begin{aligned} x &\sim \mathcal{N}(\mu, \Sigma) \\ \Rightarrow x_1|x_2 &\sim \mathcal{N}(\mu_{1|2}, \Sigma_{1|2}) \\ \mu_{1|2} &= \mu_1 + \Sigma_{12}\Sigma_{22}^{-1}(x_2 - \mu_2) \\ \Sigma_{1|2} &= \Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21} . \end{aligned} \quad (7)$$

3) The conditional density of y given x follows from Bayes' theorem (\rightarrow Proof I/5.3.1) as

$$p(y|x) = \frac{p(x|y) \cdot p(y)}{p(x)}. \quad (8)$$

The conditional distribution (\rightarrow Definition I/1.5.4) of x given y is a multivariate normal distribution (\rightarrow Proof II/4.3.3)

$$p(x|y) = \mathcal{N}(x; \mu, (y\Lambda)^{-1}) = \sqrt{\frac{|y\Lambda|}{(2\pi)^n}} \exp \left[-\frac{1}{2}(x - \mu)^T (y\Lambda)(x - \mu) \right], \quad (9)$$

the marginal distribution (\rightarrow Definition I/1.5.3) of y is a gamma distribution (\rightarrow Proof II/4.3.8)

$$p(y) = \text{Gam}(y; a, b) = \frac{b^a}{\Gamma(a)} y^{a-1} \exp[-by] \quad (10)$$

and the marginal distribution (\rightarrow Definition I/1.5.3) of x is a multivariate t-distribution (\rightarrow Proof II/4.3.8)

$$\begin{aligned} p(x) &= t \left(x; \mu, \left(\frac{a}{b} \Lambda \right)^{-1}, 2a \right) \\ &= \sqrt{\frac{\left| \frac{a}{b} \Lambda \right|}{(2a\pi)^n}} \cdot \frac{\Gamma\left(\frac{2a+n}{2}\right)}{\Gamma\left(\frac{2a}{2}\right)} \cdot \left(1 + \frac{1}{2a}(x - \mu)^T \left(\frac{a}{b} \Lambda \right) (x - \mu) \right)^{-\frac{2a+n}{2}} \\ &= \sqrt{\frac{|\Lambda|}{(2\pi)^n}} \cdot \frac{\Gamma\left(a + \frac{n}{2}\right)}{\Gamma(a)} \cdot b^a \cdot \left(b + \frac{1}{2}(x - \mu)^T \Lambda (x - \mu) \right)^{-(a + \frac{n}{2})}. \end{aligned} \quad (11)$$

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 Proof II/3.4.6) 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

$$p(y|x) = \text{Gam} \left(y; a + \frac{n}{2}, b + \frac{1}{2}(x - \mu)^T \Lambda (x - \mu) \right). \quad (14)$$

Sources:

- original work

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4.3.10 Drawing samples

Theorem: Let $Z_1 \in \mathbb{R}^n$ be a random vector (\rightarrow Definition I/1.2.3) with all entries independently following a standard normal distribution (\rightarrow Definition II/3.2.2) and let $Z_2 \in \mathbb{R}$ be a random variable (\rightarrow Definition I/1.2.2) following a standard gamma distribution (\rightarrow Definition II/3.4.2) 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 Definition II/4.3.1) with mean vector (\rightarrow Definition I/1.7.13) μ , precision matrix (\rightarrow Definition I/1.10.19) 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 Definition II/3.2.2)

$$z_{1i} \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, 1) \quad \text{for all } i = 1, \dots, n , \quad (2)$$

this implies a multivariate normal distribution with diagonal covariance matrix (\rightarrow Proof II/4.1.12):

$$Z_1 \sim \mathcal{N}(0_n, I_n) \quad (3)$$

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 Definition II/3.4.2)

$$Z_2 \sim \text{Gam}(a, 1) , \quad (4)$$

then due to the relationship between gamma and standard gamma distribution (\rightarrow Proof II/3.4.3), 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 Proof II/4.1.9), 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 Definition II/3.4.1) and the distribution of X conditional on Y is a multivariate normal distribution (\rightarrow Definition 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 Definition II/4.3.1), X and Y jointly follow a normal-gamma distribution (\rightarrow Definition II/4.3.1):

$$X, Y \sim \text{NG}(\mu, \Lambda, a, b) , \quad (8)$$

Thus, given Z_1 defined by (2) and Z_2 defined by (4), X and Y defined by (1) are a sample (\rightarrow Definition “samp”) 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.

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4.4 Dirichlet distribution

4.4.1 Definition

Definition: Let X be a $k \times 1$ random vector (\rightarrow Definition 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 Definition I/1.6.6) 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.

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4.4.2 Probability density function

Theorem: Let X be a random vector (\rightarrow Definition I/1.2.3) following a Dirichlet distribution (\rightarrow Definition II/4.4.1):

$$X \sim \text{Dir}(\alpha) . \quad (1)$$

Then, the probability density function (\rightarrow Definition I/1.6.6) 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 Definition II/4.4.1).

Sources:

- original work

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4.4.3 Kullback-Leibler divergence

Theorem: Let x be an $k \times 1$ random vector (\rightarrow Definition I/1.2.3). Assume two Dirichlet distributions (\rightarrow Definition II/4.4.1) 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 Definition 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 Definition 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 Definition 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 Proof II/4.4.2), this becomes:

$$\begin{aligned}
\text{KL}[P \parallel Q] &= \left\langle \ln \frac{\frac{\Gamma(\sum_{i=1}^k \alpha_{1i})}{\prod_{i=1}^k \Gamma(\alpha_{1i})} \prod_{i=1}^k x_i^{\alpha_{1i}-1}}{\frac{\Gamma(\sum_{i=1}^k \alpha_{2i})}{\prod_{i=1}^k \Gamma(\alpha_{2i})} \prod_{i=1}^k x_i^{\alpha_{2i}-1}} \right\rangle_{p(x)} \\
&= \left\langle \ln \left(\frac{\Gamma(\sum_{i=1}^k \alpha_{1i})}{\Gamma(\sum_{i=1}^k \alpha_{2i})} \cdot \frac{\prod_{i=1}^k \Gamma(\alpha_{2i})}{\prod_{i=1}^k \Gamma(\alpha_{1i})} \cdot \prod_{i=1}^k x_i^{\alpha_{1i}-\alpha_{2i}} \right) \right\rangle_{p(x)} \\
&= \left\langle \ln \frac{\Gamma(\sum_{i=1}^k \alpha_{1i})}{\Gamma(\sum_{i=1}^k \alpha_{2i})} + \sum_{i=1}^k \ln \frac{\Gamma(\alpha_{2i})}{\Gamma(\alpha_{1i})} + \sum_{i=1}^k (\alpha_{1i} - \alpha_{2i}) \cdot \ln(x_i) \right\rangle_{p(x)} \\
&= \ln \frac{\Gamma(\sum_{i=1}^k \alpha_{1i})}{\Gamma(\sum_{i=1}^k \alpha_{2i})} + \sum_{i=1}^k \ln \frac{\Gamma(\alpha_{2i})}{\Gamma(\alpha_{1i})} + \sum_{i=1}^k (\alpha_{1i} - \alpha_{2i}) \cdot \langle \ln x_i \rangle_{p(x)} .
\end{aligned} \tag{5}$$

Using the expected value of a logarithmized Dirichlet variate (\rightarrow Proof “dir-logmean”)

$$x \sim \text{Dir}(\alpha) \quad \Rightarrow \quad \langle \ln x_i \rangle = \psi(\alpha_i) - \psi\left(\sum_{i=1}^k \alpha_i\right) , \tag{6}$$

the Kullback-Leibler divergence from (5) becomes:

$$\text{KL}[P \parallel Q] = \ln \frac{\Gamma(\sum_{i=1}^k \alpha_{1i})}{\Gamma(\sum_{i=1}^k \alpha_{2i})} + \sum_{i=1}^k \ln \frac{\Gamma(\alpha_{2i})}{\Gamma(\alpha_{1i})} + \sum_{i=1}^k (\alpha_{1i} - \alpha_{2i}) \cdot \left[\psi(\alpha_{1i}) - \psi\left(\sum_{i=1}^k \alpha_{1i}\right) \right] \tag{7}$$

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>.

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4.4.4 Exceedance probabilities

Theorem: Let $r = [r_1, \dots, r_k]$ be a random vector (\rightarrow Definition I/1.2.3) following a Dirichlet distribution (\rightarrow Definition II/4.4.1) with concentration parameters $\alpha = [\alpha_1, \dots, \alpha_k]$:

$$r \sim \text{Dir}(\alpha) . \tag{1}$$

1) If $k = 2$, then the exceedance probability (\rightarrow Definition I/1.3.10) for r_1 is

$$\varphi_1 = 1 - \frac{B\left(\frac{1}{2}; \alpha_1, \alpha_2\right)}{B(\alpha_1, \alpha_2)} \tag{2}$$

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 Definition I/1.3.10) for r_i is

$$\varphi_i = \int_0^\infty \prod_{j \neq i} \left(\frac{\gamma(\alpha_j, q_i)}{\Gamma(\alpha_j)} \right) \frac{q_i^{\alpha_i-1} \exp[-q_i]}{\Gamma(\alpha_i)} dq_i . \quad (3)$$

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 Definition II/4.4.1), the exceedance probability (\rightarrow Definition I/1.3.10) 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 Proof II/4.4.2) 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

$$r_i \in [0, 1] \quad \text{for} \quad i = 1, \dots, k \quad \text{and} \quad \sum_{i=1}^k r_i = 1 , \quad (6)$$

and defined to be zero otherwise (\rightarrow Definition II/4.4.1).

1) If $k = 2$, the probability density function of the Dirichlet distribution (\rightarrow Proof II/4.4.2) 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 Proof II/3.9.3)

$$p(r_1) = \frac{r_1^{\alpha_1-1} (1 - r_1)^{\alpha_2-1}}{B(\alpha_1, \alpha_2)} \quad (8)$$

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 Proof II/3.9.5), it evaluates to

$$\varphi_1 = 1 - \int_0^{\frac{1}{2}} p(r_1) dr_1 = 1 - \frac{B\left(\frac{1}{2}; \alpha_1, \alpha_2\right)}{B(\alpha_1, \alpha_2)} \quad (11)$$

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 (\rightarrow Proof “gam-dir”) 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 Proof II/3.4.6) 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 Definition 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 Definition II/4.4.1)

$$r = (r_1, \dots, r_k) = \left(\frac{q_1}{q_s}, \dots, \frac{q_k}{q_s} \right) \sim \text{Dir}(\alpha_1, \dots, \alpha_k) . \quad (17)$$

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 Proof II/3.4.7) 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 Definition 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 Definition I/1.3.10) for one element from a Dirichlet-distributed (\rightarrow Definition II/4.4.1) random vector (\rightarrow Definition 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 Definition II/3.4.1) cumulative distribution functions (\rightarrow Definition I/1.6.13) and the second term is a gamma (\rightarrow Definition II/3.4.1) probability density function (\rightarrow Definition I/1.6.6).

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>.

Metadata: ID: P181 | shortcut: dir-ep | author: JoramSoch | date: 2020-10-22, 08:04.

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 Definition I/1.2.4). Then, X is said to be matrix-normally distributed with mean M , covariance (\rightarrow Definition I/1.10.9) across rows U and covariance (\rightarrow Definition I/1.10.9) across columns V

$$X \sim \mathcal{MN}(M, U, V), \quad (1)$$

if and only if its probability density function (\rightarrow Definition I/1.6.6) 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.

Metadata: ID: D6 | shortcut: matn | author: JoramSoch | date: 2020-01-27, 14:37.

5.1.2 Equivalence to multivariate normal distribution

Theorem: The matrix X is matrix-normally distributed (\rightarrow Definition 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 Definition 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 Proof 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 Proof 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 Definition I/1.6.6) are identical, it is proven that the associated probability distributions (\rightarrow Definition 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.

Metadata: ID: P26 | shortcut: matn-mvn | author: JoramSoch | date: 2020-01-20, 21:09.

5.1.3 Probability density function

Theorem: Let X be a random matrix (\rightarrow Definition I/1.2.4) following a matrix-normal distribution (\rightarrow Definition II/5.1.1):

$$X \sim \mathcal{MN}(M, U, V) . \quad (1)$$

Then, the probability density function (\rightarrow Definition I/1.6.6) 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 Definition II/5.1.1).

Sources:

- original work

Metadata: ID: P70 | shortcut: matn-pdf | author: JoramSoch | date: 2020-03-02, 21:03.

5.1.4 Mean

Theorem: Let X be a random matrix (\rightarrow Definition I/1.2.4) following a matrix-normal distribution (\rightarrow Definition II/5.1.1):

$$X \sim \mathcal{MN}(M, U, V) . \quad (1)$$

Then, the mean or expected value (\rightarrow Definition I/1.7.1) of X is

$$\mathbb{E}(X) = M . \quad (2)$$

Proof: When X follows a matrix-normal distribution (\rightarrow Definition II/5.1.1), its vectorized version follows a multivariate normal distribution (\rightarrow Proof 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 Proof II/4.1.5)

$$\mathbb{E}[\text{vec}(X)] = \text{vec}(M) . \quad (4)$$

Since the expected value of a random matrix is calculated element-wise (\rightarrow Definition I/1.7.14), we can invert the vectorization operator to get:

$$\mathbb{E}[X] = M . \quad (5)$$

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.

Metadata: ID: P341 | shortcut: matn-mean | author: JoramSoch | date: 2022-09-15, 12:05.

5.1.5 Covariance

Theorem: Let X be an $n \times p$ random matrix (\rightarrow Definition I/1.2.4) following a matrix-normal distribution (\rightarrow Definition II/5.1.1):

$$X \sim \mathcal{MN}(M, U, V) . \quad (1)$$

Then,

- 1) the covariance matrix (\rightarrow Definition I/1.10.9) 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 Definition I/1.10.9) 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 Definition I/1.5.3) of a given row of X is a multivariate normal distribution (\rightarrow Proof 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 Proof II/4.1.6) is

$$\text{Cov}(x_{i,\bullet}^T) = u_{ii}V \propto V . \quad (5)$$

2) The marginal distribution (\rightarrow Definition I/1.5.3) of a given column of X is a multivariate normal distribution (\rightarrow Proof 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 Proof II/4.1.6) 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.

Metadata: ID: P342 | shortcut: matn-cov | author: JoramSoch | date: 2022-09-15, 12:23.

5.1.6 Differential entropy

Theorem: Let X be an $n \times p$ random matrix (\rightarrow Definition I/1.2.4) following a matrix-normal distribution (\rightarrow Definition II/5.1.1)

$$X \sim \mathcal{MN}(M, U, V) . \quad (1)$$

Then, the differential entropy (\rightarrow Definition 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 Proof 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 differential entropy for the multivariate normal distribution (\rightarrow Proof II/4.1.7) 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 $n \times 1$ random vector (\rightarrow Definition 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

$$|A \otimes B| = |A|^m |B|^n \quad \text{where } A \in \mathbb{R}^{n \times n} \quad \text{and} \quad B \in \mathbb{R}^{m \times m}, \quad (6)$$

the differential entropy from (5) becomes:

$$\begin{aligned} h(X) &= \frac{np}{2} \ln(2\pi) + \frac{1}{2} \ln (|V|^n |U|^p) + \frac{1}{2} np \\ &= \frac{np}{2} \ln(2\pi) + \frac{n}{2} \ln |V| + \frac{p}{2} \ln |U| + \frac{np}{2}. \end{aligned} \quad (7)$$

Sources:

- original work

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5.1.7 Kullback-Leibler divergence

Theorem: Let X be an $n \times p$ random matrix (\rightarrow Definition I/1.2.4). Assume two matrix-normal distributions (\rightarrow Definition 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 Definition I/2.5.1) of P from Q is given by

$$\begin{aligned} \text{KL}[P || Q] &= \frac{1}{2} \left[\text{vec}(M_2 - M_1)^T \text{vec} (U_2^{-1} (M_2 - M_1) V_2^{-1}) \right. \\ &\quad \left. + \text{tr} ((V_2^{-1} V_1) \otimes (U_2^{-1} U_1)) - n \ln \frac{|V_1|}{|V_2|} - p \ln \frac{|U_1|}{|U_2|} - np \right]. \end{aligned} \quad (2)$$

Proof: The matrix-normal distribution is equivalent to the multivariate normal distribution (\rightarrow Proof 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 Kullback-Leibler divergence for the multivariate normal distribution (\rightarrow Proof II/4.1.8) 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 $n \times 1$ random vector (\rightarrow Definition 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)

$$\begin{aligned} \text{KL}[P \parallel Q] = \frac{1}{2} & \left[(\text{vec}(M_2) - \text{vec}(M_1))^T (V_2 \otimes U_2)^{-1} (\text{vec}(M_2) - \text{vec}(M_1)) \right. \\ & \left. + \text{tr}((V_2 \otimes U_2)^{-1} (V_1 \otimes U_1)) - \ln \frac{|V_1 \otimes U_1|}{|V_2 \otimes U_2|} - np \right]. \end{aligned} \quad (5)$$

Using the vectorization operator and Kronecker product properties

$$\text{vec}(A) + \text{vec}(B) = \text{vec}(A + B) \quad (6)$$

$$(A \otimes B)^{-1} = A^{-1} \otimes B^{-1} \quad (7)$$

$$(A \otimes B)(C \otimes D) = (AC) \otimes (BD) \quad (8)$$

$$|A \otimes B| = |A|^m |B|^n \quad \text{where } A \in \mathbb{R}^{n \times n} \quad \text{and } B \in \mathbb{R}^{m \times m}, \quad (9)$$

the Kullback-Leibler divergence from (5) becomes:

$$\begin{aligned} \text{KL}[P \parallel Q] = \frac{1}{2} & \left[\text{vec}(M_2 - M_1)^T (V_2^{-1} \otimes U_2^{-1}) \text{vec}(M_2 - M_1) \right. \\ & \left. + \text{tr}((V_2^{-1} V_1) \otimes (U_2^{-1} U_1)) - n \ln \frac{|V_1|}{|V_2|} - p \ln \frac{|U_1|}{|U_2|} - np \right]. \end{aligned} \quad (10)$$

Using the relationship between Kronecker product and vectorization operator

$$(C^T \otimes A) \text{vec}(B) = \text{vec}(ABC), \quad (11)$$

we finally have:

$$\begin{aligned} \text{KL}[P \parallel Q] = \frac{1}{2} & \left[\text{vec}(M_2 - M_1)^T \text{vec}(U_2^{-1} (M_2 - M_1) V_2^{-1}) \right. \\ & \left. + \text{tr}((V_2^{-1} V_1) \otimes (U_2^{-1} U_1)) - n \ln \frac{|V_1|}{|V_2|} - p \ln \frac{|U_1|}{|U_2|} - np \right]. \end{aligned} \quad (12)$$

Sources:

- original work

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5.1.8 Transposition

Theorem: Let X be a random matrix (\rightarrow Definition I/1.2.4) following a matrix-normal distribution (\rightarrow Definition 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: The probability density function of the matrix-normal distribution (\rightarrow Proof II/5.1.3) is:

$$f(X) = \mathcal{MN}(X; M, U, V) = \frac{1}{\sqrt{(2\pi)^{np}|V|^n|U|^p}} \cdot \exp \left[-\frac{1}{2} \text{tr} (V^{-1}(X - M)^T U^{-1}(X - M)) \right] . \quad (3)$$

Define $Y = X^T$. Then, $X = Y^T$ and we can substitute:

$$f(Y) = \frac{1}{\sqrt{(2\pi)^{np}|V|^n|U|^p}} \cdot \exp \left[-\frac{1}{2} \text{tr} (V^{-1}(Y^T - M)^T U^{-1}(Y^T - M)) \right] . \quad (4)$$

Using $(A + B)^T = (A^T + B^T)$, we have:

$$f(Y) = \frac{1}{\sqrt{(2\pi)^{np}|V|^n|U|^p}} \cdot \exp \left[-\frac{1}{2} \text{tr} (V^{-1}(Y - M^T) U^{-1}(Y - M^T)^T) \right] . \quad (5)$$

Using $\text{tr}(ABC) = \text{tr}(CAB)$, we obtain

$$f(Y) = \frac{1}{\sqrt{(2\pi)^{np}|V|^n|U|^p}} \cdot \exp \left[-\frac{1}{2} \text{tr} (U^{-1}(Y - M^T)^T V^{-1}(Y - M^T)) \right] \quad (6)$$

which is the probability density function of a matrix-normal distribution (\rightarrow Proof II/5.1.3) with mean M^T , covariance across rows V and covariance across columns U .

Sources:

- original work

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5.1.9 Linear transformation

Theorem: Let X be an $n \times p$ random matrix (\rightarrow Definition I/1.2.4) following a matrix-normal distribution (\rightarrow Definition II/5.1.1):

$$X \sim \mathcal{MN}(M, U, V) . \quad (1)$$

Then, a linear transformation of X is also matrix-normally distributed

$$Y = AXB + C \sim \mathcal{MN}(AMB + C, AUA^T, B^T V B) \quad (2)$$

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 Proof 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 Proof II/4.1.9) 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

$$\begin{aligned} \text{vec}(Y) &= \text{vec}(AXB + C) \\ &= \text{vec}(AXB) + \text{vec}(C) \\ &= (B^T \otimes A)\text{vec}(X) + \text{vec}(C). \end{aligned} \quad (5)$$

Using (3) and (4), we have

$$\begin{aligned} \text{vec}(Y) &\sim \mathcal{N}((B^T \otimes A)\text{vec}(M) + \text{vec}(C), (B^T \otimes A)(V \otimes U)(B^T \otimes A)^T) \\ &= \mathcal{N}(\text{vec}(AMB) + \text{vec}(C), (B^T V \otimes AU)(B^T \otimes A)^T) \\ &= \mathcal{N}(\text{vec}(AMB + C), B^T V B \otimes AU A^T). \end{aligned} \quad (6)$$

Using (3), we finally have:

$$Y \sim \mathcal{MN}(AMB + C, AU A^T, B^T V B). \quad (7)$$

Sources:

- original work

Metadata: ID: P145 | shortcut: matn-ltt | author: JoramSoch | date: 2020-08-03, 22:24.

5.1.10 Marginal distributions

Theorem: Let X be an $n \times p$ random matrix (\rightarrow Definition I/1.2.4) following a matrix-normal distribution (\rightarrow Definition II/5.1.1):

$$X \sim \mathcal{MN}(M, U, V). \quad (1)$$

Then,

1) the marginal distribution (\rightarrow Definition 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 Definition 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 Definition I/1.5.3) of each row vector is a multivariate normal distribution (\rightarrow Definition 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 Definition I/1.5.3) of each column vector is a multivariate normal distribution (\rightarrow Definition 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 Definition I/1.5.3) of one element of X is a univariate normal distribution (\rightarrow Definition 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 Proof II/5.1.9) to give

$$X_{I,J} \sim \mathcal{MN}(AMB, AU A^T, B^T V B) \quad (9)$$

Finally, we see that $AMB = M_{I,J}$, $AU A^T = U_{I,I}$ and $B^T V B = V_{J,J}$.

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 Proof 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 Proof 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 Proof 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 Definition II/3.2.1) as a special case (\rightarrow Proof II/3.2.8) of the matrix-normal distribution (\rightarrow Proof II/4.1.3):

$$x_{ij} \sim \mathcal{N}(m_{ij}, u_{ii}v_{jj}) . \quad (19)$$

Sources:

- original work

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5.1.11 Drawing samples

Theorem: Let $X \in \mathbb{R}^{n \times p}$ be a random matrix (\rightarrow Definition I/1.2.4) with all entries independently following a standard normal distribution (\rightarrow Definition II/3.2.2). 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 Definition II/5.1.1) with mean (\rightarrow Definition I/1.7.14) M , covariance (\rightarrow Definition I/1.10.9) across rows U and covariance (\rightarrow Definition I/1.10.9) 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 Definition II/3.2.2)

$$x_{ij} \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, 1) \quad \text{for all } i = 1, \dots, n \quad \text{and} \quad j = 1, \dots, p , \quad (2)$$

this implies a multivariate normal distribution with diagonal covariance matrix (\rightarrow Proof II/4.1.12):

$$\begin{aligned} \text{vec}(X) &\sim \mathcal{N}(\text{vec}(0_{np}), I_{np}) \\ &\sim \mathcal{N}(\text{vec}(0_{np}), I_p \otimes I_n) \end{aligned} \quad (3)$$

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 Proof 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 Proof 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 Definition “samp”) 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.

Metadata: ID: P297 | shortcut: matn-samp | author: JoramSoch | date: 2021-12-07, 08:43.

5.2 Wishart distribution

5.2.1 Definition

Definition: Let X be an $n \times p$ matrix following a matrix-normal distribution (\rightarrow Definition 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.

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5.2.2 Kullback-Leibler divergence

Theorem: Let S be a $p \times p$ random matrix (\rightarrow Definition I/1.2.4). Assume two Wishart distributions (\rightarrow Definition 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 Definition 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 Definition 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 Definition 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 (\rightarrow Proof “wish-pdf”), this becomes:

$$\begin{aligned} \text{KL}[P \parallel Q] &= \left\langle \ln \frac{\frac{1}{\sqrt{2^{n_1 p} |V_1|^{n_1} \Gamma_p(\frac{n_1}{2})}} \cdot |S|^{(n_1 - p - 1)/2} \cdot \exp \left[-\frac{1}{2} \text{tr}(V_1^{-1} S) \right]}{\frac{1}{\sqrt{2^{n_2 p} |V_2|^{n_2} \Gamma_p(\frac{n_2}{2})}} \cdot |S|^{(n_2 - p - 1)/2} \cdot \exp \left[-\frac{1}{2} \text{tr}(V_2^{-1} S) \right]} \right\rangle_{p(S)} \\ &= \left\langle \ln \left(\sqrt{2^{(n_2 - n_1)p}} \cdot \frac{|V_2|^{n_2}}{|V_1|^{n_1}} \cdot \frac{\Gamma_p(\frac{n_2}{2})}{\Gamma_p(\frac{n_1}{2})} \cdot |S|^{(n_1 - n_2)/2} \cdot \exp \left[-\frac{1}{2} \text{tr}(V_1^{-1} S) + \frac{1}{2} \text{tr}(V_2^{-1} S) \right] \right) \right\rangle_{p(S)} \\ &= \left\langle \frac{(n_2 - n_1)p}{2} \ln 2 + \frac{n_2}{2} \ln |V_2| - \frac{n_1}{2} \ln |V_1| + \ln \frac{\Gamma_p(\frac{n_2}{2})}{\Gamma_p(\frac{n_1}{2})} \right. \\ &\quad \left. + \frac{n_1 - n_2}{2} \ln |S| - \frac{1}{2} \text{tr}(V_1^{-1} S) + \frac{1}{2} \text{tr}(V_2^{-1} S) \right\rangle_{p(S)} \\ &= \frac{(n_2 - n_1)p}{2} \ln 2 + \frac{n_2}{2} \ln |V_2| - \frac{n_1}{2} \ln |V_1| + \ln \frac{\Gamma_p(\frac{n_2}{2})}{\Gamma_p(\frac{n_1}{2})} \\ &\quad + \frac{n_1 - n_2}{2} \langle \ln |S| \rangle_{p(S)} - \frac{1}{2} \langle \text{tr}(V_1^{-1} S) \rangle_{p(S)} + \frac{1}{2} \langle \text{tr}(V_2^{-1} S) \rangle_{p(S)} . \end{aligned} \quad (7)$$

Using the expected value of a Wishart random matrix (\rightarrow Proof “wish-mean”)

$$S \sim \mathcal{W}(V, n) \quad \Rightarrow \quad \langle S \rangle = nV , \quad (8)$$

such that the expected value of the matrix trace (\rightarrow Proof I/1.7.8) becomes

$$\langle \text{tr}(AS) \rangle = \text{tr}(\langle AS \rangle) = \text{tr}(A \langle S \rangle) = \text{tr}(A \cdot (nV)) = n \cdot \text{tr}(AV) , \quad (9)$$

and the expected value of a Wishart log-determinant (\rightarrow Proof “wish-logdetmean”)

$$S \sim \mathcal{W}(V, n) \quad \Rightarrow \quad \langle \ln |S| \rangle = \psi_p \left(\frac{n}{2} \right) + p \cdot \ln 2 + \ln |V| , \quad (10)$$

the Kullback-Leibler divergence from (7) becomes:

$$\begin{aligned}
\text{KL}[P \parallel Q] &= \frac{(n_2 - n_1)p}{2} \ln 2 + \frac{n_2}{2} \ln |V_2| - \frac{n_1}{2} \ln |V_1| + \ln \frac{\Gamma_p\left(\frac{n_2}{2}\right)}{\Gamma_p\left(\frac{n_1}{2}\right)} \\
&\quad + \frac{n_1 - n_2}{2} \left[\psi_p\left(\frac{n_1}{2}\right) + p \cdot \ln 2 + \ln |V_1| \right] - \frac{n_1}{2} \text{tr}(V_1^{-1}V_1) + \frac{n_1}{2} \text{tr}(V_2^{-1}V_1) \\
&= \frac{n_2}{2} (\ln |V_2| - \ln |V_1|) + \ln \frac{\Gamma_p\left(\frac{n_2}{2}\right)}{\Gamma_p\left(\frac{n_1}{2}\right)} + \frac{n_1 - n_2}{2} \psi_p\left(\frac{n_1}{2}\right) - \frac{n_1}{2} \text{tr}(I_p) + \frac{n_1}{2} \text{tr}(V_2^{-1}V_1) \\
&= \frac{1}{2} \left[n_2 (\ln |V_2| - \ln |V_1|) + n_1 \text{tr}(V_2^{-1}V_1) + 2 \ln \frac{\Gamma_p\left(\frac{n_2}{2}\right)}{\Gamma_p\left(\frac{n_1}{2}\right)} + (n_1 - n_2) \psi_p\left(\frac{n_1}{2}\right) - n_1 p \right].
\end{aligned} \tag{11}$$

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.

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5.3 Normal-Wishart distribution

5.3.1 Definition

Definition: Let X be an $n \times p$ random matrix (\rightarrow Definition 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

$$X, Y \sim \text{NW}(M, U, V, \nu), \tag{1}$$

if the distribution of X conditional on Y is a matrix-normal distribution (\rightarrow Definition II/5.1.1) with mean M , covariance across rows U , covariance across columns Y^{-1} and Y follows a Wishart distribution (\rightarrow Definition II/5.2.1) with scale matrix V and degrees of freedom ν :

$$\begin{aligned}
X|Y &\sim \mathcal{MN}(M, U, Y^{-1}) \\
Y &\sim \mathcal{W}(V, \nu).
\end{aligned} \tag{2}$$

The $p \times p$ matrix Y can be seen as the precision matrix (\rightarrow Definition I/1.10.19) across the columns of the $n \times p$ matrix X .

Sources:

- original work

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5.3.2 Probability density function

Theorem: Let X and Y follow a normal-Wishart distribution (\rightarrow Definition II/5.3.1):

$$X, Y \sim \text{NW}(M, U, V, \nu) . \quad (1)$$

Then, the joint probability (\rightarrow Definition I/1.3.2) density function (\rightarrow Definition I/1.6.6) of X and Y is

$$p(X, Y) = \frac{1}{\sqrt{(2\pi)^{np}|U|^p|V|^\nu}} \cdot \frac{\sqrt{2^{-\nu p}}}{\Gamma_p\left(\frac{\nu}{2}\right)} \cdot |Y|^{(\nu+n-p-1)/2} \cdot \exp \left[-\frac{1}{2} \text{tr} \left(Y \left[(X - M)^T U^{-1} (X - M) + V^{-1} \right] \right) \right] . \quad (2)$$

Proof: The normal-Wishart distribution (\rightarrow Definition II/5.3.1) is defined as X conditional on Y following a matrix-normal distribution (\rightarrow Definition II/5.1.1) and Y following a Wishart distribution (\rightarrow Definition 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 Proof II/5.1.3) and the probability density function of the Wishart distribution (\rightarrow Proof “wish-pdf”), we have the following probabilities:

$$\begin{aligned} p(X|Y) &= \mathcal{MN}(X; M, U, Y^{-1}) \\ &= \sqrt{\frac{|Y|^n}{(2\pi)^{np}|U|^p}} \cdot \exp \left[-\frac{1}{2} \text{tr} \left(Y (X - M)^T U^{-1} (X - M) \right) \right] \\ p(Y) &= \mathcal{W}(Y; V, \nu) \\ &= \frac{1}{\Gamma_p\left(\frac{\nu}{2}\right)} \cdot \frac{1}{\sqrt{2^{\nu p}|V|^\nu}} \cdot |Y|^{(\nu-p-1)/2} \cdot \exp \left[-\frac{1}{2} \text{tr} \left(V^{-1} Y \right) \right] . \end{aligned} \quad (4)$$

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

$$p(X, Y) = p(X|Y) p(Y) , \quad (5)$$

such that the normal-Wishart density function becomes:

$$\begin{aligned}
p(X, Y) &= \mathcal{MN}(X; M, U, Y^{-1}) \cdot \mathcal{W}(Y; V, \nu) \\
&= \sqrt{\frac{|Y|^n}{(2\pi)^{np}|U|^p}} \cdot \exp \left[-\frac{1}{2} \text{tr} (Y(X - M)^T U^{-1}(X - M)) \right] \cdot \\
&\quad \frac{1}{\Gamma_p \left(\frac{\nu}{2} \right)} \cdot \frac{1}{\sqrt{2^{\nu p} |V|^\nu}} \cdot |Y|^{(\nu-p-1)/2} \cdot \exp \left[-\frac{1}{2} \text{tr} (V^{-1}Y) \right] \\
&= \frac{1}{\sqrt{(2\pi)^{np}|U|^p|V|^\nu}} \cdot \frac{\sqrt{2^{-\nu p}}}{\Gamma_p \left(\frac{\nu}{2} \right)} \cdot |Y|^{(\nu+n-p-1)/2} \cdot \\
&\quad \exp \left[-\frac{1}{2} \text{tr} (Y [(X - M)^T U^{-1}(X - M) + V^{-1}]) \right] .
\end{aligned} \tag{6}$$

Sources:

- original work

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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 Definition II/5.3.1):

$$X, Y \sim \text{NW}(M, U, V, \nu) . \tag{1}$$

Then, the expected value (\rightarrow Definition I/1.7.1) of X and Y is

$$\mathbb{E}[(X, Y)] = (M, \nu V) . \tag{2}$$

Proof: Consider the random matrix (\rightarrow Definition I/1.2.4)

$$\begin{bmatrix} X \\ Y \end{bmatrix} = \begin{bmatrix} x_{11} & \dots & x_{1p} \\ \vdots & \ddots & \vdots \\ x_{n1} & \dots & x_{np} \\ y_{11} & \dots & y_{1p} \\ \vdots & \ddots & \vdots \\ y_{p1} & \dots & y_{pp} \end{bmatrix} . \tag{3}$$

According to the expected value of a random matrix (\rightarrow Definition I/1.7.14), its expected value is

$$\mathbb{E} \left(\begin{bmatrix} X \\ Y \end{bmatrix} \right) = \begin{bmatrix} \mathbb{E}(x_{11}) & \dots & \mathbb{E}(x_{1p}) \\ \vdots & \ddots & \vdots \\ \mathbb{E}(x_{n1}) & \dots & \mathbb{E}(x_{np}) \\ \mathbb{E}(y_{11}) & \dots & \mathbb{E}(y_{1p}) \\ \vdots & \ddots & \vdots \\ \mathbb{E}(y_{p1}) & \dots & \mathbb{E}(y_{pp}) \end{bmatrix} = \begin{bmatrix} \mathbb{E}(X) \\ \mathbb{E}(Y) \end{bmatrix}. \quad (4)$$

When X and Y are jointly normal-Wishart distributed, then (\rightarrow Definition II/5.3.1) by definition X follows a matrix-normal distribution (\rightarrow Definition II/5.1.1) conditional on Y and Y follows a Wishart distribution (\rightarrow Definition 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 Proof II/5.1.4) and the law of conditional probability (\rightarrow Definition I/1.3.4), $\mathbb{E}(X)$ becomes

$$\begin{aligned} \mathbb{E}(X) &= \iint X \cdot p(X, Y) \, dX \, dY \\ &= \iint X \cdot p(X|Y) \cdot p(Y) \, dX \, dY \\ &= \int p(Y) \int X \cdot p(X|Y) \, dX \, dY \\ &= \int p(Y) \langle X \rangle_{\mathcal{MN}(M, U, Y^{-1})} \, dY \\ &= \int p(Y) \cdot M \, dY \\ &= M \int p(Y) \, dY \\ &= M, \end{aligned} \quad (6)$$

and with the expected value of the Wishart distribution (\rightarrow Proof “wish-mean”), $\mathbb{E}(Y)$ becomes

$$\begin{aligned} \mathbb{E}(Y) &= \int Y \cdot p(Y) \, dY \\ &= \langle Y \rangle_{\mathcal{W}(V, \nu)} \\ &= \nu V. \end{aligned} \quad (7)$$

Thus, the expectation of the random matrix in equations (3) and (4) is

$$\mathbb{E} \left(\begin{bmatrix} X \\ Y \end{bmatrix} \right) = \begin{bmatrix} M \\ \nu V \end{bmatrix}, \quad (8)$$

as indicated by equation (2).

Sources:

- original work

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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 according to a normal distribution (\rightarrow Definition 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>.

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1.1.2 Maximum likelihood estimation

Theorem: Let there be a univariate Gaussian data set (\rightarrow Definition 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 Definition 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 Definition I/5.1.2) for each observation is given by the probability density function of the normal distribution (\rightarrow Proof 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 Definition 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 Definition 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>.

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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 Definition III/1.1.1) with unknown mean μ and unknown variance σ^2 . Then, the test statistic (\rightarrow Definition I/4.3.5)

$$t = \frac{\bar{y} - \mu_0}{s/\sqrt{n}} \tag{2}$$

with sample mean (\rightarrow Definition I/1.7.2) \bar{y} and sample variance (\rightarrow Definition I/1.8.2) s^2 follows a Student’s t-distribution (\rightarrow Definition II/3.3.1) with $n - 1$ degrees of freedom (\rightarrow Definition “dof”)

$$t \sim t(n - 1) \tag{3}$$

under the null hypothesis (\rightarrow Definition I/4.3.2)

$$H_0 : \mu = \mu_0 . \tag{4}$$

Proof: The sample mean (\rightarrow Definition I/1.7.2) is given by

$$\bar{y} = \frac{1}{n} \sum_{i=1}^n y_i \quad (5)$$

and the sample variance (\rightarrow Definition I/1.8.2) 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 Proof II/3.2.26), the sample mean follows a normal distribution (\rightarrow Definition 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 Definition II/3.2.2)

$$Z = \frac{\sqrt{n}(\bar{y} - \mu_0)}{\sigma} \sim \mathcal{N} \left(\frac{\sqrt{n}}{\sigma}(\mu - \mu_0), \left(\frac{\sqrt{n}}{\sigma} \right)^2 \frac{\sigma^2}{n} \right) \stackrel{H_0}{=} \mathcal{N} (0, 1) . \quad (8)$$

Because sample variances calculated from independent normal random variables follow a chi-squared distribution (\rightarrow Proof II/3.2.6), 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 Definition II/3.3.1), the distribution of the test statistic (\rightarrow Definition 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 Definition I/4.3.2) can be rejected when t is as extreme or more extreme than the critical value (\rightarrow Definition I/4.3.9) obtained from the Student's t-distribution (\rightarrow Definition II/3.3.1) with $n-1$ degrees of freedom (\rightarrow Definition “dof”) using a significance level (\rightarrow Definition 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.

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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 Definition 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 Definition 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 Definition I/1.7.2) \bar{y}_1 and \bar{y}_2 and pooled standard deviation (\rightarrow Definition “std-pool”) s_p follows a Student’s t-distribution (\rightarrow Definition II/3.3.1) with $n_1 + n_2 - 2$ degrees of freedom (\rightarrow Definition “dof”)

$$t \sim t(n_1 + n_2 - 2) \quad (3)$$

under the null hypothesis (\rightarrow Definition I/4.3.2)

$$H_0 : \mu_1 - \mu_2 = \mu_\Delta . \quad (4)$$

Proof: The sample means (\rightarrow Definition I/1.7.2) 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 Definition “std-pool”) 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 Definition I/1.8.2)

$$\begin{aligned} s_1^2 &= \frac{1}{n_1 - 1} \sum_{i=1}^{n_1} (y_{1i} - \bar{y}_1)^2 \\ s_2^2 &= \frac{1}{n_2 - 1} \sum_{i=1}^{n_2} (y_{2i} - \bar{y}_2)^2 . \end{aligned} \quad (7)$$

Using the linear combination formula for normal random variables (\rightarrow Proof II/3.2.26), the sample means follows normal distributions (\rightarrow Definition 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 Definition II/3.2.2)

$$Z = \frac{(\bar{y}_1 - \bar{y}_2) - \mu_\Delta}{\sigma \cdot \sqrt{\frac{1}{n_1} + \frac{1}{n_2}}} \sim \mathcal{N} \left(\frac{(\mu_1 - \mu_2) - \mu_\Delta}{\sigma \cdot \sqrt{\frac{1}{n_1} + \frac{1}{n_2}}}, \left(\frac{1}{\sigma \cdot \sqrt{\frac{1}{n_1} + \frac{1}{n_2}}} \right)^2 \left(\frac{\sigma^2}{n_1} + \frac{\sigma^2}{n_2} \right) \right) \stackrel{H_0}{=} \mathcal{N}(0, 1) . \quad (9)$$

Because sample variances calculated from independent normal random variables follow a chi-squared distribution (\rightarrow Proof II/3.2.6), 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 Definition II/3.3.1), the distribution of the test statistic (\rightarrow Definition 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 Definition I/4.3.2) can be rejected when t is as extreme or more extreme than the critical value (\rightarrow Definition I/4.3.9) obtained from the Student's t-distribution (\rightarrow Definition II/3.3.1) with $n_1 + n_2 - 2$ degrees of freedom (\rightarrow Definition “dof”) using a significance level (\rightarrow Definition 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)).

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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 Definition III/1.1.1) with unknown shift μ and unknown variance σ^2 . Then, the test statistic (\rightarrow Definition 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 Definition I/1.7.2) \bar{d} and sample variance (\rightarrow Definition I/1.8.2) s_d^2 follows a Student's t-distribution (\rightarrow Definition II/3.3.1) with $n - 1$ degrees of freedom (\rightarrow Definition “dof”)

$$t \sim t(n-1) \quad (3)$$

under the null hypothesis (\rightarrow Definition I/4.3.2)

$$H_0 : \mu = \mu_0 . \quad (4)$$

Proof: Define the pair-wise difference $d_i = y_{i1} - y_{i2}$ which is, according to the linearity of the expected value (\rightarrow Proof I/1.7.5) and the invariance of the variance under addition (\rightarrow Proof I/1.8.6), 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 Proof 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.

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1.1.6 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 Definition III/1.1.1) with unknown mean μ and unknown variance σ^2 . Then, the conjugate prior (\rightarrow Definition I/5.2.5) for this model is a normal-gamma distribution (\rightarrow Definition II/4.3.1)

$$p(\mu, \tau) = \mathcal{N}(\mu; \mu_0, (\tau \lambda_0)^{-1}) \cdot \text{Gam}(\tau; a_0, b_0) \quad (2)$$

where $\tau = 1/\sigma^2$ is the inverse variance or precision.

Proof: By definition, a conjugate prior (\rightarrow Definition I/5.2.5) is a prior distribution (\rightarrow Definition I/5.1.3) that, when combined with the likelihood function (\rightarrow Definition I/5.1.2), leads to a posterior distribution (\rightarrow Definition I/5.1.7) that belongs to the same family of probability distributions (\rightarrow Definition 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 Definition I/5.1.2)

$$\begin{aligned}
p(y|\mu, \sigma^2) &= \prod_{i=1}^n \mathcal{N}(y_i; \mu, \sigma^2) \\
&= \prod_{i=1}^n \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp \left[-\frac{1}{2} \left(\frac{y_i - \mu}{\sigma} \right)^2 \right] \\
&= \frac{1}{(\sqrt{2\pi}\sigma^2)^n} \cdot \exp \left[-\frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \mu)^2 \right]
\end{aligned} \tag{3}$$

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 Definition 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 :

$$p(y|\mu, \tau) \propto \tau^{n/2} \cdot \exp \left[-\frac{\tau}{2} (y^T y - n\bar{y}^2) \right] \cdot \exp \left[-\frac{\tau n}{2} (\mu - \bar{y})^2 \right]. \quad (8)$$

The same is true for a normal-gamma distribution (\rightarrow Definition II/4.3.1) over μ and τ

$$p(\mu, \tau) = \mathcal{N}(\mu; \mu_0, (\tau \lambda_0)^{-1}) \cdot \text{Gam}(\tau; a_0, b_0) \quad (9)$$

the probability density function of which (\rightarrow Proof II/4.3.3)

$$p(\mu, \tau) = \sqrt{\frac{\tau \lambda_0}{2\pi}} \cdot \exp \left[-\frac{\tau \lambda_0}{2} (\mu - \mu_0)^2 \right] \cdot \frac{b_0^{a_0}}{\Gamma(a_0)} \tau^{a_0-1} \exp[-b_0 \tau] \quad (10)$$

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>.

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1.1.7 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 Definition III/1.1.1) with unknown mean μ and unknown variance σ^2 . Moreover, assume a normal-gamma prior distribution (\rightarrow Proof III/1.1.6) 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 Definition I/5.1.7) is also a normal-gamma distribution (\rightarrow Definition II/4.3.1)

$$p(\mu, \tau|y) = \mathcal{N}(\mu; \mu_n, (\tau \lambda_n)^{-1}) \cdot \text{Gam}(\tau; a_n, b_n) \quad (3)$$

and the posterior hyperparameters (\rightarrow Definition I/5.1.7) are given by

$$\begin{aligned}
\mu_n &= \frac{\lambda_0 \mu_0 + n \bar{y}}{\lambda_0 + n} \\
\lambda_n &= \lambda_0 + n \\
a_n &= a_0 + \frac{n}{2} \\
b_n &= b_0 + \frac{1}{2} (y^T y + \lambda_0 \mu_0^2 - \lambda_n \mu_n^2) .
\end{aligned} \tag{4}$$

Proof: According to Bayes' theorem (\rightarrow Proof I/5.3.1), the posterior distribution (\rightarrow Definition I/5.1.7) is given by

$$p(\mu, \tau | y) = \frac{p(y | \mu, \tau) p(\mu, \tau)}{p(y)} . \tag{5}$$

Since $p(y)$ is just a normalization factor, the posterior is proportional (\rightarrow Proof I/5.1.8) to the numerator:

$$p(\mu, \tau | y) \propto p(y | \mu, \tau) p(\mu, \tau) = p(y, \mu, \tau) . \tag{6}$$

Equation (1) implies the following likelihood function (\rightarrow Definition 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 Definition I/5.1.2) (8) with the prior distribution (\rightarrow Definition I/5.1.3) (2), the joint likelihood (\rightarrow Definition I/5.1.5) 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 Proof III/1.1.6) gives

$$\begin{aligned}
p(y, \mu, \tau) &= \sqrt{\frac{\tau^{n+1} \lambda_0}{(2\pi)^{n+1}}} \frac{b_0^{a_0}}{\Gamma(a_0)} \tau^{a_0-1} \exp[-b_0 \tau] \cdot \\
&\quad \exp \left[-\frac{\tau}{2} ((y^T y - 2\mu n \bar{y} + n\mu^2) + \lambda_0 (\mu^2 - 2\mu\mu_0 + \mu_0^2)) \right]
\end{aligned} \tag{11}$$

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

$$\begin{aligned}
p(y, \mu, \tau) &= \sqrt{\frac{\tau^{n+1} \lambda_0}{(2\pi)^{n+1}}} \frac{b_0^{a_0}}{\Gamma(a_0)} \tau^{a_0-1} \exp[-b_0 \tau] \cdot \\
&\quad \exp \left[-\frac{\tau}{2} (\mu^2 (\lambda_0 + n) - 2\mu (\lambda_0 \mu_0 + n \bar{y}) + (y^T y + \lambda_0 \mu_0^2)) \right]
\end{aligned} \tag{12}$$

Completing the square over μ , we finally have

$$\begin{aligned}
p(y, \mu, \tau) &= \sqrt{\frac{\tau^{n+1} \lambda_0}{(2\pi)^{n+1}}} \frac{b_0^{a_0}}{\Gamma(a_0)} \tau^{a_0-1} \exp[-b_0 \tau] \cdot \\
&\quad \exp \left[-\frac{\tau \lambda_n}{2} (\mu - \mu_n)^2 - \frac{\tau}{2} (y^T y + \lambda_0 \mu_0^2 - \lambda_n \mu_n^2) \right]
\end{aligned} \tag{13}$$

with the posterior hyperparameters (\rightarrow Definition I/5.1.7)

$$\begin{aligned}
\mu_n &= \frac{\lambda_0 \mu_0 + n \bar{y}}{\lambda_0 + n} \\
\lambda_n &= \lambda_0 + n .
\end{aligned} \tag{14}$$

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 Definition I/5.1.7)

$$\begin{aligned} a_n &= a_0 + \frac{n}{2} \\ b_n &= b_0 + \frac{1}{2} (y^T y + \lambda_0 \mu_0^2 - \lambda_n \mu_n^2) . \end{aligned} \quad (16)$$

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 Definition I/1.3.2) posterior distribution (\rightarrow Definition I/5.1.7) 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>.

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1.1.8 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 Definition III/1.1.1) with unknown mean μ and unknown variance σ^2 . Moreover, assume a normal-gamma prior distribution (\rightarrow Proof III/1.1.6) 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 Definition 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 Definition I/5.1.7) are given by

$$\begin{aligned}
\mu_n &= \frac{\lambda_0 \mu_0 + n \bar{y}}{\lambda_0 + n} \\
\lambda_n &= \lambda_0 + n \\
a_n &= a_0 + \frac{n}{2} \\
b_n &= b_0 + \frac{1}{2}(y^T y + \lambda_0 \mu_0^2 - \lambda_n \mu_n^2) .
\end{aligned} \tag{4}$$

Proof: According to the law of marginal probability (\rightarrow Definition I/1.3.3), the model evidence (\rightarrow Definition I/5.1.9) for this model is:

$$p(y|m) = \iint p(y|\mu, \tau) p(\mu, \tau) d\mu d\tau . \tag{5}$$

According to the law of conditional probability (\rightarrow Definition I/1.3.4), the integrand is equivalent to the joint likelihood (\rightarrow Definition I/5.1.5):

$$p(y|m) = \iint p(y, \mu, \tau) d\mu d\tau . \tag{6}$$

Equation (1) implies the following likelihood function (\rightarrow Definition 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 Proof III/1.1.7) $p(\mu, \tau|y)$, the joint likelihood $p(y, \mu, \tau)$ is obtained as

$$p(y, \mu, \tau) = \sqrt{\frac{\tau^{n+1} \lambda_0}{(2\pi)^{n+1}}} \frac{b_0^{a_0}}{\Gamma(a_0)} \tau^{a_0-1} \exp[-b_0 \tau] \cdot \exp \left[-\frac{\tau \lambda_n}{2} (\mu - \mu_n)^2 - \frac{\tau}{2} (y^T y + \lambda_0 \mu_0^2 - \lambda_n \mu_n^2) \right] . \quad (9)$$

Using the probability density function of the normal distribution (\rightarrow Proof II/3.2.10), we can rewrite this as

$$p(y, \mu, \tau) = \sqrt{\frac{\tau^n}{(2\pi)^n}} \sqrt{\frac{\tau \lambda_0}{2\pi}} \sqrt{\frac{2\pi}{\tau \lambda_n}} \frac{b_0^{a_0}}{\Gamma(a_0)} \tau^{a_0-1} \exp[-b_0 \tau] \cdot \mathcal{N}(\mu; \mu_n, (\tau \lambda_n)^{-1}) \exp \left[-\frac{\tau}{2} (y^T y + \lambda_0 \mu_0^2 - \lambda_n \mu_n^2) \right] . \quad (10)$$

Now, μ can be integrated out easily:

$$\int p(y, \mu, \tau) d\mu = \sqrt{\frac{1}{(2\pi)^n}} \sqrt{\frac{\lambda_0}{\lambda_n}} \frac{b_0^{a_0}}{\Gamma(a_0)} \tau^{a_0+n/2-1} \exp[-b_0 \tau] \cdot \exp \left[-\frac{\tau}{2} (y^T y + \lambda_0 \mu_0^2 - \lambda_n \mu_n^2) \right] . \quad (11)$$

Using the probability density function of the gamma distribution (\rightarrow Proof II/3.4.6), 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 Definition 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>.

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1.1.9 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 Definition III/1.1.1) with unknown mean μ and unknown variance σ^2 . Moreover, assume a normal-gamma prior distribution (\rightarrow Proof III/1.1.6) 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 Proof 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 Proof III/1.1.7) and \bar{y} is the sample mean (\rightarrow Definition I/1.7.2).

Proof: Model accuracy and complexity are defined as (\rightarrow Proof 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 Definition I/1.7.1) of the log-likelihood function (\rightarrow Definition I/4.1.2) $\log p(y|\mu, \tau)$ with respect to the posterior distribution (\rightarrow Definition I/5.1.7) $p(\mu, \tau|y)$. With the log-likelihood function for the univariate Gaussian (\rightarrow Proof III/1.1.2) and the posterior distribution for the univariate Gaussian (\rightarrow Proof III/1.1.7), the model accuracy of m evaluates to:

$$\begin{aligned} \text{Acc}(m) &= \langle \log p(y|\mu, \tau) \rangle_{p(\mu, \tau|y)} \\ &= \left\langle \langle \log p(y|\mu, \tau) \rangle_{p(\mu|\tau, y)} \right\rangle_{p(\tau|y)} \\ &= \left\langle \left\langle \frac{n}{2} \log(\tau) - \frac{n}{2} \log(2\pi) - \frac{\tau}{2} (y^T y - 2n\bar{y}\mu + n\mu^2) \right\rangle_{\mathcal{N}(\mu_n, (\tau \lambda_n)^{-1})} \right\rangle_{\text{Gam}(a_n, b_n)} \\ &= \left\langle \frac{n}{2} \log(\tau) - \frac{n}{2} \log(2\pi) - \frac{\tau}{2} (y^T y - 2n\bar{y}\mu_n + n\mu_n^2) - \frac{1}{2} n\lambda_n^{-1} \right\rangle_{\text{Gam}(a_n, b_n)} \\ &= \frac{n}{2} (\psi(a_n) - \log(b_n)) - \frac{n}{2} \log(2\pi) - \frac{1}{2} \frac{a_n}{b_n} (y^T y - 2n\bar{y}\mu_n + n\mu_n^2) - \frac{1}{2} n\lambda_n^{-1} \\ &= -\frac{1}{2} \frac{a_n}{b_n} (y^T y - 2n\bar{y}\mu_n + n\mu_n^2) - \frac{1}{2} n\lambda_n^{-1} + \frac{n}{2} (\psi(a_n) - \log(b_n)) - \frac{n}{2} \log(2\pi) \end{aligned} \quad (5)$$

The complexity penalty is the Kullback-Leibler divergence (\rightarrow Definition I/2.5.1) of the posterior distribution (\rightarrow Definition I/5.1.7) $p(\mu, \tau|y)$ from the prior distribution (\rightarrow Definition I/5.1.3) $p(\mu, \tau)$. With the prior distribution (\rightarrow Proof III/1.1.6) given by (2), the posterior distribution for the univariate Gaussian (\rightarrow Proof III/1.1.7) and the Kullback-Leibler divergence of the normal-gamma distribution (\rightarrow Proof II/4.3.7), the model complexity of m evaluates to:

$$\begin{aligned}
\text{Com}(m) &= \text{KL} [p(\mu, \tau|y) || p(\mu, \tau)] \\
&= \text{KL} [\text{NG}(\mu_n, \lambda_n^{-1}, a_n, b_n) || \text{NG}(\mu_0, \lambda_0^{-1}, a_0, b_0)] \\
&= \frac{1}{2} \frac{a_n}{b_n} [\lambda_0(\mu_0 - \mu_n)^2] + \frac{1}{2} \frac{\lambda_0}{\lambda_n} - \frac{1}{2} \log \frac{\lambda_0}{\lambda_n} - \frac{1}{2} \\
&\quad + a_0 \cdot \log \frac{b_n}{b_0} - \log \frac{\Gamma(a_n)}{\Gamma(a_0)} + (a_n - a_0) \cdot \psi(a_n) - (b_n - b_0) \cdot \frac{a_n}{b_n} \\
&= \frac{1}{2} \frac{a_n}{b_n} [\lambda_0(\mu_0 - \mu_n)^2 - 2(b_n - b_0)] + \frac{1}{2} \frac{\lambda_0}{\lambda_n} - \frac{1}{2} \log \frac{\lambda_0}{\lambda_n} - \frac{1}{2} \\
&\quad + a_0 \cdot \log \frac{b_n}{b_0} - \log \frac{\Gamma(a_n)}{\Gamma(a_0)} + (a_n - a_0) \cdot \psi(a_n) .
\end{aligned} \tag{6}$$

A control calculation confirms that

$$\text{Acc}(m) - \text{Com}(m) = \text{LME}(m) \tag{7}$$

where $\text{LME}(m)$ is the log model evidence for the univariate Gaussian (\rightarrow Proof III/1.1.8).

Sources:

- original work

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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 according to a normal distribution (\rightarrow Definition 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>.

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1.2.2 Maximum likelihood estimation

Theorem: Let there be univariate Gaussian data with known variance (\rightarrow Definition III/1.2.1) $y = \{y_1, \dots, y_n\}$:

$$y_i \sim \mathcal{N}(\mu, \sigma^2), \quad i = 1, \dots, n. \quad (1)$$

Then, the maximum likelihood estimate (\rightarrow Definition I/4.1.3) for the mean μ is given by

$$\hat{\mu} = \bar{y} \quad (2)$$

where \bar{y} is the sample mean (\rightarrow Definition I/1.7.2)

$$\bar{y} = \frac{1}{n} \sum_{i=1}^n y_i. \quad (3)$$

Proof: The likelihood function (\rightarrow Definition I/5.1.2) for each observation is given by the probability density function of the normal distribution (\rightarrow Proof 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 Definition 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 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 Definition 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:

$$\begin{aligned}
\frac{dLL(\hat{\mu})}{d\mu} &= 0 \\
0 &= \frac{n}{\sigma^2}(\bar{y} - \hat{\mu}) \\
0 &= \bar{y} - \hat{\mu} \\
\hat{\mu} &= \bar{y}
\end{aligned} \tag{9}$$

Plugging this value into the second derivative, we confirm:

$$\frac{d^2LL(\hat{\mu})}{d\mu^2} = -\frac{n}{\sigma^2} < 0 . \tag{10}$$

This demonstrates that the estimate $\hat{\mu} = \bar{y}$ maximizes the likelihood $p(y|\mu)$.

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>.

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1.2.3 One-sample z-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 Definition III/1.2.1) with unknown mean μ and known variance σ^2 . Then, the test statistic (\rightarrow Definition I/4.3.5)

$$z = \sqrt{n} \frac{\bar{y} - \mu_0}{\sigma} \tag{2}$$

with sample mean (\rightarrow Definition I/1.7.2) \bar{y} follows a standard normal distribution (\rightarrow Definition II/3.2.2)

$$z \sim \mathcal{N}(0, 1) \tag{3}$$

under the null hypothesis (\rightarrow Definition I/4.3.2)

$$H_0 : \mu = \mu_0 . \tag{4}$$

Proof: The sample mean (\rightarrow Definition I/1.7.2) is given by

$$\bar{y} = \frac{1}{n} \sum_{i=1}^n y_i . \tag{5}$$

Using the linear combination formula for normal random variables (\rightarrow Proof II/3.2.26), the sample mean follows a normal distribution (\rightarrow Definition 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 Definition I/4.3.2) can be rejected when z is as extreme or more extreme than the critical value (\rightarrow Definition I/4.3.9) obtained from the standard normal distribution (\rightarrow Definition II/3.2.2) using a significance level (\rightarrow Definition 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>.

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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 Definition 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 Definition 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 Definition I/1.7.2) \bar{y}_1 and \bar{y}_2 follows a standard normal distribution (\rightarrow Definition II/3.2.2)

$$z \sim \mathcal{N}(0, 1) \quad (3)$$

under the null hypothesis (\rightarrow Definition I/4.3.2)

$$H_0 : \mu_1 - \mu_2 = \mu_\Delta . \quad (4)$$

Proof: The sample means (\rightarrow Definition I/1.7.2) are given by

$$\begin{aligned}\bar{y}_1 &= \frac{1}{n_1} \sum_{i=1}^{n_1} y_{1i} \\ \bar{y}_2 &= \frac{1}{n_2} \sum_{i=1}^{n_2} y_{2i} .\end{aligned}\tag{5}$$

Using the linear combination formula for normal random variables (\rightarrow Proof II/3.2.26), the sample means follows normal distributions (\rightarrow Definition II/3.2.1) with the following parameters:

$$\begin{aligned}\bar{y}_1 &= \frac{1}{n_1} \sum_{i=1}^{n_1} y_{1i} \sim \mathcal{N} \left(\frac{1}{n_1} n_1 \mu_1, \left(\frac{1}{n_1} \right)^2 n_1 \sigma^2 \right) = \mathcal{N} (\mu_1, \sigma_1^2/n_1) \\ \bar{y}_2 &= \frac{1}{n_2} \sum_{i=1}^{n_2} y_{2i} \sim \mathcal{N} \left(\frac{1}{n_2} n_2 \mu_2, \left(\frac{1}{n_2} \right)^2 n_2 \sigma^2 \right) = \mathcal{N} (\mu_2, \sigma_2^2/n_2) .\end{aligned}\tag{6}$$

Again employing the linear combination theorem, the distribution of $z = [(\bar{y}_1 - \bar{y}_2) - \mu_\Delta]/\sigma_\Delta$ becomes

$$z = \frac{(\bar{y}_1 - \bar{y}_2) - \mu_\Delta}{\sigma_\Delta} \sim \mathcal{N} \left(\frac{(\mu_1 - \mu_2) - \mu_\Delta}{\sigma_\Delta}, \left(\frac{1}{\sigma_\Delta} \right)^2 \sigma_\Delta^2 \right) = \mathcal{N} \left(\frac{(\mu_1 - \mu_2) - \mu_\Delta}{\sigma_\Delta}, 1 \right)\tag{7}$$

where σ_Δ is the pooled standard deviation (\rightarrow Definition “std-pool”)

$$\sigma_\Delta = \sqrt{\frac{\sigma_1^2}{n_1} + \frac{\sigma_2^2}{n_2}} ,\tag{8}$$

such that, under the null hypothesis in (4), we have:

$$z \sim \mathcal{N}(0, 1), \quad \text{if } \mu_\Delta = \mu_1 - \mu_2 .\tag{9}$$

This means that the null hypothesis (\rightarrow Definition I/4.3.2) can be rejected when z is as extreme or more extreme than the critical value (\rightarrow Definition I/4.3.9) obtained from the standard normal distribution (\rightarrow Definition II/3.2.2) using a significance level (\rightarrow Definition 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.

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1.2.5 Paired z-test

Theorem: Let y_{i1} and y_{i2} with $i = 1, \dots, n$ be paired observations, such that

$$y_{i1} \sim \mathcal{N}(y_{i2} + \mu, \sigma^2), \quad i = 1, \dots, n\tag{1}$$

is a univariate Gaussian data set (\rightarrow Definition III/1.2.1) with unknown shift μ and known variance σ^2 . Then, the test statistic (\rightarrow Definition 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 Definition I/1.7.2) \bar{d} follows a standard normal distribution (\rightarrow Definition II/3.2.2)

$$z \sim \mathcal{N}(0, 1) \quad (3)$$

under the null hypothesis (\rightarrow Definition I/4.3.2)

$$H_0 : \mu = \mu_0 . \quad (4)$$

Proof: Define the pair-wise difference $d_i = y_{i1} - y_{i2}$ which is, according to the linearity of the expected value (\rightarrow Proof I/1.7.5) and the invariance of the variance under addition (\rightarrow Proof I/1.8.6), 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 Proof 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).

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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 Definition III/1.2.1) with unknown mean μ and known variance σ^2 . Then, the conjugate prior (\rightarrow Definition I/5.2.5) for this model is a normal distribution (\rightarrow Definition II/3.2.1)

$$p(\mu) = \mathcal{N}(\mu; \mu_0, \lambda_0^{-1}) \quad (2)$$

with prior (\rightarrow Definition I/5.1.3) mean (\rightarrow Definition I/1.7.1) μ_0 and prior (\rightarrow Definition I/5.1.3) precision (\rightarrow Definition I/1.8.12) λ_0 .

Proof: By definition, a conjugate prior (\rightarrow Definition I/5.2.5) is a prior distribution (\rightarrow Definition I/5.1.3) that, when combined with the likelihood function (\rightarrow Definition I/5.1.2), leads to a posterior distribution (\rightarrow Definition I/5.1.7) that belongs to the same family of probability distributions (\rightarrow

Definition 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 Definition 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

$$\begin{aligned} p(y|\mu) &= \left(\frac{\tau}{2\pi} \right)^{n/2} \cdot \exp \left[-\frac{\tau}{2} \sum_{i=1}^n (y_i^2 - 2\mu y_i + \mu^2) \right] \\ &= \left(\frac{\tau}{2\pi} \right)^{n/2} \cdot \exp \left[-\frac{\tau}{2} \left(\sum_{i=1}^n y_i^2 - 2\mu \sum_{i=1}^n y_i + n\mu^2 \right) \right] \\ &= \left(\frac{\tau}{2\pi} \right)^{n/2} \cdot \exp \left[-\frac{\tau}{2} (y^T y - 2\mu n\bar{y} + n\mu^2) \right] \\ &= \left(\frac{\tau}{2\pi} \right)^{n/2} \cdot \exp \left[-\frac{\tau n}{2} \left(\frac{1}{n} y^T y - 2\mu\bar{y} + \mu^2 \right) \right] \end{aligned} \quad (5)$$

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

$$p(y|\mu) = \left(\frac{\tau}{2\pi} \right)^{n/2} \cdot \exp \left[-\frac{\tau n}{2} \left((\mu - \bar{y})^2 - \bar{y}^2 + \frac{1}{n} y^T y \right) \right] \quad (6)$$

In other words, the likelihood function (\rightarrow Definition I/5.1.2) is proportional to an exponential of a squared form of μ , weighted by some constant:

$$p(y|\mu) \propto \exp \left[-\frac{\tau n}{2} (\mu - \bar{y})^2 \right] . \quad (7)$$

The same is true for a normal distribution (\rightarrow Definition II/3.2.1) over μ

$$p(\mu) = \mathcal{N}(\mu; \mu_0, \lambda_0^{-1}) \quad (8)$$

the probability density function of which (\rightarrow Proof II/3.2.10)

$$p(\mu) = \sqrt{\frac{\lambda_0}{2\pi}} \cdot \exp \left[-\frac{\lambda_0}{2} (\mu - \mu_0)^2 \right] \quad (9)$$

exhibits the same proportionality

$$p(\mu) \propto \exp \left[-\frac{\lambda_0}{2} (\mu - \mu_0)^2 \right] \quad (10)$$

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>.

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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 Definition III/1.2.1) with unknown mean μ and known variance σ^2 . Moreover, assume a normal distribution (\rightarrow Proof 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 Definition I/5.1.7) is also a normal distribution (\rightarrow Definition II/3.2.1)

$$p(\mu|y) = \mathcal{N}(\mu; \mu_n, \lambda_n^{-1}) \quad (3)$$

and the posterior hyperparameters (\rightarrow Definition I/5.1.7) 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 Definition I/1.7.2) \bar{y} and the inverse variance or precision (\rightarrow Definition I/1.8.12) $\tau = 1/\sigma^2$.

Proof: According to Bayes' theorem (\rightarrow Proof I/5.3.1), the posterior distribution (\rightarrow Definition I/5.1.7) 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 Proof I/5.1.8) 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 Definition 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 Definition I/5.1.2) (8) with the prior distribution (\rightarrow Definition I/5.1.3) (2), the joint likelihood (\rightarrow Definition I/5.1.5) 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 Proof III/1.2.6) gives

$$\begin{aligned}
p(y, \mu) &= \left(\frac{\tau}{2\pi}\right)^{\frac{n}{2}} \cdot \left(\frac{\lambda_0}{2\pi}\right)^{\frac{1}{2}} \cdot \exp \left[-\frac{1}{2} \left(\sum_{i=1}^n \tau(y_i - \mu)^2 + \lambda_0(\mu - \mu_0)^2 \right) \right] \\
&= \left(\frac{\tau}{2\pi}\right)^{\frac{n}{2}} \cdot \left(\frac{\lambda_0}{2\pi}\right)^{\frac{1}{2}} \cdot \exp \left[-\frac{1}{2} \left(\sum_{i=1}^n \tau(y_i^2 - 2y_i\mu + \mu^2) + \lambda_0(\mu^2 - 2\mu\mu_0 + \mu_0^2) \right) \right] \\
&= \left(\frac{\tau}{2\pi}\right)^{\frac{n}{2}} \cdot \left(\frac{\lambda_0}{2\pi}\right)^{\frac{1}{2}} \cdot \exp \left[-\frac{1}{2} (\tau(y^T y - 2n\bar{y}\mu + n\mu^2) + \lambda_0(\mu^2 - 2\mu\mu_0 + \mu_0^2)) \right] \\
&= \left(\frac{\tau}{2\pi}\right)^{\frac{n}{2}} \cdot \left(\frac{\lambda_0}{2\pi}\right)^{\frac{1}{2}} \cdot \exp \left[-\frac{1}{2} (\mu^2(\tau n + \lambda_0) - 2\mu(\tau n\bar{y} + \lambda_0\mu_0) + (\tau y^T y + \lambda_0\mu_0^2)) \right]
\end{aligned} \tag{11}$$

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

$$p(y, \mu) = \left(\frac{\tau}{2\pi}\right)^{\frac{n}{2}} \cdot \left(\frac{\lambda_0}{2\pi}\right)^{\frac{1}{2}} \cdot \exp \left[-\frac{\lambda_n}{2} (\mu - \mu_n)^2 + f_n \right] \tag{12}$$

with the posterior hyperparameters (\rightarrow Definition I/5.1.7)

$$\begin{aligned}
\mu_n &= \frac{\lambda_0\mu_0 + \tau n\bar{y}}{\lambda_0 + \tau n} \\
\lambda_n &= \lambda_0 + \tau n
\end{aligned} \tag{13}$$

and the remaining independent term

$$f_n = -\frac{1}{2} (\tau y^T y + \lambda_0\mu_0^2 - \lambda_n\mu_n^2) . \tag{14}$$

Ergo, the joint likelihood in (12) is proportional to

$$p(y, \mu) \propto \exp \left[-\frac{\lambda_n}{2} (\mu - \mu_n)^2 \right] , \tag{15}$$

such that the posterior distribution over μ is given by

$$p(\mu|y) = \mathcal{N}(\mu; \mu_n, \lambda_n^{-1}) . \tag{16}$$

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%20%202006.pdf>.

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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 Definition III/1.2.1) with unknown mean μ and known variance σ^2 . Moreover, assume a normal distribution (\rightarrow Proof 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 Definition 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 Definition I/5.1.7) 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 Definition I/1.7.2) \bar{y} and the inverse variance or precision (\rightarrow Definition I/1.8.12) $\tau = 1/\sigma^2$.

Proof: According to the law of marginal probability (\rightarrow Definition I/1.3.3), the model evidence (\rightarrow Definition I/5.1.9) 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 Definition I/1.3.4), the integrand is equivalent to the joint likelihood (\rightarrow Definition I/5.1.5):

$$p(y|m) = \int p(y, \mu) d\mu . \quad (6)$$

Equation (1) implies the following likelihood function (\rightarrow Definition I/5.1.2)

$$\begin{aligned} p(y|\mu, \sigma^2) &= \prod_{i=1}^n \mathcal{N}(y_i; \mu, \sigma^2) \\ &= \prod_{i=1}^n \frac{1}{\sqrt{2\pi\sigma^2}} \cdot \exp \left[-\frac{1}{2} \left(\frac{y_i - \mu}{\sigma} \right)^2 \right] \\ &= \left(\sqrt{\frac{1}{2\pi\sigma^2}} \right)^n \cdot \exp \left[-\frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \mu)^2 \right] \end{aligned} \quad (7)$$

which, for mathematical convenience, can also be parametrized as

$$\begin{aligned}
p(y|\mu, \tau) &= \prod_{i=1}^n \mathcal{N}(y_i; \mu, \tau^{-1}) \\
&= \prod_{i=1}^n \sqrt{\frac{\tau}{2\pi}} \cdot \exp \left[-\frac{\tau}{2} (y_i - \mu)^2 \right] \\
&= \left(\sqrt{\frac{\tau}{2\pi}} \right)^n \cdot \exp \left[-\frac{\tau}{2} \sum_{i=1}^n (y_i - \mu)^2 \right]
\end{aligned} \tag{8}$$

using the inverse variance or precision $\tau = 1/\sigma^2$.

When deriving the posterior distribution (\rightarrow Proof III/1.2.7) $p(\mu|y)$, the joint likelihood $p(y, \mu)$ is obtained as

$$p(y, \mu) = \left(\frac{\tau}{2\pi} \right)^{\frac{n}{2}} \cdot \sqrt{\frac{\lambda_0}{2\pi}} \cdot \exp \left[-\frac{\lambda_n}{2} (\mu - \mu_n)^2 - \frac{1}{2} (\tau y^T y + \lambda_0 \mu_0^2 - \lambda_n \mu_n^2) \right]. \tag{9}$$

Using the probability density function of the normal distribution (\rightarrow Proof II/3.2.10), we can rewrite this as

$$p(y, \mu) = \left(\frac{\tau}{2\pi} \right)^{\frac{n}{2}} \cdot \sqrt{\frac{\lambda_0}{2\pi}} \cdot \sqrt{\frac{2\pi}{\lambda_n}} \cdot \mathcal{N}(\mu; \lambda_n^{-1}) \cdot \exp \left[-\frac{1}{2} (\tau y^T y + \lambda_0 \mu_0^2 - \lambda_n \mu_n^2) \right]. \tag{10}$$

Now, μ can be integrated out using the properties of the probability density function (\rightarrow Definition I/1.6.6):

$$p(y|m) = \int p(y, \mu) d\mu = \left(\frac{\tau}{2\pi} \right)^{\frac{n}{2}} \cdot \sqrt{\frac{\lambda_0}{\lambda_n}} \cdot \exp \left[-\frac{1}{2} (\tau y^T y + \lambda_0 \mu_0^2 - \lambda_n \mu_n^2) \right]. \tag{11}$$

Thus, the log model evidence (\rightarrow Definition IV/3.1.3) of this model is given by

$$\log p(y|m) = \frac{n}{2} \log \left(\frac{\tau}{2\pi} \right) + \frac{1}{2} \log \left(\frac{\lambda_0}{\lambda_n} \right) - \frac{1}{2} (\tau y^T y + \lambda_0 \mu_0^2 - \lambda_n \mu_n^2). \tag{12}$$

Sources:

- original work

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1.2.9 Accuracy and complexity

Theorem: Let

$$y = \{y_1, \dots, y_n\}, \quad y_i \sim \mathcal{N}(\mu, \sigma^2), \quad i = 1, \dots, n \tag{1}$$

be a univariate Gaussian data set (\rightarrow Definition III/1.2.1) with unknown mean μ and known variance σ^2 . Moreover, assume a statistical model (\rightarrow Definition I/5.1.4) imposing a normal distribution (\rightarrow Proof III/1.2.6) as the prior distribution (\rightarrow Definition I/5.1.3) on the model parameter μ :

$$m : y_i \sim \mathcal{N}(\mu, \sigma^2), \quad \mu \sim \mathcal{N}(\mu_0, \lambda_0^{-1}). \tag{2}$$

Then, accuracy and complexity (\rightarrow Proof 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 Proof III/1.2.7), $\tau = 1/\sigma^2$ is the inverse variance or precision (\rightarrow Definition I/1.8.12) and \bar{y} is the sample mean (\rightarrow Definition I/1.7.2).

Proof: Model accuracy and complexity are defined as (\rightarrow Proof 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 Definition I/1.7.1) of the log-likelihood function (\rightarrow Definition I/4.1.2) $\log p(y|\mu)$ with respect to the posterior distribution (\rightarrow Definition I/5.1.7) $p(\mu|y)$. With the log-likelihood function for the univariate Gaussian with known variance (\rightarrow Proof III/1.2.2) and the posterior distribution for the univariate Gaussian with known variance (\rightarrow Proof 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 Definition I/2.5.1) of the posterior distribution (\rightarrow Definition I/5.1.7) $p(\mu|y)$ from the prior distribution (\rightarrow Definition I/5.1.3) $p(\mu)$. With the prior distribution (\rightarrow Proof III/1.2.6) given by (2), the posterior distribution for the univariate Gaussian with known variance (\rightarrow Proof III/1.2.7) and the Kullback-Leibler divergence of the normal distribution (\rightarrow Proof 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 Proof III/1.2.8).

Sources:

- original work

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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 Definition III/1.2.1) with unknown mean μ and known variance σ^2 . Moreover, assume two statistical models (\rightarrow Definition I/5.1.4), one assuming that μ is zero (null model (\rightarrow Definition I/4.3.2)), the other imposing a normal distribution (\rightarrow Proof III/1.2.6) as the prior distribution (\rightarrow Definition I/5.1.3) on the model parameter μ (alternative (\rightarrow Definition 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 Definition 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 Proof III/1.2.7) which are functions of the inverse variance or precision (\rightarrow Definition I/1.8.12) $\tau = 1/\sigma^2$ and the sample mean (\rightarrow Definition I/1.7.2) \bar{y} .

Proof: The log Bayes factor is equal to the difference of two log model evidences (\rightarrow Proof 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 Proof 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 Definition IV/3.1.3) (logarithmized marginal likelihood (\rightarrow Definition I/5.1.9)) is equal to the log-likelihood function for the univariate Gaussian with known variance (\rightarrow Proof 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 Definition I/5.1.7) are given by (\rightarrow Proof 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 Definition I/1.7.2) \bar{y} and the inverse variance or precision (\rightarrow Definition I/1.8.12) $\tau = 1/\sigma^2$.

Sources:

- original work

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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 Definition III/1.2.1) with unknown mean μ and known variance σ^2 . Moreover, assume two statistical models (\rightarrow Definition I/5.1.4), one assuming that μ is zero (null model (\rightarrow Definition I/4.3.2)), the other imposing a normal distribution (\rightarrow Proof III/1.2.6) as the prior distribution (\rightarrow Definition I/5.1.3) on the model parameter μ (alternative (\rightarrow Definition 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 Definition I/4.3.2) that m_0 generated the data, the expectation (\rightarrow Definition I/1.7.1) of the log Bayes factor (\rightarrow Definition 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 Proof III/1.2.7).

Proof: The log Bayes factor for the univariate Gaussian with known variance (\rightarrow Proof 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 Definition I/5.1.7) are given by (\rightarrow Proof 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 Definition I/1.7.2) \bar{y} and the inverse variance or precision (\rightarrow Definition I/1.8.12) $\tau = 1/\sigma^2$. 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 Definition I/5.1.3) with prior mean (\rightarrow Definition I/1.7.1) $\mu_0 = 0$ 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 Definition I/1.7.1) 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 Definition I/1.7.1) 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 Definition 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:

$$\langle \text{LBF}_{10} \rangle = \frac{1}{2} \log \left(\frac{\lambda_0}{\lambda_n} \right) + \frac{1}{2} \left(\frac{\lambda_n - \lambda_0}{\lambda_n} \right).\tag{11}$$

Sources:

- original work

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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 Definition III/1.2.1) with unknown mean μ and known variance σ^2 . Moreover, assume two statistical models (\rightarrow Definition I/5.1.4), one assuming that μ is zero (null model (\rightarrow Definition I/4.3.2)), the other imposing a normal distribution (\rightarrow Proof III/1.2.6) as the prior distribution (\rightarrow Definition I/5.1.3) on the model parameter μ (alternative (\rightarrow Definition 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 Definition IV/3.1.8) 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 Definition I/1.7.2), $\tau = 1/\sigma^2$ is the inverse variance or precision (\rightarrow Definition I/1.8.12), $y_1^{(i)}$ are the training data in the i -th cross-validation fold and S is the number of data subsets (\rightarrow Definition IV/3.1.8).

Proof: For evaluation of the cross-validated log model evidences (\rightarrow Definition IV/3.1.8) (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 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 Definition “ooslme”) (oosLME) is equal to the log-likelihood function (\rightarrow Proof III/1.2.2) of the test data at $\mu = 0$:

$$\text{oosLME}_i(m_0) = \log p\left(y_2^{(i)} \middle| \mu = 0\right) = \frac{n_2}{2} \log\left(\frac{\tau}{2\pi}\right) - \frac{1}{2} \left[\tau y_2^{(i)\top} y_2^{(i)} \right]. \quad (6)$$

By definition, the cross-validated log model evidence is the sum of out-of-sample log model evidences (\rightarrow Definition IV/3.1.8) over cross-validation folds, such that the cvLME of m_0 is:

$$\begin{aligned} \text{cvLME}(m_0) &= \sum_{i=1}^S \text{oosLME}_i(m_0) \\ &= \sum_{i=1}^S \left(\frac{n_2}{2} \log\left(\frac{\tau}{2\pi}\right) - \frac{1}{2} \left[\tau y_2^{(i)\top} y_2^{(i)} \right] \right) \\ &= \frac{n}{2} \log\left(\frac{\tau}{2\pi}\right) - \frac{1}{2} [\tau y^\top y]. \end{aligned} \quad (7)$$

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 Definition I/5.2.3) and applying the posterior distribution for the univariate Gaussian with known variance (\rightarrow Proof 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 Definition I/5.2.3), again applying the posterior distribution for the univariate Gaussian with known variance (\rightarrow Proof 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 Proof III/1.2.8), the out-of-sample log model evidence (\rightarrow Definition “ooslme”) (oosLME) therefore follows as

$$\begin{aligned} \text{oosLME}_i(m_1) &= \frac{n_2}{2} \log\left(\frac{\tau}{2\pi}\right) + \frac{1}{2} \log\left(\frac{\lambda_0^{(2)}}{\lambda_n^{(2)}}\right) - \frac{1}{2} \left[\tau y_2^{(i)\top} y_2^{(i)} + \lambda_0^{(2)} \mu_0^{(2)2} - \lambda_n^{(2)} \mu_n^{(2)2} \right] \\ &= \frac{n_2}{2} \log\left(\frac{\tau}{2\pi}\right) + \frac{1}{2} \log\left(\frac{n_1}{n}\right) - \frac{1}{2} \left[\tau y_2^{(i)\top} y_2^{(i)} + \frac{\tau}{n_1} \left(n_1 \bar{y}_1^{(i)} \right)^2 - \frac{\tau}{n} (n \bar{y})^2 \right]. \end{aligned} \quad (10)$$

Again, because the cross-validated log model evidence is the sum of out-of-sample log model evidences (\rightarrow Definition IV/3.1.8) over cross-validation folds, the cvLME of m_1 becomes:

$$\begin{aligned}
 \text{cvLME}(m_1) &= \sum_{i=1}^S \text{oosLME}_i(m_1) \\
 &= \sum_{i=1}^S \left(\frac{n_2}{2} \log \left(\frac{\tau}{2\pi} \right) + \frac{1}{2} \log \left(\frac{n_1}{n} \right) - \frac{1}{2} \left[\tau y_2^{(i)\top} y_2^{(i)} + \frac{\tau}{n_1} \left(n_1 \bar{y}_1^{(i)} \right)^2 - \frac{\tau}{n} (n\bar{y})^2 \right] \right) \\
 &= \frac{S \cdot n_2}{2} \log \left(\frac{\tau}{2\pi} \right) + \frac{S}{2} \log \left(\frac{n_1}{n} \right) - \frac{\tau}{2} \sum_{i=1}^S \left[y_2^{(i)\top} y_2^{(i)} + \frac{\left(n_1 \bar{y}_1^{(i)} \right)^2}{n_1} - \frac{(n\bar{y})^2}{n} \right] \\
 &= \frac{n}{2} \log \left(\frac{\tau}{2\pi} \right) + \frac{S}{2} \log \left(\frac{S-1}{S} \right) - \frac{\tau}{2} \left[y^\top y + \sum_{i=1}^S \left(\frac{\left(n_1 \bar{y}_1^{(i)} \right)^2}{n_1} - \frac{(n\bar{y})^2}{n} \right) \right].
 \end{aligned} \tag{11}$$

Together, (7) and (11) conform to the results given in (3).

Sources:

- original work

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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 Definition III/1.2.1) with unknown mean μ and known variance σ^2 . Moreover, assume two statistical models (\rightarrow Definition I/5.1.4), one assuming that μ is zero (null model (\rightarrow Definition I/4.3.2)), the other imposing a normal distribution (\rightarrow Proof III/1.2.6) as the prior distribution (\rightarrow Definition I/5.1.3) on the model parameter μ (alternative (\rightarrow Definition 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 Definition IV/3.1.8) log Bayes factor (\rightarrow Definition 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 Definition I/1.7.2), $\tau = 1/\sigma^2$ is the inverse variance or precision (\rightarrow Definition I/1.8.12), $y_1^{(i)}$ are the training data in the i -th cross-validation fold and S is the number of data subsets (\rightarrow Definition IV/3.1.8).

Proof: The relationship between log Bayes factor and log model evidences (\rightarrow Proof IV/3.3.8) also holds for cross-validated log bayes factor (\rightarrow Definition IV/3.3.6) (cvLBF) and cross-validated log model evidences (\rightarrow Definition IV/3.1.8) (cvLME):

$$\text{cvLBF}_{12} = \text{cvLME}(m_1) - \text{cvLME}(m_2) . \quad (4)$$

The cross-validated log model evidences (\rightarrow Definition IV/3.1.8) of m_0 and m_1 are given by (\rightarrow Proof 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

$$\begin{aligned} \text{cvLBF}_{10} &= \text{cvLME}(m_1) - \text{LME}(m_0) \\ &= \left(\frac{n}{2} \log \left(\frac{\tau}{2\pi} \right) + \frac{S}{2} \log \left(\frac{S-1}{S} \right) - \frac{\tau}{2} \left[y^T y + \sum_{i=1}^S \left(\frac{(n_1 \bar{y}_1^{(i)})^2}{n_1} - \frac{(n \bar{y})^2}{n} \right) \right] \right) \\ &\quad - \left(\frac{n}{2} \log \left(\frac{\tau}{2\pi} \right) - \frac{1}{2} (\tau y^T y) \right) \\ &= \frac{S}{2} \log \left(\frac{S-1}{S} \right) - \frac{\tau}{2} \sum_{i=1}^S \left(\frac{(n_1 \bar{y}_1^{(i)})^2}{n_1} - \frac{(n \bar{y})^2}{n} \right) . \end{aligned} \quad (6)$$

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- original work

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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 Definition III/1.2.1) with unknown mean μ and known variance σ^2 . Moreover, assume two statistical models (\rightarrow Definition I/5.1.4), one assuming that μ is zero (null model (\rightarrow Definition I/4.3.2)), the other imposing a normal distribution (\rightarrow Proof III/1.2.6) as the prior distribution (\rightarrow Definition I/5.1.3) on the model parameter μ (alternative (\rightarrow Definition 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 Definition I/1.7.1) of the cross-validated (\rightarrow Definition IV/3.1.8) log Bayes factor (\rightarrow Definition 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 Definition I/1.8.12) and S is the number of data subsets (\rightarrow Definition IV/3.1.8).

Proof: The cross-validated log Bayes factor for the univariate Gaussian with known variance (\rightarrow Proof 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 Definition I/1.7.1) 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 Definition I/1.7.1) 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 Proof III/1.2.12) $n_1 + n_2 = n$ and $n_2 = n/S$, we finally have:

$$\begin{aligned}
\langle \text{cvLBF}_{10} \rangle &= \frac{S}{2} \log \left(\frac{S-1}{S} \right) - \frac{\tau}{2} \sum_{i=1}^S (-n_i) \mu^2 \\
&= \frac{S}{2} \log \left(\frac{S-1}{S} \right) + \frac{1}{2} [\tau n \mu^2] .
\end{aligned} \tag{7}$$

Sources:

- original work

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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 Definition II/3.2.1)

$$y_{ij} \sim \mathcal{N}(\mu_i, \sigma^2) \quad \text{for all } i = 1, \dots, k \quad \text{and } j = 1, \dots, n_i \tag{1}$$

where

- μ_i is the expected value (\rightarrow Definition I/1.7.1) in group i and
- σ^2 is the common variance (\rightarrow Definition I/1.8.1) across groups.

Alternatively, the model may be written as

$$\begin{aligned}
y_{ij} &= \mu_i + \varepsilon_{ij} \\
\varepsilon_{ij} &\stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2)
\end{aligned} \tag{2}$$

where ε_{ij} is the error term (\rightarrow Definition III/1.4.1) belonging to observation j in category i and ε_{ij} are the independent and identically distributed (\rightarrow Definition “iid”).

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 CrossValidated*, retrieved on 2022-11-06; URL: <https://stats.stackexchange.com/questions/355594/derive-the-distribution-of-the-anova-f-statistic-under-the-alternative-hypothesis>.

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1.3.2 Treatment sum of squares

Definition: Let there be an analysis of variance (ANOVA) model with one (\rightarrow Definition III/1.3.1), two (\rightarrow Definition III/1.3.8) or multiple (\rightarrow Definition “anovan”) factors influencing the measured data y (here, using the reparametrized version (\rightarrow Proof III/1.3.7) of one-way ANOVA (\rightarrow Definition 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] (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.

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1.3.3 Ordinary least squares for one-way ANOVA

Theorem: Given the one-way analysis of variance (\rightarrow Definition 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 Definition III/1.5.7) are given by

$$\hat{\mu}_i = \bar{y}_i \quad (2)$$

where \bar{y}_i is the sample mean (\rightarrow Definition I/1.7.2) of all observations in group (\rightarrow Definition III/1.3.1) i :

$$\hat{\mu}_i = \bar{y}_i = \frac{1}{n_i} \sum_{j=1}^{n_i} y_{ij} . \quad (3)$$

Proof: The residual sum of squares (\rightarrow Definition III/1.5.7) 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

$$\begin{aligned}
\frac{d\text{RSS}(\mu)}{d\mu_i} &= \sum_{j=1}^{n_i} \frac{d}{d\mu_i} (y_{ij} - \mu_i)^2 \\
&= \sum_{j=1}^{n_i} 2(y_{ij} - \mu_i)(-1) \\
&= 2 \sum_{j=1}^{n_i} (\mu_i - y_{ij}) \\
&= 2n_i\mu_i - 2 \sum_{j=1}^{n_i} y_{ij} \quad \text{for } i = 1, \dots, k.
\end{aligned} \tag{5}$$

Setting these derivatives to zero, we obtain the estimates of μ_i :

$$\begin{aligned}
0 &= 2n_i\hat{\mu}_i - 2 \sum_{j=1}^{n_i} y_{ij} \\
\hat{\mu}_i &= \frac{1}{n_i} \sum_{j=1}^{n_i} y_{ij} \quad \text{for } i = 1, \dots, k.
\end{aligned} \tag{6}$$

Sources:

- original work

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1.3.4 Sums of squares in one-way ANOVA

Theorem: Given one-way analysis of variance (\rightarrow Definition III/1.3.1),

$$y_{ij} = \mu_i + \varepsilon_{ij}, \quad \varepsilon_{ij} \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2) \tag{1}$$

sums of squares can be partitioned as follows

$$\text{SS}_{\text{tot}} = \text{SS}_{\text{treat}} + \text{SS}_{\text{res}} \tag{2}$$

where SS_{tot} is the total sum of squares (\rightarrow Definition III/1.5.5), SS_{treat} is the treatment sum of squares (\rightarrow Definition III/1.3.2) (equivalent to explained sum of squares (\rightarrow Definition III/1.5.6)) and SS_{res} is the residual sum of squares (\rightarrow Definition III/1.5.7).

Proof: The total sum of squares (\rightarrow Definition III/1.5.5) for one-way ANOVA (\rightarrow Definition III/1.3.1) is given by

$$\text{SS}_{\text{tot}} = \sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \bar{y})^2 \tag{3}$$

where \bar{y} is the mean across all values y_{ij} . This can be rewritten as

$$\begin{aligned}
\sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \bar{y})^2 &= \sum_{i=1}^k \sum_{j=1}^{n_i} [(y_{ij} - \bar{y}_i) + (\bar{y}_i - \bar{y})]^2 \\
&= \sum_{i=1}^k \sum_{j=1}^{n_i} [(y_{ij} - \bar{y}_i)^2 + (\bar{y}_i - \bar{y})^2 + 2(y_{ij} - \bar{y}_i)(\bar{y}_i - \bar{y})] \\
&= \sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_i)^2 + \sum_{i=1}^k \sum_{j=1}^{n_i} (\bar{y}_i - \bar{y})^2 + 2 \sum_{i=1}^k (\bar{y}_i - \bar{y}) \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_i) .
\end{aligned} \tag{4}$$

Note that the following sum is zero

$$\sum_{j=1}^{n_i} (y_{ij} - \bar{y}_i) = \sum_{j=1}^{n_i} y_{ij} - n_i \cdot \bar{y}_i = \sum_{j=1}^{n_i} y_{ij} - n_i \cdot \frac{1}{n_i} \sum_{j=1}^{n_i} y_{ij} , \tag{5}$$

so that the sum in (4) reduces to

$$\sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \bar{y})^2 = \sum_{i=1}^k \sum_{j=1}^{n_i} (\bar{y}_i - \bar{y})^2 + \sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_i)^2 . \tag{6}$$

With the treatment sum of squares (\rightarrow Definition III/1.3.2) for one-way ANOVA (\rightarrow Definition III/1.3.1)

$$SS_{\text{treat}} = \sum_{i=1}^k \sum_{j=1}^{n_i} (\bar{y}_i - \bar{y})^2 \tag{7}$$

and the residual sum of squares (\rightarrow Definition III/1.5.7) for one-way ANOVA (\rightarrow Definition III/1.3.1)

$$SS_{\text{res}} = \sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_i)^2 , \tag{8}$$

we finally have:

$$SS_{\text{tot}} = SS_{\text{treat}} + SS_{\text{res}} . \tag{9}$$

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.

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1.3.5 F-test for main effect in one-way ANOVA

Theorem: Assume the one-way analysis of variance (\rightarrow Definition III/1.3.1) model

$$y_{ij} = \mu_i + \varepsilon_{ij}, \quad \varepsilon_{ij} \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2), \quad i = 1, \dots, k, \quad j = 1, \dots, n_i . \tag{1}$$

Then, the test statistic (\rightarrow Definition 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 Definition II/3.8.1)

$$F \sim F(k-1, n-k) \quad (3)$$

under the null hypothesis (\rightarrow Definition 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 Definition I/1.7.1) 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 Definition I/1.2.2) $U_{ij} = (y_{ij} - \mu)/\sigma$ follows a standard normal distribution (\rightarrow Proof II/3.2.3)

$$U_{ij} = \frac{y_{ij} - \mu}{\sigma} \sim \mathcal{N}(0, 1). \quad (8)$$

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

$$\begin{aligned}\sum_{j=1}^{n_i} (y_{ij} - \bar{y}_i) &= \sum_{j=1}^{n_i} y_{ij} - n_i \bar{y}_i \\ &= \sum_{j=1}^{n_i} y_{ij} - n_i \cdot \frac{1}{n_i} \sum_{j=1}^{n_i} y_{ij} \\ &= 0, \quad i = 1, \dots, k\end{aligned}\tag{10}$$

and the following sum over i and j is also zero

$$\begin{aligned}\sum_{i=1}^k \sum_{j=1}^{n_i} (\bar{y}_i - \bar{y}) &= \sum_{i=1}^k n_i (\bar{y}_i - \bar{y}) \\ &= \sum_{i=1}^k n_i \bar{y}_i - \bar{y} \sum_{i=1}^k n_i \\ &= \sum_{i=1}^k n_i \cdot \frac{1}{n_i} \sum_{j=1}^{n_i} y_{ij} - n \cdot \frac{1}{n} \sum_{i=1}^k \sum_{j=1}^{n_i} y_{ij} \\ &= 0,\end{aligned}\tag{11}$$

non-square products in (9) disappear and the sum reduces to

$$\begin{aligned}\sum_{i=1}^k \sum_{j=1}^{n_i} U_{ij}^2 &= \sum_{i=1}^k \sum_{j=1}^{n_i} \left[\left(\frac{y_{ij} - \bar{y}_i}{\sigma} \right)^2 + \left(\frac{\bar{y}_i - \bar{y}}{\sigma} \right)^2 + \left(\frac{\bar{y} - \mu}{\sigma} \right)^2 \right] \\ &= \sum_{i=1}^k \sum_{j=1}^{n_i} \left(\frac{y_{ij} - \bar{y}_i}{\sigma} \right)^2 + \sum_{i=1}^k \sum_{j=1}^{n_i} \left(\frac{\bar{y}_i - \bar{y}}{\sigma} \right)^2 + \sum_{i=1}^k \sum_{j=1}^{n_i} \left(\frac{\bar{y} - \mu}{\sigma} \right)^2.\end{aligned}\tag{12}$$

Cochran's theorem (\rightarrow Proof "snorm-cochran") states that, if a sum of squared standard normal (\rightarrow Definition II/3.2.2) random variables (\rightarrow Definition 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 Definition I/1.3.6) and each term Q_j follows a chi-squared distribution (\rightarrow Definition 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 $n \times 1$ column vector of all observations

$$U = \begin{bmatrix} u_1 \\ \vdots \\ u_k \end{bmatrix} \quad (15)$$

where the group-wise $n_i \times 1$ column vectors are

$$u_1 = \begin{bmatrix} (y_{1,1} - \mu)/\sigma \\ \vdots \\ (y_{1,n_1} - \mu)/\sigma \end{bmatrix}, \quad \dots, \quad u_k = \begin{bmatrix} (y_{k,1} - \mu)/\sigma \\ \vdots \\ (y_{k,n_k} - \mu)/\sigma \end{bmatrix}. \quad (16)$$

Then, we observe that the sum in (12) can be represented in the form of (13) using the matrices

$$\begin{aligned} B^{(1)} &= I_n - \text{diag} \left(\frac{1}{n_1} J_{n_1}, \dots, \frac{1}{n_k} J_{n_k} \right) \\ B^{(2)} &= \text{diag} \left(\frac{1}{n_1} J_{n_1}, \dots, \frac{1}{n_k} J_{n_k} \right) - \frac{1}{n} J_n \\ B^{(3)} &= \frac{1}{n} J_n \end{aligned} \quad (17)$$

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

$$\sum_{i=1}^k \sum_{j=1}^{n_i} U_{ij}^2 = Q_1 + Q_2 + Q_3 = U^T B^{(1)} U + U^T B^{(2)} U + U^T B^{(3)} U \quad (18)$$

as well as

$$B^{(1)} + B^{(2)} + B^{(3)} = I_n \quad (19)$$

and their ranks are:

$$\begin{aligned} \text{rank}(B^{(1)}) &= n - k \\ \text{rank}(B^{(2)}) &= k - 1 \\ \text{rank}(B^{(3)}) &= 1. \end{aligned} \quad (20)$$

Let's write down the explained sum of squares (\rightarrow Definition III/1.5.6) and the residual sum of squares (\rightarrow Definition III/1.5.7) for one-way analysis of variance (\rightarrow Definition III/1.3.1) as

$$\begin{aligned} \text{ESS} &= \sum_{i=1}^k \sum_{j=1}^{n_i} (\bar{y}_i - \bar{y})^2 \\ \text{RSS} &= \sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_i)^2. \end{aligned} \quad (21)$$

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 Definition II/3.7.1) random variables (\rightarrow Definition 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 Definition II/3.8.1), is distributed as

$$F \sim F(k-1, n-k)\tag{24}$$

under the null hypothesis (\rightarrow Definition 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>.

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1.3.6 F-statistic in terms of OLS estimates

Theorem: Given the one-way analysis of variance (\rightarrow Definition III/1.3.1) assumption

$$y_{ij} = \mu_i + \varepsilon_{ij}, \quad \varepsilon_{ij} \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2),\tag{1}$$

1) the F-statistic for the main effect (\rightarrow Proof III/1.3.5) can be expressed in terms of ordinary least squares parameter estimates (\rightarrow Proof III/1.3.3) as

$$F = \frac{\frac{1}{k-1} \sum_{i=1}^k n_i (\hat{\mu}_i - \bar{y})^2}{\frac{1}{n-k} \sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \hat{\mu}_i)^2}\tag{2}$$

2) or, when using the reparametrized version of one-way ANOVA (\rightarrow Proof III/1.3.7), the F-statistic can be expressed as

$$F = \frac{\frac{1}{k-1} \sum_{i=1}^k n_i \hat{\delta}_i^2}{\frac{1}{n-k} \sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \hat{\mu} - \hat{\delta}_i)^2} . \quad (3)$$

Theorem: The F-statistic for the main effect in one-way ANOVA (\rightarrow Proof III/1.3.5) is given in terms of the sample means (\rightarrow Definition I/1.7.2) 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 Proof 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 Proof 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

$$F = \frac{\frac{1}{k-1} \sum_{i=1}^k n_i \hat{\delta}_i^2}{\frac{1}{n-k} \sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \hat{\mu} - \hat{\delta}_i)^2} . \quad (8)$$

Sources:

- original work

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1.3.7 Reparametrization of one-way ANOVA

Theorem: The one-way analysis of variance (\rightarrow Definition 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 Proof 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 Proof III/1.3.4) is chi-square distributed (\rightarrow Definition 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 Definition I/4.3.5) is F-distributed (\rightarrow Definition 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 Definition “anova1-f”)

$$H_0 : \delta_1 = \dots = \delta_k = 0. \quad (8)$$

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) Equation (2) is a special case of the two-way analysis of variance (\rightarrow Definition III/1.3.8) with (i) just one factor A and (ii) no interaction term. Thus, OLS estimates are identical to that of two-way ANOVA (\rightarrow Proof III/1.3.10), i.e. given by

$$\begin{aligned} \hat{\mu} &= \bar{y}_{\bullet\bullet} = \frac{1}{n} \sum_{i=1}^k \sum_{j=1}^{n_i} y_{ij} \\ \hat{\delta}_i &= \bar{y}_{i\bullet} - \bar{y}_{\bullet\bullet} = \frac{1}{n_i} \sum_{j=1}^{n_i} y_{ij} - \frac{1}{n} \sum_{i=1}^k \sum_{j=1}^{n_i} y_{ij}. \end{aligned} \quad (10)$$

3) Let $U_{ij} = (y_{ij} - \mu - \delta_i)/\sigma$, such that (\rightarrow Proof II/3.2.3) $U_{ij} \sim \mathcal{N}(0, 1)$ and consider the sum of all squared random variables (\rightarrow Definition I/1.2.2) U_{ij} :

$$\begin{aligned}
\sum_{i=1}^k \sum_{j=1}^{n_i} U_{ij}^2 &= \sum_{i=1}^k \sum_{j=1}^{n_i} \left(\frac{y_{ij} - \mu - \delta_i}{\sigma} \right)^2 \\
&= \frac{1}{\sigma^2} \sum_{i=1}^k \sum_{j=1}^{n_i} [(y_{ij} - \bar{y}_i) + ([\bar{y}_i - \bar{y}] - \delta_i) + (\bar{y} - \mu)]^2.
\end{aligned} \tag{11}$$

This square of sums, using a number of intermediate steps, can be developed (\rightarrow Proof III/1.3.5) into a sum of squares:

$$\begin{aligned}
\sum_{i=1}^k \sum_{j=1}^{n_i} U_{ij}^2 &= \frac{1}{\sigma^2} \sum_{i=1}^k \sum_{j=1}^{n_i} [(y_{ij} - \bar{y}_i)^2 + ([\bar{y}_i - \bar{y}] - \delta_i)^2 + (\bar{y} - \mu)^2] \\
&= \frac{1}{\sigma^2} \left[\sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_i)^2 + \sum_{i=1}^k \sum_{j=1}^{n_i} ([\bar{y}_i - \bar{y}] - \delta_i)^2 + \sum_{i=1}^k \sum_{j=1}^{n_i} (\bar{y} - \mu)^2 \right].
\end{aligned} \tag{12}$$

To this sum, Cochran's theorem for one-way analysis of variance can be applied (\rightarrow Proof III/1.3.5), yielding the distributions:

$$\begin{aligned}
\frac{1}{\sigma^2} \sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_i)^2 &\sim \chi^2(n - k) \\
\frac{1}{\sigma^2} \sum_{i=1}^k \sum_{j=1}^{n_i} ([\bar{y}_i - \bar{y}] - \delta_i)^2 &\stackrel{(10)}{=} \frac{1}{\sigma^2} \sum_{i=1}^k \sum_{j=1}^{n_i} (\hat{\delta}_i - \delta_i)^2 \sim \chi^2(k - 1).
\end{aligned} \tag{13}$$

4) The ratio of two chi-square distributed (\rightarrow Definition II/3.7.1) random variables (\rightarrow Definition I/1.2.2), divided by their degrees of freedom (\rightarrow Definition "dof"), is defined to be F-distributed (\rightarrow Definition II/3.8.1), so that

$$\begin{aligned}
F &= \frac{\left(\frac{1}{\sigma^2} \sum_{i=1}^k \sum_{j=1}^{n_i} (\hat{\delta}_i - \delta_i)^2 \right) / (k - 1)}{\left(\frac{1}{\sigma^2} \sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_i)^2 \right) / (n - k)} \\
&= \frac{\frac{1}{k-1} \sum_{i=1}^k \sum_{j=1}^{n_i} (\hat{\delta}_i - \delta_i)^2}{\frac{1}{n-k} \sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_i)^2} \\
&= \frac{\frac{1}{k-1} \sum_{i=1}^k n_i (\hat{\delta}_i - \delta_i)^2}{\frac{1}{n-k} \sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_i)^2} \\
&\stackrel{(8)}{=} \frac{\frac{1}{k-1} \sum_{i=1}^k n_i \hat{\delta}_i^2}{\frac{1}{n-k} \sum_{i=1}^k \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_i)^2}
\end{aligned} \tag{14}$$

follows the F-distribution

$$F \sim F(k - 1, n - k) \tag{15}$$

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.

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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 Definition II/3.2.1)

$$y_{ij} \sim \mathcal{N}(\mu_{ij}, \sigma^2) \quad \text{for all } i = 1, \dots, a, \quad j = 1, \dots, b, \quad \text{and } k = 1, \dots, n_{ij} \quad (1)$$

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 Definition I/1.7.1) in category (i, j) ; and
- σ^2 is common variance (\rightarrow Definition I/1.8.1) 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 Definition 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 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>.

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1.3.9 Interaction sum of squares

Definition: Let there be an analysis of variance (ANOVA) model with two (\rightarrow Definition III/1.3.8) or more (\rightarrow Definition “anovan”) factors influencing the measured data y (here, using the standard formulation (\rightarrow Proof III/1.3.11) of two-way ANOVA (\rightarrow Definition 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] (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 Definition 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>.

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1.3.10 Ordinary least squares for two-way ANOVA

Theorem: Given the two-way analysis of variance (\rightarrow Definition 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 Definition III/1.5.7) and satisfying the constraints for the model parameters (\rightarrow Definition 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 Definition I/1.7.2):

$$\begin{aligned}\bar{y}_{\bullet\bullet\bullet} &= \frac{1}{n} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} y_{ijk} \\ \bar{y}_{i\bullet\bullet} &= \frac{1}{n_{i\bullet}} \sum_{j=1}^b \sum_{k=1}^{n_{ij}} y_{ijk} \\ \bar{y}_{\bullet j\bullet} &= \frac{1}{n_{\bullet j}} \sum_{i=1}^a \sum_{k=1}^{n_{ij}} y_{ijk} \\ \bar{y}_{ij\bullet} &= \frac{1}{n_{ij}} \sum_{k=1}^{n_{ij}} y_{ijk}\end{aligned}\tag{3}$$

with the sample size 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 Definition 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 Definition III/1.5.7) 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_i :

$$\begin{aligned}
0 &= 2n\hat{\mu} + 2 \left(\sum_{i=1}^a n_{i\bullet} \alpha_i + \sum_{j=1}^b n_{\bullet j} \beta_j + \sum_{i=1}^a \sum_{j=1}^b n_{ij} \gamma_{ij} \right) - 2 \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} y_{ijk} \\
\hat{\mu} &= \frac{1}{n} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} y_{ijk} - \sum_{i=1}^a \frac{n_{i\bullet}}{n} \alpha_i - \sum_{j=1}^b \frac{n_{\bullet j}}{n} \beta_j - \sum_{i=1}^a \sum_{j=1}^b \frac{n_{ij}}{n} \gamma_{ij} \\
&\stackrel{(4)}{=} \frac{1}{n} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} y_{ijk} - \sum_{j=1}^b \sum_{i=1}^a \frac{n_{ij}}{n} \alpha_i - \sum_{i=1}^a \sum_{j=1}^b \frac{n_{ij}}{n} \beta_j - \sum_{i=1}^a \sum_{j=1}^b \frac{n_{ij}}{n} \gamma_{ij} \\
&\stackrel{(5)}{=} \frac{1}{n} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} y_{ijk} \\
&\stackrel{(3)}{=} \bar{y}_{\bullet\bullet\bullet}
\end{aligned} \tag{11}$$

$$\begin{aligned}
0 &= 2n_{i\bullet} \hat{\mu} + 2n_{i\bullet} \hat{\alpha}_i + 2 \left(\sum_{j=1}^b n_{ij} \beta_j + \sum_{j=1}^b n_{ij} \gamma_{ij} \right) - 2 \sum_{j=1}^b \sum_{k=1}^{n_{ij}} y_{ijk} \\
\hat{\alpha}_i &= \frac{1}{n_{i\bullet}} \sum_{j=1}^b \sum_{k=1}^{n_{ij}} y_{ijk} - \hat{\mu} - \sum_{j=1}^b \frac{n_{ij}}{n_{i\bullet}} \beta_j - \sum_{j=1}^b \frac{n_{ij}}{n_{i\bullet}} \gamma_{ij} \\
&= \frac{1}{n_{i\bullet}} \sum_{j=1}^b \sum_{k=1}^{n_{ij}} y_{ijk} - \hat{\mu} - \frac{n}{n_{i\bullet}} \sum_{j=1}^b \frac{n_{ij}}{n} \beta_j - \frac{n}{n_{i\bullet}} \sum_{j=1}^b \frac{n_{ij}}{n} \gamma_{ij} \\
&\stackrel{(5)}{=} \frac{1}{n_{i\bullet}} \sum_{j=1}^b \sum_{k=1}^{n_{ij}} y_{ijk} - \frac{1}{n} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} y_{ijk} \\
&\stackrel{(3)}{=} \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet}
\end{aligned} \tag{12}$$

$$\begin{aligned}
0 &= 2n_{\bullet j} \hat{\mu} + 2n_{\bullet j} \hat{\beta}_j + 2 \left(\sum_{i=1}^a n_{ij} \alpha_i + \sum_{i=1}^a n_{ij} \gamma_{ij} \right) - 2 \sum_{i=1}^a \sum_{k=1}^{n_{ij}} y_{ijk} \\
\hat{\beta}_j &= \frac{1}{n_{\bullet j}} \sum_{i=1}^a \sum_{k=1}^{n_{ij}} y_{ijk} - \hat{\mu} - \sum_{i=1}^a \frac{n_{ij}}{n_{\bullet j}} \alpha_i - \sum_{i=1}^a \frac{n_{ij}}{n_{\bullet j}} \gamma_{ij} \\
&= \frac{1}{n_{\bullet j}} \sum_{i=1}^a \sum_{k=1}^{n_{ij}} y_{ijk} - \hat{\mu} - \frac{n}{n_{\bullet j}} \sum_{i=1}^a \frac{n_{ij}}{n} \alpha_i - \frac{n}{n_{\bullet j}} \sum_{i=1}^a \frac{n_{ij}}{n} \gamma_{ij} \\
&\stackrel{(5)}{=} \frac{1}{n_{\bullet j}} \sum_{i=1}^a \sum_{k=1}^{n_{ij}} y_{ijk} - \frac{1}{n} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} y_{ijk} \\
&\stackrel{(3)}{=} \bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet}
\end{aligned} \tag{13}$$

$$\begin{aligned}
0 &= 2n_{ij}(\hat{\mu} + \hat{\alpha}_i + \hat{\beta}_j + \hat{\gamma}_{ij}) - 2 \sum_{k=1}^{n_{ij}} y_{ijk} \\
\hat{\gamma}_{ij} &= \frac{1}{n_{ij}} \sum_{k=1}^{n_{ij}} y_{ijk} - \hat{\alpha}_i - \hat{\beta}_j - \hat{\mu} \\
&= \frac{1}{n_{ij}} \sum_{k=1}^{n_{ij}} y_{ijk} - \frac{1}{n_{i\bullet}} \sum_{j=1}^b \sum_{k=1}^{n_{ij}} y_{ijk} - \frac{1}{n_{\bullet j}} \sum_{i=1}^a \sum_{k=1}^{n_{ij}} y_{ijk} + \frac{1}{n} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} y_{ijk} \\
&\stackrel{(3)}{=} \bar{y}_{ij\bullet} - \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet j\bullet} + \bar{y}_{\bullet\bullet\bullet} .
\end{aligned} \tag{14}$$

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.

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1.3.11 Sums of squares in two-way ANOVA

Theorem: Given two-way analysis of variance (\rightarrow Definition 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 Definition III/1.5.5), SS_A , SS_B and $\text{SS}_{A \times B}$ are treatment (\rightarrow Definition III/1.3.2) and interaction sum of squares (\rightarrow Definition III/1.3.9) (summing into the explained sum of squares (\rightarrow Definition III/1.5.6)) and SS_{res} is the residual sum of squares (\rightarrow Definition III/1.5.7).

Proof: The total sum of squares (\rightarrow Definition III/1.5.5) for two-way ANOVA (\rightarrow Definition 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

$$\begin{aligned}
\sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{\bullet\bullet\bullet})^2 &= \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} [(y_{ijk} - \bar{y}_{ij\bullet}) + (\bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet}) + (\bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet}) + \\
&\quad (\bar{y}_{ij\bullet} - \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet j\bullet} + \bar{y}_{\bullet\bullet\bullet})]^2
\end{aligned} \tag{4}$$

It can be shown (\rightarrow Proof 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

$$\begin{aligned}
 \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{\bullet\bullet\bullet})^2 &= \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} [(y_{ijk} - \bar{y}_{ij\bullet})^2 + (\bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet})^2 + (\bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet})^2 + \\
 &\quad (\bar{y}_{ij\bullet} - \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet j\bullet} + \bar{y}_{\bullet\bullet\bullet})^2] \\
 &= \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2 + \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (\bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet})^2 + \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (\bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet})^2 + \\
 &\quad \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (\bar{y}_{ij\bullet} - \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet j\bullet} + \bar{y}_{\bullet\bullet\bullet})^2.
 \end{aligned} \tag{6}$$

With the treatment sums of squares (\rightarrow Definition 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 Definition 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 Definition III/1.5.7) for two-way ANOVA (\rightarrow Definition 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.

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1.3.12 Cochran’s theorem for two-way ANOVA

Theorem: Assume the two-way analysis of variance (\rightarrow Definition III/1.3.8) model

$$\begin{aligned} y_{ijk} &= \mu + \alpha_i + \beta_j + \gamma_{ij} + \varepsilon_{ijk} \\ \varepsilon_{ijk} &\stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2), \quad i = 1, \dots, a, \quad j = 1, \dots, b, \quad k = 1, \dots, n_{ij} \end{aligned} \quad (1)$$

under the well-known constraints for the model parameters (\rightarrow Definition 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 Proof III/1.3.11) are chi-square distributed (\rightarrow Definition II/3.7.1)

$$\begin{aligned}
\frac{1}{\sigma^2} n(\bar{y}_{\bullet\bullet\bullet} - \mu)^2 &= \frac{\text{SS}_M}{\sigma^2} \sim \chi^2(1) \\
\frac{1}{\sigma^2} \sum_{i=1}^a n_{i\bullet} ([\bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet}] - \alpha_i)^2 &= \frac{\text{SS}_A}{\sigma^2} \sim \chi^2(a-1) \\
\frac{1}{\sigma^2} \sum_{j=1}^b n_{\bullet j} ([\bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet}] - \beta_j)^2 &= \frac{\text{SS}_B}{\sigma^2} \sim \chi^2(b-1) \\
\frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b n_{ij} ([\bar{y}_{ij\bullet} - \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet j\bullet} + \bar{y}_{\bullet\bullet\bullet}] - \gamma_{ij})^2 &= \frac{\text{SS}_{A \times B}}{\sigma^2} \sim \chi^2((a-1)(b-1)) \\
\frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2 &= \frac{\text{SS}_{\text{res}}}{\sigma^2} \sim \chi^2(n - ab) .
\end{aligned} \tag{3}$$

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 Definition I/1.2.2) $U_{ijk} = (y_{ijk} - \mu - \alpha_i - \beta_j - \gamma_{ij})/\sigma$ follows a standard normal distribution (\rightarrow Proof II/3.2.3)

$$U_{ijk} = \frac{y_{ijk} - \mu - \alpha_i - \beta_j - \gamma_{ij}}{\sigma} \sim \mathcal{N}(0, 1) . \quad (7)$$

Now consider the following sum

$$\sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} U_{ijk}^2 = \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} \left(\frac{y_{ijk} - \mu - \alpha_i - \beta_j - \gamma_{ij}}{\sigma} \right)^2 \quad (8)$$

which can be rewritten as follows:

$$\begin{aligned} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} U_{ijk}^2 &= \frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} [(y_{ijk} - \mu - \alpha_i - \beta_j - \gamma_{ij}) - \\ &\quad [\bar{y}_{\bullet\bullet\bullet} + (\bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet}) + (\bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet}) + (\bar{y}_{ij\bullet} - \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet j\bullet} + \bar{y}_{\bullet\bullet\bullet})] + \\ &\quad [\bar{y}_{\bullet\bullet\bullet} + (\bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet}) + (\bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet}) + (\bar{y}_{ij\bullet} - \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet j\bullet} + \bar{y}_{\bullet\bullet\bullet})]]^2 \\ &= \frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} [(y_{ijk} - [\bar{y}_{\bullet\bullet\bullet} + (\bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet}) + (\bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet}) + (\bar{y}_{ij\bullet} - \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet j\bullet} + \bar{y}_{\bullet\bullet\bullet})]) + \\ &\quad (\bar{y}_{\bullet\bullet\bullet} - \mu) + ([\bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet}] - \alpha_i) + ([\bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet}] - \beta_j) + \\ &\quad ([\bar{y}_{ij\bullet} - \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet j\bullet} + \bar{y}_{\bullet\bullet\bullet}] - \gamma_{ij})]^2 \\ &= \frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} [(y_{ijk} - \bar{y}_{ij\bullet}) + (\bar{y}_{\bullet\bullet\bullet} - \mu) + ([\bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet}] - \alpha_i) + \\ &\quad ([\bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet}] - \beta_j) + ([\bar{y}_{ij\bullet} - \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet j\bullet} + \bar{y}_{\bullet\bullet\bullet}] - \gamma_{ij})]^2 \end{aligned} \quad (9)$$

Note that the following sums are all zero

$$\begin{aligned} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet}) &= \sum_{i=1}^a \sum_{j=1}^b \left[\sum_{k=1}^{n_{ij}} y_{ijk} - n_{ij} \cdot \bar{y}_{ij\bullet} \right] \\ &\stackrel{(5)}{=} \sum_{i=1}^a \sum_{j=1}^b \left[\sum_{k=1}^{n_{ij}} y_{ijk} - n_{ij} \cdot \frac{1}{n_{ij}} \sum_{k=1}^{n_{ij}} y_{ijk} \right] \\ &= \sum_{i=1}^a \sum_{j=1}^b 0 = 0 \end{aligned} \quad (10)$$

$$\begin{aligned} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} ([\bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet}] - \alpha_i) &= \sum_{i=1}^a n_{i\bullet\bullet} \cdot (\bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet} - \alpha_i) \\ &= \sum_{i=1}^a n_{i\bullet\bullet} \cdot \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet} \sum_{i=1}^a n_{i\bullet\bullet} - \sum_{i=1}^a n_{i\bullet\bullet} \alpha_i \\ &\stackrel{(5)}{=} \sum_{i=1}^a n_{i\bullet\bullet} \cdot \frac{1}{n_{i\bullet\bullet}} \sum_{j=1}^b \sum_{k=1}^{n_{ij}} y_{ijk} - n \cdot \frac{1}{n} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} y_{ijk} - \sum_{i=1}^a n_{i\bullet\bullet} \alpha_i \\ &= - \sum_{i=1}^a n_{i\bullet\bullet} \alpha_i \stackrel{(4)}{=} -n \sum_{i=1}^a \sum_{j=1}^b \frac{n_{ij}}{n} \alpha_i \stackrel{(2)}{=} 0 \end{aligned} \quad (11)$$

$$\begin{aligned}
\sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} ([\bar{y}_{\bullet j \bullet} - \bar{y}_{\bullet \bullet \bullet}] - \beta_j) &= \sum_{j=1}^b n_{\bullet j} \cdot (\bar{y}_{\bullet j \bullet} - \bar{y}_{\bullet \bullet \bullet} - \beta_j) \\
&= \sum_{j=1}^b n_{\bullet j} \cdot \bar{y}_{\bullet j \bullet} - \bar{y}_{\bullet \bullet \bullet} \sum_{j=1}^b n_{\bullet j} - \sum_{j=1}^b n_{\bullet j} \beta_j \\
&\stackrel{(5)}{=} \sum_{j=1}^b n_{\bullet j} \cdot \frac{1}{n_{\bullet j}} \sum_{i=1}^a \sum_{k=1}^{n_{ij}} y_{ijk} - n \cdot \frac{1}{n} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} y_{ijk} - \sum_{j=1}^b n_{\bullet j} \beta_j \\
&= - \sum_{j=1}^b n_{\bullet j} \beta_j \stackrel{(4)}{=} -n \sum_{j=1}^b \sum_{i=1}^a \frac{n_{ij}}{n} \beta_j \stackrel{(2)}{=} 0
\end{aligned} \tag{12}$$

$$\begin{aligned}
&\sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} ([\bar{y}_{ij \bullet} - \bar{y}_{i \bullet \bullet} - \bar{y}_{\bullet j \bullet} + \bar{y}_{\bullet \bullet \bullet}] - \gamma_{ij}) \\
&= \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} [(\bar{y}_{ij \bullet} - \bar{y}_{\bullet \bullet \bullet}) - (\bar{y}_{i \bullet \bullet} - \bar{y}_{\bullet \bullet \bullet}) - (\bar{y}_{\bullet j \bullet} - \bar{y}_{\bullet \bullet \bullet}) - \gamma_{ij}] \\
&= \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (\bar{y}_{ij \bullet} - \bar{y}_{\bullet \bullet \bullet} - \gamma_{ij}) - \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (\bar{y}_{i \bullet \bullet} - \bar{y}_{\bullet \bullet \bullet}) - \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (\bar{y}_{\bullet j \bullet} - \bar{y}_{\bullet \bullet \bullet}) \\
&\stackrel{(12)}{=} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (\bar{y}_{ij \bullet} - \bar{y}_{\bullet \bullet \bullet} - \gamma_{ij}) - \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (\bar{y}_{i \bullet \bullet} - \bar{y}_{\bullet \bullet \bullet}) \\
&\stackrel{(11)}{=} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (\bar{y}_{ij \bullet} - \bar{y}_{\bullet \bullet \bullet} - \gamma_{ij}) \\
&= \sum_{i=1}^a \sum_{j=1}^b n_{ij} \bar{y}_{ij \bullet} - \bar{y}_{\bullet \bullet \bullet} \sum_{i=1}^a \sum_{j=1}^b n_{ij} - \sum_{i=1}^a \sum_{j=1}^b n_{ij} \gamma_{ij} \\
&\stackrel{(5)}{=} \sum_{i=1}^a \sum_{j=1}^b n_{ij} \cdot \frac{1}{n_{ij}} \sum_{k=1}^{n_{ij}} y_{ijk} - n \cdot \frac{1}{n} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} y_{ijk} - \sum_{i=1}^a \sum_{j=1}^b n_{ij} \gamma_{ij} \\
&= - \sum_{i=1}^a \sum_{j=1}^b n_{ij} \gamma_{ij} = - \frac{1}{n} \sum_{i=1}^a \sum_{j=1}^b \frac{n_{ij}}{n} \gamma_{ij} \stackrel{(2)}{=} 0 .
\end{aligned} \tag{13}$$

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 (\rightarrow Proof "snorm-cochran") states that, if a sum of squared standard normal (\rightarrow Definition II/3.2.2) random variables (\rightarrow Definition 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 Definition I/1.3.6) and each term Q_j follows a chi-squared distribution (\rightarrow Definition 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 $n \times 1$ 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 (\rightarrow Proof "snorm-cochran") 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 Proof III/1.3.11) and simplify them to reach the expressions given by (3):

$$\begin{aligned}
\frac{SS_M}{\sigma^2} &= \frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (\bar{y}_{\bullet\bullet\bullet} - \mu)^2 = \frac{1}{\sigma^2} n (\bar{y}_{\bullet\bullet\bullet} - \mu)^2 \\
\frac{SS_A}{\sigma^2} &= \frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} ([\bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet}] - \alpha_i)^2 = \frac{1}{\sigma^2} \sum_{i=1}^a n_{i\bullet} ([\bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet}] - \alpha_i)^2 \\
\frac{SS_B}{\sigma^2} &= \frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} ([\bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet}] - \beta_j)^2 = \frac{1}{\sigma^2} \sum_{j=1}^b n_{\bullet j} ([\bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet}] - \beta_j)^2 \\
\frac{SS_{A \times B}}{\sigma^2} &= \frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} ([\bar{y}_{ij\bullet} - \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet j\bullet} + \bar{y}_{\bullet\bullet\bullet}] - \gamma_{ij})^2 = \frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b n_{ij} ([\bar{y}_{ij\bullet} - \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet j\bullet} + \bar{y}_{\bullet\bullet\bullet}] - \gamma_{ij})^2 \\
\frac{SS_{\text{res}}}{\sigma^2} &= \frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2 = \frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2 .
\end{aligned} \tag{25}$$

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>.

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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 Definition III/1.3.8) model

$$y_{ijk} = \mu + \alpha_i + \beta_j + \gamma_{ij} + \varepsilon_{ijk} \quad (1)$$

$$\varepsilon_{ijk} \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2), \quad i = 1, \dots, a, \quad j = 1, \dots, b, \quad k = 1, \dots, n_{ij}.$$

Then, the test statistic (\rightarrow Definition 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 Definition II/3.8.1)

$$F_A \sim F(a-1, n-ab) \quad (3)$$

under the null hypothesis (\rightarrow Definition I/4.3.2) for the main effect (\rightarrow Definition III/1.3.8) of factor A

$$H_0 : \alpha_1 = \dots = \alpha_a = 0$$

$$H_1 : \alpha_i \neq 0 \quad \text{for at least one } i \in \{1, \dots, a\} \quad (4)$$

and the test statistic (\rightarrow Definition 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 Definition II/3.8.1)

$$F_B \sim F(b-1, n-ab) \quad (6)$$

under the null hypothesis (\rightarrow Definition I/4.3.2) for the main effect (\rightarrow Definition III/1.3.8) of factor B

$$H_0 : \beta_1 = \dots = \beta_b = 0$$

$$H_1 : \beta_j \neq 0 \quad \text{for at least one } j \in \{1, \dots, b\} \quad (7)$$

Proof: Applying Cochran's theorem for two-analysis of variance (\rightarrow Proof III/1.3.12), we find that the following squared sums

$$\frac{SS_A}{\sigma^2} = \frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} ([\bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet}] - \alpha_i)^2 = \frac{1}{\sigma^2} \sum_{i=1}^a n_{i\bullet} ([\bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet}] - \alpha_i)^2$$

$$\frac{SS_B}{\sigma^2} = \frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} ([\bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet}] - \beta_j)^2 = \frac{1}{\sigma^2} \sum_{j=1}^b n_{\bullet j} ([\bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet}] - \beta_j)^2 \quad (8)$$

$$\frac{SS_{\text{res}}}{\sigma^2} = \frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2 = \frac{1}{\sigma^2} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2$$

are independent (\rightarrow Definition I/1.3.6) and chi-squared distributed (\rightarrow Definition II/3.7.1):

$$\begin{aligned}
\frac{SS_A}{\sigma^2} &\sim \chi^2(a-1) \\
\frac{SS_B}{\sigma^2} &\sim \chi^2(b-1) \\
\frac{SS_{\text{res}}}{\sigma^2} &\sim \chi^2(n-ab) .
\end{aligned} \tag{9}$$

1) Thus, the F-statistic from (2) is equal to the ratio of two independent (\rightarrow Definition I/1.3.6) chi-squared distributed (\rightarrow Definition II/3.7.1) random variables (\rightarrow Definition I/1.2.2) divided by their degrees of freedom

$$\begin{aligned}
F_A &= \frac{(SS_A/\sigma^2)/(a-1)}{(SS_{\text{res}}/\sigma^2)/(n-ab)} \\
&= \frac{SS_A/(a-1)}{SS_{\text{res}}/(n-ab)} \\
&\stackrel{(8)}{=} \frac{\frac{1}{a-1} \sum_{i=1}^a n_{i\bullet} ([\bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet}] - \alpha_i)^2}{\frac{1}{n-ab} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2} \\
&\stackrel{(3)}{=} \frac{\frac{1}{a-1} \sum_{i=1}^a n_{i\bullet} (\bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet})^2}{\frac{1}{n-ab} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2}
\end{aligned} \tag{10}$$

which, by definition of the F-distribution (\rightarrow Definition II/3.8.1), is distributed as

$$F_A \sim F(a-1, n-ab) \tag{11}$$

under the null hypothesis (\rightarrow Definition 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 Definition II/3.7.1) random variables (\rightarrow Definition I/1.2.2) divided by their degrees of freedom

$$\begin{aligned}
F_B &= \frac{(SS_B/\sigma^2)/(b-1)}{(SS_{\text{res}}/\sigma^2)/(n-ab)} \\
&= \frac{SS_B/(b-1)}{SS_{\text{res}}/(n-ab)} \\
&\stackrel{(8)}{=} \frac{\frac{1}{b-1} \sum_{j=1}^b n_{\bullet j} ([\bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet}] - \beta_j)^2}{\frac{1}{n-ab} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2} \\
&\stackrel{(6)}{=} \frac{\frac{1}{b-1} \sum_{j=1}^b n_{\bullet j} (\bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet})^2}{\frac{1}{n-ab} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2}
\end{aligned} \tag{12}$$

which, by definition of the F-distribution (\rightarrow Definition II/3.8.1), is distributed as

$$F_B \sim F(b-1, n-ab) \tag{13}$$

under the null hypothesis (\rightarrow Definition I/4.3.2) for main effect of B .

Sources:

- 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-1j-1-under-the-null-hypothesis>.
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1.3.14 F-test for interaction in two-way ANOVA

Theorem: Assume the two-way analysis of variance (\rightarrow Definition 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 Definition 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 Definition II/3.8.1)

$$F_{A \times B} \sim F((a-1)(b-1), n-ab) \quad (3)$$

under the null hypothesis (\rightarrow Definition I/4.3.2) for the interaction effect (\rightarrow Definition 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 Proof 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 Definition I/1.3.6) and chi-squared distributed (\rightarrow Definition II/3.7.1):

$$\begin{aligned}\frac{SS_{A \times B}}{\sigma^2} &\sim \chi^2((a-1)(b-1)) \\ \frac{SS_{\text{res}}}{\sigma^2} &\sim \chi^2(n-ab) .\end{aligned}\tag{6}$$

Thus, the F-statistic from (2) is equal to the ratio of two independent (\rightarrow Definition I/1.3.6) chi-squared distributed (\rightarrow Definition II/3.7.1) random variables (\rightarrow Definition I/1.2.2) divided by their degrees of freedom

$$\begin{aligned}F_{A \times B} &= \frac{(SS_{A \times B}/\sigma^2)/((a-1)(b-1))}{(SS_{\text{res}}/\sigma^2)/(n-ab)} \\ &= \frac{SS_{A \times B}/((a-1)(b-1))}{SS_{\text{res}}/(n-ab)} \\ &\stackrel{(5)}{=} \frac{\frac{1}{(a-1)(b-1)} \sum_{i=1}^a \sum_{j=1}^b n_{ij} ([\bar{y}_{ij\bullet} - \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet j\bullet} + \bar{y}_{\bullet\bullet\bullet}] - \gamma_{ij})^2}{\frac{1}{n-ab} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2} \\ &\stackrel{(3)}{=} \frac{\frac{1}{(a-1)(b-1)} \sum_{i=1}^a \sum_{j=1}^b n_{ij} (\bar{y}_{ij\bullet} - \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet j\bullet} + \bar{y}_{\bullet\bullet\bullet})^2}{\frac{1}{n-ab} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2}\end{aligned}\tag{7}$$

which, by definition of the F-distribution (\rightarrow Definition 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 Definition 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-1j-1-under-the-null-hypothesis>.

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1.3.15 F-test for grand mean in two-way ANOVA

Theorem: Assume the two-way analysis of variance (\rightarrow Definition 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 Definition I/4.3.5)

$$F_M = \frac{n(\bar{y}_{\bullet\bullet\bullet})^2}{\frac{1}{n-ab} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2} \quad (2)$$

follows an F-distribution (\rightarrow Definition II/3.8.1)

$$F_M \sim F(1, n - ab) \quad (3)$$

under the null hypothesis (\rightarrow Definition I/4.3.2) for the grand mean (\rightarrow Definition III/1.3.8)

$$\begin{aligned} H_0 : \mu &= 0 \\ H_1 : \mu &\neq 0 . \end{aligned} \quad (4)$$

Proof: Applying Cochran's theorem for two-analysis of variance (\rightarrow Proof 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 Definition I/1.3.6) and chi-squared distributed (\rightarrow Definition 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 Definition I/1.3.6) chi-squared distributed (\rightarrow Definition II/3.7.1) random variables (\rightarrow Definition I/1.2.2) divided by their degrees of freedom

$$\begin{aligned} F_M &= \frac{(SS_M/\sigma^2)/(1)}{(SS_{\text{res}}/\sigma^2)/(n - ab)} \\ &= \frac{SS_M/(1)}{SS_{\text{res}}/(n - ab)} \\ &\stackrel{(5)}{=} \frac{n(\bar{y}_{\bullet\bullet\bullet} - \mu)^2}{\frac{1}{n-ab} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2} \\ &\stackrel{(2)}{=} \frac{n(\bar{y}_{\bullet\bullet\bullet})^2}{\frac{1}{n-ab} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \bar{y}_{ij\bullet})^2} \end{aligned} \quad (7)$$

which, by definition of the F-distribution (\rightarrow Definition II/3.8.1), is distributed as

$$F_M \sim F(1, n - ab) \quad (8)$$

under the null hypothesis (\rightarrow Definition 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.

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1.3.16 F-statistics in terms of OLS estimates

Theorem: Given the two-way analysis of variance (\rightarrow Definition 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 Proof III/1.3.15), the main effects (\rightarrow Proof III/1.3.13) and the interaction (\rightarrow Proof III/1.3.14) can be expressed in terms of ordinary least squares parameter estimates (\rightarrow Proof 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 Proof III/1.3.15), the main effects (\rightarrow Proof III/1.3.13) and the interaction (\rightarrow Proof III/1.3.14) in two-way ANOVA (\rightarrow Definition 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 Proof III/1.3.10) are

$$\begin{aligned}\hat{\mu} &= \bar{y}_{\bullet\bullet\bullet} \\ \hat{\alpha}_i &= \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet} \\ \hat{\beta}_j &= \bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet\bullet} \\ \hat{\gamma}_{ij} &= \bar{y}_{ij\bullet} - \bar{y}_{i\bullet\bullet} - \bar{y}_{\bullet j\bullet} + \bar{y}_{\bullet\bullet\bullet}\end{aligned}\tag{5}$$

where the sample means (\rightarrow Definition I/1.7.2) 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:

$$\begin{aligned}F_M &= \frac{n\hat{\mu}^2}{\frac{1}{n-ab} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \hat{y}_{ijk})^2} \\ F_A &= \frac{\frac{1}{a-1} \sum_{i=1}^a n_{i\bullet} \hat{\alpha}_i^2}{\frac{1}{n-ab} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \hat{y}_{ijk})^2} \\ F_B &= \frac{\frac{1}{b-1} \sum_{j=1}^b n_{\bullet j} \hat{\beta}_j^2}{\frac{1}{n-ab} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \hat{y}_{ijk})^2} \\ F_{A \times B} &= \frac{\frac{1}{(a-1)(b-1)} \sum_{i=1}^a \sum_{j=1}^b n_{ij} \hat{\gamma}_{ij}^2}{\frac{1}{n-ab} \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^{n_{ij}} (y_{ijk} - \hat{y}_{ijk})^2} .\end{aligned}\tag{8}$$

Sources:

- original work

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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

$$y = \beta_0 + \beta_1 x + \varepsilon, \quad (1)$$

together with a statement asserting a normal distribution (\rightarrow Definition II/4.1.1) for ε

$$\varepsilon \sim \mathcal{N}(0, \sigma^2 V) \quad (2)$$

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 Definition III/1.4.10)”;
- β_0 is called “intercept of the regression line (\rightarrow Definition 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 (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.

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.

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1.4.2 Special case of multiple linear regression

Theorem: Simple linear regression (\rightarrow Definition III/1.4.1) is a special case of multiple linear regression (\rightarrow Definition 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 Definition III/1.4.10).

Proof: Without loss of generality, consider the simple linear regression case with uncorrelated errors (\rightarrow Definition 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 Definition II/4.1.1), this can also be written as

$$\begin{aligned} y &= \beta_0 \mathbf{1}_n + \beta_1 x + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, I_n) \\ y &= \begin{bmatrix} \mathbf{1}_n & x \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, I_n). \end{aligned} \quad (3)$$

Comparing with the multiple linear regression equations for uncorrelated errors (\rightarrow Definition III/1.5.1), we finally note:

$$y = X\beta + \varepsilon \quad \text{with} \quad X = \begin{bmatrix} \mathbf{1}_n & x \end{bmatrix} \quad \text{and} \quad \beta = \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}. \quad (4)$$

In the case of correlated observations (\rightarrow Definition III/1.4.1), the error distribution changes to (\rightarrow Definition III/1.5.1):

$$\varepsilon \sim \mathcal{N}(0, \sigma^2 V). \quad (5)$$

Sources:

- original work

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1.4.3 Ordinary least squares

Theorem: Given a simple linear regression model (\rightarrow Definition 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 Definition III/1.5.7) 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 Definition I/1.7.2), s_x^2 is the sample variance (\rightarrow Definition I/1.8.2) of x and s_{xy} is the sample covariance (\rightarrow Definition I/1.10.2) between x and y .

Proof: The residual sum of squares (\rightarrow Definition III/1.5.7) 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

$$\begin{aligned} 0 &= -2 \sum_{i=1}^n (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i) \\ 0 &= -2 \sum_{i=1}^n (x_i y_i - \hat{\beta}_0 x_i - \hat{\beta}_1 x_i^2) \end{aligned} \quad (5)$$

yields the following equations:

$$\begin{aligned} \hat{\beta}_1 \sum_{i=1}^n x_i + \hat{\beta}_0 \cdot n &= \sum_{i=1}^n y_i \\ \hat{\beta}_1 \sum_{i=1}^n x_i^2 + \hat{\beta}_0 \sum_{i=1}^n x_i &= \sum_{i=1}^n x_i y_i. \end{aligned} \quad (6)$$

From the first equation, we can derive the estimate for the intercept:

$$\begin{aligned} \hat{\beta}_0 &= \frac{1}{n} \sum_{i=1}^n y_i - \hat{\beta}_1 \cdot \frac{1}{n} \sum_{i=1}^n x_i \\ &= \bar{y} - \hat{\beta}_1 \bar{x}. \end{aligned} \quad (7)$$

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.

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1.4.4 Ordinary least squares

Theorem: Given a simple linear regression model (\rightarrow Definition 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 Definition III/1.5.7) 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 Definition I/1.7.2), s_x^2 is the sample variance (\rightarrow Definition I/1.8.2) of x and s_{xy} is the sample covariance (\rightarrow Definition I/1.10.2) between x and y .

Proof: Simple linear regression is a special case of multiple linear regression (\rightarrow Proof 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 Proof 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 Proof 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:

$$\begin{aligned}
 \hat{\beta}_0 &= \frac{n\bar{y} x^T x - n\bar{x} x^T y}{nx^T x - (n\bar{x})^2} \\
 &= \frac{\bar{y} x^T x - \bar{x} x^T y}{x^T x - n\bar{x}^2} \\
 &= \frac{\bar{y} x^T x - \bar{x} x^T y + n\bar{x}^2 \bar{y} - n\bar{x}^2 \bar{y}}{x^T x - n\bar{x}^2} \\
 &= \frac{\bar{y}(x^T x - n\bar{x}^2) - \bar{x}(x^T y - n\bar{x}\bar{y})}{x^T x - n\bar{x}^2} \\
 &= \frac{\bar{y}(x^T x - n\bar{x}^2)}{x^T x - n\bar{x}^2} - \frac{\bar{x}(x^T y - n\bar{x}\bar{y})}{x^T x - n\bar{x}^2} \\
 &= \bar{y} - \bar{x} \frac{\sum_{i=1}^n x_i y_i - \sum_{i=1}^n \bar{x} \bar{y}}{\sum_{i=1}^n x_i^2 - \sum_{i=1}^n \bar{x}^2} \\
 &= \bar{y} - \hat{\beta}_1 \bar{x}.
 \end{aligned} \tag{7}$$

Sources:

- original work

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1.4.5 Expectation of estimates

Theorem: Assume a simple linear regression model (\rightarrow Definition 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 Proof III/1.4.3). Then, the expected values (\rightarrow Definition I/1.7.1) of the estimated parameters are

$$\begin{aligned} \mathbb{E}(\hat{\beta}_0) &= \beta_0 \\ \mathbb{E}(\hat{\beta}_1) &= \beta_1 \end{aligned} \quad (2)$$

which means that the ordinary least squares solution (\rightarrow Proof III/1.4.3) produces unbiased estimators (\rightarrow Definition “est-unb”).

Proof: According to the simple linear regression model in (1), the expectation of a single data point is

$$\mathbb{E}(y_i) = \beta_0 + \beta_1 x_i. \quad (3)$$

The ordinary least squares estimates for simple linear regression (\rightarrow Proof III/1.4.3) are given by

$$\begin{aligned} \hat{\beta}_0 &= \frac{1}{n} \sum_{i=1}^n y_i - \hat{\beta}_1 \cdot \frac{1}{n} \sum_{i=1}^n x_i \\ \hat{\beta}_1 &= \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2}. \end{aligned} \quad (4)$$

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

$$\begin{aligned} \sum_{i=1}^n c_i &= \frac{\sum_{i=1}^n (x_i - \bar{x})}{\sum_{i=1}^n (x_i - \bar{x})^2} = \frac{\sum_{i=1}^n x_i - n\bar{x}}{\sum_{i=1}^n (x_i - \bar{x})^2} \\ &= \frac{n\bar{x} - n\bar{x}}{\sum_{i=1}^n (x_i - \bar{x})^2} = 0, \end{aligned} \quad (6)$$

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:

$$\begin{aligned}
E(\hat{\beta}_1) &= E\left(\sum_{i=1}^n c_i y_i - \bar{y} \sum_{i=1}^n c_i\right) \\
&= \sum_{i=1}^n c_i E(y_i) - \bar{y} \sum_{i=1}^n c_i \\
&= \beta_1 \sum_{i=1}^n c_i x_i + \beta_0 \sum_{i=1}^n c_i - \bar{y} \sum_{i=1}^n c_i \\
&= \beta_1 .
\end{aligned} \tag{9}$$

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_%22F%22%60UNIQ--postMath-00000037-QINU%60%22%27%7F.

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1.4.6 Variance of estimates

Theorem: Assume a simple linear regression model (\rightarrow Definition 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 Proof III/1.4.3). Then, the variances (\rightarrow Definition I/1.8.1) of the estimated parameters are

$$\begin{aligned} \text{Var}(\hat{\beta}_0) &= \frac{x^T x}{n} \cdot \frac{\sigma^2}{(n-1)s_x^2} \\ \text{Var}(\hat{\beta}_1) &= \frac{\sigma^2}{(n-1)s_x^2} \end{aligned} \quad (2)$$

where s_x^2 is the sample variance (\rightarrow Definition I/1.8.2) 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

$$\text{Var}(y_i) = \text{Var}(\varepsilon_i) = \sigma^2. \quad (3)$$

The ordinary least squares estimates for simple linear regression (\rightarrow Proof III/1.4.3) are given by

$$\begin{aligned} \hat{\beta}_0 &= \frac{1}{n} \sum_{i=1}^n y_i - \hat{\beta}_1 \cdot \frac{1}{n} \sum_{i=1}^n x_i \\ \hat{\beta}_1 &= \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2}. \end{aligned} \quad (4)$$

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

$$\begin{aligned}
\sum_{i=1}^n c_i^2 &= \sum_{i=1}^n \left(\frac{x_i - \bar{x}}{\sum_{i=1}^n (x_i - \bar{x})^2} \right)^2 \\
&= \frac{\sum_{i=1}^n (x_i - \bar{x})^2}{[\sum_{i=1}^n (x_i - \bar{x})^2]^2} \\
&= \frac{1}{\sum_{i=1}^n (x_i - \bar{x})^2} .
\end{aligned} \tag{6}$$

With (5), the estimate for the slope from (4) becomes

$$\begin{aligned}
\hat{\beta}_1 &= \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2} \\
&= \sum_{i=1}^n c_i (y_i - \bar{y}) \\
&= \sum_{i=1}^n c_i y_i - \bar{y} \sum_{i=1}^n c_i
\end{aligned} \tag{7}$$

and with (3) and (6) as well as invariance (\rightarrow Proof I/1.8.6), scaling (\rightarrow Proof I/1.8.7) and additivity (\rightarrow Proof I/1.8.10) of the variance, the variance of $\hat{\beta}_1$ is:

$$\begin{aligned}
\text{Var}(\hat{\beta}_1) &= \text{Var} \left(\sum_{i=1}^n c_i y_i - \bar{y} \sum_{i=1}^n c_i \right) \\
&= \text{Var} \left(\sum_{i=1}^n c_i y_i \right) \\
&= \sum_{i=1}^n c_i^2 \text{Var}(y_i) \\
&= \sigma^2 \sum_{i=1}^n c_i^2 \\
&= \sigma^2 \frac{1}{\sum_{i=1}^n (x_i - \bar{x})^2} \\
&= \frac{\sigma^2}{(n-1) \frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x})^2} \\
&= \frac{\sigma^2}{(n-1) s_x^2} .
\end{aligned} \tag{8}$$

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 Definition I/1.8.2) s_x^2 , we finally get:

$$\begin{aligned}
\text{Var}(\hat{\beta}_0) &= \sigma^2 \left(\frac{1}{n} + \frac{\bar{x}^2}{\sum_{i=1}^n (x_i - \bar{x})^2} \right) \\
&= \sigma^2 \left(\frac{\frac{1}{n} \sum_{i=1}^n (x_i - \bar{x})^2}{\sum_{i=1}^n (x_i - \bar{x})^2} + \frac{\bar{x}^2}{\sum_{i=1}^n (x_i - \bar{x})^2} \right) \\
&= \sigma^2 \left(\frac{\frac{1}{n} \sum_{i=1}^n (x_i^2 - 2\bar{x}x_i + \bar{x}^2) + \bar{x}^2}{\sum_{i=1}^n (x_i - \bar{x})^2} \right) \\
&= \sigma^2 \left(\frac{(\frac{1}{n} \sum_{i=1}^n x_i^2 - 2\bar{x} \frac{1}{n} \sum_{i=1}^n x_i + \bar{x}^2) + \bar{x}^2}{\sum_{i=1}^n (x_i - \bar{x})^2} \right) \\
&= \sigma^2 \left(\frac{\frac{1}{n} \sum_{i=1}^n x_i^2 - 2\bar{x}^2 + 2\bar{x}^2}{\sum_{i=1}^n (x_i - \bar{x})^2} \right) \\
&= \sigma^2 \left(\frac{\frac{1}{n} \sum_{i=1}^n x_i^2}{(n-1) \frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x})^2} \right) \\
&= \frac{x^T x}{n} \cdot \frac{\sigma^2}{(n-1)s_x^2}.
\end{aligned} \tag{10}$$

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.
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1.4.7 Distribution of estimates

Theorem: Assume a simple linear regression model (\rightarrow Definition III/1.4.1) with independent observations

$$y = \beta_0 + \beta_1 x + \varepsilon, \quad \varepsilon_i \sim \mathcal{N}(0, \sigma^2) \quad (1)$$

and consider estimation using ordinary least squares (\rightarrow Proof III/1.4.3). Then, the estimated parameters are normally distributed (\rightarrow Definition 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 Definition I/1.7.2) and s_x^2 is the sample variance (\rightarrow Definition I/1.8.2) of x .

Proof: Simple linear regression is a special case of multiple linear regression (\rightarrow Proof 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 Proof 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 Proof II/4.1.9), 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 Proof II/4.1.9), 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 Definition II/4.1.1) can be further developed as follows:

$$\begin{aligned}
\sigma^2(X^T X)^{-1} &= \sigma^2 \left(\begin{bmatrix} 1_n^T \\ x^T \end{bmatrix} \begin{bmatrix} 1_n & x \end{bmatrix} \right)^{-1} \\
&= \sigma^2 \left(\begin{bmatrix} n & n\bar{x} \\ n\bar{x} & x^T x \end{bmatrix} \right)^{-1} \\
&= \frac{\sigma^2}{nx^T x - (n\bar{x})^2} \begin{bmatrix} x^T x & -n\bar{x} \\ -n\bar{x} & n \end{bmatrix} \\
&= \frac{\sigma^2}{x^T x - n\bar{x}^2} \begin{bmatrix} x^T x/n & -\bar{x} \\ -\bar{x} & 1 \end{bmatrix}.
\end{aligned} \tag{8}$$

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.

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1.4.8 Correlation of estimates

Theorem: In simple linear regression (\rightarrow Definition III/1.4.1), when the independent variable x is mean-centered (\rightarrow Definition I/1.7.1), the ordinary least squares (\rightarrow Proof III/1.4.3) estimates for slope and intercept are uncorrelated (\rightarrow Definition I/1.11.1).

Proof: The parameter estimates for simple linear regression are bivariate normally distributed under ordinary least squares (\rightarrow Proof 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 Definition I/1.10.9) of the multivariate normal distribution (\rightarrow Definition II/4.1.1) contains the pairwise covariances of the random variables (\rightarrow Definition I/1.2.2), we can deduce that the covariance (\rightarrow Definition I/1.10.1) 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 Definition III/1.4.1), s_x^2 is the sample variance (\rightarrow Definition I/1.8.2) 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 Definition I/1.11.1), we can conclude that the correlation of $\hat{\beta}_0$ and $\hat{\beta}_1$ is also zero:

$$\text{Corr}(\hat{\beta}_0, \hat{\beta}_1) = 0. \quad (4)$$

Sources:

- original work

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1.4.9 Effects of mean-centering

Theorem: In simple linear regression (\rightarrow Definition III/1.4.1), when the dependent variable y and/or the independent variable x are mean-centered (\rightarrow Definition I/1.7.1), the ordinary least squares (\rightarrow Proof 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 Proof 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 Definition I/1.7.2) \bar{x} and \bar{y} , sample variance (\rightarrow Definition I/1.8.2) s_x^2 and sample covariance (\rightarrow Definition I/1.10.2) s_{xy} , such that β_0 estimates “the mean y at $x = 0$ ”.

2) Let \tilde{x} be the mean-centered covariate vector (\rightarrow Definition 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 Definition 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.

Sources:

- original work

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1.4.10 Regression line

Definition: Let there be a simple linear regression with independent observations (\rightarrow Definition 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 Proof 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.

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1.4.11 Regression line includes center of mass

Theorem: In simple linear regression (\rightarrow Definition III/1.4.1), the regression line (\rightarrow Definition III/1.4.10) estimated using ordinary least squares (\rightarrow Proof III/1.4.3) includes the point $M(\bar{x}, \bar{y})$.

Proof: The fitted regression line (\rightarrow Definition 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 Proof 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 Definition III/1.4.10) goes through the center of mass point (\bar{x}, \bar{y}) , if the model (\rightarrow Definition 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.

Metadata: ID: P275 | shortcut: slr-comp | author: JoramSoch | date: 2021-10-27, 12:52.

1.4.12 Projection of data point to regression line

Theorem: Consider simple linear regression (\rightarrow Definition III/1.4.1) and an estimated regression line (\rightarrow Definition 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:

$$P(w \mid \hat{\beta}_0 + \hat{\beta}_1 w) \quad \text{with} \quad w = \frac{x_o + (y_o - \hat{\beta}_0)\hat{\beta}_1}{1 + \hat{\beta}_1^2} . \quad (2)$$

Proof: The intersection point of the regression line (\rightarrow Definition 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

$$\begin{aligned}
a^T(b - p) &= 0 \\
a^T(b - w \cdot a) &= 0 \\
a^T b - w \cdot a^T a &= 0 \\
w \cdot a^T a &= a^T b \\
w &= \frac{a^T b}{a^T a} .
\end{aligned} \tag{8}$$

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.

Metadata: ID: P283 | shortcut: slr-proj | author: JoramSoch | date: 2021-11-09, 10:16.

1.4.13 Sums of squares

Theorem: Under ordinary least squares (\rightarrow Proof III/1.4.3) for simple linear regression (\rightarrow Definition III/1.4.1), total (\rightarrow Definition III/1.5.5), explained (\rightarrow Definition III/1.5.6) and residual (\rightarrow Definition III/1.5.7) 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 Definition I/1.8.2) of x and y and s_{xy} is the sample covariance (\rightarrow Definition I/1.10.2) between x and y .

Proof: The ordinary least squares parameter estimates (\rightarrow Proof III/1.4.3) are given by

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x} \quad \text{and} \quad \hat{\beta}_1 = \frac{s_{xy}}{s_x^2}. \quad (2)$$

1) The total sum of squares (\rightarrow Definition III/1.5.5) is defined as

$$\text{TSS} = \sum_{i=1}^n (y_i - \bar{y})^2 \quad (3)$$

which can be reformulated as follows:

$$\begin{aligned} \text{TSS} &= \sum_{i=1}^n (y_i - \bar{y})^2 \\ &= (n-1) \frac{1}{n-1} \sum_{i=1}^n (y_i - \bar{y})^2 \\ &= (n-1) s_y^2. \end{aligned} \quad (4)$$

2) The explained sum of squares (\rightarrow Definition III/1.5.6) is defined as

$$\text{ESS} = \sum_{i=1}^n (\hat{y}_i - \bar{y})^2 \quad \text{where} \quad \hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i \quad (5)$$

which, with the OLS parameter estimates, becomes:

$$\begin{aligned} \text{ESS} &= \sum_{i=1}^n (\hat{y}_i - \bar{y})^2 \\ &= \sum_{i=1}^n (\hat{\beta}_0 + \hat{\beta}_1 x_i - \bar{y})^2 \\ &\stackrel{(2)}{=} \sum_{i=1}^n (\bar{y} - \hat{\beta}_1 \bar{x} + \hat{\beta}_1 x_i - \bar{y})^2 \\ &= \sum_{i=1}^n \left(\hat{\beta}_1 (x_i - \bar{x}) \right)^2 \\ &\stackrel{(2)}{=} \sum_{i=1}^n \left(\frac{s_{xy}}{s_x^2} (x_i - \bar{x}) \right)^2 \\ &= \left(\frac{s_{xy}}{s_x^2} \right)^2 \sum_{i=1}^n (x_i - \bar{x})^2 \\ &= \left(\frac{s_{xy}}{s_x^2} \right)^2 (n-1) s_x^2 \\ &= (n-1) \frac{s_{xy}^2}{s_x^2}. \end{aligned} \quad (6)$$

3) The residual sum of squares (\rightarrow Definition III/1.5.7) is defined as

$$\text{RSS} = \sum_{i=1}^n (y_i - \hat{y}_i)^2 \quad \text{where} \quad \hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i \quad (7)$$

which, with the OLS parameter estimates, becomes:

$$\begin{aligned} \text{RSS} &= \sum_{i=1}^n (y_i - \hat{y}_i)^2 \\ &= \sum_{i=1}^n (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2 \\ &\stackrel{(2)}{=} \sum_{i=1}^n (y_i - \bar{y} + \hat{\beta}_1 \bar{x} - \hat{\beta}_1 x_i)^2 \\ &= \sum_{i=1}^n \left((y_i - \bar{y}) - \hat{\beta}_1 (x_i - \bar{x}) \right)^2 \\ &= \sum_{i=1}^n \left((y_i - \bar{y})^2 - 2\hat{\beta}_1 (x_i - \bar{x})(y_i - \bar{y}) + \hat{\beta}_1^2 (x_i - \bar{x})^2 \right) \\ &= \sum_{i=1}^n (y_i - \bar{y})^2 - 2\hat{\beta}_1 \sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y}) + \hat{\beta}_1^2 \sum_{i=1}^n (x_i - \bar{x})^2 \\ &= (n-1) s_y^2 - 2(n-1) \hat{\beta}_1 s_{xy} + (n-1) \hat{\beta}_1^2 s_x^2 \\ &\stackrel{(2)}{=} (n-1) s_y^2 - 2(n-1) \left(\frac{s_{xy}}{s_x^2} \right) s_{xy} + (n-1) \left(\frac{s_{xy}}{s_x^2} \right)^2 s_x^2 \\ &= (n-1) s_y^2 - (n-1) \frac{s_{xy}^2}{s_x^2} \\ &= (n-1) \left(s_y^2 - \frac{s_{xy}^2}{s_x^2} \right) . \end{aligned} \quad (8)$$

Sources:

- original work

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1.4.14 Transformation matrices

Theorem: Under ordinary least squares (\rightarrow Proof III/1.4.3) for simple linear regression (\rightarrow Definition III/1.4.1), estimation (\rightarrow Definition III/1.5.9), projection (\rightarrow Definition III/1.5.10) and residual-forming (\rightarrow Definition III/1.5.11) matrices are given by

$$\begin{aligned}
E &= \frac{1}{(n-1)s_x^2} \begin{bmatrix} (x^T x/n) 1_n^T - \bar{x} x^T \\ -\bar{x} 1_n^T + x^T \end{bmatrix} \\
P &= \frac{1}{(n-1)s_x^2} \begin{bmatrix} (x^T x/n) - 2\bar{x}x_1 + x_1^2 & \cdots & (x^T x/n) - \bar{x}(x_1 + x_n) + x_1x_n \\ \vdots & \ddots & \vdots \\ (x^T x/n) - \bar{x}(x_1 + x_n) + x_1x_n & \cdots & (x^T x/n) - 2\bar{x}x_n + x_n^2 \end{bmatrix} \\
R &= \frac{1}{(n-1)s_x^2} \begin{bmatrix} (n-1)(x^T x/n) + \bar{x}(2x_1 - n\bar{x}) - x_1^2 & \cdots & -(x^T x/n) + \bar{x}(x_1 + x_n) - x_1x_n \\ \vdots & \ddots & \vdots \\ -(x^T x/n) + \bar{x}(x_1 + x_n) - x_1x_n & \cdots & (n-1)(x^T x/n) + \bar{x}(2x_n - n\bar{x}) - x_n^2 \end{bmatrix}
\end{aligned} \tag{1}$$

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 Definition I/1.7.2) of x and s_x^2 is the sample variance (\rightarrow Definition I/1.8.2) of x .

Proof: Simple linear regression is a special case of multiple linear regression (\rightarrow Proof III/1.4.2) with

$$X = \begin{bmatrix} 1_n & x \end{bmatrix} \quad \text{and} \quad \beta = \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}, \tag{2}$$

such that the simple linear regression model can also be written as

$$y = X\beta + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 I_n). \tag{3}$$

Moreover, we note the following equality (\rightarrow Proof III/1.4.7):

$$x^T x - n\bar{x}^2 = (n-1)s_x^2. \tag{4}$$

1) The estimation matrix is given by (\rightarrow Proof III/1.5.12)

$$E = (X^T X)^{-1} X^T \tag{5}$$

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 Proof III/1.5.12)

$$P = X(X^T X)^{-1} X^T = X E \tag{7}$$

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 Proof III/1.5.12)

$$R = I_n - X(X^T X)^{-1} X^T = I_n - P \tag{9}$$

which also is an $n \times n$ matrix and can be reformulated as follows:

$$\begin{aligned}
R = I_n - P &= \begin{bmatrix} 1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 1 \end{bmatrix} - \begin{bmatrix} p_{11} & \cdots & p_{1n} \\ \vdots & \ddots & \vdots \\ p_{n1} & \cdots & p_{nn} \end{bmatrix} \\
&\stackrel{(4)}{=} \frac{1}{(n-1)s_x^2} \begin{bmatrix} x^T x - n\bar{x}^2 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & x^T x - n\bar{x}^2 \end{bmatrix} \\
&\quad - \frac{1}{(n-1)s_x^2} \begin{bmatrix} (x^T x/n) - 2\bar{x}x_1 + x_1^2 & \cdots & (x^T x/n) - \bar{x}(x_1 + x_n) + x_1 x_n \\ \vdots & \ddots & \vdots \\ (x^T x/n) - \bar{x}(x_1 + x_n) + x_1 x_n & \cdots & (x^T x/n) - 2\bar{x}x_n + x_n^2 \end{bmatrix} \\
&= \frac{1}{(n-1)s_x^2} \begin{bmatrix} (n-1)(x^T x/n) + \bar{x}(2x_1 - n\bar{x}) - x_1^2 & \cdots & -(x^T x/n) + \bar{x}(x_1 + x_n) - x_1 x_n \\ \vdots & \ddots & \vdots \\ -(x^T x/n) + \bar{x}(x_1 + x_n) - x_1 x_n & \cdots & (n-1)(x^T x/n) + \bar{x}(2x_n - n\bar{x}) - x_n^2 \end{bmatrix}.
\end{aligned} \tag{10}$$

Sources:

- original work

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1.4.15 Weighted least squares

Theorem: Given a simple linear regression model (\rightarrow Definition 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 Definition III/1.5.7) 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

$$WVW^T = I_n. \tag{3}$$

Since V is a covariance matrix and thus symmetric, W is also symmetric and can be expressed as the matrix square root of the inverse of V :

$$WVW = I_n \quad \Leftrightarrow \quad V = W^{-1}W^{-1} \quad \Leftrightarrow \quad V^{-1} = WW \quad \Leftrightarrow \quad W = V^{-1/2}. \quad (4)$$

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 Proof II/4.1.9) implies that

$$Wy = \beta_0 W\mathbf{1}_n + \beta_1 Wx + W\varepsilon, \quad W\varepsilon \sim \mathcal{N}(0, \sigma^2 WVW^T). \quad (6)$$

Applying (3), we see that (6) is actually a linear regression model (\rightarrow Definition 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 Proof 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:

$$\begin{aligned} \hat{\beta} &= \frac{1}{\tilde{x}_0^T \tilde{x}_0 \tilde{x}^T \tilde{x} - \tilde{x}_0^T \tilde{x} \tilde{x}^T \tilde{x}_0} \begin{bmatrix} \tilde{x}^T \tilde{x} & -\tilde{x}_0^T \tilde{x} \\ -\tilde{x}^T \tilde{x}_0 & \tilde{x}_0^T \tilde{x}_0 \end{bmatrix}^{-1} \begin{bmatrix} \tilde{x}_0^T \\ \tilde{x}^T \end{bmatrix} \tilde{y} \\ &= \frac{1}{\tilde{x}_0^T \tilde{x}_0 \tilde{x}^T \tilde{x} - \tilde{x}_0^T \tilde{x} \tilde{x}^T \tilde{x}_0} \begin{bmatrix} \tilde{x}^T \tilde{x} \tilde{x}_0^T - \tilde{x}_0^T \tilde{x} \tilde{x}^T \\ \tilde{x}_0^T \tilde{x}_0 \tilde{x}^T - \tilde{x}^T \tilde{x}_0 \tilde{x}_0^T \end{bmatrix} \tilde{y} \\ &= \frac{1}{\tilde{x}_0^T \tilde{x}_0 \tilde{x}^T \tilde{x} - \tilde{x}_0^T \tilde{x} \tilde{x}^T \tilde{x}_0} \begin{bmatrix} \tilde{x}^T \tilde{x} \tilde{x}_0^T \tilde{y} - \tilde{x}_0^T \tilde{x} \tilde{x}^T \tilde{y} \\ \tilde{x}_0^T \tilde{x}_0 \tilde{x}^T \tilde{y} - \tilde{x}^T \tilde{x}_0 \tilde{x}_0^T \tilde{y} \end{bmatrix}. \end{aligned} \quad (9)$$

Applying $\tilde{x}_0 = W\mathbf{1}_n$, $\tilde{x} = Wx$ and $W^T W = WW = V^{-1}$, we finally have

$$\begin{aligned}
\hat{\beta} &= \frac{1}{1_n^T W^T W 1_n x^T W^T W x - 1_n^T W^T W x x^T W^T W 1_n} \begin{bmatrix} x^T W^T W x 1_n^T W^T W y - 1_n^T W^T W x x^T W^T W y \\ 1_n^T W^T W 1_n x^T W^T W y - x^T W^T W 1_n 1_n^T W^T W y \end{bmatrix} \\
&= \frac{1}{x^T V^{-1} x 1_n^T V^{-1} 1_n - 1_n^T V^{-1} x x^T V^{-1} 1_n} \begin{bmatrix} x^T V^{-1} x 1_n^T V^{-1} y - 1_n^T V^{-1} x x^T V^{-1} y \\ 1_n^T V^{-1} 1_n x^T V^{-1} y - x^T V^{-1} 1_n 1_n^T V^{-1} y \end{bmatrix} \\
&= \begin{bmatrix} \frac{x^T V^{-1} x 1_n^T V^{-1} y - 1_n^T V^{-1} x x^T V^{-1} y}{x^T V^{-1} x 1_n^T V^{-1} 1_n - 1_n^T V^{-1} x x^T V^{-1} 1_n} \\ \frac{1_n^T V^{-1} 1_n x^T V^{-1} y - x^T V^{-1} 1_n 1_n^T V^{-1} y}{1_n^T V^{-1} 1_n x^T V^{-1} x - x^T V^{-1} 1_n 1_n^T V^{-1} x} \end{bmatrix}
\end{aligned} \tag{10}$$

which corresponds to the weighted least squares solution (2).

Sources:

- original work

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1.4.16 Weighted least squares

Theorem: Given a simple linear regression model (\rightarrow Definition 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 Definition III/1.5.7) are given by

$$\begin{aligned}
\hat{\beta}_0 &= \frac{x^T V^{-1} x 1_n^T V^{-1} y - 1_n^T V^{-1} x x^T V^{-1} y}{x^T V^{-1} x 1_n^T V^{-1} 1_n - 1_n^T V^{-1} x x^T V^{-1} 1_n} \\
\hat{\beta}_1 &= \frac{1_n^T V^{-1} 1_n x^T V^{-1} y - x^T V^{-1} 1_n 1_n^T V^{-1} y}{1_n^T V^{-1} 1_n x^T V^{-1} x - x^T V^{-1} 1_n 1_n^T V^{-1} x}
\end{aligned} \tag{2}$$

where 1_n is an $n \times 1$ vector of ones.

Proof: Simple linear regression is a special case of multiple linear regression (\rightarrow Proof 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 weighted least squares estimates (\rightarrow Proof III/1.5.19) are given by

$$\hat{\beta} = (X^T V^{-1} X)^{-1} X^T V^{-1} y. \tag{4}$$

Writing out equation (4), we have

$$\begin{aligned}
\hat{\beta} &= \left(\begin{bmatrix} 1_n^T \\ x^T \end{bmatrix} V^{-1} \begin{bmatrix} 1_n & x \end{bmatrix} \right)^{-1} \begin{bmatrix} 1_n^T \\ x^T \end{bmatrix} V^{-1} y \\
&= \begin{bmatrix} 1_n^T V^{-1} 1_n & 1_n^T V^{-1} x \\ x^T V^{-1} 1_n & x^T V^{-1} x \end{bmatrix}^{-1} \begin{bmatrix} 1_n^T V^{-1} y \\ x^T V^{-1} y \end{bmatrix} \\
&= \frac{1}{x^T V^{-1} x 1_n^T V^{-1} 1_n - 1_n^T V^{-1} x x^T V^{-1} 1_n} \begin{bmatrix} x^T V^{-1} x & -1_n^T V^{-1} x \\ -x^T V^{-1} 1_n & 1_n^T V^{-1} 1_n \end{bmatrix} \begin{bmatrix} 1_n^T V^{-1} y \\ x^T V^{-1} y \end{bmatrix} \\
&= \frac{1}{x^T V^{-1} x 1_n^T V^{-1} 1_n - 1_n^T V^{-1} x x^T V^{-1} 1_n} \begin{bmatrix} x^T V^{-1} x 1_n^T V^{-1} y - 1_n^T V^{-1} x x^T V^{-1} y \\ 1_n^T V^{-1} 1_n x^T V^{-1} y - x^T V^{-1} 1_n 1_n^T V^{-1} y \end{bmatrix}.
\end{aligned} \tag{5}$$

Thus, the first entry of $\hat{\beta}$ is equal to:

$$\hat{\beta}_0 = \frac{x^T V^{-1} x 1_n^T V^{-1} y - 1_n^T V^{-1} x x^T V^{-1} y}{x^T V^{-1} x 1_n^T V^{-1} 1_n - 1_n^T V^{-1} x x^T V^{-1} 1_n}. \tag{6}$$

Moreover, the second entry of $\hat{\beta}$ is equal to (\rightarrow Proof III/1.4.15):

$$\hat{\beta}_1 = \frac{1_n^T V^{-1} 1_n x^T V^{-1} y - x^T V^{-1} 1_n 1_n^T V^{-1} y}{1_n^T V^{-1} 1_n x^T V^{-1} x - x^T V^{-1} 1_n 1_n^T V^{-1} x}. \tag{7}$$

Sources:

- original work

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1.4.17 Maximum likelihood estimation

Theorem: Given a simple linear regression model (\rightarrow Definition III/1.5.1) with independent observations

$$y_i = \beta_0 + \beta_1 x_i + \varepsilon_i, \quad \varepsilon_i \sim \mathcal{N}(0, \sigma^2), \quad i = 1, \dots, n, \tag{1}$$

the maximum likelihood estimates (\rightarrow Definition I/4.1.3) of β_0 , β_1 and σ^2 are given by

$$\begin{aligned}
\hat{\beta}_0 &= \bar{y} - \hat{\beta}_1 \bar{x} \\
\hat{\beta}_1 &= \frac{s_{xy}}{s_x^2} \\
\hat{\sigma}^2 &= \frac{1}{n} \sum_{i=1}^n (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2
\end{aligned} \tag{2}$$

where \bar{x} and \bar{y} are the sample means (\rightarrow Definition I/1.7.2), s_x^2 is the sample variance (\rightarrow Definition I/1.8.2) of x and s_{xy} is the sample covariance (\rightarrow Definition I/1.10.2) between x and y .

Proof: With the probability density function of the normal distribution (\rightarrow Proof II/3.2.10) and probability under independence (\rightarrow Definition I/1.3.6), the linear regression equation (1) implies the following likelihood function (\rightarrow Definition I/5.1.2)

$$\begin{aligned}
 p(y|\beta_0, \beta_1, \sigma^2) &= \prod_{i=1}^n p(y_i|\beta_0, \beta_1, \sigma^2) \\
 &= \prod_{i=1}^n \mathcal{N}(y_i; \beta_0 + \beta_1 x_i, \sigma^2) \\
 &= \prod_{i=1}^n \frac{1}{\sqrt{2\pi\sigma}} \cdot \exp \left[-\frac{(y_i - \beta_0 - \beta_1 x_i)^2}{2\sigma^2} \right] \\
 &= \frac{1}{\sqrt{(2\pi\sigma^2)^n}} \cdot \exp \left[-\frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)^2 \right]
 \end{aligned} \tag{3}$$

and the log-likelihood function (\rightarrow Definition I/4.1.2)

$$\begin{aligned}
 \text{LL}(\beta_0, \beta_1, \sigma^2) &= \log p(y|\beta_0, \beta_1, \sigma^2) \\
 &= -\frac{n}{2} \log(2\pi) - \frac{n}{2} \log(\sigma^2) - \frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)^2 .
 \end{aligned} \tag{4}$$

The derivative of the log-likelihood function (4) with respect to β_0 is

$$\frac{\text{dLL}(\beta_0, \beta_1, \sigma^2)}{\text{d}\beta_0} = \frac{1}{\sigma^2} \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i) \tag{5}$$

and setting this derivative to zero gives the MLE for β_0 :

$$\begin{aligned}
 \frac{\text{dLL}(\hat{\beta}_0, \hat{\beta}_1, \hat{\sigma}^2)}{\text{d}\beta_0} &= 0 \\
 0 &= \frac{1}{\hat{\sigma}^2} \sum_{i=1}^n (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i) \\
 0 &= \sum_{i=1}^n y_i - n\hat{\beta}_0 - \hat{\beta}_1 \sum_{i=1}^n x_i \\
 \hat{\beta}_0 &= \frac{1}{n} \sum_{i=1}^n y_i - \hat{\beta}_1 \frac{1}{n} \sum_{i=1}^n x_i \\
 \hat{\beta}_0 &= \bar{y} - \hat{\beta}_1 \bar{x} .
 \end{aligned} \tag{6}$$

The derivative of the log-likelihood function (4) at $\hat{\beta}_0$ with respect to β_1 is

$$\frac{\text{dLL}(\hat{\beta}_0, \beta_1, \sigma^2)}{\text{d}\beta_1} = \frac{1}{\sigma^2} \sum_{i=1}^n (x_i y_i - \hat{\beta}_0 x_i - \beta_1 x_i^2) \tag{7}$$

and setting this derivative to zero gives the MLE for β_1 :

$$\begin{aligned}
 \frac{dLL(\hat{\beta}_0, \hat{\beta}_1, \hat{\sigma}^2)}{d\beta_1} &= 0 \\
 0 &= \frac{1}{\hat{\sigma}^2} \sum_{i=1}^n (x_i y_i - \hat{\beta}_0 x_i - \hat{\beta}_1 x_i^2) \\
 0 &= \sum_{i=1}^n x_i y_i - \hat{\beta}_0 \sum_{i=1}^n x_i - \hat{\beta}_1 \sum_{i=1}^n x_i^2 \\
 0 &\stackrel{(6)}{=} \sum_{i=1}^n x_i y_i - (\bar{y} - \hat{\beta}_1 \bar{x}) \sum_{i=1}^n x_i - \hat{\beta}_1 \sum_{i=1}^n x_i^2 \\
 0 &= \sum_{i=1}^n x_i y_i - \bar{y} \sum_{i=1}^n x_i + \hat{\beta}_1 \bar{x} \sum_{i=1}^n x_i - \hat{\beta}_1 \sum_{i=1}^n x_i^2 \\
 0 &= \sum_{i=1}^n x_i y_i - n \bar{x} \bar{y} + \hat{\beta}_1 n \bar{x}^2 - \hat{\beta}_1 \sum_{i=1}^n x_i^2 \\
 \hat{\beta}_1 &= \frac{\sum_{i=1}^n x_i y_i - \sum_{i=1}^n \bar{x} \bar{y}}{\sum_{i=1}^n x_i^2 - \sum_{i=1}^n \bar{x}^2} \\
 \hat{\beta}_1 &= \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2} \\
 \hat{\beta}_1 &= \frac{s_{xy}}{s_x^2} .
 \end{aligned} \tag{8}$$

The derivative of the log-likelihood function (4) at $(\hat{\beta}_0, \hat{\beta}_1)$ with respect to σ^2 is

$$\frac{dLL(\hat{\beta}_0, \hat{\beta}_1, \sigma^2)}{d\sigma^2} = -\frac{n}{2\sigma^2} + \frac{1}{2(\sigma^2)^2} \sum_{i=1}^n (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2 \tag{9}$$

and setting this derivative to zero gives the MLE for σ^2 :

$$\begin{aligned}
 \frac{dLL(\hat{\beta}_0, \hat{\beta}_1, \hat{\sigma}^2)}{d\sigma^2} &= 0 \\
 0 &= -\frac{n}{2\hat{\sigma}^2} + \frac{1}{2(\hat{\sigma}^2)^2} \sum_{i=1}^n (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2 \\
 \frac{n}{2\hat{\sigma}^2} &= \frac{1}{2(\hat{\sigma}^2)^2} \sum_{i=1}^n (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2 \\
 \hat{\sigma}^2 &= \frac{1}{n} \sum_{i=1}^n (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2 .
 \end{aligned} \tag{10}$$

Together, (6), (8) and (10) constitute the MLE for simple linear regression.

Sources:

- original work

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1.4.18 Maximum likelihood estimation

Theorem: Given a simple linear regression model (\rightarrow Definition 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 Definition 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 Definition I/1.7.2), s_x^2 is the sample variance (\rightarrow Definition I/1.8.2) of x and s_{xy} is the sample covariance (\rightarrow Definition I/1.10.2) between x and y .

Proof: Simple linear regression is a special case of multiple linear regression (\rightarrow Proof 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 weighted least squares estimates (\rightarrow Proof III/1.5.25) 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 Proof III/1.4.4):

$$\begin{aligned}\hat{\beta}_0 &= \bar{y} - \hat{\beta}_1 \bar{x} \\ \hat{\beta}_1 &= \frac{s_{xy}}{s_x^2} .\end{aligned}\tag{7}$$

Additionally, we can write out the estimate of σ^2 :

$$\begin{aligned}\hat{\sigma}^2 &= \frac{1}{n}(y - X\hat{\beta})^T V^{-1}(y - X\hat{\beta}) \\ &= \frac{1}{n} \left(y - \begin{bmatrix} 1_n & x \end{bmatrix} \begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \end{bmatrix} \right)^T \left(y - \begin{bmatrix} 1_n & x \end{bmatrix} \begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \end{bmatrix} \right) \\ &= \frac{1}{n} (y - \hat{\beta}_0 - \hat{\beta}_1 x)^T (y - \hat{\beta}_0 - \hat{\beta}_1 x) \\ &= \frac{1}{n} \sum_{i=1}^n (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2 .\end{aligned}\tag{8}$$

Sources:

- original work

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1.4.19 Sum of residuals is zero

Theorem: In simple linear regression (\rightarrow Definition III/1.4.1), the sum of the residuals (\rightarrow Definition III/1.5.7) is zero when estimated using ordinary least squares (\rightarrow Proof III/1.4.3).

Proof: The residuals are defined as the estimated error terms (\rightarrow Definition III/1.4.1)

$$\hat{\varepsilon}_i = y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i \tag{1}$$

where $\hat{\beta}_0$ and $\hat{\beta}_1$ are parameter estimates obtained using ordinary least squares (\rightarrow Proof III/1.4.3):

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x} \quad \text{and} \quad \hat{\beta}_1 = \frac{s_{xy}}{s_x^2} . \tag{2}$$

With that, we can calculate the sum of the residuals:

$$\begin{aligned}\sum_{i=1}^n \hat{\varepsilon}_i &= \sum_{i=1}^n (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i) \\ &= \sum_{i=1}^n (y_i - \bar{y} + \hat{\beta}_1 \bar{x} - \hat{\beta}_1 x_i) \\ &= \sum_{i=1}^n y_i - n\bar{y} + \hat{\beta}_1 n\bar{x} - \hat{\beta}_1 \sum_{i=1}^n x_i \\ &= n\bar{y} - n\bar{y} + \hat{\beta}_1 n\bar{x} - \hat{\beta}_1 n\bar{x} \\ &= 0 .\end{aligned}\tag{3}$$

Thus, the sum of the residuals (\rightarrow Definition III/1.5.7) is zero under ordinary least squares (\rightarrow Proof III/1.4.3), if the model (\rightarrow Definition 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.

Metadata: ID: P276 | shortcut: slr-ressum | author: JoramSoch | date: 2021-10-27, 13:07.

1.4.20 Correlation with covariate is zero

Theorem: In simple linear regression (\rightarrow Definition III/1.4.1), the residuals (\rightarrow Definition III/1.5.7) and the covariate (\rightarrow Definition III/1.4.1) are uncorrelated (\rightarrow Definition I/1.11.1) when estimated using ordinary least squares (\rightarrow Proof III/1.4.3).

Proof: The residuals are defined as the estimated error terms (\rightarrow Definition 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 Proof 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 Definition I/1.11.1), this demonstrates that residuals (\rightarrow Definition III/1.5.7) and covariate (\rightarrow Definition III/1.4.1) values are uncorrelated under ordinary least squares (\rightarrow Proof 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.

Metadata: ID: P277 | shortcut: slr-rescorr | author: JoramSoch | date: 2021-10-27, 13:07.

1.4.21 Residual variance in terms of sample variance

Theorem: Assume a simple linear regression model (\rightarrow Definition 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 Proof III/1.4.3). Then, residual variance (\rightarrow Definition IV/1.1.1) and sample variance (\rightarrow Definition I/1.8.2) are related to each other via the correlation coefficient (\rightarrow Definition I/1.11.1):

$$\hat{\sigma}^2 = (1 - r_{xy}^2) s_y^2 . \quad (2)$$

Proof: The residual variance (\rightarrow Definition IV/1.1.1) can be expressed in terms of the residual sum of squares (\rightarrow Definition III/1.5.7):

$$\hat{\sigma}^2 = \frac{1}{n-1} \text{RSS}(\hat{\beta}_0, \hat{\beta}_1) \quad (3)$$

and the residual sum of squares for simple linear regression (\rightarrow Proof 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 Definition I/1.11.1)

$$\text{Corr}(X, Y) = \frac{\text{Cov}(X, Y)}{\sqrt{\text{Var}(X)} \sqrt{\text{Var}(Y)}} \quad (6)$$

which also holds for sample correlation, sample covariance (\rightarrow Definition I/1.10.2) and sample standard deviation (\rightarrow Definition I/1.13.1)

$$r_{xy} = \frac{s_{xy}}{s_x s_y} , \quad (7)$$

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.

Metadata: ID: P278 | shortcut: slr-resvar | author: JoramSoch | date: 2021-10-27, 14:37.

1.4.22 Correlation coefficient in terms of slope estimate

Theorem: Assume a simple linear regression model (\rightarrow Definition 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 Proof III/1.4.3). Then, correlation coefficient (\rightarrow Definition I/1.11.1) and the estimated value of the slope parameter (\rightarrow Definition III/1.4.1) are related to each other via the sample standard deviations (\rightarrow Definition I/1.13.1):

$$r_{xy} = \frac{s_x}{s_y} \hat{\beta}_1. \quad (2)$$

Proof: The ordinary least squares estimate of the slope (\rightarrow Proof 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 Proof I/1.10.7)

$$\text{Cov}(X, Y) = \sigma_X \text{Corr}(X, Y) \sigma_Y \quad (4)$$

which also holds for sample correlation (\rightarrow Definition I/1.11.1) and sample covariance (\rightarrow Definition I/1.10.2)

$$s_{xy} = s_x r_{xy} s_y, \quad (5)$$

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.

Metadata: ID: P279 | shortcut: slr-corr | author: JoramSoch | date: 2021-10-27, 14:58.

1.4.23 Coefficient of determination in terms of correlation coefficient

Theorem: Assume a simple linear regression model (\rightarrow Definition 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 Proof III/1.4.3). Then, the coefficient of determination (\rightarrow Definition IV/1.2.1) is equal to the squared correlation coefficient (\rightarrow Definition I/1.11.1) between x and y :

$$R^2 = r_{xy}^2. \quad (2)$$

Proof: The ordinary least squares estimates for simple linear regression (\rightarrow Proof 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 Definition 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 Definition III/1.5.6) to total sum of squares (\rightarrow Definition III/1.5.5):

$$R^2 = \frac{\text{ESS}}{\text{TSS}}. \quad (4)$$

Using the explained and total sum of squares for simple linear regression (\rightarrow Proof 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:

$$\begin{aligned} R^2 &= \frac{\sum_{i=1}^n (\bar{y} - \hat{\beta}_1 \bar{x} + \hat{\beta}_1 x_i - \bar{y})^2}{\sum_{i=1}^n (y_i - \bar{y})^2} \\ &= \frac{\sum_{i=1}^n (\hat{\beta}_1 (x_i - \bar{x}))^2}{\sum_{i=1}^n (y_i - \bar{y})^2} \\ &= \hat{\beta}_1^2 \frac{\frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x})^2}{\frac{1}{n-1} \sum_{i=1}^n (y_i - \bar{y})^2} \\ &= \hat{\beta}_1^2 \frac{s_x^2}{s_y^2} \\ &= \left(\frac{s_x}{s_y} \hat{\beta}_1 \right)^2. \end{aligned} \quad (6)$$

Using the relationship between correlation coefficient and slope estimate (\rightarrow Proof III/1.4.22), 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.

Metadata: ID: P280 | shortcut: slr-rsq | author: JoramSoch | date: 2021-10-27, 15:31.

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 Definition 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 (i.i.d.) observations:

$$V = I_n \Rightarrow \varepsilon \sim \mathcal{N}(0, \sigma^2 I_n) \Rightarrow \varepsilon_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2) . \quad (5)$$

Otherwise, it is called multiple linear regression with correlated observations.

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.

Metadata: ID: D36 | shortcut: mlr | author: JoramSoch | date: 2020-03-21, 20:09.

1.5.2 Special case of general linear model

Theorem: Multiple linear regression (\rightarrow Definition III/1.5.1) is a special case of the general linear model (\rightarrow Definition III/1.5.1) 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 Definition III/1.5.1).

Proof: The linear regression model with correlated errors (\rightarrow Definition 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 $n \times 1$ 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 Proof 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 Definition III/2.1.1)

$$Y = XB + E, \quad E \sim \mathcal{MN}(0, V, \Sigma) , \quad (5)$$

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.

Metadata: ID: P329 | shortcut: mlr-glm | author: JoramSoch | date: 2022-07-21, 08:28.

1.5.3 Ordinary least squares

Theorem: Given a linear regression model (\rightarrow Definition 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 Definition III/1.5.7) 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>.

Metadata: ID: P2 | shortcut: mlr-ols | author: JoramSoch | date: 2019-09-27, 07:18.

1.5.4 Ordinary least squares

Theorem: Given a linear regression model (\rightarrow Definition 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 Definition III/1.5.7) are given by

$$\hat{\beta} = (X^T X)^{-1} X^T y. \quad (2)$$

Proof: The residual sum of squares (\rightarrow Definition III/1.5.7) 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:

$$\begin{aligned} \frac{d\text{RSS}(\hat{\beta})}{d\beta} &= 0 \\ 0 &= -2X^T y + 2X^T X \hat{\beta} \\ X^T X \hat{\beta} &= X^T y \\ \hat{\beta} &= (X^T X)^{-1} X^T y . \end{aligned} \quad (6)$$

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/.

Metadata: ID: P40 | shortcut: mlr-ols2 | author: JoramSoch | date: 2020-02-03, 18:43.

1.5.5 Total sum of squares

Definition: Let there be a multiple linear regression with independent observations (\rightarrow Definition 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 total sum of squares (TSS) is defined as the sum of squared deviations of the measured signal from the average signal:

$$\text{TSS} = \sum_{i=1}^n (y_i - \bar{y})^2 \quad \text{where} \quad \bar{y} = \frac{1}{n} \sum_{i=1}^n y_i . \quad (2)$$

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.

Metadata: ID: D37 | shortcut: tss | author: JoramSoch | date: 2020-03-21, 21:44.

1.5.6 Explained sum of squares

Definition: Let there be a multiple linear regression with independent observations (\rightarrow Definition 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 explained sum of squares (ESS) is defined as the sum of squared deviations of the fitted signal from the average signal:

$$\text{ESS} = \sum_{i=1}^n (\hat{y}_i - \bar{y})^2 \quad \text{where} \quad \hat{y} = X\hat{\beta} \quad \text{and} \quad \bar{y} = \frac{1}{n} \sum_{i=1}^n y_i \quad (2)$$

with estimated regression coefficients $\hat{\beta}$, e.g. obtained via ordinary least squares (\rightarrow Proof 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.

Metadata: ID: D38 | shortcut: ess | author: JoramSoch | date: 2020-03-21, 21:57.

1.5.7 Residual sum of squares

Definition: Let there be a multiple linear regression with independent observations (\rightarrow Definition 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 Proof 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.

Metadata: ID: D39 | shortcut: rss | author: JoramSoch | date: 2020-03-21, 22:03.

1.5.8 Total, explained and residual sum of squares

Theorem: Assume a linear regression model (\rightarrow Definition 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 Definition III/1.5.5), ESS is the explained sum of squares (\rightarrow Definition III/1.5.6) and RSS is the residual sum of squares (\rightarrow Definition III/1.5.7).

Proof: The total sum of squares (\rightarrow Definition III/1.5.5) 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

$$\begin{aligned} \text{TSS} &= \sum_{i=1}^n (y_i - \bar{y} + \hat{y}_i - \hat{y}_i)^2 \\ &= \sum_{i=1}^n ((\hat{y}_i - \bar{y}) + (y_i - \hat{y}_i))^2 \\ &= \sum_{i=1}^n ((\hat{y}_i - \bar{y}) + \hat{\varepsilon}_i)^2 \\ &= \sum_{i=1}^n ((\hat{y}_i - \bar{y})^2 + 2\hat{\varepsilon}_i(\hat{y}_i - \bar{y}) + \hat{\varepsilon}_i^2) \\ &= \sum_{i=1}^n (\hat{y}_i - \bar{y})^2 + \sum_{i=1}^n \hat{\varepsilon}_i^2 + 2 \sum_{i=1}^n \hat{\varepsilon}_i(\hat{y}_i - \bar{y}) \\ &= \sum_{i=1}^n (\hat{y}_i - \bar{y})^2 + \sum_{i=1}^n \hat{\varepsilon}_i^2 + 2 \sum_{i=1}^n \hat{\varepsilon}_i(x_i\hat{\beta} - \bar{y}) \\ &= \sum_{i=1}^n (\hat{y}_i - \bar{y})^2 + \sum_{i=1}^n \hat{\varepsilon}_i^2 + 2 \sum_{i=1}^n \hat{\varepsilon}_i \left(\sum_{j=1}^p x_{ij}\hat{\beta}_j \right) - 2 \sum_{i=1}^n \hat{\varepsilon}_i \bar{y} \\ &= \sum_{i=1}^n (\hat{y}_i - \bar{y})^2 + \sum_{i=1}^n \hat{\varepsilon}_i^2 + 2 \sum_{j=1}^p \hat{\beta}_j \sum_{i=1}^n \hat{\varepsilon}_i x_{ij} - 2\bar{y} \sum_{i=1}^n \hat{\varepsilon}_i \end{aligned} \quad (4)$$

The fact that the design matrix includes a constant regressor ensures that

$$\sum_{i=1}^n \hat{\varepsilon}_i = \hat{\varepsilon}^T \mathbf{1}_n = 0 \quad (5)$$

and because the residuals are orthogonal to the design matrix (\rightarrow Proof III/1.5.3), we have

$$\sum_{i=1}^n \hat{\varepsilon}_i x_{ij} = \hat{\varepsilon}^T \mathbf{x}_j = 0. \quad (6)$$

Applying (5) and (6) to (4), this becomes

$$\text{TSS} = \sum_{i=1}^n (\hat{y}_i - \bar{y})^2 + \sum_{i=1}^n \hat{\varepsilon}_i^2 \quad (7)$$

and, with the definitions of explained (\rightarrow Definition III/1.5.6) and residual sum of squares (\rightarrow Definition III/1.5.7), it is

$$\text{TSS} = \text{ESS} + \text{RSS} . \quad (8)$$

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.

Metadata: ID: P76 | shortcut: mlr-pss | author: JoramSoch | date: 2020-03-09, 22:18.

1.5.9 Estimation matrix

Definition: In multiple linear regression (\rightarrow Definition III/1.5.1), the estimation matrix is the matrix E that results in ordinary least squares (\rightarrow Proof III/1.5.3) or weighted least squares (\rightarrow Proof III/1.5.19) parameter estimates when right-multiplied with the measured data:

$$Ey = \hat{\beta} . \quad (1)$$

Sources:

- original work

Metadata: ID: D81 | shortcut: emat | author: JoramSoch | date: 2020-07-22, 05:17.

1.5.10 Projection matrix

Definition: In multiple linear regression (\rightarrow Definition III/1.5.1), the projection matrix is the matrix P that results in the fitted signal explained by estimated parameters (\rightarrow Definition III/1.5.9) 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.

Metadata: ID: D82 | shortcut: pmat | author: JoramSoch | date: 2020-07-22, 05:25.

1.5.11 Residual-forming matrix

Definition: In multiple linear regression (\rightarrow Definition 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 Definition III/1.5.9) 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.

Metadata: ID: D83 | shortcut: rformat | author: JoramSoch | date: 2020-07-22, 05:35.

1.5.12 Estimation, projection and residual-forming matrix

Theorem: Assume a linear regression model (\rightarrow Definition 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 Proof 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

$$\begin{aligned} E &= (X^T X)^{-1} X^T \\ P &= X(X^T X)^{-1} X^T \\ R &= I_n - X(X^T X)^{-1} X^T \end{aligned} \quad (3)$$

are the estimation matrix (\rightarrow Definition III/1.5.9), projection matrix (\rightarrow Definition III/1.5.10) and residual-forming matrix (\rightarrow Definition III/1.5.11) 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 Definition III/1.5.7)

$$\hat{\beta} = \arg \min_{\beta} [(y - X\beta)^T (y - X\beta)] \quad (4)$$

and the solution to this (\rightarrow Proof III/1.5.3) is given by

$$\begin{aligned} \hat{\beta} &= (X^T X)^{-1} X^T y \\ &\stackrel{(3)}{=} Ey. \end{aligned} \quad (5)$$

2) The fitted signal is given by multiplying the design matrix with the estimated regression coefficients

$$\hat{y} = X\hat{\beta} \quad (6)$$

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>.

Metadata: ID: P75 | shortcut: mlr-mat | author: JoramSoch | date: 2020-03-09, 21:18.

1.5.13 Symmetry of projection and residual-forming matrix

Theorem: The projection matrix (\rightarrow Definition III/1.5.10) and the residual-forming matrix (\rightarrow Definition III/1.5.11) 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 Definition 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 Proof III/1.5.12)

$$P = X(X^T X)^{-1} X^T ,\tag{4}$$

such that

$$\begin{aligned}
P^T &= (X(X^T X)^{-1} X^T)^T \\
&= X^{TT} ((X^T X)^{-1})^T X^T \\
&= X(X^T X)^{-1} X^T .
\end{aligned} \tag{5}$$

2) The residual-forming matrix for ordinary least squares is given by (\rightarrow Proof III/1.5.12)

$$R = I_n - X(X^T X)^{-1} X^T = I_n - P , \tag{6}$$

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.

Metadata: ID: P399 | shortcut: mlr-symm | author: JoramSoch | date: 2022-12-22, 13:17.

1.5.14 Idempotence of projection and residual-forming matrix

Theorem: The projection matrix (\rightarrow Definition III/1.5.10) and the residual-forming matrix (\rightarrow Definition III/1.5.11) 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 Proof III/1.5.12)

$$P = X(X^T X)^{-1} X^T , \tag{2}$$

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 Proof III/1.5.12)

$$R = I_n - X(X^T X)^{-1} X^T = I_n - P, \quad (4)$$

such that

$$\begin{aligned} R^2 &= (I_n - P)(I_n - P) \\ &= I_n - P - P + P^2 \\ &\stackrel{(3)}{=} I_n - 2P + P \\ &= I_n - P \\ &\stackrel{(4)}{=} R. \end{aligned} \quad (5)$$

Sources:

- Wikipedia (2020): “Projection matrix”; in: *Wikipedia, the free encyclopedia*, retrieved on 2020-07-22; URL: https://en.wikipedia.org/wiki/Projection_matrix#Properties.

Metadata: ID: P135 | shortcut: mlr-idem | author: JoramSoch | date: 2020-07-22, 06:28.

1.5.15 Independence of estimated parameters and residuals

Theorem: Assume a linear regression model (\rightarrow Definition 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 Proof III/1.5.19). Then, the estimated parameters and the vector of residuals (\rightarrow Proof III/1.5.17) are independent from each other:

$$\begin{aligned} \hat{\beta} &= (X^T V^{-1} X)^{-1} X^T V^{-1} y \quad \text{and} \\ \hat{\varepsilon} &= y - X\hat{\beta} \quad \text{ind.} \end{aligned} \quad (2)$$

Proof: Equation (1) implies the following distribution (\rightarrow Proof III/1.5.17) for the random vector (\rightarrow Definition I/1.2.3) y :

$$\begin{aligned} y &\sim \mathcal{N}(X\beta, \sigma^2 V) \\ &\sim \mathcal{N}(X\beta, \Sigma) \\ \text{with } \Sigma &= \sigma^2 V. \end{aligned} \quad (3)$$

Note that the estimated parameters and residuals can be written as projections from the same random vector (\rightarrow Proof III/1.5.12) y :

$$\begin{aligned} \hat{\beta} &= (X^T V^{-1} X)^{-1} X^T V^{-1} y \\ &= Ay \\ \text{with } A &= (X^T V^{-1} X)^{-1} X^T V^{-1} \end{aligned} \quad (4)$$

$$\begin{aligned}
\hat{\varepsilon} &= y - X\hat{\beta} \\
&= (I_n - X(X^T V^{-1} X)^{-1} X^T V^{-1})y \\
&= By
\end{aligned} \tag{5}$$

$$\text{with } B = (I_n - X(X^T V^{-1} X)^{-1} X^T V^{-1}) .$$

Two projections AZ and BZ from the same multivariate normal (\rightarrow Definition II/4.1.1) random vector (\rightarrow Definition I/1.2.3) $Z \sim \mathcal{N}(\mu, \Sigma)$ are independent, if and only if the following condition holds (\rightarrow Proof III/1.5.15):

$$A\Sigma B^T = 0 . \tag{6}$$

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 Proof III/1.5.23) from $\hat{\beta}$ and $\hat{\varepsilon}$ – are statistically independent (\rightarrow Definition 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>.

Metadata: ID: P393 | shortcut: mlr-ind | author: JoramSoch | date: 2022-12-13, 16:18.

1.5.16 Distribution of OLS estimates, signal and residuals

Theorem: Assume a linear regression model (\rightarrow Definition III/1.5.1) with independent observations

$$y = X\beta + \varepsilon, \quad \varepsilon_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2) \tag{1}$$

and consider estimation using ordinary least squares (\rightarrow Proof III/1.5.3). Then, the estimated parameters, fitted signal and residuals are distributed as

$$\begin{aligned}
\hat{\beta} &\sim \mathcal{N}(\beta, \sigma^2 (X^T X)^{-1}) \\
\hat{y} &\sim \mathcal{N}(X\beta, \sigma^2 P) \\
\hat{\varepsilon} &\sim \mathcal{N}(0, \sigma^2 (I_n - P))
\end{aligned} \tag{2}$$

where P is the projection matrix (\rightarrow Definition III/1.5.10) for ordinary least squares (\rightarrow Proof III/1.5.3)

$$P = X(X^T X)^{-1} X^T . \tag{3}$$

Proof: We will use the linear transformation theorem for the multivariate normal distribution (\rightarrow Proof II/4.1.9):

$$x \sim \mathcal{N}(\mu, \Sigma) \quad \Rightarrow \quad y = Ax + b \sim \mathcal{N}(A\mu + b, A\Sigma A^T) . \quad (4)$$

The distributional assumption in (1) is equivalent to (\rightarrow Proof II/4.1.12):

$$y = X\beta + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 I_n) . \quad (5)$$

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 Proof 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 Proof III/1.5.12) 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 Proof III/1.5.12) 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

$$\begin{aligned} \hat{\varepsilon} &\sim \mathcal{N}([I_n - X(X^T X)^{-1} X^T] X\beta, \sigma^2 [I_n - P] I_n [I_n - P]^T) \\ &\sim \mathcal{N}(X\beta - X\beta, \sigma^2 [I_n - P] [I_n - P]^T) . \end{aligned} \quad (12)$$

Because the residual-forming matrix (\rightarrow Definition “rfm”) is symmetric (\rightarrow Proof III/1.5.13) and idempotent (\rightarrow Proof III/1.5.14), 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.

- Penny, William (2006): “Multiple Regression”; in: *Mathematics for Brain Imaging*, ch. 1.5, pp. 39-41, eqs. 1.106-1.110; URL: https://ueapsylabs.co.uk/sites/wpenny/mbi/mbi_course.pdf.

Metadata: ID: P400 | shortcut: mlr-olsdist | author: JoramSoch | date: 2022-12-23, 16:36.

1.5.17 Distribution of WLS estimates, signal and residuals

Theorem: Assume a linear regression model (\rightarrow Definition 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 Proof III/1.5.19). Then, the estimated parameters, fitted signal and residuals are distributed as

$$\begin{aligned} \hat{\beta} &\sim \mathcal{N}(\beta, \sigma^2 (X^T V^{-1} X)^{-1}) \\ \hat{y} &\sim \mathcal{N}(X\beta, \sigma^2 (PV)) \\ \hat{\varepsilon} &\sim \mathcal{N}(0, \sigma^2 (I_n - P)V) \end{aligned} \quad (2)$$

where P is the projection matrix (\rightarrow Definition III/1.5.10) for weighted least squares (\rightarrow Proof III/1.5.19)

$$P = X(X^T V^{-1} X)^{-1} X^T V^{-1} . \quad (3)$$

Proof: We will use the linear transformation theorem for the multivariate normal distribution (\rightarrow Proof II/4.1.9):

$$x \sim \mathcal{N}(\mu, \Sigma) \quad \Rightarrow \quad y = Ax + b \sim \mathcal{N}(A\mu + b, A\Sigma A^T) . \quad (4)$$

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 Proof III/1.5.19) 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 Proof III/1.5.12) 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 Proof III/1.5.12) 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

$$\begin{aligned} \hat{\varepsilon} &\sim \mathcal{N} \left([I_n - X(X^T V^{-1} X)^{-1} X^T V^{-1}] X\beta, \sigma^2 [I_n - P] V [I_n - P]^T \right) \\ &\sim \mathcal{N} (X\beta - X\beta, \sigma^2 [V - V P^T - P V + P V P^T]) \\ &\sim \mathcal{N} (0, \sigma^2 [V - V V^{-1} X (X^T V^{-1} X)^{-1} X^T - X (X^T V^{-1} X)^{-1} X^T V^{-1} V + P V P^T]) \\ &\sim \mathcal{N} (0, \sigma^2 [V - 2 P V + X (X^T V^{-1} X)^{-1} X^T V^{-1} V V^{-1} X (X^T V^{-1} X)^{-1} X^T]) \\ &\sim \mathcal{N} (0, \sigma^2 [V - 2 P V + P V]) \\ &\sim \mathcal{N} (0, \sigma^2 [V - P V]) \\ &\sim \mathcal{N} (0, \sigma^2 [I_n - P] V) . \end{aligned} \quad (11)$$

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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- 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, eq. A.10; URL: <https://www.sciencedirect.com/science/article/pii/S1053811919310407>; DOI: 10.1016/j.neuroimage.2019.116449.
- 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. A.2; URL: <https://www.sciencedirect.com/science/article/pii/S105381191730527X>; DOI: 10.1016/j.neuroimage.2017.06.056.

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1.5.18 Distribution of residual sum of squares

Theorem: Assume a linear regression model (\rightarrow Definition 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 Proof III/1.5.19). Then, the residual sum of squares (\rightarrow Definition III/1.5.7) $\hat{\varepsilon}^T \hat{\varepsilon}$, divided by the true error variance (\rightarrow Definition III/1.5.1) σ^2 , follows a chi-squared distribution (\rightarrow Definition II/3.7.1) with $n - p$ degrees of freedom (\rightarrow Definition “dof”)

$$\frac{\hat{\varepsilon}^T \hat{\varepsilon}}{\sigma^2} \sim \chi^2(n - p) \quad (2)$$

where n and p are the dimensions of the $n \times p$ design matrix (\rightarrow Definition 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 Proof II/4.1.9)

$$\tilde{y} \sim \mathcal{N}(\tilde{X}\beta, \sigma^2 I_n) . \quad (6)$$

With that, we have obtained a linear regression model (\rightarrow Definition III/1.5.1) with independent observations. Cochran's theorem for multivariate normal variables (\rightarrow Proof "mvn-cochran") states that, for an $n \times 1$ normal random vector (\rightarrow Definition II/4.1.1) whose covariance matrix (\rightarrow Definition I/1.10.9) is a scalar multiple of the identity matrix, a specific squared form will follow a non-central chi-squared distribution (\rightarrow Definition "ncchi2") where the degrees of freedom and the non-centrality parameter depend on the matrix in the quadratic form:

$$x \sim \mathcal{N}(\mu, \sigma^2 I_n) \quad \Rightarrow \quad y = x^T A x / \sigma^2 \sim \chi^2(\text{tr}(A), \mu^T A \mu) . \quad (7)$$

First, we formulate the residuals (\rightarrow Proof III/1.5.12) in terms of transformed measurements \tilde{y} :

$$\begin{aligned} \hat{\varepsilon} &= \tilde{y} - \tilde{X}\hat{\beta} & \text{where} & \quad \hat{\beta} = (\tilde{X}^T \tilde{X})^{-1} \tilde{X}^T \tilde{y} \\ &= (I_n - \tilde{P})\tilde{y} & \text{where} & \quad \tilde{P} = \tilde{X}(\tilde{X}^T \tilde{X})^{-1} \tilde{X}^T \\ &= \tilde{R}\tilde{y} & \text{where} & \quad \tilde{R} = I_n - \tilde{P} . \end{aligned} \quad (8)$$

Next, we observe that the residual sum of squares can be represented as a quadratic form:

$$\frac{1}{\sigma^2} \sum_{i=1}^n \hat{\varepsilon}_i^2 = \frac{\hat{\varepsilon}^T \hat{\varepsilon}}{\sigma^2} = \tilde{y}^T \tilde{R}^T \tilde{R} \tilde{y} / \sigma^2 \quad (9)$$

Because the residual-forming matrix (\rightarrow Definition III/1.5.11) \tilde{R} is symmetric (\rightarrow Proof III/1.5.13) and idempotent (\rightarrow Proof III/1.5.14), we have $\tilde{R}^T = \tilde{R}$ and $\tilde{R}^2 = \tilde{R}$, such that:

$$\frac{\hat{\varepsilon}^T \hat{\varepsilon}}{\sigma^2} = \tilde{y}^T \tilde{R} \tilde{y} / \sigma^2 . \quad (10)$$

With that, we can apply Cochran's theorem given by (7) which yields

$$\begin{aligned}
\frac{\hat{\varepsilon}^T \hat{\varepsilon}}{\sigma^2} &\sim \chi^2 \left(\text{tr}(I_n - \tilde{P}), \beta^T \tilde{X}^T \tilde{R} \tilde{X} \beta \right) \\
&\sim \chi^2 \left(\text{tr}(I_n) - \text{tr}(\tilde{P}), \beta^T \tilde{X}^T (I_n - \tilde{P}) \tilde{X} \beta \right) \\
&\sim \chi^2 \left(\text{tr}(I_n) - \text{tr}(\tilde{X}(\tilde{X}^T \tilde{X})^{-1} \tilde{X}^T), \beta^T (\tilde{X}^T \tilde{X} - \tilde{X}^T \tilde{X}(\tilde{X}^T \tilde{X})^{-1} \tilde{X}^T \tilde{X}) \beta \right) \\
&\sim \chi^2 \left(\text{tr}(I_n) - \text{tr}(\tilde{X}^T \tilde{X}(\tilde{X}^T \tilde{X})^{-1}), \beta^T (\tilde{X}^T \tilde{X} - \tilde{X}^T \tilde{X}) \beta \right) \\
&\sim \chi^2 \left(\text{tr}(I_n) - \text{tr}(I_p), \beta^T 0_{pp} \beta \right) \\
&\sim \chi^2(n - p, 0) .
\end{aligned} \tag{11}$$

Because a non-central chi-squared distribution with non-centrality parameter of zero reduces to the central chi-squared distribution (\rightarrow Proof “ncchi2-chi2”), we obtain our final result:

$$\frac{\hat{\varepsilon}^T \hat{\varepsilon}}{\sigma^2} \sim \chi^2(n - p) . \tag{12}$$

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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- Wikipedia (2022): “Ordinary least squares”; in: *Wikipedia, the free encyclopedia*, retrieved on 2022-12-13; URL: https://en.wikipedia.org/wiki/Ordinary_least_squares#Estimation.
- 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>.

Metadata: ID: P390 | shortcut: mlr-rssdist | author: JoramSoch | date: 2022-12-13, 07:08.

1.5.19 Weighted least squares

Theorem: Given a linear regression model (\rightarrow Definition III/1.5.1) with correlated observations

$$y = X\beta + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 V) , \tag{1}$$

the parameters minimizing the weighted residual sum of squares (\rightarrow Definition III/1.5.7) are given by

$$\hat{\beta} = (X^T V^{-1} X)^{-1} X^T V^{-1} y . \tag{2}$$

Proof: Let there be an $n \times n$ square matrix W , such that

$$WVW^T = I_n . \tag{3}$$

Since V is a covariance matrix and thus symmetric, W is also symmetric and can be expressed as the matrix square root of the inverse of V :

$$WVW = I_n \Leftrightarrow V = W^{-1}W^{-1} \Leftrightarrow V^{-1} = WW \Leftrightarrow W = V^{-1/2}. \quad (4)$$

Left-multiplying the linear regression equation (1) with W , the linear transformation theorem (\rightarrow Proof II/4.1.9) 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 Definition 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 Proof III/1.5.3) giving

$$\begin{aligned} \hat{\beta} &= (\tilde{X}^T \tilde{X})^{-1} \tilde{X}^T \tilde{y} \\ &= ((WX)^T WX)^{-1} (WX)^T Wy \\ &= (X^T W^T W X)^{-1} X^T W^T Wy \\ &= (X^T W W X)^{-1} X^T W Wy \\ &\stackrel{(4)}{=} (X^T V^{-1} X)^{-1} X^T V^{-1} y \end{aligned} \quad (7)$$

which corresponds to the weighted least squares solution (2).

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>.
- Wikipedia (2021): “Weighted least squares”; in: *Wikipedia, the free encyclopedia*, retrieved on 2021-11-17; URL: https://en.wikipedia.org/wiki/Weighted_least_squares#Motivation.

Metadata: ID: P77 | shortcut: mlr-wls | author: JoramSoch | date: 2020-03-11, 11:22.

1.5.20 Weighted least squares

Theorem: Given a linear regression model (\rightarrow Definition 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 Definition III/1.5.7) 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, W is also symmetric and can be expressed the matrix square root of the inverse of V :

$$WVW = I_n \Leftrightarrow V = W^{-1}W^{-1} \Leftrightarrow V^{-1} = WW \Leftrightarrow W = V^{-1/2}. \quad (4)$$

Left-multiplying the linear regression equation (1) with W , the linear transformation theorem (\rightarrow Proof II/4.1.9) implies that

$$Wy = WX\beta + W\varepsilon, \quad W\varepsilon \sim \mathcal{N}(0, \sigma^2 WWVW^T). \quad (5)$$

Applying (3), we see that (5) is actually a linear regression model (\rightarrow Definition 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 Definition III/1.5.7) 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 $\text{wRSS}(\beta)$.

Sources:

- original work

Metadata: ID: P136 | shortcut: mlr-wls2 | author: JoramSoch | date: 2020-07-22, 06:48.

1.5.21 t-contrast

Definition: Consider a linear regression model (\rightarrow Definition III/1.5.1) with $n \times p$ design matrix X and $p \times 1$ regression coefficients β :

$$y = X\beta + \varepsilon, \varepsilon \sim \mathcal{N}(0, \sigma^2 V) . \quad (1)$$

Then, a t-contrast is specified by a $p \times 1$ vector c and it entails the null hypothesis (\rightarrow Definition 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 Definition I/4.3.3) of a two-tailed t-test (\rightarrow Definition I/4.2.4) is

$$H_1 : c^T \beta \neq 0 \quad (3)$$

and the alternative hypothesis (\rightarrow Definition I/4.3.3) of a one-sided t-test (\rightarrow Definition 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>.

Metadata: ID: D185 | shortcut: tcon | author: JoramSoch | date: 2022-12-16, 12:35.

1.5.22 F-contrast

Definition: Consider a linear regression model (\rightarrow Definition III/1.5.1) with $n \times p$ design matrix X and $p \times 1$ regression coefficients β :

$$y = X\beta + \varepsilon, \varepsilon \sim \mathcal{N}(0, \sigma^2 V) . \quad (1)$$

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 Definition 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 Definition I/4.3.3) of the statistical test (\rightarrow Definition 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/methodsspring10.html>.

Metadata: ID: D186 | shortcut: fcon | author: JoramSoch | date: 2022-12-16, 12:42.

1.5.23 Contrast-based t-test

Theorem: Consider a linear regression model (\rightarrow Definition III/1.5.1)

$$y = X\beta + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 V) \quad (1)$$

and a t-contrast (\rightarrow Definition III/1.5.21) 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 Definition 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 Proof III/1.5.25)

$$\begin{aligned} \hat{\beta} &= (X^T V^{-1} X)^{-1} X^T V^{-1} y \\ \hat{\sigma}^2 &= \frac{1}{n-p} (y - X\hat{\beta})^T V^{-1} (y - X\hat{\beta}) \end{aligned} \quad (4)$$

follows a t-distribution (\rightarrow Definition II/3.3.1)

$$t \sim t(n-p) \quad (5)$$

under the null hypothesis (\rightarrow Definition 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 Proof III/1.5.17):

$$\hat{\beta} \sim \mathcal{N}(\beta, \sigma^2 (X^T V^{-1} X)^{-1}) . \quad (7)$$

Thus, the estimated contrast value (\rightarrow Definition III/1.5.21) $\hat{\gamma} = c^T \hat{\beta}$ is distributed according to a univariate normal distribution (\rightarrow Proof II/4.1.9):

$$\hat{\gamma} \sim \mathcal{N}(c^T \beta, \sigma^2 c^T (X^T V^{-1} X)^{-1} c) . \quad (8)$$

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 Proof II/4.1.9), 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 Definition II/3.2.2) under the null hypothesis (\rightarrow Definition 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 Definition III/1.5.7), divided the true error variance (\rightarrow Definition 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 Proof III/1.5.18):

$$v \sim \chi^2(n - p). \quad (13)$$

3) Because the estimated regression coefficients and the vector of residuals are independent from each other (\rightarrow Proof III/1.5.15)

$$\hat{\beta} \quad \text{and} \quad \hat{\varepsilon} \quad \text{ind.} \quad (14)$$

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 Definition 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:

$$\begin{aligned}
t &\stackrel{(16)}{=} \frac{z}{\sqrt{v/(n-p)}} \\
&\stackrel{(15)}{=} \frac{c^T \hat{\beta}}{\sqrt{\sigma^2 c^T (X^T V^{-1} X)^{-1} c}} \cdot \sqrt{\frac{n-p}{\hat{\varepsilon}^T \hat{\varepsilon} / \sigma^2}} \\
&= \frac{c^T \hat{\beta}}{\sqrt{\frac{\hat{\varepsilon}^T \hat{\varepsilon}}{n-p} \cdot c^T (X^T V^{-1} X)^{-1} c}} \\
&\stackrel{(12)}{=} \frac{c^T \hat{\beta}}{\sqrt{\frac{(y-X\hat{\beta})^T V^{-1} (y-X\hat{\beta})}{n-p} \cdot c^T (X^T V^{-1} X)^{-1} c}} \\
&\stackrel{(4)}{=} \frac{c^T \hat{\beta}}{\sqrt{\hat{\sigma}^2 c^T (X^T V^{-1} X)^{-1} c}}.
\end{aligned} \tag{17}$$

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>.
- Walter, Henrik (ed.) (2005): “Datenanalyse für funktionell bildgebende Verfahren”; in: *Funktionelle Bildgebung in Psychiatrie und Psychotherapie*, Schattauer, Stuttgart/New York, 2005, p. 40; URL: https://books.google.de/books?id=edWzKAHi7jQC&source=gbs_navlinks_s.
- 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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1.5.24 Contrast-based F-test

Theorem: Consider a linear regression model (\rightarrow Definition III/1.5.1)

$$y = X\beta + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 V) \tag{1}$$

and an F-contrast (\rightarrow Definition III/1.5.22) on the model parameters

$$\gamma = C^T \beta \quad \text{where} \quad C \in \mathbb{R}^{p \times q}. \tag{2}$$

Then, the test statistic (\rightarrow Definition I/4.3.5)

$$F = \hat{\beta}^T C (\hat{\sigma}^2 C^T (X^T V^{-1} X)^{-1} C)^{-1} C^T \hat{\beta} / q \tag{3}$$

with the parameter estimates (\rightarrow Proof III/1.5.25)

$$\begin{aligned}\hat{\beta} &= (X^T V^{-1} X)^{-1} X^T V^{-1} y \\ \hat{\sigma}^2 &= \frac{1}{n-p} (y - X\hat{\beta})^T V^{-1} (y - X\hat{\beta})\end{aligned}\quad (4)$$

follows an F-distribution (\rightarrow Definition II/3.8.1)

$$F \sim F(q, n-p) \quad (5)$$

under the null hypothesis (\rightarrow Definition 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 Proof III/1.5.17):

$$\hat{\beta} \sim \mathcal{N}(\beta, \sigma^2 (X^T V^{-1} X)^{-1}). \quad (7)$$

Thus, the estimated contrast vector (\rightarrow Definition III/1.5.22) $\hat{\gamma} = C^T \hat{\beta}$ is also distributed according to a multivariate normal distribution (\rightarrow Proof II/4.1.9):

$$\hat{\gamma} \sim \mathcal{N}(C^T \beta, \sigma^2 C^T (X^T V^{-1} X)^{-1} C). \quad (8)$$

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 Definition 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 Definition III/1.5.7), divided the true error variance (\rightarrow Definition 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 Proof III/1.5.18):

$$\frac{\hat{\varepsilon}^T \hat{\varepsilon}}{\sigma^2} = \tau \hat{\varepsilon}^T \hat{\varepsilon} \sim \chi^2(n-p). \quad (11)$$

The chi-squared distribution is related to the gamma distribution (\rightarrow Proof II/3.7.2) in the following way:

$$X \sim \chi^2(k) \quad \Rightarrow \quad cX \sim \text{Gam}\left(\frac{k}{2}, \frac{1}{2c}\right). \quad (12)$$

Thus, applying (12) to (11), we obtain the marginal distribution (\rightarrow Definition I/1.5.3) of τ as:

$$\frac{1}{\hat{\varepsilon}^T \hat{\varepsilon}} (\tau \hat{\varepsilon}^T \hat{\varepsilon}) = \tau \sim \text{Gam}\left(\frac{n-p}{2}, \frac{\hat{\varepsilon}^T \hat{\varepsilon}}{2}\right). \quad (13)$$

3) Note that the joint distribution (\rightarrow Definition I/1.5.2) of $\hat{\gamma}$ and τ is, following from (9) and (13) and by definition, a normal-gamma distribution (\rightarrow Definition II/4.3.1):

$$\hat{\gamma}, \tau \sim \text{NG} \left(C^T \beta, Q, \frac{n-p}{2}, \frac{\hat{\varepsilon}^T \hat{\varepsilon}}{2} \right). \quad (14)$$

The marginal distribution of a normal-gamma distribution with respect to the normal random variable, is a multivariate t-distribution (\rightarrow Proof II/4.3.8):

$$X, Y \sim \text{NG}(\mu, \Lambda, a, b) \Rightarrow X \sim t \left(\mu, \left(\frac{a}{b} \Lambda \right)^{-1}, 2a \right). \quad (15)$$

Thus, the marginal distribution (\rightarrow Definition I/1.5.3) of $\hat{\gamma}$ is:

$$\hat{\gamma} \sim t \left(C^T \beta, \left(\frac{n-p}{\hat{\varepsilon}^T \hat{\varepsilon}} Q \right)^{-1}, n-p \right). \quad (16)$$

4) Because of the following relationship between the multivariate t-distribution and the F-distribution (\rightarrow Proof II/4.2.3)

$$X \sim t(\mu, \Sigma, \nu) \Rightarrow (X - \mu)^T \Sigma^{-1} (X - \mu) / \nu \sim F(\nu, \nu), \quad (17)$$

the following quantity is, by definition, F-distributed (\rightarrow Definition II/3.8.1)

$$F = \left(\hat{\gamma} - C^T \hat{\beta} \right)^T \left(\frac{n-p}{\hat{\varepsilon}^T \hat{\varepsilon}} Q \right) \left(\hat{\gamma} - C^T \hat{\beta} \right) / q \quad (18)$$

and under the null hypothesis (\rightarrow Definition I/4.3.2) (6), it can be evaluated as:

$$\begin{aligned} F &\stackrel{(18)}{=} \left(\hat{\gamma} - C^T \hat{\beta} \right)^T \left(\frac{n-p}{\hat{\varepsilon}^T \hat{\varepsilon}} Q \right) \left(\hat{\gamma} - C^T \hat{\beta} \right) / q \\ &\stackrel{(6)}{=} \hat{\gamma}^T \left(\frac{n-p}{\hat{\varepsilon}^T \hat{\varepsilon}} Q \right) \hat{\gamma} / q \\ &\stackrel{(2)}{=} \hat{\beta}^T C \left(\frac{n-p}{\hat{\varepsilon}^T \hat{\varepsilon}} Q \right) C^T \hat{\beta} / q \\ &\stackrel{(9)}{=} \hat{\beta}^T C \left(\frac{n-p}{\hat{\varepsilon}^T \hat{\varepsilon}} (C^T (X^T V^{-1} X)^{-1} C)^{-1} \right) C^T \hat{\beta} / q \\ &\stackrel{(10)}{=} \hat{\beta}^T C \left(\frac{n-p}{(y - X \hat{\beta})^T V^{-1} (y - X \hat{\beta})} (C^T (X^T V^{-1} X)^{-1} C)^{-1} \right) C^T \hat{\beta} / q \\ &\stackrel{(4)}{=} \hat{\beta}^T C \left(\frac{1}{\hat{\sigma}^2} (C^T (X^T V^{-1} X)^{-1} C)^{-1} \right) C^T \hat{\beta} / q \\ &= \hat{\beta}^T C (\hat{\sigma}^2 C^T (X^T V^{-1} X)^{-1} C)^{-1} C^T \hat{\beta} / q. \end{aligned} \quad (19)$$

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>.

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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>.
- Penny, William (2006): “Comparing nested GLMs”; in: *Mathematics for Brain Imaging*, ch. 2.3, pp. 51-52, eq. 2.9; URL: https://ueapsylabs.co.uk/sites/wpenny/mbi/mbi_course.pdf.

Metadata: ID: P392 | shortcut: mlr-f | author: JoramSoch | date: 2022-12-13, 12:36.

1.5.25 Maximum likelihood estimation

Theorem: Given a linear regression model (\rightarrow Definition 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 Definition 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 Proof II/4.1.4), the linear regression equation (1) implies the following likelihood function (\rightarrow Definition 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 Definition 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

$$\begin{aligned}
\frac{dLL(\beta, \sigma^2)}{d\beta} &= \frac{d}{d\beta} \left(-\frac{1}{2\sigma^2} (y^T Py - 2\beta^T X^T Py + \beta^T X^T PX\beta) \right) \\
&= \frac{1}{2\sigma^2} \frac{d}{d\beta} (2\beta^T X^T Py - \beta^T X^T PX\beta) \\
&= \frac{1}{2\sigma^2} (2X^T Py - 2X^T PX\beta) \\
&= \frac{1}{\sigma^2} (X^T Py - X^T PX\beta)
\end{aligned} \tag{6}$$

and setting this derivative to zero gives the MLE for β :

$$\begin{aligned}
\frac{dLL(\hat{\beta}, \sigma^2)}{d\beta} &= 0 \\
0 &= \frac{1}{\sigma^2} (X^T Py - X^T PX\hat{\beta}) \\
0 &= X^T Py - X^T PX\hat{\beta} \\
X^T PX\hat{\beta} &= X^T Py \\
\hat{\beta} &= (X^T PX)^{-1} X^T Py
\end{aligned} \tag{7}$$

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.

Sources:

- original work

Metadata: ID: P78 | shortcut: mlr-mle | author: JoramSoch | date: 2020-03-11, 12:27.

1.5.26 Maximum log-likelihood

Theorem: Consider a linear regression model (\rightarrow Definition III/1.5.1) m with correlation structure (\rightarrow Definition I/1.11.5) V

$$m : y = X\beta + \varepsilon, \varepsilon \sim \mathcal{N}(0, \sigma^2 V) . \quad (1)$$

Then, the maximum log-likelihood (\rightarrow Definition I/4.1.5) 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 Definition 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 Definition III/1.5.7) and wRSS is the weighted residual sum of squares (\rightarrow Proof III/1.5.20).

Proof: The likelihood function (\rightarrow Definition I/5.1.2) for multiple linear regression is given by (\rightarrow Proof III/1.5.25)

$$\begin{aligned} p(y|\beta, \sigma^2) &= \mathcal{N}(y; X\beta, \sigma^2 V) \\ &= \sqrt{\frac{1}{(2\pi)^n |\sigma^2 V|}} \cdot \exp \left[-\frac{1}{2} (y - X\beta)^T (\sigma^2 V)^{-1} (y - X\beta) \right] , \end{aligned} \quad (4)$$

such that, with $|\sigma^2 V| = (\sigma^2)^n |V|$, the log-likelihood function (\rightarrow Definition I/4.1.2) for this model becomes (\rightarrow Proof III/1.5.25)

$$\begin{aligned} \text{LL}(\beta, \sigma^2) &= \log p(y|\beta, \sigma^2) \\ &= -\frac{n}{2} \log(2\pi) - \frac{n}{2} \log(\sigma^2) - \frac{1}{2} \log |V| - \frac{1}{2\sigma^2} (y - X\beta)^T V^{-1} (y - X\beta) . \end{aligned} \quad (5)$$

The maximum likelihood estimate for the noise variance (\rightarrow Proof III/1.5.25) 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 Definition III/1.5.7) 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 Definition I/4.1.5) as

$$\begin{aligned}
\text{MLL}(m) &= \text{LL}(\hat{\beta}, \hat{\sigma}^2) \\
&= -\frac{n}{2} \log(2\pi) - \frac{n}{2} \log(\hat{\sigma}^2) - \frac{1}{2} \log |V| - \frac{1}{2\hat{\sigma}^2} (y - X\hat{\beta})^T V^{-1} (y - X\hat{\beta}) \\
&= -\frac{n}{2} \log(2\pi) - \frac{n}{2} \log \left(\frac{\text{wRSS}}{n} \right) - \frac{1}{2} \log |V| - \frac{1}{2} \cdot \frac{n}{\text{wRSS}} \cdot \text{wRSS} \\
&= -\frac{n}{2} \log \left(\frac{\text{wRSS}}{n} \right) - \frac{n}{2} [1 + \log(2\pi)] - \frac{1}{2} \log |V|
\end{aligned} \tag{8}$$

which proves the result in (3). Assuming $V = I_n$, we have

$$\hat{\sigma}^2 = \frac{1}{n} (y - X\hat{\beta})^T (y - X\hat{\beta}) = \frac{1}{n} \sum_{i=1}^n \hat{\varepsilon}_i^2 = \frac{\text{RSS}}{n} \tag{9}$$

and

$$\frac{1}{2} \log |V| = \frac{1}{2} \log |I_n| = \frac{1}{2} \log 1 = 0, \tag{10}$$

such that

$$\text{MLL}(m) = -\frac{n}{2} \log \left(\frac{\text{RSS}}{n} \right) - \frac{n}{2} [1 + \log(2\pi)] \tag{11}$$

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.

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1.5.27 Deviance function

Theorem: Consider a linear regression model (\rightarrow Definition III/1.5.1) m with correlation structure (\rightarrow Definition I/1.11.5) V

$$m : y = X\beta + \varepsilon, \varepsilon \sim \mathcal{N}(0, \sigma^2 V). \tag{1}$$

Then, the deviance (\rightarrow Definition 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 Definition 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 Definition III/1.5.7) and wRSS is the weighted residual sum of squares (\rightarrow Proof III/1.5.20).

Proof: The likelihood function (\rightarrow Definition I/5.1.2) for multiple linear regression is given by (\rightarrow Proof III/1.5.25)

$$\begin{aligned} p(y|\beta, \sigma^2) &= \mathcal{N}(y; X\beta, \sigma^2 V) \\ &= \sqrt{\frac{1}{(2\pi)^n |\sigma^2 V|}} \cdot \exp \left[-\frac{1}{2} (y - X\beta)^T (\sigma^2 V)^{-1} (y - X\beta) \right], \end{aligned} \quad (4)$$

such that, with $|\sigma^2 V| = (\sigma^2)^n |V|$, the log-likelihood function (\rightarrow Definition I/4.1.2) for this model becomes (\rightarrow Proof III/1.5.25)

$$\begin{aligned} \text{LL}(\beta, \sigma^2) &= \log p(y|\beta, \sigma^2) \\ &= -\frac{n}{2} \log(2\pi) - \frac{n}{2} \log(\sigma^2) - \frac{1}{2} \log |V| - \frac{1}{2\sigma^2} (y - X\beta)^T V^{-1} (y - X\beta). \end{aligned} \quad (5)$$

The last term can be expressed in terms of the (weighted) residual sum of squares (\rightarrow Definition III/1.5.7) as

$$\begin{aligned} -\frac{1}{2\sigma^2} (y - X\beta)^T V^{-1} (y - X\beta) &= -\frac{1}{2\sigma^2} (Wy - WX\beta)^T (Wy - WX\beta) \\ &= -\frac{1}{2\sigma^2} \left(\frac{1}{n} \sum_{i=1}^n (W\varepsilon_i)^2 \right) = -\frac{\text{wRSS}}{2\sigma^2} \end{aligned} \quad (6)$$

where $W = V^{-1/2}$. Plugging (6) into (5) and multiplying with -2 , we obtain the deviance (\rightarrow Definition IV/2.3.2) as

$$\begin{aligned} D(\beta, \sigma^2) &= -2 \text{LL}(\beta, \sigma^2) \\ &= -2 \left(-\frac{\text{wRSS}}{2\sigma^2} - \frac{n}{2} \log(\sigma^2) - \frac{n}{2} \log(2\pi) - \frac{1}{2} \log |V| \right) \\ &= \text{wRSS}/\sigma^2 + n \cdot [\log(\sigma^2) + \log(2\pi)] + \log |V| \end{aligned} \quad (7)$$

which proves the result in (3). Assuming $V = I_n$, we have

$$\begin{aligned} -\frac{1}{2\sigma^2} (y - X\beta)^T V^{-1} (y - X\beta) &= -\frac{1}{2\sigma^2} (y - X\beta)^T (y - X\beta) \\ &= -\frac{1}{2\sigma^2} \left(\frac{1}{n} \sum_{i=1}^n \varepsilon_i^2 \right) = -\frac{\text{RSS}}{2\sigma^2} \end{aligned} \quad (8)$$

and

$$\frac{1}{2} \log |V| = \frac{1}{2} \log |I_n| = \frac{1}{2} \log 1 = 0, \quad (9)$$

such that

$$D(\beta, \sigma^2) = \text{RSS}/\sigma^2 + n \cdot [\log(\sigma^2) + \log(2\pi)] \quad (10)$$

which proves the result in (2). This completes the proof.

Sources:

- original work

Metadata: ID: P312 | shortcut: mlr-dev | author: JoramSoch | date: 2022-03-01, 08:42.

1.5.28 Akaike information criterion

Theorem: Consider a linear regression model (\rightarrow Definition 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 Definition 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 Definition III/1.5.7), p is the number of regressors (\rightarrow Definition III/1.5.1) in the design matrix X and n is the number of observations (\rightarrow Definition III/1.5.1) in the data vector y .

Proof: The Akaike information criterion (\rightarrow Definition 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 Definition I/4.1.5) is k is the number of free parameters in m .

The maximum log-likelihood for multiple linear regression (\rightarrow Proof III/1.5.26) 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 Definition III/1.5.1) is $k = p + 1$, i.e. one for each regressor in the design matrix (\rightarrow Definition III/1.5.1) X , plus one for the noise variance (\rightarrow Definition 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.

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1.5.29 Bayesian information criterion

Theorem: Consider a linear regression model (\rightarrow Definition 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 Definition 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 Definition III/1.5.7), p is the number of regressors (\rightarrow Definition III/1.5.1) in the design matrix X and n is the number of observations (\rightarrow Definition III/1.5.1) in the data vector y .

Proof: The Bayesian information criterion (\rightarrow Definition 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 Definition I/4.1.5), 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 Proof III/1.5.26) 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 Definition III/1.5.1) is $k = p + 1$, i.e. one for each regressor in the design matrix (\rightarrow Definition III/1.5.1) X , plus one for the noise variance (\rightarrow Definition III/1.5.1) σ^2 .

Thus, the BIC of m follows from (3) and (4) as

$$\text{BIC}(m) = n \log \left(\frac{\text{wRSS}}{n} \right) + n [1 + \log(2\pi)] + \log |V| + \log(n) (p + 1) . \quad (5)$$

Sources:

- original work

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1.5.30 Corrected Akaike information criterion

Theorem: Consider a linear regression model (\rightarrow Definition 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 Definition 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 Definition III/1.5.7), p is the number of regressors (\rightarrow Definition III/1.5.1) in the design matrix X and n is the number of observations (\rightarrow Definition III/1.5.1) in the data vector y .

Proof: The corrected Akaike information criterion (\rightarrow Definition IV/2.1.2) is defined as

$$\text{AIC}_c(m) = \text{AIC}(m) + \frac{2k^2 + 2k}{n - k - 1} \quad (3)$$

where $AIC(m)$ is the Akaike information criterion (\rightarrow Definition 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 Proof III/1.5.26) is given by

$$AIC(m) = n \log \left(\frac{wRSS}{n} \right) + n [1 + \log(2\pi)] + \log |V| + 2(p+1) \quad (4)$$

and the number of free paramters in multiple linear regression (\rightarrow Definition III/1.5.1) is $k = p + 1$, i.e. one for each regressor in the design matrix (\rightarrow Definition III/1.5.1) X , plus one for the noise variance (\rightarrow Definition III/1.5.1) σ^2 .

Thus, the corrected AIC of m follows from (3) and (4) as

$$\begin{aligned} AIC_c(m) &= n \log \left(\frac{wRSS}{n} \right) + n [1 + \log(2\pi)] + \log |V| + 2k + \frac{2k^2 + 2k}{n - k - 1} \\ &= n \log \left(\frac{wRSS}{n} \right) + n [1 + \log(2\pi)] + \log |V| + \frac{2nk - 2k^2 - 2k}{n - k - 1} + \frac{2k^2 + 2k}{n - k - 1} \\ &= n \log \left(\frac{wRSS}{n} \right) + n [1 + \log(2\pi)] + \log |V| + \frac{2nk}{n - k - 1} \\ &= n \log \left(\frac{wRSS}{n} \right) + n [1 + \log(2\pi)] + \log |V| + \frac{2n(p+1)}{n - p - 2} \end{aligned} \quad (5)$$

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.

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1.6 Bayesian linear regression

1.6.1 Conjugate prior distribution

Theorem: Let

$$y = X\beta + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 V) \quad (1)$$

be a linear regression model (\rightarrow Definition III/1.5.1) with measured $n \times 1$ 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 Definition I/5.2.5) for this model is a normal-gamma distribution (\rightarrow Definition II/4.3.1)

$$p(\beta, \tau) = \mathcal{N}(\beta; \mu_0, (\tau \Lambda_0)^{-1}) \cdot \text{Gam}(\tau; a_0, b_0) \quad (2)$$

where $\tau = 1/\sigma^2$ is the inverse noise variance or noise precision.

Proof: By definition, a conjugate prior (\rightarrow Definition I/5.2.5) is a prior distribution (\rightarrow Definition I/5.1.3) that, when combined with the likelihood function (\rightarrow Definition I/5.1.2), leads to a posterior distribution (\rightarrow Definition I/5.1.7) that belongs to the same family of probability distributions (\rightarrow Definition 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 Definition I/5.1.2)

$$p(y|\beta, \sigma^2) = \mathcal{N}(y; X\beta, \sigma^2 V) = \sqrt{\frac{1}{(2\pi)^n |\sigma^2 V|}} \exp \left[-\frac{1}{2\sigma^2} (y - X\beta)^T V^{-1} (y - X\beta) \right] \quad (3)$$

which, for mathematical convenience, can also be parametrized as

$$p(y|\beta, \tau) = \mathcal{N}(y; X\beta, (\tau P)^{-1}) = \sqrt{\frac{|\tau P|}{(2\pi)^n}} \exp \left[-\frac{\tau}{2} (y - X\beta)^T P (y - X\beta) \right] \quad (4)$$

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 Definition 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 Definition II/4.3.1) 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 Proof II/4.3.3)

$$p(\beta, \tau) = \sqrt{\frac{|\tau \Lambda_0|}{(2\pi)^p}} \exp \left[-\frac{\tau}{2} (\beta - \mu_0)^T \Lambda_0 (\beta - \mu_0) \right] \cdot \frac{b_0^{a_0}}{\Gamma(a_0)} \tau^{a_0-1} \exp[-b_0 \tau] \quad (10)$$

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>.

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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 Definition III/1.5.1) with measured $n \times 1$ 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 Proof 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 Definition I/5.1.7) is also a normal-gamma distribution (\rightarrow Definition II/4.3.1)

$$p(\beta, \tau|y) = \mathcal{N}(\beta; \mu_n, (\tau \Lambda_n)^{-1}) \cdot \text{Gam}(\tau; a_n, b_n) \quad (3)$$

and the posterior hyperparameters (\rightarrow Definition I/5.1.7) 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 Proof I/5.3.1), the posterior distribution (\rightarrow Definition I/5.1.7) 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 Proof I/5.1.8) 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 Definition 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 Definition I/1.10.19) $P = V^{-1}$.

Combining the likelihood function (\rightarrow Definition I/5.1.2) (8) with the prior distribution (\rightarrow Definition I/5.1.3) (2), the joint likelihood (\rightarrow Definition I/5.1.5) of the model is given by

$$\begin{aligned} p(y, \beta, \tau) &= p(y|\beta, \tau) p(\beta, \tau) \\ &= \sqrt{\frac{|\tau P|}{(2\pi)^n}} \exp \left[-\frac{\tau}{2} (y - X\beta)^T P (y - X\beta) \right] \cdot \\ &\quad \sqrt{\frac{|\tau \Lambda_0|}{(2\pi)^p}} \exp \left[-\frac{\tau}{2} (\beta - \mu_0)^T \Lambda_0 (\beta - \mu_0) \right] \cdot \\ &\quad \frac{b_0^{a_0}}{\Gamma(a_0)} \tau^{a_0-1} \exp[-b_0 \tau] . \end{aligned} \quad (9)$$

Collecting identical variables gives:

$$\begin{aligned} p(y, \beta, \tau) &= \sqrt{\frac{\tau^{n+p}}{(2\pi)^{n+p}} |P| |\Lambda_0|} \frac{b_0^{a_0}}{\Gamma(a_0)} \tau^{a_0-1} \exp[-b_0 \tau] \cdot \\ &\quad \exp \left[-\frac{\tau}{2} ((y - X\beta)^T P (y - X\beta) + (\beta - \mu_0)^T \Lambda_0 (\beta - \mu_0)) \right] . \end{aligned} \quad (10)$$

Expanding the products in the exponent gives:

$$\begin{aligned} p(y, \beta, \tau) &= \sqrt{\frac{\tau^{n+p}}{(2\pi)^{n+p}} |P| |\Lambda_0|} \frac{b_0^{a_0}}{\Gamma(a_0)} \tau^{a_0-1} \exp[-b_0 \tau] \cdot \\ &\quad \exp \left[-\frac{\tau}{2} (y^T P y - y^T P X \beta - \beta^T X^T P y + \beta^T X^T P X \beta + \right. \\ &\quad \left. \beta^T \Lambda_0 \beta - \beta^T \Lambda_0 \mu_0 - \mu_0^T \Lambda_0 \beta + \mu_0^T \Lambda_0 \mu_0) \right] . \end{aligned} \quad (11)$$

Completing the square over β , we finally have

$$\begin{aligned} p(y, \beta, \tau) &= \sqrt{\frac{\tau^{n+p}}{(2\pi)^{n+p}} |P| |\Lambda_0|} \frac{b_0^{a_0}}{\Gamma(a_0)} \tau^{a_0-1} \exp[-b_0 \tau] \cdot \\ &\quad \exp \left[-\frac{\tau}{2} ((\beta - \mu_n)^T \Lambda_n (\beta - \mu_n) + (y^T P y + \mu_0^T \Lambda_0 \mu_0 - \mu_n^T \Lambda_n \mu_n)) \right] \end{aligned} \quad (12)$$

with the posterior hyperparameters (\rightarrow Definition I/5.1.7)

$$\begin{aligned}\mu_n &= \Lambda_n^{-1}(X^T P y + \Lambda_0 \mu_0) \\ \Lambda_n &= X^T P X + \Lambda_0 .\end{aligned}\tag{13}$$

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 Definition I/5.1.7)

$$\begin{aligned}a_n &= a_0 + \frac{n}{2} \\ b_n &= b_0 + \frac{1}{2} (y^T P y + \mu_0^T \Lambda_0 \mu_0 - \mu_n^T \Lambda_n \mu_n) .\end{aligned}\tag{15}$$

From the term in (14), we can isolate the posterior distribution over β given τ :

$$p(\beta|\tau, y) = \mathcal{N}(\beta; \mu_n, (\tau \Lambda_n)^{-1}) . \tag{16}$$

From the remaining term, we can isolate the posterior distribution over τ :

$$p(\tau|y) = \text{Gam}(\tau; a_n, b_n) . \tag{17}$$

Together, (16) and (17) constitute the joint (\rightarrow Definition I/1.3.2) posterior distribution (\rightarrow Definition I/5.1.7) 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>.

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1.6.3 Log model evidence

Theorem: Let

$$m : y = X\beta + \varepsilon, \varepsilon \sim \mathcal{N}(0, \sigma^2 V) \tag{1}$$

be a linear regression model (\rightarrow Definition III/1.5.1) with measured $n \times 1$ 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 Proof III/1.6.1) over the model parameters β and $\tau = 1/\sigma^2$:

$$p(\beta, \tau) = \mathcal{N}(\beta; \mu_0, (\tau \Lambda_0)^{-1}) \cdot \text{Gam}(\tau; a_0, b_0) . \tag{2}$$

Then, the log model evidence (\rightarrow Definition IV/3.1.3) for this model is

$$\begin{aligned}\log p(y|m) &= \frac{1}{2} \log |P| - \frac{n}{2} \log(2\pi) + \frac{1}{2} \log |\Lambda_0| - \frac{1}{2} \log |\Lambda_n| + \\ &\quad \log \Gamma(a_n) - \log \Gamma(a_0) + a_0 \log b_0 - a_n \log b_n\end{aligned}\tag{3}$$

where the posterior hyperparameters (\rightarrow Definition I/5.1.7) are given by

$$\begin{aligned}\mu_n &= \Lambda_n^{-1}(X^T P y + \Lambda_0 \mu_0) \\ \Lambda_n &= X^T P X + \Lambda_0 \\ a_n &= a_0 + \frac{n}{2} \\ b_n &= b_0 + \frac{1}{2}(y^T P y + \mu_0^T \Lambda_0 \mu_0 - \mu_n^T \Lambda_n \mu_n) .\end{aligned}\tag{4}$$

Proof: According to the law of marginal probability (\rightarrow Definition I/1.3.3), the model evidence (\rightarrow Definition I/5.1.9) for this model is:

$$p(y|m) = \iint p(y|\beta, \tau) p(\beta, \tau) d\beta d\tau .\tag{5}$$

According to the law of conditional probability (\rightarrow Definition I/1.3.4), the integrand is equivalent to the joint likelihood (\rightarrow Definition I/5.1.5):

$$p(y|m) = \iint p(y, \beta, \tau) d\beta d\tau .\tag{6}$$

Equation (1) implies the following likelihood function (\rightarrow Definition I/5.1.2)

$$p(y|\beta, \sigma^2) = \mathcal{N}(y; X\beta, \sigma^2 V) = \sqrt{\frac{1}{(2\pi)^n |\sigma^2 V|}} \exp \left[-\frac{1}{2\sigma^2} (y - X\beta)^T V^{-1} (y - X\beta) \right]\tag{7}$$

which, for mathematical convenience, can also be parametrized as

$$p(y|\beta, \tau) = \mathcal{N}(y; X\beta, (\tau P)^{-1}) = \sqrt{\frac{|\tau P|}{(2\pi)^n}} \exp \left[-\frac{\tau}{2} (y - X\beta)^T P (y - X\beta) \right]\tag{8}$$

using the noise precision $\tau = 1/\sigma^2$ and the $n \times n$ precision matrix $P = V^{-1}$.

When deriving the posterior distribution (\rightarrow Proof III/1.6.2) $p(\beta, \tau|y)$, the joint likelihood $p(y, \beta, \tau)$ is obtained as

$$\begin{aligned}p(y, \beta, \tau) &= \sqrt{\frac{\tau^n |P|}{(2\pi)^n}} \sqrt{\frac{\tau^p |\Lambda_0|}{(2\pi)^p}} \frac{b_0^{a_0}}{\Gamma(a_0)} \tau^{a_0-1} \exp[-b_0 \tau] \cdot \\ &\exp \left[-\frac{\tau}{2} ((\beta - \mu_n)^T \Lambda_n (\beta - \mu_n) + (y^T P y + \mu_0^T \Lambda_0 \mu_0 - \mu_n^T \Lambda_n \mu_n)) \right] .\end{aligned}\tag{9}$$

Using the probability density function of the multivariate normal distribution (\rightarrow Proof II/4.1.4), we can rewrite this as

$$\begin{aligned}p(y, \beta, \tau) &= \sqrt{\frac{\tau^n |P|}{(2\pi)^n}} \sqrt{\frac{\tau^p |\Lambda_0|}{(2\pi)^p}} \sqrt{\frac{(2\pi)^p}{\tau^p |\Lambda_n|}} \frac{b_0^{a_0}}{\Gamma(a_0)} \tau^{a_0-1} \exp[-b_0 \tau] \cdot \\ &\mathcal{N}(\beta; \mu_n, (\tau \Lambda_n)^{-1}) \exp \left[-\frac{\tau}{2} (y^T P y + \mu_0^T \Lambda_0 \mu_0 - \mu_n^T \Lambda_n \mu_n) \right] .\end{aligned}\tag{10}$$

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 Proof II/3.4.6), 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 Definition 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:

- Bishop CM (2006): “Bayesian linear regression”; in: *Pattern Recognition for Machine Learning*, pp. 152-161, ex. 3.23, eq. 3.118; URL: <https://www.springer.com/gp/book/9780387310732>.

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1.6.4 Deviance information criterion

Theorem: Consider a linear regression model (\rightarrow Definition 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 Proof 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 Definition 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 Definition I/5.1.7) describing the posterior distribution in Bayesian linear regression (\rightarrow Proof III/1.6.2).

Proof: The deviance for multiple linear regression (\rightarrow Proof III/1.5.27) 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 Definition 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 Definition “mlr-mll”) at the posterior expectations (\rightarrow Definition I/1.7.1) and the “effective number of parameters” p_D is the difference between the expectation of the deviance and the deviance at the expectation (\rightarrow Definition 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 Proof 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 Definition I/5.1.7) are given by

$$\begin{aligned} \mu_n &= \Lambda_n^{-1} (X^T P y + \Lambda_0 \mu_0) \\ \Lambda_n &= X^T P X + \Lambda_0 \\ a_n &= a_0 + \frac{n}{2} \\ b_n &= b_0 + \frac{1}{2} (y^T P y + \mu_0^T \Lambda_0 \mu_0 - \mu_n^T \Lambda_n \mu_n) . \end{aligned} \quad (10)$$

Thus, we have the following posterior expectations:

$$\langle \beta \rangle_{\beta, \tau | y} = \mu_n \quad (11)$$

$$\langle \tau \rangle_{\beta, \tau | y} = \frac{a_n}{b_n} \quad (12)$$

$$\langle \log \tau \rangle_{\beta, \tau | y} = \psi(a_n) - \log(b_n) \quad (13)$$

$$\begin{aligned} \langle \beta^T A \beta \rangle_{\beta | \tau, y} &= \mu_n^T A \mu_n + \text{tr} (A (\tau \Lambda_n)^{-1}) \\ &= \mu_n^T A \mu_n + \frac{1}{\tau} \text{tr} (A \Lambda_n^{-1}) . \end{aligned} \quad (14)$$

In these identities, we have used the mean of the multivariate normal distribution (\rightarrow Proof II/4.1.5), the mean of the gamma distribution (\rightarrow Proof II/3.4.9), the logarithmic expectation of the gamma distribution (\rightarrow Proof II/3.4.11), the expectation of a quadratic form (\rightarrow Proof I/1.7.9) and the covariance of the multivariate normal distribution (\rightarrow Proof II/4.1.6).

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:

$$\begin{aligned}
 \langle D(\beta, \tau) \rangle &\stackrel{(5)}{=} \langle n \cdot \log(2\pi) - n \cdot \log(\tau) - \log |P| + \tau \cdot (y - X \beta)^T P (y - X \beta) \rangle \\
 &= n \cdot \log(2\pi) - n \cdot \langle \log(\tau) \rangle - \log |P| + \langle \tau \cdot (y - X \beta)^T P (y - X \beta) \rangle \\
 &\stackrel{(13)}{=} n \cdot \log(2\pi) - n \cdot [\psi(a_n) - \log(b_n)] - \log |P| \\
 &\quad + \left\langle \tau \cdot \langle (y - X \beta)^T P (y - X \beta) \rangle_{\beta|\tau, y} \right\rangle_{\tau|y} \\
 &= n \cdot \log(2\pi) - n \cdot [\psi(a_n) - \log(b_n)] - \log |P| \\
 &\quad + \left\langle \tau \cdot \langle y^T P y - y^T P X \beta - \beta^T X^T P y + \beta^T X^T P X \beta \rangle_{\beta|\tau, y} \right\rangle_{\tau|y} \\
 &\stackrel{(14)}{=} n \cdot \log(2\pi) - n \cdot [\psi(a_n) - \log(b_n)] - \log |P| \\
 &\quad + \left\langle \tau \cdot \left[y^T P y - y^T P X \mu_n - \mu_n^T X^T P y + \mu_n^T X^T P X \mu_n + \frac{1}{\tau} \text{tr} (X^T P X \Lambda_n^{-1}) \right] \right\rangle_{\tau|y} \\
 &= n \cdot \log(2\pi) - n \cdot [\psi(a_n) - \log(b_n)] - \log |P| \\
 &\quad + \langle \tau \cdot (y - X \mu_n)^T P (y - X \mu_n) \rangle_{\tau|y} + \text{tr} (X^T P X \Lambda_n^{-1}) \\
 &\stackrel{(12)}{=} n \cdot \log(2\pi) - n \cdot [\psi(a_n) - \log(b_n)] - \log |P| \\
 &\quad + \frac{a_n}{b_n} \cdot (y - X \mu_n)^T P (y - X \mu_n) + \text{tr} (X^T P X \Lambda_n^{-1}) .
 \end{aligned} \tag{16}$$

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).

Sources:

- original work

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1.6.5 Posterior probability of alternative hypothesis

Theorem: Let there be a linear regression model (\rightarrow Definition III/1.5.1) with normally distributed (\rightarrow Definition 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 Definition II/4.3.1) prior distribution (\rightarrow Definition 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 Definition I/5.1.7) probability (\rightarrow Definition I/1.3.1) of the alternative hypothesis (\rightarrow Definition 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 Definition “con”), $T(x; \nu)$ is the cumulative distribution function (\rightarrow Definition I/1.6.13) of the t-distribution (\rightarrow Definition II/3.3.1) with ν degrees of freedom (\rightarrow Definition “dof”) and μ , Σ and ν can be obtained from the posterior hyperparameters (\rightarrow Definition I/5.1.7) of Bayesian linear regression.

Proof: The posterior distribution for Bayesian linear regression (\rightarrow Proof III/1.6.2) is given by a normal-gamma distribution (\rightarrow Definition II/4.3.1) 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 Definition I/5.1.7)

$$\begin{aligned} \mu_n &= \Lambda_n^{-1}(X^T P y + \Lambda_0 \mu_0) \\ \Lambda_n &= X^T P X + \Lambda_0 \\ a_n &= a_0 + \frac{n}{2} \\ b_n &= b_0 + \frac{1}{2}(y^T P y + \mu_0^T \Lambda_0 \mu_0 - \mu_n^T \Lambda_n \mu_n) . \end{aligned} \quad (6)$$

The marginal distribution of a normal-gamma distribution is a multivariate t-distribution (\rightarrow Proof II/4.3.8), such that the marginal (\rightarrow Definition I/1.5.3) posterior (\rightarrow Definition I/5.1.7) distribution of β is

$$p(\beta|y) = t(\beta; \mu, \Sigma, \nu) \quad (7)$$

with the posterior hyperparameters (\rightarrow Definition I/5.1.7)

$$\begin{aligned} \mu &= \mu_n \\ \Sigma &= \left(\frac{a_n}{b_n} \Lambda_n \right)^{-1} \\ \nu &= 2 a_n . \end{aligned} \quad (8)$$

Define the quantity $\gamma = c^T \beta$. According to the linear transformation theorem for the multivariate t-distribution (\rightarrow Proof “mvt-ltt”), γ also follows a multivariate t-distribution (\rightarrow Definition II/4.2.1):

$$p(\gamma|y) = t(\gamma; c^T \mu, c^T \Sigma c, \nu) . \quad (9)$$

Because c^T is a $1 \times p$ vector, γ is a scalar and actually has a non-standardized t-distribution (\rightarrow Definition II/3.3.2). 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 Proof II/3.3.3), 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.

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1.6.6 Posterior credibility region excluding null hypothesis

Theorem: Let there be a linear regression model (\rightarrow Definition III/1.5.1) with normally distributed (\rightarrow Definition 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 Definition II/4.3.1) prior distribution (\rightarrow Definition 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 Definition I/5.1.7) credibility region (\rightarrow Definition “cr”) that does not contain the omnibus null hypothesis (\rightarrow Definition I/4.3.2)

$$H_0 : C^T\beta = 0 \tag{3}$$

is given by the credibility level (\rightarrow Definition “cr”)

$$(1 - \alpha) = F([\mu^T C (C^T \Sigma C)^{-1} C^T \mu] / q; q, \nu) \tag{4}$$

where C is a $p \times q$ contrast matrix (\rightarrow Definition “con”), $F(x; v, w)$ is the cumulative distribution function (\rightarrow Definition I/1.6.13) of the F-distribution (\rightarrow Definition II/3.8.1) with v numerator degrees of freedom (\rightarrow Definition “dof”), w denominator degrees of freedom (\rightarrow Definition “dof”) and μ, Σ and ν can be obtained from the posterior hyperparameters (\rightarrow Definition I/5.1.7) of Bayesian linear regression.

Proof: The posterior distribution for Bayesian linear regression (\rightarrow Proof III/1.6.2) is given by a normal-gamma distribution (\rightarrow Definition II/4.3.1) 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 Definition I/5.1.7)

$$\begin{aligned}
\mu_n &= \Lambda_n^{-1}(X^T P y + \Lambda_0 \mu_0) \\
\Lambda_n &= X^T P X + \Lambda_0 \\
a_n &= a_0 + \frac{n}{2} \\
b_n &= b_0 + \frac{1}{2}(y^T P y + \mu_0^T \Lambda_0 \mu_0 - \mu_n^T \Lambda_n \mu_n) .
\end{aligned} \tag{6}$$

The marginal distribution of a normal-gamma distribution is a multivariate t-distribution (\rightarrow Proof II/4.3.8), such that the marginal (\rightarrow Definition I/1.5.3) posterior (\rightarrow Definition I/5.1.7) distribution of β is

$$p(\beta|y) = t(\beta; \mu, \Sigma, \nu) \tag{7}$$

with the posterior hyperparameters (\rightarrow Definition I/5.1.7)

$$\begin{aligned}
\mu &= \mu_n \\
\Sigma &= \left(\frac{a_n}{b_n} \Lambda_n \right)^{-1} \\
\nu &= 2 a_n .
\end{aligned} \tag{8}$$

Define the quantity $\gamma = C^T \beta$. According to the linear transformation theorem for the multivariate t-distribution (\rightarrow Proof “mvt-ltt”), γ also follows a multivariate t-distribution (\rightarrow Definition II/4.2.1):

$$p(\gamma|y) = t(\gamma; C^T \mu, C^T \Sigma C, \nu) . \tag{9}$$

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 Proof II/4.2.3), such that we can write:

$$\text{QF}(\gamma) = (\gamma - C^T \mu)^T (C^T \Sigma C)^{-1} (\gamma - C^T \mu) / q \sim F(q, \nu) . \tag{10}$$

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:

$$\begin{aligned}
(1 - \alpha) &= F(\text{QF}(0); q, \nu) \\
&= F([\mu^T C (C^T \Sigma C)^{-1} C^T \mu] / q; q, \nu) .
\end{aligned} \tag{11}$$

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, 2.211, 2.183; URL: <https://www.springer.com/de/book/9783540727231>; DOI: 10.1007/978-3-540-72726-2.

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2 Multivariate normal data

2.1 General linear model

2.1.1 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 Definition 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 (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.

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.

Metadata: ID: D40 | shortcut: glm | author: JoramSoch | date: 2020-03-21, 22:24.

2.1.2 Ordinary least squares

Theorem: Given a general linear model (\rightarrow Definition III/2.1.1) with independent observations

$$Y = XB + E, \quad E \sim \mathcal{MN}(0, \sigma^2 I_n, \Sigma) , \quad (1)$$

the ordinary least squares (\rightarrow Proof 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 Proof 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 Definition I/1.7.1) 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:

- original work

Metadata: ID: P106 | shortcut: glm-ols | author: JoramSoch | date: 2020-05-19, 06:02.

2.1.3 Weighted least squares

Theorem: Given a general linear model (\rightarrow Definition III/2.1.1) with correlated observations

$$Y = XB + E, \quad E \sim \mathcal{MN}(0, V, \Sigma) , \quad (1)$$

the weighted least squares (\rightarrow Proof III/1.5.19) 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, W is also symmetric and can be expressed as the matrix square root of the inverse of V :

$$WW = V^{-1} \quad \Leftrightarrow \quad W = V^{-1/2} . \quad (4)$$

Left-multiplying the linear regression equation (1) with W , the linear transformation theorem (\rightarrow Proof 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 Definition III/2.1.1) 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 Proof III/2.1.2) 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).

Sources:

- original work

Metadata: ID: P107 | shortcut: glm-wls | author: JoramSoch | date: 2020-05-19, 06:27.

2.1.4 Maximum likelihood estimation

Theorem: Given a general linear model (\rightarrow Definition III/2.1.1) with matrix-normally distributed (\rightarrow Definition II/5.1.1) errors

$$Y = XB + E, \quad E \sim \mathcal{MN}(0, V, \Sigma), \quad (1)$$

maximum likelihood estimates (\rightarrow Definition 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 Definition I/5.1.2)

$$\begin{aligned} p(Y|B, \Sigma) &= \mathcal{MN}(Y; XB, V, \Sigma) \\ &= \sqrt{\frac{1}{(2\pi)^{nv} |\Sigma|^n |V|^v}} \cdot \exp \left[-\frac{1}{2} \text{tr} (\Sigma^{-1} (Y - XB)^T V^{-1} (Y - XB)) \right] \end{aligned} \quad (3)$$

and the log-likelihood function (\rightarrow Definition 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

$$\begin{aligned}
\frac{d\text{LL}(B, \Sigma)}{dB} &= \frac{d}{dB} \left(-\frac{1}{2} \text{tr} [\Sigma^{-1} (Y^T P Y - Y^T P X B - B^T X^T P Y + B^T X^T P X B)] \right) \\
&= \frac{d}{dB} \left(-\frac{1}{2} \text{tr} [-2\Sigma^{-1} Y^T P X B] \right) + \frac{d}{dB} \left(-\frac{1}{2} \text{tr} [\Sigma^{-1} B^T X^T P X B] \right) \\
&= -\frac{1}{2} (-2X^T P Y \Sigma^{-1}) - \frac{1}{2} (X^T P X B \Sigma^{-1} + (X^T P X)^T B (\Sigma^{-1})^T) \\
&= X^T P Y \Sigma^{-1} - X^T P X B \Sigma^{-1}
\end{aligned} \tag{6}$$

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:

- original work

Metadata: ID: P7 | shortcut: glm-mle | author: JoramSoch | date: 2019-12-06, 10:40.

2.2 Transformed general linear model

2.2.1 Definition

Definition: Let there be two general linear models (\rightarrow Definition III/2.1.1) of measured data $Y \in \mathbb{R}^{n \times v}$ using design matrices (\rightarrow Definition III/2.1.1) $X \in \mathbb{R}^{n \times p}$ and $X_t \in \mathbb{R}^{n \times t}$

$$Y = XB + E, \quad E \sim \mathcal{MN}(0, V, \Sigma) \tag{1}$$

$$Y = X_t \Gamma + E_t, \quad E_t \sim \mathcal{MN}(0, V, \Sigma_t) \tag{2}$$

and assume that X_t can be transformed into X using a transformation matrix $T \in \mathbb{R}^{t \times p}$

$$X = X_t T \tag{3}$$

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 Definition III/2.1.1) 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.

Metadata: ID: D160 | shortcut: tglm | author: JoramSoch | date: 2021-10-21, 14:43.

2.2.2 Derivation of the distribution

Theorem: Let there be two general linear models (\rightarrow Definition III/2.1.1) 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 Definition III/2.2.1) is given by

$$\hat{\Gamma} = TB + H, \quad H \sim \mathcal{MN}(0, U, \Sigma) \quad (4)$$

where the covariance across rows (\rightarrow Definition 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 Proof II/5.1.9) states:

$$X \sim \mathcal{MN}(M, U, V) \quad \Rightarrow \quad Y = AXB + C \sim \mathcal{MN}(AMB + C, AU A^T, B^T V B). \quad (5)$$

The weighted least squares parameter estimates (\rightarrow Proof III/2.1.3) 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

$$\begin{aligned} \hat{\Gamma} &\sim \mathcal{MN} \left([(X_t^T V^{-1} X_t)^{-1} X_t^T V^{-1}] XB, [(X_t^T V^{-1} X_t)^{-1} X_t^T V^{-1}] V [V^{-1} X_t (X_t^T V^{-1} X_t)^{-1}], \Sigma \right) \\ &\sim \mathcal{MN} \left((X_t^T V^{-1} X_t)^{-1} X_t^T V^{-1} X_t TB, (X_t^T V^{-1} X_t)^{-1} X_t^T V^{-1} X_t (X_t^T V^{-1} X_t)^{-1}, \Sigma \right) \\ &\sim \mathcal{MN} (TB, (X_t^T V^{-1} X_t)^{-1}, \Sigma). \end{aligned} \quad (8)$$

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.

Metadata: ID: P265 | shortcut: tglm-dist | author: JoramSoch | date: 2021-10-21, 15:03.

2.2.3 Equivalence of parameter estimates

Theorem: Let there be a general linear model (\rightarrow Definition III/2.1.1)

$$Y = XB + E, \quad E \sim \mathcal{MN}(0, V, \Sigma) \quad (1)$$

and the transformed general linear model (\rightarrow Definition III/2.2.1)

$$\hat{\Gamma} = TB + H, \quad H \sim \mathcal{MN}(0, U, \Sigma) \quad (2)$$

which are linked to each other (\rightarrow Proof III/2.2.2) 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 Proof III/2.1.3) 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 Proof III/2.1.3) 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 Proof III/2.2.2) 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.

Metadata: ID: P266 | shortcut: tglm-para | author: JoramSoch | date: 2021-10-21, 15:25.

2.3 Inverse general linear model

2.3.1 Definition

Definition: Let there be a general linear model (\rightarrow Definition III/2.1.1) of measured data $Y \in \mathbb{R}^{n \times v}$ in terms of the design matrix (\rightarrow Definition III/2.1.1) $X \in \mathbb{R}^{n \times p}$:

$$Y = XB + E, \quad E \sim \mathcal{MN}(0, V, \Sigma) . \quad (1)$$

Then, a linear model (\rightarrow Definition III/2.1.1) 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.

Metadata: ID: D161 | shortcut: iglm | author: JoramSoch | date: 2021-10-21, 15:31.

2.3.2 Derivation of the distribution

Theorem: Let there be a general linear model (\rightarrow Definition III/2.1.1) 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 Definition III/2.3.1) 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 Definition II/5.1.1) is $\Sigma_x = W^T \Sigma W$.

Proof: The linear transformation theorem for the matrix-normal distribution (\rightarrow Proof 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.

Metadata: ID: P267 | shortcut: iglm-dist | author: JoramSoch | date: 2021-10-21, 16:03.

2.3.3 Best linear unbiased estimator

Theorem: Let there be a general linear model (\rightarrow Definition III/2.1.1) 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 Proof III/2.3.2) 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 Proof III/2.1.3) for W is the best linear unbiased estimator (\rightarrow Definition “blue”) of W .

Proof: The linear transformation theorem for the matrix-normal distribution (\rightarrow Proof II/5.1.9) states:

$$X \sim \mathcal{MN}(M, U, V) \quad \Rightarrow \quad Y = AXB + C \sim \mathcal{MN}(AMB + C, AUA^T, B^T V B) . \quad (4)$$

The weighted least squares parameter estimates (\rightarrow Proof III/2.1.3) 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 (\rightarrow Definition “blue”) $\hat{\theta}$ of a certain quantity θ estimated from measured data (\rightarrow Definition “data”) 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 Definition I/1.8.1).

1) First, \hat{W} is a linear estimator, because it is of the form $\tilde{W} = M\hat{X}$ 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

$$\tilde{W} = MX \sim \mathcal{MN}(MYW, MV M^T, \Sigma_x) \quad (6)$$

which requires (\rightarrow Proof 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 (\rightarrow Definition “blue”) is the one with minimum variance (\rightarrow Definition I/1.8.1), 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 Definition 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 Definition II/5.2.1)

$$X \sim \mathcal{MN}(0, U, V) \quad \Rightarrow \quad \langle XX^T \rangle = \text{tr}(V) U , \quad (10)$$

this variance (\rightarrow Definition I/1.8.1) 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:

$$\begin{aligned} \text{Var}[\tilde{W}(D)] &\stackrel{(7)}{=} \text{tr}(\Sigma_x) \text{tr} \left[((Y^T V^{-1} Y)^{-1} Y^T V^{-1} + D) V ((Y^T V^{-1} Y)^{-1} Y^T V^{-1} + D)^T \right] \\ &= \text{tr}(\Sigma_x) \text{tr} \left[(Y^T V^{-1} Y)^{-1} Y^T V^{-1} V V^{-1} Y (Y^T V^{-1} Y)^{-1} + \right. \\ &\quad \left. (Y^T V^{-1} Y)^{-1} Y^T V^{-1} V D^T + D V V^{-1} Y (Y^T V^{-1} Y)^{-1} + D V D^T \right] \\ &= \text{tr}(\Sigma_x) [\text{tr}((Y^T V^{-1} Y)^{-1}) + \text{tr}(D V D^T)] . \end{aligned} \quad (12)$$

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.

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2.3.4 Corresponding forward model

Definition: Let there be observations $Y \in \mathbb{R}^{n \times v}$ and $X \in \mathbb{R}^{n \times p}$ and consider a weight matrix $W = f(Y, X) \in \mathbb{R}^{v \times p}$ estimated from Y and X , such that right-multiplying Y with the weight matrix gives an estimate 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, 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, eq. 3; URL: <https://www.sciencedirect.com/science/article/pii/S1053811913010914>; DOI: 10.1016/j.neuroimage.2013.10.067.

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2.3.5 Derivation of parameters

Theorem: Let there be observations $Y \in \mathbb{R}^{n \times v}$ 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 Definition III/2.3.4) is equal to

$$A = \Sigma_y W \Sigma_x^{-1} \quad (2)$$

with the “sample covariances (\rightarrow Definition I/1.10.2)”

$$\begin{aligned} \Sigma_x &= \hat{X}^T \hat{X} \\ \Sigma_y &= Y^T Y . \end{aligned} \quad (3)$$

Proof: The corresponding forward model (\rightarrow Definition III/2.3.4) is given by

$$Y = \hat{X}A^T + E , \quad (4)$$

subject to the constraint that predicted X and errors E are uncorrelated:

$$\hat{X}^T E = 0 . \quad (5)$$

With that, we can directly derive the parameter matrix A :

$$\begin{aligned}
Y &\stackrel{(4)}{=} \hat{X}A^T + E \\
\hat{X}A^T &= Y - E \\
\hat{X}^T \hat{X}A^T &= \hat{X}^T(Y - E) \\
\hat{X}^T \hat{X}A^T &= \hat{X}^T Y - \hat{X}^T E \\
\hat{X}^T \hat{X}A^T &\stackrel{(5)}{=} \hat{X}^T Y \\
\hat{X}^T \hat{X}A^T &\stackrel{(1)}{=} W^T Y^T Y \\
\Sigma_x A^T &\stackrel{(3)}{=} W^T \Sigma_y \\
A^T &= \Sigma_x^{-1} W^T \Sigma_y \\
A &= \Sigma_y W \Sigma_x^{-1} .
\end{aligned} \tag{6}$$

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, Theorem 1; URL: <https://www.sciencedirect.com/science/article/pii/S1053811913010914>; DOI: 10.1016/j.neuroimage.2013.10.067.

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2.3.6 Proof of existence

Theorem: Let there be observations $Y \in \mathbb{R}^{n \times v}$ 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 :

$$\hat{X} = YW . \tag{1}$$

Then, there exists a corresponding forward model (\rightarrow Definition III/2.3.4).

Proof: The corresponding forward model (\rightarrow Definition III/2.3.4) is defined as

$$Y = \hat{X}A^T + E \quad \text{with} \quad \hat{X}^T E = 0 \tag{2}$$

and the parameters of the corresponding forward model (\rightarrow Proof III/2.3.5) are equal to

$$A = \Sigma_y W \Sigma_x^{-1} \quad \text{where} \quad \Sigma_x = \hat{X}^T \hat{X} \quad \text{and} \quad \Sigma_y = Y^T Y . \tag{3}$$

1) Because the columns of \hat{X} are assumed to be linearly independent by definition of the corresponding forward model (\rightarrow Definition III/2.3.4), 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 Definition III/2.3.4) for predicted X and errors E to be uncorrelated which can be shown as follows:

$$\begin{aligned}
\hat{X}^T E &\stackrel{(2)}{=} \hat{X}^T (Y - \hat{X} A^T) \\
&\stackrel{(3)}{=} \hat{X}^T (Y - \hat{X} \Sigma_x^{-1} W^T \Sigma_y) \\
&= \hat{X}^T Y - \hat{X}^T \hat{X} \Sigma_x^{-1} W^T \Sigma_y \\
&\stackrel{(3)}{=} \hat{X}^T Y - \hat{X}^T \hat{X} (\hat{X}^T \hat{X})^{-1} W^T (Y^T Y) \\
&\stackrel{(1)}{=} (Y W)^T Y - W^T (Y^T Y) \\
&= W^T Y^T Y - W^T Y^T Y \\
&= 0.
\end{aligned} \tag{4}$$

This completes the proof.

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, Appendix B; URL: <https://www.sciencedirect.com/science/article/pii/S1053811913010914>; DOI: 10.1016/j.neuroimage.2013.10.067.

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2.4 Multivariate Bayesian linear regression

2.4.1 Conjugate prior distribution

Theorem: Let

$$Y = XB + E, \quad E \sim \mathcal{MN}(0, V, \Sigma) \tag{1}$$

be a general linear model (\rightarrow Definition III/2.1.1) with measured $n \times v$ data matrix Y , known $n \times p$ design matrix X , known $n \times n$ covariance structure (\rightarrow Definition II/5.1.1) V as well as unknown $p \times v$ regression coefficients B and unknown $v \times v$ noise covariance (\rightarrow Definition II/5.1.1) Σ .

Then, the conjugate prior (\rightarrow Definition I/5.2.5) for this model is a normal-Wishart distribution (\rightarrow Definition II/5.3.1)

$$p(B, T) = \mathcal{MN}(B; M_0, \Lambda_0^{-1}, T^{-1}) \cdot \mathcal{W}(T; \Omega_0^{-1}, \nu_0) \tag{2}$$

where $T = \Sigma^{-1}$ is the inverse noise covariance (\rightarrow Definition I/1.10.9) or noise precision matrix (\rightarrow Definition I/1.10.19).

Proof: By definition, a conjugate prior (\rightarrow Definition I/5.2.5) is a prior distribution (\rightarrow Definition I/5.1.3) that, when combined with the likelihood function (\rightarrow Definition I/5.1.2), leads to a posterior distribution (\rightarrow Definition I/5.1.7) that belongs to the same family of probability distributions (\rightarrow Definition 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 Definition 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 Definition I/1.10.19) $T = \Sigma^{-1}$ and the $n \times n$ precision matrix (\rightarrow Definition I/1.10.19) $P = V^{-1}$.

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 Definition 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 Definition 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 Proof II/5.3.2)

$$p(B, T) = \sqrt{\frac{|T|^p |\Lambda_0|^v}{(2\pi)^{pv}}} \exp \left[-\frac{1}{2} \text{tr} (T(B - M_0)^T \Lambda_0 (B - M_0)) \right] \cdot \frac{1}{\Gamma_v \left(\frac{\nu_0}{2} \right)} \sqrt{\frac{|\Omega_0|^{\nu_0}}{2^{\nu_0 v}}} |T|^{(\nu_0 - v - 1)/2} \exp \left[-\frac{1}{2} \text{tr} (\Omega_0 T) \right] \quad (10)$$

exhibits the same proportionality

$$p(B, T) \propto |T|^{(\nu_0 + p - v - 1)/2} \cdot \exp \left[-\frac{1}{2} \text{tr}(T \Omega_0) \right] \cdot \exp \left[-\frac{1}{2} \text{tr} \left(T [(B - M_0)^T \Lambda_0 (B - M_0)] \right) \right] \quad (11)$$

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.

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2.4.2 Posterior distribution

Theorem: Let

$$Y = XB + E, \quad E \sim \mathcal{MN}(0, V, \Sigma) \quad (1)$$

be a general linear model (\rightarrow Definition III/2.1.1) with measured $n \times v$ data matrix Y , known $n \times p$ design matrix X , known $n \times n$ covariance structure (\rightarrow Definition II/5.1.1) V as well as unknown $p \times v$ regression coefficients B and unknown $v \times v$ noise covariance (\rightarrow Definition II/5.1.1) Σ . Moreover, assume a normal-Wishart prior distribution (\rightarrow Proof III/2.4.1) 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 Definition I/5.1.7) is also a normal-Wishart distribution (\rightarrow Definition 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 Definition I/5.1.7) 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 Proof I/5.3.1), the posterior distribution (\rightarrow Definition I/5.1.7) 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 Proof I/5.1.8) 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 Definition 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 Definition I/1.10.19) $T = \Sigma^{-1}$ and the $n \times n$ precision matrix (\rightarrow Definition I/1.10.19) $P = V^{-1}$.

Combining the likelihood function (\rightarrow Definition I/5.1.2) (8) with the prior distribution (\rightarrow Definition I/5.1.3) (2), the joint likelihood (\rightarrow Definition I/5.1.5) of the model is given by

$$\begin{aligned} p(Y, B, T) &= p(Y|B, T) p(B, T) \\ &= \sqrt{\frac{|T|^n |P|^v}{(2\pi)^{nv}}} \exp \left[-\frac{1}{2} \text{tr} (T(Y - XB)^T P (Y - XB)) \right] \cdot \\ &\quad \sqrt{\frac{|T|^p |\Lambda_0|^v}{(2\pi)^{pv}}} \exp \left[-\frac{1}{2} \text{tr} (T(B - M_0)^T \Lambda_0 (B - M_0)) \right] \cdot \\ &\quad \frac{1}{\Gamma_v \left(\frac{\nu_0}{2} \right)} \sqrt{\frac{|\Omega_0|^{\nu_0}}{2^{\nu_0 v}}} |T|^{(\nu_0 - v - 1)/2} \exp \left[-\frac{1}{2} \text{tr} (\Omega_0 T) \right] . \end{aligned} \quad (9)$$

Collecting identical variables gives:

$$\begin{aligned} p(Y, B, T) &= \sqrt{\frac{|T|^n |P|^v}{(2\pi)^{nv}}} \sqrt{\frac{|T|^p |\Lambda_0|^v}{(2\pi)^{pv}}} \sqrt{\frac{|\Omega_0|^{\nu_0}}{2^{\nu_0 v}}} \frac{1}{\Gamma_v \left(\frac{\nu_0}{2} \right)} \cdot |T|^{(\nu_0 - v - 1)/2} \exp \left[-\frac{1}{2} \text{tr} (\Omega_0 T) \right] \cdot \\ &\quad \exp \left[-\frac{1}{2} \text{tr} (T [(Y - XB)^T P (Y - XB) + (B - M_0)^T \Lambda_0 (B - M_0)]) \right] . \end{aligned} \quad (10)$$

Expanding the products in the exponent gives:

$$\begin{aligned} p(Y, B, T) &= \sqrt{\frac{|T|^n |P|^v}{(2\pi)^{nv}}} \sqrt{\frac{|T|^p |\Lambda_0|^v}{(2\pi)^{pv}}} \sqrt{\frac{|\Omega_0|^{\nu_0}}{2^{\nu_0 v}}} \frac{1}{\Gamma_v \left(\frac{\nu_0}{2} \right)} \cdot |T|^{(\nu_0 - v - 1)/2} \exp \left[-\frac{1}{2} \text{tr} (\Omega_0 T) \right] \cdot \\ &\quad \exp \left[-\frac{1}{2} \text{tr} (T [Y^T P Y - Y^T P X B - B^T X^T P Y + B^T X^T P X B + \right. \\ &\quad \left. B^T \Lambda_0 B - B^T \Lambda_0 M_0 - M_0^T \Lambda_0 B + M_0^T \Lambda_0 M_0]) \right] . \end{aligned} \quad (11)$$

Completing the square over B , we finally have

$$p(Y, B, T) = \sqrt{\frac{|T|^n |P|^v}{(2\pi)^{nv}}} \sqrt{\frac{|T|^p |\Lambda_0|^v}{(2\pi)^{pv}}} \sqrt{\frac{|\Omega_0|^{\nu_0}}{2^{\nu_0 v}} \frac{1}{\Gamma_v(\frac{\nu_0}{2})}} \cdot |T|^{(\nu_0 - v - 1)/2} \exp \left[-\frac{1}{2} \text{tr}(\Omega_0 T) \right] \cdot \exp \left[-\frac{1}{2} \text{tr} \left(T \left[(B - M_n)^T \Lambda_n (B - M_n) + (Y^T P Y + M_0^T \Lambda_0 M_0 - M_n^T \Lambda_n M_n) \right] \right) \right]. \quad (12)$$

with the posterior hyperparameters (\rightarrow Definition I/5.1.7)

$$\begin{aligned} M_n &= \Lambda_n^{-1} (X^T P Y + \Lambda_0 M_0) \\ \Lambda_n &= X^T P X + \Lambda_0. \end{aligned} \quad (13)$$

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 Definition I/5.1.7)

$$\begin{aligned} \Omega_n &= \Omega_0 + Y^T P Y + M_0^T \Lambda_0 M_0 - M_n^T \Lambda_n M_n \\ \nu_n &= \nu_0 + n. \end{aligned} \quad (15)$$

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 Definition I/1.3.2) posterior distribution (\rightarrow Definition I/5.1.7) 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.

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2.4.3 Log model evidence

Theorem: Let

$$Y = X B + E, \quad E \sim \mathcal{MN}(0, V, \Sigma) \quad (1)$$

be a general linear model (\rightarrow Definition III/2.1.1) with measured $n \times v$ data matrix Y , known $n \times p$ design matrix X , known $n \times n$ covariance structure (\rightarrow Definition II/5.1.1) V as well as unknown $p \times v$

regression coefficients B and unknown $v \times v$ noise covariance (\rightarrow Definition II/5.1.1) Σ . Moreover, assume a normal-Wishart prior distribution (\rightarrow Proof III/2.4.1) 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 Definition 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 Definition I/5.1.7) 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 Definition I/1.3.3), the model evidence (\rightarrow Definition I/5.1.9) 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 Definition I/1.3.4), the integrand is equivalent to the joint likelihood (\rightarrow Definition I/5.1.5):

$$p(Y|m) = \iint p(Y, B, T) dB dT . \quad (6)$$

Equation (1) implies the following likelihood function (\rightarrow Definition I/5.1.2)

$$p(Y|B, \Sigma) = \mathcal{MN}(Y; XB, V, \Sigma) = \sqrt{\frac{1}{(2\pi)^{nv} |\Sigma| |V|^v}} \exp \left[-\frac{1}{2} \text{tr} (\Sigma^{-1} (Y - XB)^T V^{-1} (Y - XB)) \right] \quad (7)$$

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 Definition I/1.10.19) $T = \Sigma^{-1}$ and the $n \times n$ precision matrix (\rightarrow Definition I/1.10.19) $P = V^{-1}$.

When deriving the posterior distribution (\rightarrow Proof III/2.4.2) $p(B, T|Y)$, the joint likelihood $p(Y, B, T)$ is obtained as

$$p(Y, B, T) = \sqrt{\frac{|T|^n |P|^v}{(2\pi)^{nv}}} \sqrt{\frac{|T|^p |\Lambda_0|^v}{(2\pi)^{pv}}} \sqrt{\frac{|\Omega_0|^{\nu_0}}{2^{\nu_0 v}}} \frac{1}{\Gamma_v\left(\frac{\nu_0}{2}\right)} \cdot |T|^{(\nu_0 - v - 1)/2} \exp\left[-\frac{1}{2} \text{tr}(\Omega_0 T)\right] \cdot \exp\left[-\frac{1}{2} \text{tr}\left(T[(B - M_n)^T \Lambda_n (B - M_n) + (Y^T P Y + M_0^T \Lambda_0 M_0 - M_n^T \Lambda_n M_n)]\right)\right]. \quad (9)$$

Using the probability density function of the matrix-normal distribution (\rightarrow Proof II/5.1.3), we can rewrite this as

$$p(Y, B, T) = \sqrt{\frac{|T|^n |P|^v}{(2\pi)^{nv}}} \sqrt{\frac{|T|^p |\Lambda_0|^v}{(2\pi)^{pv}}} \sqrt{\frac{(2\pi)^{pv}}{|T|^p |\Lambda_n|^v}} \sqrt{\frac{|\Omega_0|^{\nu_0}}{2^{\nu_0 v}}} \frac{1}{\Gamma_v\left(\frac{\nu_0}{2}\right)} \cdot |T|^{(\nu_0 - v - 1)/2} \exp\left[-\frac{1}{2} \text{tr}(\Omega_0 T)\right] \cdot \mathcal{MN}(B; M_n, \Lambda_n^{-1}, T^{-1}) \cdot \exp\left[-\frac{1}{2} \text{tr}\left(T[Y^T P Y + M_0^T \Lambda_0 M_0 - M_n^T \Lambda_n M_n]\right)\right]. \quad (10)$$

Now, B can be integrated out easily:

$$\int p(Y, B, T) dB = \sqrt{\frac{|T|^n |P|^v}{(2\pi)^{nv}}} \sqrt{\frac{|\Lambda_0|^v}{|\Lambda_n|^v}} \sqrt{\frac{|\Omega_0|^{\nu_0}}{2^{\nu_0 v}}} \frac{1}{\Gamma_v\left(\frac{\nu_0}{2}\right)} \cdot |T|^{(\nu_0 - v - 1)/2} \cdot \exp\left[-\frac{1}{2} \text{tr}\left(T[\Omega_0 + Y^T P Y + M_0^T \Lambda_0 M_0 - M_n^T \Lambda_n M_n]\right)\right]. \quad (11)$$

Using the probability density function of the Wishart distribution (\rightarrow Proof “wish-pdf”), we can rewrite this as

$$\int p(Y, B, T) dB = \sqrt{\frac{|P|^v}{(2\pi)^{nv}}} \sqrt{\frac{|\Lambda_0|^v}{|\Lambda_n|^v}} \sqrt{\frac{|\Omega_0|^{\nu_0}}{2^{\nu_0 v}}} \sqrt{\frac{2^{\nu_n v}}{|\Omega_n|^{\nu_n}}} \frac{\Gamma_v\left(\frac{\nu_n}{2}\right)}{\Gamma_v\left(\frac{\nu_0}{2}\right)} \cdot \mathcal{W}(T; \Omega_n^{-1}, \nu_n). \quad (12)$$

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 Definition IV/3.1.3) of this model is given by

$$\begin{aligned} \log p(Y|m) &= \frac{v}{2} \log |P| - \frac{nv}{2} \log(2\pi) + \frac{v}{2} \log |\Lambda_0| - \frac{v}{2} \log |\Lambda_n| + \\ &\quad \frac{\nu_0}{2} \log \left| \frac{1}{2} \Omega_0 \right| - \frac{\nu_n}{2} \log \left| \frac{1}{2} \Omega_n \right| + \log \Gamma_v\left(\frac{\nu_n}{2}\right) - \log \Gamma_v\left(\frac{\nu_0}{2}\right). \end{aligned} \quad (14)$$

Sources:

- original work

Metadata: ID: P161 | shortcut: mblr-lme | author: JoramSoch | date: 2020-09-03, 09:23.

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.

Sources:

- original work

Metadata: ID: D78 | shortcut: bin-data | author: JoramSoch | date: 2020-07-07, 07:04.

3.1.2 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 Definition II/1.3.1):

$$y \sim \text{Bin}(n, p) . \quad (1)$$

Then, the maximum likelihood estimator (\rightarrow Definition I/4.1.3) of p is

$$\hat{p} = \frac{y}{n} . \quad (2)$$

Proof: With the probability mass function of the binomial distribution (\rightarrow Proof II/1.3.2), equation (1) implies the following likelihood function (\rightarrow Definition I/5.1.2):

$$\begin{aligned} p(y|p) &= \text{Bin}(y; n, p) \\ &= \binom{n}{y} p^y (1-p)^{n-y} . \end{aligned} \quad (3)$$

Thus, the log-likelihood function (\rightarrow Definition I/4.1.2) is given by

$$\begin{aligned} \text{LL}(p) &= \log p(y|p) \\ &= \log \binom{n}{y} + y \log p + (n-y) \log(1-p) . \end{aligned} \quad (4)$$

The derivative of the log-likelihood function (4) with respect to p is

$$\frac{d\text{LL}(p)}{dp} = \frac{y}{p} - \frac{n-y}{1-p} \quad (5)$$

and setting this derivative to zero gives the MLE for p :

$$\begin{aligned}
\frac{dLL(p)}{d\hat{p}} &= 0 \\
0 &= \frac{y}{\hat{p}} - \frac{n-y}{1-\hat{p}} \\
\frac{n-y}{1-\hat{p}} &= \frac{y}{\hat{p}} \\
(n-y)\hat{p} &= y(1-\hat{p}) \\
n\hat{p} - y\hat{p} &= y - y\hat{p} \\
n\hat{p} &= y \\
\hat{p} &= \frac{y}{n} .
\end{aligned} \tag{6}$$

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.

Metadata: ID: P381 | shortcut: bin-mle | author: JoramSoch | date: 2022-11-23, 18:17.

3.1.3 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 Definition II/1.3.1):

$$y \sim \text{Bin}(n, p) . \tag{1}$$

Then, the maximum log-likelihood (\rightarrow Definition I/4.1.5) for this model is

$$\begin{aligned}
\text{MLL} &= \log \Gamma(n+1) - \log \Gamma(y+1) - \log \Gamma(n-y+1) \\
&\quad - n \log(n) + y \log(y) + (n-y) \log(n-y) .
\end{aligned} \tag{2}$$

Proof: The log-likelihood function for binomial data (\rightarrow Proof III/3.1.2) is given by

$$LL(p) = \log \binom{n}{y} + y \log p + (n-y) \log(1-p) \tag{3}$$

and the maximum likelihood estimate of the success probability (\rightarrow Proof III/3.1.2) p is

$$\hat{p} = \frac{y}{n} . \tag{4}$$

Plugging (4) into (3), we obtain the maximum log-likelihood (\rightarrow Definition I/4.1.5) 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

$$\begin{aligned}
\text{MLL} &= \log \Gamma(n + 1) - \log \Gamma(y + 1) - \log \Gamma(n - y + 1) \\
&\quad - n \log(n) + y \log(y) + (n - y) \log(n - y) .
\end{aligned} \tag{8}$$

Sources:

- original work

Metadata: ID: P382 | shortcut: bin-ml | author: JoramSoch | date: 2022-11-24, 14:19.

3.1.4 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 Definition II/1.3.1):

$$y \sim \text{Bin}(n, p) . \tag{1}$$

Then, the conjugate prior (\rightarrow Definition I/5.2.5) for the model parameter p is a beta distribution (\rightarrow Definition II/3.9.1):

$$p(p) = \text{Bet}(p; \alpha_0, \beta_0) . \tag{2}$$

Proof: With the probability mass function of the binomial distribution (\rightarrow Proof II/1.3.2), the likelihood function (\rightarrow Definition I/5.1.2) implied by (1) is given by

$$p(y|p) = \binom{n}{y} p^y (1 - p)^{n-y} . \tag{3}$$

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 Proof II/3.9.3)

$$p(p) = \frac{1}{B(\alpha_0, \beta_0)} p^{\alpha_0-1} (1-p)^{\beta_0-1} \quad (6)$$

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.

Metadata: ID: P29 | shortcut: bin-prior | author: JoramSoch | date: 2020-01-23, 23:38.

3.1.5 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 Definition II/1.3.1):

$$y \sim \text{Bin}(n, p) . \quad (1)$$

Moreover, assume a beta prior distribution (\rightarrow Proof III/3.1.4) over the model parameter p :

$$p(p) = \text{Bet}(p; \alpha_0, \beta_0) . \quad (2)$$

Then, the posterior distribution (\rightarrow Definition I/5.1.7) is also a beta distribution (\rightarrow Definition II/3.9.1)

$$p(p|y) = \text{Bet}(p; \alpha_n, \beta_n) . \quad (3)$$

and the posterior hyperparameters (\rightarrow Definition I/5.1.7) 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 Proof II/1.3.2), the likelihood function (\rightarrow Definition 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 Definition I/5.1.5) 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 Proof I/5.1.8):

$$p(p|y) \propto p(y, p). \quad (7)$$

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 Proof II/3.9.3):

$$p(p|y) = \frac{1}{B(\alpha_n, \beta_n)} p^{\alpha_n-1} (1-p)^{\beta_n-1} = \text{Bet}(p; \alpha_n, \beta_n). \quad (9)$$

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.

Metadata: ID: P30 | shortcut: bin-post | author: JoramSoch | date: 2020-01-24, 00:20.

3.1.6 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 Definition II/1.3.1):

$$y \sim \text{Bin}(n, p). \quad (1)$$

Moreover, assume a beta prior distribution (\rightarrow Proof III/3.1.4) over the model parameter p :

$$p(p) = \text{Bet}(p; \alpha_0, \beta_0). \quad (2)$$

Then, the log model evidence (\rightarrow Definition IV/3.1.3) for this model is

$$\begin{aligned} \log p(y|m) &= \log \Gamma(n+1) - \log \Gamma(k+1) - \log \Gamma(n-k+1) \\ &\quad + \log B(\alpha_n, \beta_n) - \log B(\alpha_0, \beta_0). \end{aligned} \quad (3)$$

where the posterior hyperparameters (\rightarrow Definition I/5.1.7) 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 Proof II/1.3.2), the likelihood function (\rightarrow Definition 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 Definition I/5.1.5) 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 Definition I/5.1.9):

$$p(y) = \int p(y, p) dp . \quad (7)$$

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 Proof II/3.9.3), 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 Definition 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.

Metadata: ID: P31 | shortcut: bin-lme | author: JoramSoch | date: 2020-01-24, 00:44.

3.1.7 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 Definition II/1.3.1):

$$y \sim \text{Bin}(n, p) . \quad (1)$$

Moreover, assume two statistical models (\rightarrow Definition I/5.1.4), one assuming that p is 0.5 (null model (\rightarrow Definition I/4.3.2)), the other imposing a beta distribution (\rightarrow Proof III/3.1.4) as the prior distribution (\rightarrow Definition I/5.1.3) on the model parameter p (alternative (\rightarrow Definition 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 Definition 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 Proof III/3.1.5) which are functions of the number of trials (\rightarrow Definition II/1.3.1) n and the number of successes (\rightarrow Definition II/1.3.1) y .

Proof: The log Bayes factor is equal to the difference of two log model evidences (\rightarrow Proof 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 Proof III/3.1.6):

$$\text{LME}(m_1) = \log p(y|m_1) = \log \binom{n}{y} + \log B(\alpha_n, \beta_n) - \log B(\alpha_0, \beta_0) . \quad (5)$$

Because the null model m_0 has no free parameter, its log model evidence (\rightarrow Definition IV/3.1.3) (logarithmized marginal likelihood (\rightarrow Definition I/5.1.9)) is equal to the log-likelihood function for binomial observations (\rightarrow Proof III/3.1.2) at the value $p = 0.5$:

$$\begin{aligned}
\text{LME}(m_0) &= \log p(y|p = 0.5) = \log \binom{n}{y} + y \log(0.5) + (n - y) \log(1 - 0.5) \\
&= \log \binom{n}{y} + n \log \left(\frac{1}{2} \right) .
\end{aligned} \tag{6}$$

Subtracting the two LMEs from each other, the LBF emerges as

$$\text{LBF}_{10} = \log B(\alpha_n, \beta_n) - \log B(\alpha_0, \beta_0) - n \log \left(\frac{1}{2} \right) \tag{7}$$

where the posterior hyperparameters (\rightarrow Definition I/5.1.7) are given by (\rightarrow Proof III/3.1.5)

$$\begin{aligned}
\alpha_n &= \alpha_0 + y \\
\beta_n &= \beta_0 + (n - y)
\end{aligned} \tag{8}$$

with the number of trials (\rightarrow Definition II/1.3.1) n and the number of successes (\rightarrow Definition II/1.3.1) y .

Sources:

- original work

Metadata: ID: P383 | shortcut: bin-lbf | author: JoramSoch | date: 2022-11-25, 14:40.

3.1.8 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 Definition II/1.3.1):

$$y \sim \text{Bin}(n, p) . \tag{1}$$

Moreover, assume two statistical models (\rightarrow Definition I/5.1.4), one assuming that p is 0.5 (null model (\rightarrow Definition I/4.3.2)), the other imposing a beta distribution (\rightarrow Proof III/3.1.4) as the prior distribution (\rightarrow Definition I/5.1.3) on the model parameter p (alternative (\rightarrow Definition 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 posterior probability (\rightarrow Definition IV/3.4.1) of the alternative model (\rightarrow Definition I/4.3.3) is given by

$$p(m_1|y) = \frac{1}{1 + 2^{-n} [B(\alpha_0, \beta_0)/B(\alpha_n, \beta_n)]} \tag{3}$$

where $B(x, y)$ is the beta function and α_n and β_n are the posterior hyperparameters for binomial observations (\rightarrow Proof III/3.1.5) which are functions of the number of trials (\rightarrow Definition II/1.3.1) n and the number of successes (\rightarrow Definition 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 Proof 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 Proof III/3.1.7) 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 Definition IV/3.3.1), i.e. exponentiated log Bayes factor (\rightarrow Proof 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 Definition I/5.1.7) are given by (\rightarrow Proof III/3.1.5)

$$\begin{aligned} \alpha_n &= \alpha_0 + y \\ \beta_n &= \beta_0 + (n - y) \end{aligned} \quad (8)$$

with the number of trials (\rightarrow Definition II/1.3.1) n and the number of successes (\rightarrow Definition II/1.3.1) y .

Sources:

- original work

Metadata: ID: P384 | shortcut: bin-pp | author: JoramSoch | date: 2022-11-26, 11:42.

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.

Sources:

- original work

Metadata: ID: D79 | shortcut: mult-data | author: JoramSoch | date: 2020-07-07, 07:12.

3.2.2 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 Definition II/2.2.1):

$$y \sim \text{Mult}(n, p) . \quad (1)$$

Then, the maximum likelihood estimator (\rightarrow Proof “mle”) 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 Proof “mult-marg”)

$$X \sim \text{Mult}(n, p) \quad \Rightarrow \quad X_j \sim \text{Bin}(n, p_j) \quad \text{for all } j = 1, \dots, k . \quad (3)$$

Thus, combining (1) with (3), we have

$$y_j \sim \text{Bin}(n, p_j) \quad (4)$$

which implies the likelihood function (\rightarrow Proof III/3.1.2)

$$p(y|p_j) = \text{Bin}(y_j; n, p_j) = \binom{n}{y_j} p_j^{y_j} (1 - p_j)^{n-y_j} . \quad (5)$$

To this, we can apply maximum likelihood estimation for binomial observations (\rightarrow Proof III/3.1.2), such that the MLE for each p_j is

$$\hat{p}_j = \frac{y_j}{n} . \quad (6)$$

Sources:

- original work

Metadata: ID: P385 | shortcut: mult-mle | author: JoramSoch | date: 2022-12-02, 17:00.

3.2.3 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 Definition II/2.2.1):

$$y \sim \text{Mult}(n, p) . \quad (1)$$

Then, the maximum log-likelihood (\rightarrow Definition I/4.1.5) 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 Proof II/2.2.2), equation (1) implies the following likelihood function (\rightarrow Definition 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 Definition 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 Proof III/3.2.2) 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 Definition I/4.1.5) 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

$$\text{MLL} = \log \Gamma(n+1) - \sum_{j=1}^k \log \Gamma(y_j+1) - n \log(n) + \sum_{j=1}^k y_j \log(y_j) . \quad (9)$$

Sources:

- original work

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3.2.4 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 Definition II/2.2.1):

$$y \sim \text{Mult}(n, p) . \quad (1)$$

Then, the conjugate prior (\rightarrow Definition I/5.2.5) for the model parameter p is a Dirichlet distribution (\rightarrow Definition II/4.4.1):

$$p(p) = \text{Dir}(p; \alpha_0) . \quad (2)$$

Proof: With the probability mass function of the multinomial distribution (\rightarrow Proof II/2.2.2), the likelihood function (\rightarrow Definition 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 Proof II/4.4.2)

$$p(p) = \frac{\Gamma\left(\sum_{j=1}^k \alpha_{0j}\right)}{\prod_{j=1}^k \Gamma(\alpha_{0j})} \prod_{j=1}^k p_j^{\alpha_{0j}-1} \quad (6)$$

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

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3.2.5 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 Definition II/2.2.1):

$$y \sim \text{Mult}(n, p) . \quad (1)$$

Moreover, assume a Dirichlet prior distribution (\rightarrow Proof III/3.2.4) over the model parameter p :

$$p(p) = \text{Dir}(p; \alpha_0) . \quad (2)$$

Then, the posterior distribution (\rightarrow Definition I/5.1.7) is also a Dirichlet distribution (\rightarrow Definition II/4.4.1)

$$p(p|y) = \text{Dir}(p; \alpha_n) . \quad (3)$$

and the posterior hyperparameters (\rightarrow Definition I/5.1.7) 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 Proof II/2.2.2), the likelihood function (\rightarrow Definition 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 Definition I/5.1.5) of the model is given by

$$\begin{aligned} p(y, p) &= p(y|p) p(p) \\ &= \binom{n}{y_1, \dots, y_k} \prod_{j=1}^k p_j^{y_j} \cdot \frac{\Gamma\left(\sum_{j=1}^k \alpha_{0j}\right)}{\prod_{j=1}^k \Gamma(\alpha_{0j})} \prod_{j=1}^k p_j^{\alpha_{0j}-1} \\ &= \frac{\Gamma\left(\sum_{j=1}^k \alpha_{0j}\right)}{\prod_{j=1}^k \Gamma(\alpha_{0j})} \binom{n}{y_1, \dots, y_k} \prod_{j=1}^k p_j^{\alpha_{0j}+y_j-1} . \end{aligned} \quad (6)$$

Note that the posterior distribution is proportional to the joint likelihood (\rightarrow Proof I/5.1.8):

$$p(p|y) \propto p(y, p) . \quad (7)$$

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 Proof II/4.4.2):

$$p(p|y) = \frac{\Gamma\left(\sum_{j=1}^k \alpha_{nj}\right)}{\prod_{j=1}^k \Gamma(\alpha_{nj})} \prod_{j=1}^k p_j^{\alpha_{nj}-1} = \text{Dir}(p; \alpha_n) . \quad (9)$$

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

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3.2.6 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 Definition II/2.2.1):

$$y \sim \text{Mult}(n, p) . \quad (1)$$

Moreover, assume a Dirichlet prior distribution (\rightarrow Proof III/3.2.4) over the model parameter p :

$$p(p) = \text{Dir}(p; \alpha_0) . \quad (2)$$

Then, the log model evidence (\rightarrow Definition IV/3.1.3) for this model is

$$\begin{aligned} \log p(y|m) &= \log \Gamma(n+1) - \sum_{j=1}^k \log \Gamma(k_j+1) \\ &\quad + \log \Gamma\left(\sum_{j=1}^k \alpha_{0j}\right) - \log \Gamma\left(\sum_{j=1}^k \alpha_{nj}\right) \\ &\quad + \sum_{j=1}^k \log \Gamma(\alpha_{nj}) - \sum_{j=1}^k \log \Gamma(\alpha_{0j}) . \end{aligned} \quad (3)$$

and the posterior hyperparameters (\rightarrow Definition I/5.1.7) 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 Proof II/2.2.2), the likelihood function (\rightarrow Definition 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 Definition I/5.1.5) 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 Proof II/4.4.2), 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 Definition 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

$$\begin{aligned} \log p(y|m) &= \log \Gamma(n+1) - \sum_{j=1}^k \log \Gamma(k_j+1) \\ &+ \log \Gamma\left(\sum_{j=1}^k \alpha_{0j}\right) - \log \Gamma\left(\sum_{j=1}^k \alpha_{nj}\right) \\ &+ \sum_{j=1}^k \log \Gamma(\alpha_{nj}) - \sum_{j=1}^k \log \Gamma(\alpha_{0j}) . \end{aligned} \quad (13)$$

Sources:

- original work

Metadata: ID: P81 | shortcut: mult-lme | author: JoramSoch | date: 2020-03-11, 15:17.

3.2.7 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 Definition II/2.2.1):

$$y \sim \text{Mult}(n, p) . \quad (1)$$

Moreover, assume two statistical models (\rightarrow Definition I/5.1.4), one assuming that each p_j is $1/k$ (null model (\rightarrow Definition I/4.3.2)), the other imposing a Dirichlet distribution (\rightarrow Proof III/3.2.4) as the prior distribution (\rightarrow Definition I/5.1.3) on the model parameters p_1, \dots, p_k (alternative (\rightarrow Definition 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 log Bayes factor (\rightarrow Definition IV/3.3.6) in favor of m_1 against m_0 is

$$\begin{aligned} \text{LBF}_{10} &= \log \Gamma\left(\sum_{j=1}^k \alpha_{0j}\right) - \log \Gamma\left(\sum_{j=1}^k \alpha_{nj}\right) \\ &+ \sum_{j=1}^k \log \Gamma(\alpha_{nj}) - \sum_{j=1}^k \log \Gamma(\alpha_{0j}) - n \log \left(\frac{1}{k}\right) \end{aligned} \quad (3)$$

where $\Gamma(x)$ is the gamma function and α_n are the posterior hyperparameters for multinomial observations (\rightarrow Proof III/3.2.5) which are functions of the numbers of observations (\rightarrow Definition 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 Proof 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 multinomial observations (\rightarrow Proof III/3.2.6):

$$\begin{aligned} \text{LME}(m_1) = \log p(y|m_1) &= \log \Gamma(n+1) - \sum_{j=1}^k \log \Gamma(k_j+1) \\ &+ \log \Gamma\left(\sum_{j=1}^k \alpha_{0j}\right) - \log \Gamma\left(\sum_{j=1}^k \alpha_{nj}\right) \\ &+ \sum_{j=1}^k \log \Gamma(\alpha_{nj}) - \sum_{j=1}^k \log \Gamma(\alpha_{0j}) . \end{aligned} \quad (5)$$

Because the null model m_0 has no free parameter, its log model evidence (\rightarrow Definition IV/3.1.3) (logarithmized marginal likelihood (\rightarrow Definition I/5.1.9)) is equal to the log-likelihood function for multinomial observations (\rightarrow Proof III/3.2.2) at the value $p_0 = [1/k, \dots, 1/k]$:

$$\begin{aligned} \text{LME}(m_0) = \log p(y|p=p_0) &= \log \binom{n}{y_1, \dots, y_k} + \sum_{j=1}^k y_j \log \left(\frac{1}{k}\right) \\ &= \log \binom{n}{y_1, \dots, y_k} + n \log \left(\frac{1}{k}\right) . \end{aligned} \quad (6)$$

Subtracting the two LMEs from each other, the LBF emerges as

$$\begin{aligned} \text{LBF}_{10} &= \log \Gamma\left(\sum_{j=1}^k \alpha_{0j}\right) - \log \Gamma\left(\sum_{j=1}^k \alpha_{nj}\right) \\ &+ \sum_{j=1}^k \log \Gamma(\alpha_{nj}) - \sum_{j=1}^k \log \Gamma(\alpha_{0j}) - n \log \left(\frac{1}{k}\right) \end{aligned} \quad (7)$$

where the posterior hyperparameters (\rightarrow Definition I/5.1.7) are given by (\rightarrow Proof III/3.2.5)

$$\begin{aligned} \alpha_n &= \alpha_0 + y \\ &= [\alpha_{01}, \dots, \alpha_{0k}] + [y_1, \dots, y_k] \\ &= [\alpha_{01} + y_1, \dots, \alpha_{0k} + y_k] \\ \text{i.e. } \alpha_{nj} &= \alpha_{0j} + y_j \quad \text{for all } j = 1, \dots, k \end{aligned} \quad (8)$$

with the numbers of observations (\rightarrow Definition II/2.2.1) y_1, \dots, y_k .

Sources:

- original work

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3.2.8 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 Definition II/2.2.1):

$$y \sim \text{Mult}(n, p) . \quad (1)$$

Moreover, assume two statistical models (\rightarrow Definition I/5.1.4), one assuming that each p_j is $1/k$ (null model (\rightarrow Definition I/4.3.2)), the other imposing a Dirichlet distribution (\rightarrow Proof III/3.2.4) as the prior distribution (\rightarrow Definition I/5.1.3) on the model parameters p_1, \dots, p_k (alternative (\rightarrow Definition 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 Definition IV/3.4.1) of the alternative model (\rightarrow Definition 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 Proof III/3.2.5) which are functions of the numbers of observations (\rightarrow Definition 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 Proof 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 Proof III/3.2.7) 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 Definition IV/3.3.1), i.e. exponentiated log Bayes factor (\rightarrow Proof 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

$$\begin{aligned} p(m_1|y) &\stackrel{(4)}{=} \frac{\exp(\text{LBF}_{10})}{\exp(\text{LBF}_{10}) + 1} \\ &\stackrel{(6)}{=} \frac{k^n \cdot \frac{\Gamma\left(\sum_{j=1}^k \alpha_{0j}\right)}{\Gamma\left(\sum_{j=1}^k \alpha_{nj}\right)} \cdot \frac{\prod_{j=1}^k \Gamma(\alpha_{nj})}{\prod_{j=1}^k \Gamma(\alpha_{0j})}}{k^n \cdot \frac{\Gamma\left(\sum_{j=1}^k \alpha_{0j}\right)}{\Gamma\left(\sum_{j=1}^k \alpha_{nj}\right)} \cdot \frac{\prod_{j=1}^k \Gamma(\alpha_{nj})}{\prod_{j=1}^k \Gamma(\alpha_{0j})} + 1} \\ &= \frac{k^n \cdot \frac{\Gamma\left(\sum_{j=1}^k \alpha_{0j}\right)}{\Gamma\left(\sum_{j=1}^k \alpha_{nj}\right)} \cdot \frac{\prod_{j=1}^k \Gamma(\alpha_{nj})}{\prod_{j=1}^k \Gamma(\alpha_{0j})}}{k^n \cdot \frac{\Gamma\left(\sum_{j=1}^k \alpha_{0j}\right)}{\Gamma\left(\sum_{j=1}^k \alpha_{nj}\right)} \cdot \frac{\prod_{j=1}^k \Gamma(\alpha_{nj})}{\prod_{j=1}^k \Gamma(\alpha_{0j})} \left(1 + k^{-n} \cdot \frac{\Gamma\left(\sum_{j=1}^k \alpha_{nj}\right)}{\Gamma\left(\sum_{j=1}^k \alpha_{0j}\right)} \cdot \frac{\prod_{j=1}^k \Gamma(\alpha_{0j})}{\prod_{j=1}^k \Gamma(\alpha_{nj})}\right)} \\ &= \frac{1}{1 + k^{-n} \cdot \frac{\Gamma\left(\sum_{j=1}^k \alpha_{nj}\right)}{\Gamma\left(\sum_{j=1}^k \alpha_{0j}\right)} \cdot \frac{\prod_{j=1}^k \Gamma(\alpha_{0j})}{\prod_{j=1}^k \Gamma(\alpha_{nj})}} \end{aligned} \quad (7)$$

where the posterior hyperparameters (\rightarrow Definition I/5.1.7) are given by (\rightarrow Proof III/3.2.5)

$$\alpha_n = \alpha_0 + y, \quad \text{i.e.} \quad \alpha_{nj} = \alpha_{0j} + y_j \quad (8)$$

with the numbers of observations (\rightarrow Definition II/2.2.1) y_1, \dots, y_k .

Sources:

- original work

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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 according to a Poisson distribution (\rightarrow Definition II/1.5.1) with rate λ :

$$y_i \sim \text{Pois}(\lambda), \quad i = 1, \dots, n. \quad (1)$$

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.

Metadata: ID: D41 | shortcut: poiss-data | author: JoramSoch | date: 2020-03-22, 22:50.

3.3.2 Maximum likelihood estimation

Theorem: Let there be a Poisson-distributed data (\rightarrow Definition 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 maximum likelihood estimate (\rightarrow Definition I/4.1.3) for the rate parameter λ is given by

$$\hat{\lambda} = \bar{y} \quad (2)$$

where \bar{y} is the sample mean (\rightarrow Definition I/1.7.2)

$$\bar{y} = \frac{1}{n} \sum_{i=1}^n y_i. \quad (3)$$

Proof: The likelihood function (\rightarrow Definition I/5.1.2) for each observation is given by the probability mass function of the Poisson distribution (\rightarrow Proof II/1.5.2)

$$p(y_i|\lambda) = \text{Pois}(y_i; \lambda) = \frac{\lambda^{y_i} \cdot \exp(-\lambda)}{y_i!} \quad (4)$$

and because observations are independent (\rightarrow Definition 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 Definition 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:

$$\begin{aligned}\frac{dLL(\hat{\lambda})}{d\lambda} &= 0 \\ 0 &= \frac{1}{\hat{\lambda}} \sum_{i=1}^n y_i - n \\ \hat{\lambda} &= \frac{1}{n} \sum_{i=1}^n y_i = \bar{y} .\end{aligned}\tag{9}$$

Plugging this value into the second derivative, we confirm:

$$\begin{aligned}\frac{d^2LL(\hat{\lambda})}{d\lambda^2} &= -\frac{1}{\bar{y}^2} \sum_{i=1}^n y_i \\ &= -\frac{n \cdot \bar{y}}{\bar{y}^2} \\ &= -\frac{n}{\bar{y}} < 0 .\end{aligned}\tag{10}$$

This demonstrates that the estimate $\hat{\lambda} = \bar{y}$ maximizes the likelihood $p(y|\lambda)$.

Sources:

- original work

Metadata: ID: P27 | shortcut: poiss-mle | author: JoramSoch | date: 2020-01-20, 21:53.

3.3.3 Conjugate prior distribution

Theorem: Let there be a Poisson-distributed data (\rightarrow Definition 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 conjugate prior (\rightarrow Definition I/5.2.5) for the model parameter λ is a gamma distribution (\rightarrow Definition 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 Proof II/1.5.2), the likelihood function (\rightarrow Definition I/5.1.2) for each observation implied by (1) is given by

$$p(y_i|\lambda) = \text{Poiss}(y_i; \lambda) = \frac{\lambda^{y_i} \cdot \exp[-\lambda]}{y_i!}\tag{3}$$

and because observations are independent (\rightarrow Definition I/1.3.6), the likelihood function for all observations is the product of the individual ones:

$$p(y|\lambda) = \prod_{i=1}^n p(y_i|\lambda) = \prod_{i=1}^n \frac{\lambda^{y_i} \cdot \exp[-\lambda]}{y_i!} .\tag{4}$$

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 Definition I/1.7.2) 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 Proof II/3.4.6)

$$p(\lambda) = \frac{b_0^{a_0}}{\Gamma(a_0)} \lambda^{a_0-1} \exp[-b_0\lambda] \quad (9)$$

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/>.

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3.3.4 Posterior distribution

Theorem: Let there be a Poisson-distributed data (\rightarrow Definition III/3.3.1) set $y = \{y_1, \dots, y_n\}$:

$$y_i \sim \text{Pois}(\lambda), \quad i = 1, \dots, n . \quad (1)$$

Moreover, assume a gamma prior distribution (\rightarrow Proof 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 Definition I/5.1.7) is also a gamma distribution (\rightarrow Definition II/3.4.1)

$$p(\lambda|y) = \text{Gam}(\lambda; a_n, b_n) \quad (3)$$

and the posterior hyperparameters (\rightarrow Definition I/5.1.7) 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 Proof II/1.5.2), the likelihood function (\rightarrow Definition 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 Definition 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 Definition I/5.1.5) 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 Definition I/1.7.2) of y :

$$\bar{y} = \frac{1}{n} \sum_{i=1}^n y_i . \quad (9)$$

Note that the posterior distribution is proportional to the joint likelihood (\rightarrow Proof I/5.1.8):

$$p(\lambda|y) \propto p(y, \lambda) . \quad (10)$$

Setting $a_n = a_0 + n\bar{y}$ and $b_n = b_0 + n$, the posterior distribution is therefore proportional to

$$p(\lambda|y) \propto \lambda^{a_n-1} \cdot \exp[-b_n\lambda] \quad (11)$$

which, when normalized to one, results in the probability density function of the gamma distribution (\rightarrow Proof II/3.4.6):

$$p(\lambda|y) = \frac{b_n^{a_n}}{\Gamma(a_n)} \lambda^{a_n-1} \exp[-b_n\lambda] = \text{Gam}(\lambda; a_n, b_n) . \quad (12)$$

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/>.

Metadata: ID: P226 | shortcut: poiss-post | author: JoramSoch | date: 2020-04-21, 08:48.

3.3.5 Log model evidence

Theorem: Let there be a Poisson-distributed data (\rightarrow Definition 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 Proof III/3.3.3) over the model parameter λ :

$$p(\lambda) = \text{Gam}(\lambda; a_0, b_0) . \quad (2)$$

Then, the log model evidence (\rightarrow Definition IV/3.1.3) for this model is

$$\log p(y|m) = - \sum_{i=1}^n \log y_i! + \log \Gamma(a_n) - \log \Gamma(a_0) + a_0 \log b_0 - a_n \log b_n . \quad (3)$$

and the posterior hyperparameters (\rightarrow Definition I/5.1.7) 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 Proof II/1.5.2), the likelihood function (\rightarrow Definition 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 Definition 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 Definition I/5.1.5) of the model is given by

$$\begin{aligned}
p(y, \lambda) &= p(y|\lambda) p(\lambda) \\
&= \prod_{i=1}^n \frac{\lambda^{y_i} \cdot \exp[-\lambda]}{y_i!} \cdot \frac{b_0^{a_0}}{\Gamma(a_0)} \lambda^{a_0-1} \exp[-b_0 \lambda] .
\end{aligned} \tag{7}$$

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 Definition I/1.7.2) of y :

$$\bar{y} = \frac{1}{n} \sum_{i=1}^n y_i . \tag{9}$$

Note that the model evidence is the marginal density of the joint likelihood (\rightarrow Definition I/5.1.9):

$$p(y) = \int p(y, \lambda) d\lambda . \tag{10}$$

Setting $a_n = a_0 + n\bar{y}$ and $b_n = b_0 + n$, the joint likelihood can also be written as

$$p(y, \lambda) = \prod_{i=1}^n \left(\frac{1}{y_i!} \right) \frac{b_0^{a_0}}{\Gamma(a_0)} \frac{\Gamma(a_n)}{b_n^{a_n}} \cdot \frac{b_n^{a_n}}{\Gamma(a_n)} \lambda^{a_n-1} \exp[-b_n \lambda] . \tag{11}$$

Using the probability density function of the gamma distribution (\rightarrow Proof II/3.4.6), λ can now be integrated out easily

$$\begin{aligned}
p(y) &= \int \prod_{i=1}^n \left(\frac{1}{y_i!} \right) \frac{b_0^{a_0}}{\Gamma(a_0)} \frac{\Gamma(a_n)}{b_n^{a_n}} \cdot \frac{b_n^{a_n}}{\Gamma(a_n)} \lambda^{a_n-1} \exp[-b_n \lambda] d\lambda \\
&= \prod_{i=1}^n \left(\frac{1}{y_i!} \right) \frac{\Gamma(a_n)}{\Gamma(a_0)} \frac{b_0^{a_0}}{b_n^{a_n}} \int \text{Gam}(\lambda; a_n, b_n) d\lambda \\
&= \prod_{i=1}^n \left(\frac{1}{y_i!} \right) \frac{\Gamma(a_n)}{\Gamma(a_0)} \frac{b_0^{a_0}}{b_n^{a_n}} ,
\end{aligned} \tag{12}$$

such that the log model evidence (\rightarrow Definition IV/3.1.3) is shown to be

$$\log p(y|m) = - \sum_{i=1}^n \log y_i! + \log \Gamma(a_n) - \log \Gamma(a_0) + a_0 \log b_0 - a_n \log b_n . \tag{13}$$

Sources:

- original work

Metadata: ID: P227 | shortcut: poiss-lme | author: JoramSoch | date: 2020-04-21, 09:09.

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 distributed according to a Poisson distribution (\rightarrow Definition II/1.5.1) with common rate 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/>.

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3.4.2 Maximum likelihood estimation

Theorem: Consider data $y = \{y_1, \dots, y_n\}$ following a Poisson distribution with exposure values (\rightarrow Definition 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 Definition 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 Definition “mean-sample”)

$$\begin{aligned} \bar{y} &= \frac{1}{n} \sum_{i=1}^n y_i \\ \bar{x} &= \frac{1}{n} \sum_{i=1}^n x_i. \end{aligned} \quad (3)$$

Proof: With the probability mass function of the Poisson distribution (\rightarrow Proof II/1.5.2), the likelihood function (\rightarrow Definition I/5.1.2) for each observation implied by (1) is given by

$$p(y_i|\lambda) = \text{Poiss}(y_i; \lambda x_i) = \frac{(\lambda x_i)^{y_i} \cdot \exp[-\lambda x_i]}{y_i!} \quad (4)$$

and because observations are independent (\rightarrow Definition I/1.3.6), the likelihood function for all observations is the product of the individual ones:

$$p(y|\lambda) = \prod_{i=1}^n p(y_i|\lambda) = \prod_{i=1}^n \frac{(\lambda x_i)^{y_i} \cdot \exp[-\lambda x_i]}{y_i!} . \quad (5)$$

Thus, the log-likelihood function (\rightarrow Definition I/4.1.2) is

$$\text{LL}(\lambda) = \log p(y|\lambda) = \log \left[\prod_{i=1}^n \frac{(\lambda x_i)^{y_i} \cdot \exp[-\lambda x_i]}{y_i!} \right] \quad (6)$$

which can be developed into

$$\begin{aligned} \text{LL}(\lambda) &= \sum_{i=1}^n \log \left[\frac{(\lambda x_i)^{y_i} \cdot \exp[-\lambda x_i]}{y_i!} \right] \\ &= \sum_{i=1}^n [y_i \cdot \log(\lambda x_i) - \lambda x_i - \log(y_i!)] \\ &= -\sum_{i=1}^n \lambda x_i + \sum_{i=1}^n y_i \cdot [\log(\lambda) + \log(x_i)] - \sum_{i=1}^n \log(y_i!) \\ &= -\lambda \sum_{i=1}^n x_i + \log(\lambda) \sum_{i=1}^n y_i + \sum_{i=1}^n y_i \log(x_i) - \sum_{i=1}^n \log(y_i!) \\ &= -n\bar{x}\lambda + n\bar{y} \log(\lambda) + \sum_{i=1}^n y_i \log(x_i) - \sum_{i=1}^n \log(y_i!) \end{aligned} \quad (7)$$

where \bar{x} and \bar{y} are the sample means from equation (3).

The derivatives of the log-likelihood with respect to λ are

$$\begin{aligned} \frac{d\text{LL}(\lambda)}{d\lambda} &= -n\bar{x} + \frac{n\bar{y}}{\lambda} \\ \frac{d^2\text{LL}(\lambda)}{d\lambda^2} &= -\frac{n\bar{y}}{\lambda^2} . \end{aligned} \quad (8)$$

Setting the first derivative to zero, we obtain:

$$\begin{aligned} \frac{d\text{LL}(\hat{\lambda})}{d\lambda} &= 0 \\ 0 &= -n\bar{x} + \frac{n\bar{y}}{\hat{\lambda}} \\ \hat{\lambda} &= \frac{n\bar{y}}{n\bar{x}} = \frac{\bar{y}}{\bar{x}} . \end{aligned} \quad (9)$$

Plugging this value into the second derivative, we confirm:

$$\begin{aligned} \frac{d^2\text{LL}(\hat{\lambda})}{d\lambda^2} &= -\frac{n\bar{y}}{\hat{\lambda}^2} \\ &= -\frac{n \cdot \bar{y}}{(\bar{y}/\bar{x})^2} \\ &= -\frac{n \cdot \bar{x}^2}{\bar{y}} < 0 . \end{aligned} \quad (10)$$

This demonstrates that the estimate $\hat{\lambda} = \bar{y}/\bar{x}$ maximizes the likelihood $p(y|\lambda)$.

Sources:

- original work

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3.4.3 Conjugate prior distribution

Theorem: Consider data $y = \{y_1, \dots, y_n\}$ following a Poisson distribution with exposure values (\rightarrow Definition III/3.4.1):

$$y_i \sim \text{Poiss}(\lambda x_i), \quad i = 1, \dots, n. \quad (1)$$

Then, the conjugate prior (\rightarrow Definition I/5.2.5) for the model parameter λ is a gamma distribution (\rightarrow Definition 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 Proof II/1.5.2), the likelihood function (\rightarrow Definition I/5.1.2) for each observation implied by (1) is given by

$$p(y_i|\lambda) = \text{Poiss}(y_i; \lambda x_i) = \frac{(\lambda x_i)^{y_i} \cdot \exp[-\lambda x_i]}{y_i!} \quad (3)$$

and because observations are independent (\rightarrow Definition I/1.3.6), the likelihood function for all observations is the product of the individual ones:

$$p(y|\lambda) = \prod_{i=1}^n p(y_i|\lambda) = \prod_{i=1}^n \frac{(\lambda x_i)^{y_i} \cdot \exp[-\lambda x_i]}{y_i!}. \quad (4)$$

Resolving the product in the likelihood function, we have

$$\begin{aligned} p(y|\lambda) &= \prod_{i=1}^n \frac{x_i^{y_i}}{y_i!} \cdot \prod_{i=1}^n \lambda^{y_i} \cdot \prod_{i=1}^n \exp[-\lambda x_i] \\ &= \prod_{i=1}^n \left(\frac{x_i^{y_i}}{y_i!} \right) \cdot \lambda^{\sum_{i=1}^n y_i} \cdot \exp \left[-\lambda \sum_{i=1}^n x_i \right] \\ &= \prod_{i=1}^n \left(\frac{x_i^{y_i}}{y_i!} \right) \cdot \lambda^{n\bar{y}} \cdot \exp[-n\bar{x}\lambda] \end{aligned} \quad (5)$$

where \bar{y} and \bar{x} are the means (\rightarrow Definition I/1.7.2) of y and x respectively:

$$\begin{aligned} \bar{y} &= \frac{1}{n} \sum_{i=1}^n y_i \\ \bar{x} &= \frac{1}{n} \sum_{i=1}^n x_i. \end{aligned} \quad (6)$$

In other words, the likelihood function is proportional to a power of λ times an exponential of λ :

$$p(y|\lambda) \propto \lambda^{n\bar{y}} \cdot \exp[-n\bar{x}\lambda] . \quad (7)$$

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 Proof II/3.4.6)

$$p(\lambda) = \frac{b_0^{a_0}}{\Gamma(a_0)} \lambda^{a_0-1} \exp[-b_0\lambda] \quad (9)$$

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/>.

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3.4.4 Posterior distribution

Theorem: Consider data $y = \{y_1, \dots, y_n\}$ following a Poisson distribution with exposure values (\rightarrow Definition III/3.4.1):

$$y_i \sim \text{Poiss}(\lambda x_i), \quad i = 1, \dots, n . \quad (1)$$

Moreover, assume a gamma prior distribution (\rightarrow Proof 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 Definition I/5.1.7) is also a gamma distribution (\rightarrow Definition II/3.4.1)

$$p(\lambda|y) = \text{Gam}(\lambda; a_n, b_n) \quad (3)$$

and the posterior hyperparameters (\rightarrow Definition I/5.1.7) 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 Proof II/1.5.2), the likelihood function (\rightarrow Definition 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 Definition 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 Definition I/5.1.5) 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 Definition I/1.7.2) 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 posterior distribution is proportional to the joint likelihood (\rightarrow Proof I/5.1.8):

$$p(\lambda|y) \propto p(y, \lambda) . \quad (10)$$

Setting $a_n = a_0 + n\bar{y}$ and $b_n = b_0 + n\bar{x}$, the posterior distribution is therefore proportional to

$$p(\lambda|y) \propto \lambda^{a_n-1} \cdot \exp[-b_n \lambda] \quad (11)$$

which, when normalized to one, results in the probability density function of the gamma distribution (\rightarrow Proof II/3.4.6):

$$p(\lambda|y) = \frac{b_n^{a_n}}{\Gamma(a_n)} \lambda^{a_n-1} \exp[-b_n \lambda] = \text{Gam}(\lambda; a_n, b_n) . \quad (12)$$

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/>.

Metadata: ID: P42 | shortcut: poissexp-post | author: JoramSoch | date: 2020-02-04, 14:42.

3.4.5 Log model evidence

Theorem: Consider data $y = \{y_1, \dots, y_n\}$ following a Poisson distribution with exposure values (\rightarrow Definition III/3.4.1):

$$y_i \sim \text{Poiss}(\lambda x_i), \quad i = 1, \dots, n. \quad (1)$$

Moreover, assume a gamma prior distribution (\rightarrow Proof III/3.4.3) over the model parameter λ :

$$p(\lambda) = \text{Gam}(\lambda; a_0, b_0). \quad (2)$$

Then, the log model evidence (\rightarrow Definition IV/3.1.3) for this model is

$$\begin{aligned} \log p(y|m) &= \sum_{i=1}^n y_i \log(x_i) - \sum_{i=1}^n \log y_i! + \\ &\quad \log \Gamma(a_n) - \log \Gamma(a_0) + a_0 \log b_0 - a_n \log b_n. \end{aligned} \quad (3)$$

where the posterior hyperparameters (\rightarrow Definition I/5.1.7) are given by

$$\begin{aligned} a_n &= a_0 + n\bar{y} \\ a_n &= a_0 + n\bar{x}. \end{aligned} \quad (4)$$

Proof: With the probability mass function of the Poisson distribution (\rightarrow Proof II/1.5.2), the likelihood function (\rightarrow Definition 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 Definition 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 Definition I/5.1.5) 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

$$\begin{aligned}
 p(y, \lambda) &= \prod_{i=1}^n \frac{x_i^{y_i}}{y_i!} \prod_{i=1}^n \lambda^{y_i} \prod_{i=1}^n \exp[-\lambda x_i] \cdot \frac{b_0^{a_0}}{\Gamma(a_0)} \lambda^{a_0-1} \exp[-b_0 \lambda] \\
 &= \prod_{i=1}^n \left(\frac{x_i^{y_i}}{y_i!} \right) \lambda^{\sum_{i=1}^n y_i} \exp \left[-\lambda \sum_{i=1}^n x_i \right] \cdot \frac{b_0^{a_0}}{\Gamma(a_0)} \lambda^{a_0-1} \exp[-b_0 \lambda] \\
 &= \prod_{i=1}^n \left(\frac{x_i^{y_i}}{y_i!} \right) \lambda^{n\bar{y}} \exp[-n\bar{x}\lambda] \cdot \frac{b_0^{a_0}}{\Gamma(a_0)} \lambda^{a_0-1} \exp[-b_0 \lambda] \\
 &= \prod_{i=1}^n \left(\frac{x_i^{y_i}}{y_i!} \right) \frac{b_0^{a_0}}{\Gamma(a_0)} \cdot \lambda^{a_0+n\bar{y}-1} \cdot \exp[-(b_0 + n\bar{x})\lambda]
 \end{aligned} \tag{8}$$

where \bar{y} and \bar{x} are the means (\rightarrow Definition I/1.7.2) 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 model evidence is the marginal density of the joint likelihood (\rightarrow Definition I/5.1.9):

$$p(y) = \int p(y, \lambda) d\lambda . \tag{10}$$

Setting $a_n = a_0 + n\bar{y}$ and $b_n = b_0 + n\bar{x}$, the joint likelihood can also be written as

$$p(y, \lambda) = \prod_{i=1}^n \left(\frac{x_i^{y_i}}{y_i!} \right) \frac{b_0^{a_0}}{\Gamma(a_0)} \frac{\Gamma(a_n)}{b_n^{a_n}} \cdot \frac{b_n^{a_n}}{\Gamma(a_n)} \lambda^{a_n-1} \exp[-b_n \lambda] . \tag{11}$$

Using the probability density function of the gamma distribution (\rightarrow Proof II/3.4.6), 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 Definition IV/3.1.3) is shown to be

$$\begin{aligned}
 \log p(y|m) &= \sum_{i=1}^n y_i \log(x_i) - \sum_{i=1}^n \log y_i! + \\
 &\quad \log \Gamma(a_n) - \log \Gamma(a_0) + a_0 \log b_0 - a_n \log b_n .
 \end{aligned} \tag{13}$$

Sources:

- original work

Metadata: ID: P43 | shortcut: poissexp-lme | author: JoramSoch | date: 2020-02-04, 15:12.

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 according to a beta distribution (\rightarrow Definition II/3.9.1) with shapes α and β :

$$y_i \sim \text{Bet}(\alpha, \beta), \quad i = 1, \dots, n. \quad (1)$$

Sources:

- original work

Metadata: ID: D77 | shortcut: beta-data | author: JoramSoch | date: 2020-06-28, 21:16.

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 Definition “iid”) according to a beta distribution (\rightarrow Definition 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 Definition I/4.1.6) 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 Definition I/1.7.2) and \bar{v} is the unbiased sample variance (\rightarrow Definition I/1.8.2):

$$\begin{aligned} \bar{y} &= \frac{1}{n} \sum_{i=1}^n y_i \\ \bar{v} &= \frac{1}{n-1} \sum_{i=1}^n (y_i - \bar{y})^2. \end{aligned} \quad (3)$$

Proof: Mean (\rightarrow Proof II/3.9.6) and variance (\rightarrow Proof II/3.9.7) of the beta distribution (\rightarrow Definition II/3.9.1) in terms of the parameters α and β are given by

$$\begin{aligned} \text{E}(X) &= \frac{\alpha}{\alpha + \beta} \\ \text{Var}(X) &= \frac{\alpha\beta}{(\alpha + \beta)^2(\alpha + \beta + 1)}. \end{aligned} \quad (4)$$

Thus, matching the moments (\rightarrow Definition I/4.1.6) requires us to solve the following equation system for α and β :

$$\begin{aligned}\bar{y} &= \frac{\alpha}{\alpha + \beta} \\ \bar{v} &= \frac{\alpha\beta}{(\alpha + \beta)^2(\alpha + \beta + 1)}.\end{aligned}\tag{5}$$

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.

Metadata: ID: P28 | shortcut: beta-mome | author: JoramSoch | date: 2020-01-22, 02:53.

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

$$\begin{aligned}
y_i &= [y_{i1}, \dots, y_{ik}], \\
y_{ij} &\in [0, 1] \quad \text{and} \\
\sum_{j=1}^k y_{ij} &= 1
\end{aligned} \tag{1}$$

for all $i = 1, \dots, n$ (and $j = 1, \dots, k$) and each y_i is independent and identically distributed according to a Dirichlet distribution (\rightarrow Definition II/4.4.1) with concentration parameters $\alpha = [\alpha_1, \dots, \alpha_k]$:

$$y_i \sim \text{Dir}(\alpha), \quad i = 1, \dots, n. \tag{2}$$

Sources:

- original work

Metadata: ID: D104 | shortcut: dir-data | author: JoramSoch | date: 2020-10-22, 05:06.

4.2.2 Maximum likelihood estimation

Theorem: Let there be a Dirichlet-distributed data (\rightarrow Definition III/4.2.1) set $y = \{y_1, \dots, y_n\}$:

$$y_i \sim \text{Dir}(\alpha), \quad i = 1, \dots, n. \tag{1}$$

Then, the maximum likelihood estimate (\rightarrow Definition I/4.1.3) for the concentration parameters α can be obtained by iteratively computing

$$\alpha_j^{(\text{new})} = \psi^{-1} \left[\psi \left(\sum_{j=1}^k \alpha_j^{(\text{old})} \right) + \log \bar{y}_j \right] \tag{2}$$

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 Definition I/5.1.2) for each observation is given by the probability density function of the Dirichlet distribution (\rightarrow Proof II/4.4.2)

$$p(y_i|\alpha) = \frac{\Gamma\left(\sum_{j=1}^k \alpha_j\right)}{\prod_{j=1}^k \Gamma(\alpha_j)} \prod_{j=1}^k y_{ij}^{\alpha_j-1} \quad (4)$$

and because observations are independent (\rightarrow Definition 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 Definition 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:

$$\begin{aligned} \frac{dLL(\alpha)}{d\alpha_j} &= 0 \\ 0 &= n\psi\left(\sum_{j=1}^k \alpha_j\right) - n\psi(\alpha_j) + n \log \bar{y}_j \\ 0 &= \psi\left(\sum_{j=1}^k \alpha_j\right) - \psi(\alpha_j) + \log \bar{y}_j \\ \psi(\alpha_j) &= \psi\left(\sum_{j=1}^k \alpha_j\right) + \log \bar{y}_j \\ \alpha_j &= \psi^{-1}\left[\psi\left(\sum_{j=1}^k \alpha_j\right) + \log \bar{y}_j\right]. \end{aligned} \quad (11)$$

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 Definition II/4.4.1) belongs to the exponential family (\rightarrow Definition “dist-expfam”), 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

$$\begin{aligned} \Gamma(x) &\geq \Gamma(\hat{x}) \cdot \exp[(x - \hat{x})\psi(\hat{x})] \\ \log \Gamma(x) &\geq \log \Gamma(\hat{x}) + (x - \hat{x})\psi(\hat{x}) \end{aligned} \quad (12)$$

and apply it to $\Gamma\left(\sum_{j=1}^k \alpha_j\right)$ in (7) to yield

$$\begin{aligned} \frac{1}{n}LL(\alpha) &= \log \Gamma\left(\sum_{j=1}^k \alpha_j\right) - \sum_{j=1}^k \log \Gamma(\alpha_j) + \sum_{j=1}^k (\alpha_j - 1) \log \bar{y}_j \\ \frac{1}{n}LL(\alpha) &\geq \log \Gamma\left(\sum_{j=1}^k \hat{\alpha}_j\right) + \left(\sum_{j=1}^k \alpha_j - \sum_{j=1}^k \hat{\alpha}_j\right) \psi\left(\sum_{j=1}^k \hat{\alpha}_j\right) - \sum_{j=1}^k \log \Gamma(\alpha_j) + \sum_{j=1}^k (\alpha_j - 1) \log \bar{y}_j \\ \frac{1}{n}LL(\alpha) &\geq \left(\sum_{j=1}^k \alpha_j\right) \psi\left(\sum_{j=1}^k \hat{\alpha}_j\right) - \sum_{j=1}^k \log \Gamma(\alpha_j) + \sum_{j=1}^k (\alpha_j - 1) \log \bar{y}_j + \text{const.} \end{aligned} \quad (13)$$

which leads to the following fixed-point iteration using (11):

$$\alpha_j^{(\text{new})} = \psi^{-1} \left[\psi \left(\sum_{j=1}^k \alpha_j^{(\text{old})} \right) + \log \bar{y}_j \right] . \quad (14)$$

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>.

Metadata: ID: P182 | shortcut: dir-mle | author: JoramSoch | date: 2020-10-22, 09:31.

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 according to a beta-binomial distribution (\rightarrow Definition II/1.4.1) with number of trials n as well as shapes α and β :

$$y_i \sim \text{BetBin}(n, \alpha, \beta), \quad i = 1, \dots, N . \quad (1)$$

Sources:

- original work

Metadata: ID: D178 | shortcut: betabin-data | author: JoramSoch | date: 2022-10-20, 08:20.

4.3.2 Method of moments

Theorem: Let $y = \{y_1, \dots, y_N\}$ be a set of observed counts independent and identically distributed according to a beta-binomial distribution (\rightarrow Definition 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 Definition I/4.1.6) 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 Definition I/1.15.3):

$$\begin{aligned}
m_1 &= \frac{1}{N} \sum_{i=1}^N y_i \\
m_2 &= \frac{1}{N} \sum_{i=1}^N y_i^2.
\end{aligned} \tag{3}$$

Proof: The first two raw moments of the beta-binomial distribution (\rightarrow Definition “betabin-mom”) in terms of the parameters α and β are given by

$$\begin{aligned}
\mu_1 &= \frac{n\alpha}{\alpha + \beta} \\
\mu_2 &= \frac{n\alpha(n\alpha + \beta + n)}{(\alpha + \beta)(n\alpha + \beta + 1)}
\end{aligned} \tag{4}$$

Thus, matching the moments (\rightarrow Definition I/4.1.6) requires us to solve the following equation system for α and β :

$$\begin{aligned}
m_1 &= \frac{n\alpha}{\alpha + \beta} \\
m_2 &= \frac{n\alpha(n\alpha + \beta + n)}{(\alpha + \beta)(n\alpha + \beta + 1)}.
\end{aligned} \tag{5}$$

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:

$$\begin{aligned}
m_2 &= \frac{n \left(\alpha \left(\frac{n}{m_1} + n - 1 \right) + n \right)}{n \left(\alpha \frac{n}{m_1^2} + \frac{1}{m_1} \right)} \\
m_2 &= \frac{\alpha (n + nm_1 - m_1) + nm_1}{\alpha \frac{n}{m_1} + 1} \\
m_2 \left(\frac{\alpha n}{m_1} + 1 \right) &= \alpha (n + nm_1 - m_1) + nm_1 \\
\alpha \left(n \frac{m_2}{m_1} - (n + nm_1 - m_1) \right) &= nm_1 - m_2 \\
\alpha \left(n \left(\frac{m_2}{m_1} - m_1 - 1 \right) + m_1 \right) &= nm_1 - m_2 \\
\alpha &= \frac{nm_1 - m_2}{n \left(\frac{m_2}{m_1} - m_1 - 1 \right) + m_1}.
\end{aligned} \tag{8}$$

Plugging this into equation (6), one obtains for β :

$$\begin{aligned}
\beta &= \alpha \left(\frac{n}{m_1} - 1 \right) \\
\beta &= \left(\frac{nm_1 - m_2}{n \left(\frac{m_2}{m_1} - m_1 - 1 \right) + m_1} \right) \left(\frac{n}{m_1} - 1 \right) \\
\beta &= \frac{n^2 - nm_1 - n \frac{m_2}{m_1} + m_2}{n \left(\frac{m_2}{m_1} - m_1 - 1 \right) + m_1} \\
\hat{\beta} &= \frac{(n - m_1) \left(n - \frac{m_2}{m_1} \right)}{n \left(\frac{m_2}{m_1} - m_1 - 1 \right) + m_1}.
\end{aligned} \tag{9}$$

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.

Metadata: ID: P357 | shortcut: betabin-mome | author: JoramSoch | date: 2022-10-07, 15:13.

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.

Metadata: ID: D76 | shortcut: logreg | author: JoramSoch | date: 2020-06-28, 20:51.

5.1.2 Probability and log-odds

Theorem: Assume a logistic regression model (\rightarrow Definition 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 Definition I/5.1.2) consistent with (1), $p(y_i)$ are prior probabilities (\rightarrow Definition 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 Proof I/5.3.1) and the law of marginal probability (\rightarrow Definition I/1.3.3), the posterior probabilities (\rightarrow Definition I/5.1.7) for $y_i = 1$ and $y_i = 0$ are given by

$$\begin{aligned} p(y_i = 1|x_i) &= \frac{p(x_i|y_i = 1) p(y_i = 1)}{p(x_i|y_i = 1) p(y_i = 1) + p(x_i|y_i = 0) p(y_i = 0)} \\ p(y_i = 0|x_i) &= \frac{p(x_i|y_i = 0) p(y_i = 0)}{p(x_i|y_i = 1) p(y_i = 1) + p(x_i|y_i = 0) p(y_i = 0)} . \end{aligned} \quad (3)$$

Calculating the log-odds from the posterior probabilities, we have

$$\begin{aligned} l_i &= \log_b \frac{p(y_i = 1|x_i)}{p(y_i = 0|x_i)} \\ &= \log_b \frac{p(x_i|y_i = 1) p(y_i = 1)}{p(x_i|y_i = 0) p(y_i = 0)} . \end{aligned} \quad (4)$$

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>.

Metadata: ID: P105 | shortcut: logreg-pnlo | author: JoramSoch | date: 2020-05-19, 05:08.

5.1.3 Log-odds and probability

Theorem: Assume a logistic regression model (\rightarrow Definition 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 probability that $y_i = 1$ is given by

$$\Pr(y_i = 1) = \frac{1}{1 + b^{-(x_i \beta + \varepsilon_i)}} \quad (2)$$

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

$$l_i = \log_b \frac{p_i}{1 - p_i} \quad (3)$$

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.

Metadata: ID: P72 | shortcut: logreg-lonp | author: JoramSoch | date: 2020-03-03, 12:01.

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 Definition 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 Definition I/4.1.3).

Sources:

- original work

Metadata: ID: D20 | shortcut: resvar | author: JoramSoch | date: 2020-02-25, 11:21.

1.1.2 Maximum likelihood estimator is biased ($p = 1$)

Theorem: Let $x = \{x_1, \dots, x_n\}$ be a set of independent normally distributed (\rightarrow Definition II/3.2.1) observations with unknown mean (\rightarrow Definition I/1.7.1) μ and variance (\rightarrow Definition I/1.8.1) σ^2 :

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

Then,

1) the maximum likelihood estimator (\rightarrow Definition I/4.1.3) of σ^2 is

$$\hat{\sigma}^2 = \frac{1}{n} \sum_{i=1}^n (x_i - \bar{x})^2 \quad (2)$$

where

$$\bar{x} = \frac{1}{n} \sum_{i=1}^n x_i \quad (3)$$

2) and $\hat{\sigma}^2$ is a biased estimator (\rightarrow Definition “est-unb”) 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 Proof III/1.1.2) and a special case of the maximum likelihood estimator for multiple linear regression (\rightarrow Proof III/1.5.25) in which $y = x$, $X = 1_n$ and $\hat{\beta} = \bar{x}$:

$$\begin{aligned}
\hat{\sigma}^2 &= \frac{1}{n}(y - X\hat{\beta})^T(y - X\hat{\beta}) \\
&= \frac{1}{n}(x - 1_n\bar{x})^T(x - 1_n\bar{x}) \\
&= \frac{1}{n} \sum_{i=1}^n (x_i - \bar{x})^2 .
\end{aligned} \tag{6}$$

2) The expectation (\rightarrow Definition I/1.7.1) of the maximum likelihood estimator (\rightarrow Definition I/4.1.3) can be developed as follows:

$$\begin{aligned}
E[\hat{\sigma}^2] &= E\left[\frac{1}{n} \sum_{i=1}^n (x_i - \bar{x})^2\right] \\
&= \frac{1}{n} E\left[\sum_{i=1}^n (x_i - \bar{x})^2\right] \\
&= \frac{1}{n} E\left[\sum_{i=1}^n (x_i^2 - 2x_i\bar{x} + \bar{x}^2)\right] \\
&= \frac{1}{n} E\left[\sum_{i=1}^n x_i^2 - 2 \sum_{i=1}^n x_i\bar{x} + \sum_{i=1}^n \bar{x}^2\right] \\
&= \frac{1}{n} E\left[\sum_{i=1}^n x_i^2 - 2n\bar{x}^2 + n\bar{x}^2\right] \\
&= \frac{1}{n} E\left[\sum_{i=1}^n x_i^2 - n\bar{x}^2\right] \\
&= \frac{1}{n} \left(\sum_{i=1}^n E[x_i^2] - nE[\bar{x}^2]\right) \\
&= \frac{1}{n} \sum_{i=1}^n E[x_i^2] - E[\bar{x}^2]
\end{aligned} \tag{7}$$

Due to the partition of variance into expected values (\rightarrow Proof I/1.8.3)

$$\text{Var}(X) = E(X^2) - E(X)^2 , \tag{8}$$

we have

$$\begin{aligned}
\text{Var}(x_i) &= E(x_i^2) - E(x_i)^2 \\
\text{Var}(\bar{x}) &= E(\bar{x}^2) - E(\bar{x})^2 ,
\end{aligned} \tag{9}$$

such that (7) becomes

$$E[\hat{\sigma}^2] = \frac{1}{n} \sum_{i=1}^n (\text{Var}(x_i) + E(x_i)^2) - (\text{Var}(\bar{x}) + E(\bar{x})^2) . \tag{10}$$

From (1), it follows that

$$\mathbb{E}(x_i) = \mu \quad \text{and} \quad \text{Var}(x_i) = \sigma^2. \quad (11)$$

The expectation (\rightarrow Definition I/1.7.1) of \bar{x} given by (3) is

$$\begin{aligned} \mathbb{E}[\bar{x}] &= \mathbb{E}\left[\frac{1}{n} \sum_{i=1}^n x_i\right] = \frac{1}{n} \sum_{i=1}^n \mathbb{E}[x_i] \\ &\stackrel{(11)}{=} \frac{1}{n} \sum_{i=1}^n \mu = \frac{1}{n} \cdot n \cdot \mu \\ &= \mu. \end{aligned} \quad (12)$$

The variance of \bar{x} given by (3) is

$$\begin{aligned} \text{Var}[\bar{x}] &= \text{Var}\left[\frac{1}{n} \sum_{i=1}^n x_i\right] = \frac{1}{n^2} \sum_{i=1}^n \text{Var}[x_i] \\ &\stackrel{(11)}{=} \frac{1}{n^2} \sum_{i=1}^n \sigma^2 = \frac{1}{n^2} \cdot n \cdot \sigma^2 \\ &= \frac{1}{n} \sigma^2. \end{aligned} \quad (13)$$

Plugging (11), (12) and (13) into (10), we have

$$\begin{aligned} \mathbb{E}[\hat{\sigma}^2] &= \frac{1}{n} \sum_{i=1}^n (\sigma^2 + \mu^2) - \left(\frac{1}{n} \sigma^2 + \mu^2\right) \\ \mathbb{E}[\hat{\sigma}^2] &= \frac{1}{n} \cdot n \cdot (\sigma^2 + \mu^2) - \left(\frac{1}{n} \sigma^2 + \mu^2\right) \\ \mathbb{E}[\hat{\sigma}^2] &= \sigma^2 + \mu^2 - \frac{1}{n} \sigma^2 - \mu^2 \\ \mathbb{E}[\hat{\sigma}^2] &= \frac{n-1}{n} \sigma^2 \end{aligned} \quad (14)$$

which proves the bias (\rightarrow Definition “est-unb”) given by (5).

Sources:

- Liang, Dawen (????): “Maximum Likelihood Estimator for Variance is Biased: Proof”, retrieved on 2020-02-24; URL: https://dawenl.github.io/files/mle_biased.pdf.

Metadata: ID: P61 | shortcut: resvar-bias | author: JoramSoch | date: 2020-02-24, 23:44.

1.1.3 Maximum likelihood estimator is biased ($p > 1$)

Theorem: Consider a linear regression model (\rightarrow Definition III/1.5.1) with known design matrix X , known covariance structure V , unknown regression parameters β and unknown noise variance σ^2 :

$$y = X\beta + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2 V) . \quad (1)$$

Then,

1) the maximum likelihood estimator (\rightarrow Definition 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 Definition “est-unb”) of σ^2

$$\mathbb{E} [\hat{\sigma}^2] \neq \sigma^2 , \quad (4)$$

more precisely:

$$\mathbb{E} [\hat{\sigma}^2] = \frac{n-p}{n} \sigma^2 . \quad (5)$$

Proof:

1) This follows from maximum likelihood estimation for multiple linear regression (\rightarrow Proof III/1.5.25) and is a special case (\rightarrow Proof III/1.5.2) of maximum likelihood estimation for the general linear model (\rightarrow Proof III/2.1.4) 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 Proof III/1.5.18):

$$\begin{aligned} \frac{\hat{\varepsilon}^T \hat{\varepsilon}}{\sigma^2} &\sim \chi^2(n-p) \\ \text{where } \hat{\varepsilon}^T \hat{\varepsilon} &= (y - X\hat{\beta})^T V^{-1} (y - X\hat{\beta}) . \end{aligned} \quad (7)$$

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 Proof 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 Proof II/3.4.9)

$$X \sim \text{Gam}(a, b) \quad \Rightarrow \quad \mathbb{E}(X) = \frac{a}{b}, \quad (11)$$

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:

- ocrum (2022): “Why is RSS distributed chi square times n-p?”; in: *StackExchange CrossValidated*, retrieved on 2022-12-21; URL: <https://stats.stackexchange.com/a/20230>.

Metadata: ID: P398 | shortcut: resvar-biasp | author: JoramSoch | date: 2022-12-21, 14:15.

1.1.4 Construction of unbiased estimator

Theorem: Let $x = \{x_1, \dots, x_n\}$ be a set of independent normally distributed (\rightarrow Definition II/3.2.1) observations with unknown mean (\rightarrow Definition I/1.7.1) μ and variance (\rightarrow Definition I/1.8.1) σ^2 :

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

An unbiased estimator (\rightarrow Definition “est-unb”) of σ^2 is given by

$$\hat{\sigma}_{\text{unb}}^2 = \frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x})^2. \quad (2)$$

Proof: It can be shown that (\rightarrow Proof IV/1.1.2) the maximum likelihood estimator (\rightarrow Definition I/4.1.3) of σ^2

$$\hat{\sigma}_{\text{MLE}}^2 = \frac{1}{n} \sum_{i=1}^n (x_i - \bar{x})^2 \quad (3)$$

is a biased estimator (\rightarrow Definition “est-unb”) 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 Definition “est-unb”) can be constructed as

$$\begin{aligned}
\hat{\sigma}_{\text{unb}}^2 &= \frac{n}{n-1} \hat{\sigma}_{\text{MLE}}^2 \\
&\stackrel{(3)}{=} \frac{n}{n-1} \cdot \frac{1}{n} \sum_{i=1}^n (x_i - \bar{x})^2 \\
&= \frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x})^2 .
\end{aligned} \tag{6}$$

Sources:

- Liang, Dawen (????): “Maximum Likelihood Estimator for Variance is Biased: Proof”, retrieved on 2020-02-25; URL: https://dawenl.github.io/files/mle_biased.pdf.

Metadata: ID: P62 | shortcut: resvar-unb | author: JoramSoch | date: 2020-02-25, 15:38.

1.2 R-squared

1.2.1 Definition

Definition: Let there be a linear regression model (\rightarrow Definition III/1.5.1) with independent (\rightarrow Definition 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 .

Then, the proportion of the variance of the dependent variable y (“total variance (\rightarrow Definition III/1.5.5)”) that can be predicted from the independent variables X (“explained variance (\rightarrow Definition III/1.5.6)”) 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.

Metadata: ID: D21 | shortcut: rsq | author: JoramSoch | date: 2020-02-25, 11:41.

1.2.2 Derivation of R^2 and adjusted R^2

Theorem: Given a linear regression model (\rightarrow Definition III/1.5.1)

$$y = X\beta + \varepsilon, \quad \varepsilon_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2) \tag{1}$$

with n independent observations and p independent variables,

1) the coefficient of determination (\rightarrow Definition IV/1.2.1) is given by

$$R^2 = 1 - \frac{\text{RSS}}{\text{TSS}} \tag{2}$$

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 Definition III/1.5.7) and total sum of squares (\rightarrow Definition III/1.5.5) 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 Proof III/1.5.3) estimates.

Proof: The coefficient of determination (\rightarrow Definition 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 Definition III/1.5.6) 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 (\rightarrow Proof III/1.5.8) $\text{TSS} = \text{ESS} + \text{RSS}$.

2) Using (4), the coefficient of determination can be also written as:

$$R^2 = 1 - \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2} = 1 - \frac{\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2}{\frac{1}{n} \sum_{i=1}^n (y_i - \bar{y})^2}. \quad (8)$$

If we replace the variance estimates by their unbiased estimators (\rightarrow Proof IV/1.1.4), we obtain

$$R_{\text{adj}}^2 = 1 - \frac{\frac{1}{n-p} \sum_{i=1}^n (y_i - \hat{y}_i)^2}{\frac{1}{n-1} \sum_{i=1}^n (y_i - \bar{y})^2} = 1 - \frac{\text{RSS}/\text{df}_r}{\text{TSS}/\text{df}_t} \quad (9)$$

where $\text{df}_r = n - p$ and $\text{df}_t = n - 1$ are the residual and total degrees of freedom (\rightarrow Definition “dof”).

This gives the adjusted R^2 which adjusts R^2 for the number of explanatory variables.

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.

Metadata: ID: P8 | shortcut: rsq-der | author: JoramSoch | date: 2019-12-06, 11:19.

1.2.3 Relationship to maximum log-likelihood

Theorem: Given a linear regression model (\rightarrow Definition 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 coefficient of determination (\rightarrow Definition IV/1.2.1) can be expressed in terms of the maximum log-likelihood (\rightarrow Definition I/4.1.5) 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 Definition I/4.1.5) (MLL) of a linear regression model in terms of its residual sum of squares (\rightarrow Definition III/1.5.7) (RSS). The model in (1) implies the following log-likelihood function (\rightarrow Definition 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 Proof III/1.5.25)

$$\hat{\beta} = (X^T X)^{-1} X^T y \quad (4)$$

$$\hat{\sigma}^2 = \frac{1}{n} (y - X\hat{\beta})^T (y - X\hat{\beta}) \quad (5)$$

and the residual sum of squares (\rightarrow Definition III/1.5.7) 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 Definition 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 Definition III/1.5.5):

$$\text{TSS} = \sum_{i=1}^n (y_i - \bar{y})^2 . \quad (10)$$

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:

$$\begin{aligned} \exp[\Delta\text{MLL}] &= \exp \left[-\frac{n}{2} \log(\text{RSS}) + \frac{n}{2} \log(\text{TSS}) \right] \\ &= (\exp [\log(\text{RSS}) - \log(\text{TSS})])^{-n/2} \\ &= \left(\frac{\exp[\log(\text{RSS})]}{\exp[\log(\text{TSS})]} \right)^{-n/2} \\ &= \left(\frac{\text{RSS}}{\text{TSS}} \right)^{-n/2} . \end{aligned} \quad (12)$$

Taking both sides to the power of $-2/n$ and subtracting from 1, we have

$$\begin{aligned} (\exp[\Delta\text{MLL}])^{-2/n} &= \frac{\text{RSS}}{\text{TSS}} \\ 1 - (\exp[\Delta\text{MLL}])^{-2/n} &= 1 - \frac{\text{RSS}}{\text{TSS}} = R^2 \end{aligned} \quad (13)$$

which proves the identity given above.

Sources:

- original work

Metadata: ID: P14 | shortcut: rsq-mll | author: JoramSoch | date: 2020-01-08, 04:46.

1.3 Signal-to-noise ratio

1.3.1 Definition

Definition: Let there be a linear regression model (\rightarrow Definition III/1.5.1) with independent (\rightarrow Definition I/1.3.6) observations

$$y = X\beta + \varepsilon, \quad \varepsilon_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2) \quad (1)$$

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 Proof III/1.5.25) $\hat{\beta}$ and residual variance (\rightarrow Definition 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:

$$\text{SNR} = \frac{\text{Var}(X\hat{\beta})}{\hat{\sigma}^2} . \quad (2)$$

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. 6; URL: <https://www.sciencedirect.com/science/article/pii/S0165027018301468>; DOI: 10.1016/j.jneumeth.2018.05.017.

Metadata: ID: D22 | shortcut: snr | author: JoramSoch | date: 2020-02-25, 12:01.

1.3.2 Relationship with R^2

Theorem: Let there be a linear regression model (\rightarrow Definition III/1.5.1) with independent (\rightarrow Definition 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 Definition “est”) obtained with ordinary least squares (\rightarrow Proof III/1.5.3)

$$\hat{\beta} = (X^T X)^{-1} X^T y. \quad (2)$$

Then, the signal-to noise ratio (\rightarrow Definition IV/1.3.1) can be expressed in terms of the coefficient of determination (\rightarrow Definition 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 Definition IV/1.3.1) (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 variances, 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 Proof IV/1.1.2) (dividing by n) or the unbiased estimator for the variance (\rightarrow Proof 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 Definition III/1.5.6), residual (\rightarrow Definition III/1.5.7) and total sum of squares (\rightarrow Definition III/1.5.5):

$$\text{SNR} = \frac{\text{ESS}}{\text{RSS}} = \frac{\text{ESS}/\text{TSS}}{\text{RSS}/\text{TSS}} . \quad (8)$$

With the derivation of the coefficient of determination (\rightarrow Proof 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 Definition IV/1.2.1), we have

$$R^2 = \frac{\text{SNR}}{1 + \text{SNR}} , \quad (10)$$

Sources:

- original work

Metadata: ID: P63 | shortcut: snr-rsq | author: JoramSoch | date: 2020-02-26, 10:37.

2 Classical information criteria

2.1 Akaike information criterion

2.1.1 Definition

Definition: Let m be a generative model (\rightarrow Definition I/5.1.1) with likelihood function (\rightarrow Definition I/5.1.2) $p(y|\theta, m)$ and maximum likelihood estimates (\rightarrow Definition 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.

Metadata: ID: D23 | shortcut: aic | author: JoramSoch | date: 2020-02-25, 12:31.

2.1.2 Corrected AIC

Definition: Let m be a generative model (\rightarrow Definition I/5.1.1) with likelihood function (\rightarrow Definition I/5.1.2) $p(y|\theta, m)$ and maximum likelihood estimates (\rightarrow Definition I/4.1.3)

$$\hat{\theta} = \arg \max_{\theta} \log p(y|\theta, m) . \quad (1)$$

Then, the corrected Akaike information criterion (\rightarrow Definition 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 Definition 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.

Metadata: ID: D171 | shortcut: aicc | author: JoramSoch | date: 2022-02-11, 06:49.

2.1.3 Corrected AIC and uncorrected AIC

Theorem: In the infinite data limit, the corrected Akaike information criterion (\rightarrow Definition IV/2.1.2) converges to the uncorrected Akaike information criterion (\rightarrow Definition IV/2.1.1)

$$\lim_{n \rightarrow \infty} \text{AIC}_c(m) = \text{AIC}(m) . \quad (1)$$

Proof: The corrected Akaike information criterion (\rightarrow Definition 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.

Metadata: ID: P316 | shortcut: aicc-aic | author: JoramSoch | date: 2022-03-18, 17:00.

2.1.4 Corrected AIC and maximum log-likelihood

Theorem: The corrected Akaike information criterion (\rightarrow Definition IV/2.1.2) of a generative model (\rightarrow Definition I/5.1.1) with likelihood function (\rightarrow Definition 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 Definition I/4.1.5), k is the number of free parameters and n is the number of observations.

Proof: The Akaike information criterion (\rightarrow Definition 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 Definition 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:

$$\begin{aligned}
\text{AIC}_c(m) &= -2 \log p(y|\hat{\theta}, m) + 2k + \frac{2k^2 + 2k}{n - k - 1} \\
&= -2 \log p(y|\hat{\theta}, m) + \frac{2k(n - k - 1)}{n - k - 1} + \frac{2k^2 + 2k}{n - k - 1} \\
&= -2 \log p(y|\hat{\theta}, m) + \frac{2nk - 2k^2 - 2k}{n - k - 1} + \frac{2k^2 + 2k}{n - k - 1} \\
&= -2 \log p(y|\hat{\theta}, m) + \frac{2nk}{n - k - 1} .
\end{aligned} \tag{4}$$

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.

Metadata: ID: P315 | shortcut: aicc-ml | author: JoramSoch | date: 2022-03-11, 16:53.

2.2 Bayesian information criterion

2.2.1 Definition

Definition: Let m be a generative model (\rightarrow Definition I/5.1.1) with likelihood function (\rightarrow Definition I/5.1.2) $p(y|\theta, m)$ and maximum likelihood estimates (\rightarrow Definition I/4.1.3)

$$\hat{\theta} = \arg \max_{\theta} \log p(y|\theta, m) . \tag{1}$$

Then, the Bayesian information criterion (BIC) of this model is defined as

$$\text{BIC}(m) = -2 \log p(y|\hat{\theta}, m) + k \log n \tag{2}$$

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>.

Metadata: ID: D24 | shortcut: bic | author: JoramSoch | date: 2020-02-25, 12:21.

2.2.2 Derivation

Theorem: Let $p(y|\theta, m)$ be the likelihood function (\rightarrow Definition I/5.1.2) of a generative model (\rightarrow Definition I/5.1.1) $m \in \mathcal{M}$ with model parameters $\theta \in \Theta$ describing measured data $y \in \mathbb{R}^n$. Let $p(\theta|m)$ be a prior distribution (\rightarrow Definition 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 goes to infinity, an approximation to the log-marginal likelihood (\rightarrow Definition I/5.1.9) $\log p(y|m)$, up to constant terms not depending on the model, is given by the Bayesian information criterion (\rightarrow Definition 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 Definition 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 Definition 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 Definition I/5.1.9) 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 Definition 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>; DOI: 10.1017/CBO9780511790485.

Metadata: ID: P32 | shortcut: bic-der | author: JoramSoch | date: 2020-01-26, 23:36.

2.3 Deviance information criterion

2.3.1 Definition

Definition: Let m be a full probability model (\rightarrow Definition I/5.1.4) with likelihood function (\rightarrow Definition I/5.1.2) $p(y|\theta, m)$ and prior distribution (\rightarrow Definition I/5.1.3) $p(\theta|m)$. Together, likelihood function and prior distribution imply a posterior distribution (\rightarrow Proof I/5.1.8) $p(\theta|y, m)$. Consider the deviance (\rightarrow Definition IV/2.3.2) which is minus two times the log-likelihood function (\rightarrow Definition 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 Definition I/4.1.2) at the posterior (\rightarrow Definition I/5.1.7) expectation (\rightarrow Definition I/1.7.1) and the “effective number of parameters” p_D is the difference between the expectation of the deviance and the deviance at the expectation (\rightarrow Definition 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 Definition I/1.7.1) across the posterior distribution (\rightarrow Definition I/5.1.7).

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.

Metadata: ID: D25 | shortcut: dic | author: JoramSoch | date: 2020-02-25, 12:46.

2.3.2 Deviance

Definition: Let there be a generative model (\rightarrow Definition 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 Definition 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 Definition 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.

Metadata: ID: D172 | shortcut: dev | author: JoramSoch | date: 2022-03-01, 07:48.

3 Bayesian model selection

3.1 Model evidence

3.1.1 Definition

Definition: Let m be a generative model (\rightarrow Definition I/5.1.1) with likelihood function (\rightarrow Definition I/5.1.2) $p(y|\theta, m)$ and prior distribution (\rightarrow Definition I/5.1.3) $p(\theta|m)$. Then, the model evidence (ME) of m is defined as the marginal likelihood (\rightarrow Definition I/5.1.9) 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.

Metadata: ID: D179 | shortcut: me | author: JoramSoch | date: 2022-10-20, 09:43.

3.1.2 Derivation

Theorem: Let $p(y|\theta, m)$ be a likelihood function (\rightarrow Definition I/5.1.2) of a generative model (\rightarrow Definition 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 Definition I/5.1.3) on model parameters θ in the parameter space Θ . Then, the model evidence (\rightarrow Definition IV/3.1.1) (ME) can be expressed in terms of likelihood (\rightarrow Definition I/5.1.2) and prior (\rightarrow Definition I/5.1.3) as

$$\text{ME}(m) = \int_{\Theta} p(y|\theta, m) p(\theta|m) d\theta . \quad (1)$$

Proof: This a consequence of the law of marginal probability (\rightarrow Definition I/1.3.3) for continuous variables (\rightarrow Definition I/1.2.6)

$$p(y|m) = \int_{\Theta} p(y, \theta|m) d\theta \quad (2)$$

and the law of conditional probability (\rightarrow Definition 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:

$$\text{ME}(m) = p(y|m) = \int_{\Theta} p(y|\theta, m) p(\theta|m) d\theta . \quad (4)$$

Sources:

- original work

Metadata: ID: P367 | shortcut: me-der | author: JoramSoch | date: 2022-10-20, 10:11.

3.1.3 Log model evidence

Definition: Let m be a full probability model (\rightarrow Definition I/5.1.4) with likelihood function (\rightarrow Definition I/5.1.2) $p(y|\theta, m)$ and prior distribution (\rightarrow Definition 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 Definition I/5.1.9) 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.

Metadata: ID: D26 | shortcut: lme | author: JoramSoch | date: 2020-02-25, 12:56.

3.1.4 Derivation of the LME

Theorem: Let $p(y|\theta, m)$ be a likelihood function (\rightarrow Definition I/5.1.2) of a generative model (\rightarrow Definition 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 Definition I/5.1.3) on model parameters θ . Then, the log model evidence (\rightarrow Definition 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 Definition I/5.1.2) and prior (\rightarrow Definition I/5.1.3) as

$$\text{LME}(m) = \log \int p(y|\theta, m) p(\theta|m) d\theta . \quad (2)$$

Proof: This a consequence of the law of marginal probability (\rightarrow Definition I/1.3.3) for continuous variables (\rightarrow Definition I/1.2.6)

$$p(y|m) = \int p(y, \theta|m) d\theta \quad (3)$$

and the law of conditional probability (\rightarrow Definition 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:

$$\text{LME}(m) = \log p(y|m) = \log \int p(y|\theta, m) p(\theta|m) d\theta . \quad (5)$$

Sources:

- original work

Metadata: ID: P13 | shortcut: lme-der | author: JoramSoch | date: 2020-01-06, 21:27.

3.1.5 Expression using prior and posterior

Theorem: Let $p(y|\theta, m)$ be a likelihood function (\rightarrow Definition I/5.1.2) of a generative model (\rightarrow Definition 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 Definition I/5.1.3) on model parameters θ . Then, the log model evidence (\rightarrow Definition 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 Definition I/5.1.3) and posterior (\rightarrow Definition I/5.1.7) 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 Definition I/5.1.4), Bayes' theorem (\rightarrow Proof I/5.3.1) makes a statement about the posterior distribution (\rightarrow Definition I/5.1.7):

$$p(\theta|y, m) = \frac{p(y|\theta, m) p(\theta|m)}{p(y|m)} . \quad (3)$$

Rearranging for $p(y|m)$ and logarithmizing, we have:

$$\begin{aligned} \text{LME}(m) = \log p(y|m) &= \log \frac{p(y|\theta, m) p(\theta|m)}{p(\theta|y, m)} \\ &= \log p(y|\theta, m) + \log p(\theta|m) - \log p(\theta|y, m) . \end{aligned} \quad (4)$$

Sources:

- original work

Metadata: ID: P314 | shortcut: lme-pnp | author: JoramSoch | date: 2022-03-11, 16:25.

3.1.6 Partition into accuracy and complexity

Theorem: The log model evidence (\rightarrow Definition 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 Definition I/5.1.7) expectation (\rightarrow Proof I/1.7.12) of the log-likelihood function (\rightarrow Definition 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 Definition I/2.5.1) of posterior (\rightarrow Definition I/5.1.7) from prior (\rightarrow Definition 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 Definition “data”) y using model (\rightarrow Definition I/5.1.1) m with parameters θ . Then, Bayes' theorem (\rightarrow Proof I/5.3.1) makes a statement about the

posterior distribution (\rightarrow Definition I/5.1.7), 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 Proof 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:

- 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.
- 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.

Metadata: ID: P3 | shortcut: lme-anc | author: JoramSoch | date: 2019-09-27, 16:13.

3.1.7 Uniform-prior log model evidence

Definition: Assume a generative model (\rightarrow Definition I/5.1.1) m with likelihood function (\rightarrow Definition I/5.1.2) $p(y|\theta, m)$ and a uniform (\rightarrow Definition I/5.2.2) prior distribution (\rightarrow Definition I/5.1.3) $p_{\text{uni}}(\theta|m)$. Then, the log model evidence (\rightarrow Definition IV/3.1.3) of this model is called “log model evidence with uniform prior” or “uniform-prior log model evidence” (upLME):

$$\text{upLME}(m) = \log \int p(y|\theta, m) p_{\text{uni}}(\theta|m) d\theta . \quad (1)$$

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.

Metadata: ID: D113 | shortcut: uplme | author: JoramSoch | date: 2020-11-25, 07:28.

3.1.8 Cross-validated log model evidence

Definition: Let there be a data set (\rightarrow Definition “data”) y with mutually exclusive and collectively exhaustive subsets y_1, \dots, y_S . Assume a generative model (\rightarrow Definition I/5.1.1) m with model parameters θ implying a likelihood function (\rightarrow Definition I/5.1.2) $p(y|\theta, m)$ and a non-informative (\rightarrow Definition I/5.2.3) prior density (\rightarrow Definition I/5.1.3) $p_{\text{ni}}(\theta|m)$.

Then, the cross-validated log model evidence 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 Definition I/5.1.7) obtained from y_{-i} when using the prior distribution (\rightarrow Definition I/5.1.3) $p_{\text{ni}}(\theta|m)$:

$$p(\theta|y_{-i}, m) = \frac{p(y_{-i}|\theta, m) p_{\text{ni}}(\theta|m)}{p(y_{-i}|m)}. \quad (2)$$

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*, arXiv:1807.01585; URL: <https://arxiv.org/abs/1807.01585>.

Metadata: ID: D111 | shortcut: cvlme | author: JoramSoch | date: 2020-11-19, 04:55.

3.1.9 Empirical Bayesian log model evidence

Definition: Let m be a generative model (\rightarrow Definition I/5.1.1) with model parameters θ and hyper-parameters λ implying the likelihood function (\rightarrow Definition I/5.1.2) $p(y|\theta, \lambda, m)$ and prior distribution (\rightarrow Definition I/5.1.3) $p(\theta|\lambda, m)$. Then, the Empirical Bayesian (\rightarrow Definition I/5.3.3) log model evidence (\rightarrow Definition IV/3.1.3) is the logarithm of the marginal likelihood (\rightarrow Definition I/5.1.9), maximized with respect to the hyper-parameters:

$$\text{ebLME}(m) = \log p(y|\hat{\lambda}, m) \quad (1)$$

where

$$p(y|\lambda, m) = \int p(y|\theta, \lambda, m) (\theta|\lambda, m) d\theta \quad (2)$$

and (\rightarrow Definition 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.

Metadata: ID: D114 | shortcut: eblme | author: JoramSoch | date: 2020-11-25, 07:43.

3.1.10 Variational Bayesian log model evidence

Definition: Let m be a generative model (\rightarrow Definition I/5.1.1) with model parameters θ implying the likelihood function (\rightarrow Definition I/5.1.2) $p(y|\theta, m)$ and prior distribution (\rightarrow Definition I/5.1.3) $p(\theta|m)$. Moreover, assume an approximate (\rightarrow Definition I/5.3.4) posterior distribution (\rightarrow Definition I/5.1.7) $q(\theta)$. Then, the Variational Bayesian (\rightarrow Definition I/5.3.4) log model evidence (\rightarrow Definition IV/3.1.3), also referred to as the “negative free energy”, is the expectation of the log-likelihood function (\rightarrow Definition I/4.1.2) with respect to the approximate posterior, minus the Kullback-Leibler divergence (\rightarrow Definition I/2.5.1) between approximate posterior and the prior distribution:

$$\text{vbLME}(m) = \langle \log p(y|\theta, m) \rangle_{q(\theta)} - \text{KL} [q(\theta)||p(\theta|m)] \quad (1)$$

where

$$\langle \log p(y|\theta, m) \rangle_{q(\theta)} = \int q(\theta) \log p(y|\theta, m) d\theta \quad (2)$$

and

$$\text{KL} [q(\theta)||p(\theta|m)] = \int q(\theta) \log \frac{q(\theta)}{p(\theta|m)} d\theta . \quad (3)$$

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.

Metadata: ID: D115 | shortcut: vblme | author: JoramSoch | date: 2020-11-25, 08:10.

3.2 Family evidence

3.2.1 Definition

Definition: Let f be a family of M generative models (\rightarrow Definition 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 Definition I/1.3.3) relative to the model evidences (\rightarrow Definition 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.

Metadata: ID: D180 | shortcut: fe | author: JoramSoch | date: 2022-10-20, 09:57.

3.2.2 Derivation

Theorem: Let f be a family of M generative models (\rightarrow Definition I/5.1.1) m_1, \dots, m_M with model evidences (\rightarrow Definition IV/3.1.1) $p(y|m_1), \dots, p(y|m_M)$. Then, the family evidence (\rightarrow Definition 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 Definition IV/3.2.3) prior (\rightarrow Definition I/5.1.3) model (\rightarrow Definition I/5.1.1) probabilities (\rightarrow Definition I/1.3.1).

Proof: This a consequence of the law of marginal probability (\rightarrow Definition I/1.3.3) for discrete variables (\rightarrow Definition 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 Definition 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 Definition 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:

$$\text{FE}(f) = p(y|f) = \sum_{i=1}^M p(y|m_i) p(m_i|f) . \quad (5)$$

Sources:

- original work

Metadata: ID: P368 | shortcut: fe-der | author: JoramSoch | date: 2022-10-20, 10:47.

3.2.3 Log family evidence

Definition: Let f be a family of M generative models (\rightarrow Definition 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 Definition 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.

Metadata: ID: D80 | shortcut: lfe | author: JoramSoch | date: 2020-07-13, 22:31.

3.2.4 Derivation of the LFE

Theorem: Let f be a family of M generative models (\rightarrow Definition I/5.1.1) m_1, \dots, m_M with model evidences (\rightarrow Definition I/5.1.9) $p(y|m_1), \dots, p(y|m_M)$. Then, the log family evidence (\rightarrow Definition 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 Definition IV/3.2.3) prior (\rightarrow Definition I/5.1.3) model (\rightarrow Definition I/5.1.1) probabilities (\rightarrow Definition 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 Proof I/5.3.1) for the family evidence (\rightarrow Definition 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 Proof I/5.3.1) for the model evidence (\rightarrow Definition 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

$$\begin{aligned} p(y|f) &= \frac{\sum_{i=1}^M p(y|m_i) p(m_i)}{\sum_{i=1}^M p(m_i)} \\ &= \sum_{i=1}^M p(y|m_i) \cdot \frac{p(m_i)}{\sum_{i=1}^M p(m_i)} \\ &= \sum_{i=1}^M p(y|m_i) \cdot \frac{p(m_i, f)}{p(f)} \\ &= \sum_{i=1}^M p(y|m_i) \cdot p(m_i|f) . \end{aligned} \quad (9)$$

Equation (2) follows by logarithmizing both sides of (9).

Sources:

- original work

Metadata: ID: P132 | shortcut: lfe-der | author: JoramSoch | date: 2020-07-13, 22:58.

3.2.5 Calculation from log model evidences

Theorem: Let m_1, \dots, m_M be M statistical models with log model evidences (\rightarrow Definition IV/3.1.3) $\text{LME}(m_1), \dots, \text{LME}(m_M)$ and belonging to F mutually exclusive model families f_1, \dots, f_F . Then, the log family evidences (\rightarrow Definition IV/3.2.3) are given by:

$$\text{LFE}(f_j) = \log \sum_{m_i \in f_j} [\exp[\text{LME}(m_i)] \cdot p(m_i|f_j)], \quad j = 1, \dots, F, \quad (1)$$

where $p(m_i|f_j)$ are within-family (\rightarrow Definition IV/3.2.3) prior (\rightarrow Definition I/5.1.3) model (\rightarrow Definition I/5.1.1) probabilities (\rightarrow Definition I/1.3.1).

Proof: Let us consider the (unlogarithmized) family evidence $p(y|f_j)$. According to the law of marginal probability (\rightarrow Definition I/1.3.3), this conditional probability is given by

$$p(y|f_j) = \sum_{m_i \in f_j} [p(y|m_i, f_j) \cdot p(m_i|f_j)] . \quad (2)$$

Because model families are mutually exclusive, it holds that $p(y|m_i, f_j) = p(y|m_i)$, such that

$$p(y|f_j) = \sum_{m_i \in f_j} [p(y|m_i) \cdot p(m_i|f_j)] . \quad (3)$$

Logarithmizing transforms the family evidence $p(y|f_j)$ into the log family evidence $\text{LFE}(f_j)$:

$$\text{LFE}(f_j) = \log \sum_{m_i \in f_j} [p(y|m_i) \cdot p(m_i|f_j)] . \quad (4)$$

The definition of the log model evidence (\rightarrow Definition IV/3.1.3)

$$\text{LME}(m) = \log p(y|m) \quad (5)$$

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.

Metadata: ID: P65 | shortcut: lfe-lme | author: JoramSoch | date: 2020-02-27, 21:16.

3.3 Bayes factor

3.3.1 Definition

Definition: Consider two competing generative models (\rightarrow Definition 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 Definition I/5.1.9) of m_1 and m_2 :

$$\text{BF}_{12} = \frac{p(y \mid m_1)}{p(y \mid m_2)}. \quad (1)$$

Note that by Bayes' theorem (\rightarrow Proof I/5.3.1), the ratio of posterior model probabilities (\rightarrow Definition IV/3.4.1) (i.e., the posterior model odds) can be written as

$$\frac{p(m_1 \mid y)}{p(m_2 \mid y)} = \frac{p(m_1)}{p(m_2)} \cdot \frac{p(y \mid m_1)}{p(y \mid m_2)}, \quad (2)$$

or equivalently by (1),

$$\frac{p(m_1 \mid y)}{p(m_2 \mid y)} = \frac{p(m_1)}{p(m_2)} \cdot \text{BF}_{12}. \quad (3)$$

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 Proof I/5.3.2).

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.

Metadata: ID: D92 | shortcut: bf | author: tomfaulkenberry | date: 2020-08-26, 12:00.

3.3.2 Transitivity

Theorem: Consider three competing models (\rightarrow Definition I/5.1.1) m_1 , m_2 , and m_3 for observed data y . Then the Bayes factor (\rightarrow Definition IV/3.3.1) for m_1 over m_3 can be written as:

$$\text{BF}_{13} = \text{BF}_{12} \cdot \text{BF}_{23}. \quad (1)$$

Proof: By definition (\rightarrow Definition IV/3.3.1), the Bayes factor BF_{13} is the ratio of marginal likelihoods of data y over m_1 and m_3 , respectively. That is,

$$\text{BF}_{13} = \frac{p(y \mid m_1)}{p(y \mid m_3)}. \quad (2)$$

We can equivalently write

$$\begin{aligned} \text{BF}_{13} &\stackrel{(2)}{=} \frac{p(y \mid m_1)}{p(y \mid m_3)} \\ &= \frac{p(y \mid m_1)}{p(y \mid m_3)} \cdot \frac{p(y \mid m_2)}{p(y \mid m_2)} \\ &= \frac{p(y \mid m_1)}{p(y \mid m_2)} \cdot \frac{p(y \mid m_2)}{p(y \mid m_3)} \\ &\stackrel{(2)}{=} \text{BF}_{12} \cdot \text{BF}_{23}, \end{aligned} \quad (3)$$

which completes the proof of (1).

Sources:

- original work

Metadata: ID: P163 | shortcut: bf-trans | author: tomfaulkenberry | date: 2020-09-07, 12:00.

3.3.3 Computation using Savage-Dickey density ratio

Theorem: Consider two competing models (\rightarrow Definition 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 Definition 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 Definition 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 Definition I/5.1.9) 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 Proof I/5.3.1), 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

$$\begin{aligned}
\text{BF}_{01} &\stackrel{(2)}{=} \frac{p(y \mid m_0)}{p(y \mid m_1)} \\
&= p(y \mid m_0) \cdot \frac{1}{p(y \mid m_1)} \\
&\stackrel{(3)}{=} p(y \mid \delta = \delta_0, m_1) \cdot \frac{1}{p(y \mid m_1)} \\
&\stackrel{(4)}{=} \frac{p(\delta = \delta_0 \mid y, m_1) p(y \mid m_1)}{p(\delta = \delta_0 \mid m_1)} \cdot \frac{1}{p(y \mid m_1)} \\
&= \frac{p(\delta = \delta_0 \mid y, m_1)}{p(\delta = \delta_0 \mid m_1)},
\end{aligned} \tag{5}$$

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.

Metadata: ID: P156 | shortcut: bf-sddr | author: tomfaulkenberry | date: 2020-08-26, 12:00.

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 Definition 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 Definition IV/3.3.1) is

$$\text{BF}_{1e} = \frac{c}{d} = \frac{1/d}{1/c} \tag{1}$$

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 Proof I/5.3.1) implies

$$p(\theta \mid y, m_1) = \frac{p(y \mid \theta, m_1) \cdot p(\theta \mid m_1)}{p(y \mid m_1)}. \tag{2}$$

Rearranging equation (2) allows us to write the marginal likelihood (\rightarrow Definition I/5.1.9) for y under m_1 as

$$p(y \mid m_1) = \frac{p(y \mid \theta, m_1) \cdot p(\theta \mid m_1)}{p(\theta \mid y, m_1)}. \tag{3}$$

Taking the ratio of the marginal likelihoods for m_1 and the encompassing model (\rightarrow Definition IV/3.3.5) m_e yields the following Bayes factor (\rightarrow Definition 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 Definition 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,

$$\begin{aligned} p(\theta' \mid m_1) &= \frac{p(\theta' \mid m_e) \cdot I_{\theta' \in m_1}}{\int p(\theta' \mid m_e) \cdot I_{\theta' \in m_1} d\theta'} \\ &= \left(\frac{I_{\theta' \in m_1}}{\int p(\theta' \mid m_e) \cdot I_{\theta' \in m_1} d\theta'} \right) \cdot p(\theta' \mid m_e), \end{aligned} \quad (6)$$

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

$$p(\theta' \mid m_1) = c \cdot p(\theta' \mid m_e). \quad (7)$$

By similar reasoning, we can write the posterior as

$$p(\theta' \mid y, m_1) = \left(\frac{I_{\theta' \in m_1}}{\int p(\theta' \mid y, m_e) \cdot I_{\theta' \in m_1} d\theta'} \right) \cdot p(\theta' \mid y, m_e) = d \cdot p(\theta' \mid y, m_e). \quad (8)$$

Plugging (7) and (8) into (5), this gives us

$$\text{BF}_{1e} = \frac{c \cdot p(\theta' \mid m_e) / d \cdot p(\theta' \mid y, m_e)}{p(\theta' \mid m_e) / p(\theta' \mid y, m_e)} = \frac{c}{d} = \frac{1/d}{1/c}, \quad (9)$$

which completes the proof. Note that by definition, $1/d$ represents the proportion of the posterior distribution for θ under the encompassing model (\rightarrow Definition 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 Definition 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.

Metadata: ID: P157 | shortcut: bf-ep | author: tomfaulkenberry | date: 2020-09-02, 12:00.

3.3.5 Encompassing model

Definition: Consider a family f of generative models (\rightarrow Definition 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 Hoijtink, 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.

Metadata: ID: D93 | shortcut: encm | author: tomfaulkenberry | date: 2020-09-02, 12:00.

3.3.6 Log Bayes factor

Definition: Let there be two generative models (\rightarrow Definition 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 Definition I/5.1.9) 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.

Metadata: ID: D84 | shortcut: lbf | author: JoramSoch | date: 2020-07-22, 07:02.

3.3.7 Derivation of the LBF

Theorem: Let there be two generative models (\rightarrow Definition I/5.1.1) m_1 and m_2 with model evidences (\rightarrow Definition I/5.1.9) $p(y|m_1)$ and $p(y|m_2)$. Then, the log Bayes factor (\rightarrow Definition 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 Definition IV/3.3.1) is defined as the posterior (\rightarrow Definition I/5.1.7) odds ratio (\rightarrow Definition “odds”) when both models (\rightarrow Definition I/5.1.1) are equally likely apriori (\rightarrow Definition 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 Proof I/5.3.2), 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 Definition I/5.1.3) odds ratio (\rightarrow Definition “odds”) 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).

Sources:

- original work

Metadata: ID: P137 | shortcut: lbf-der | author: JoramSoch | date: 2020-07-22, 07:27.

3.3.8 Calculation from log model evidences

Theorem: Let m_1 and m_2 be two statistical models with log model evidences (\rightarrow Definition IV/3.1.3) $\text{LME}(m_1)$ and $\text{LME}(m_2)$. Then, the log Bayes factor (\rightarrow Definition 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 Definition IV/3.3.1) is defined as the ratio of the model evidences (\rightarrow Definition I/5.1.9) 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 Definition 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 Definition 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.

Metadata: ID: P64 | shortcut: lbf-lme | author: JoramSoch | date: 2020-02-27, 20:51.

3.4 Posterior model probability

3.4.1 Definition

Definition: Let m_1, \dots, m_M be M statistical models (\rightarrow Definition I/5.1.4) with model evidences (\rightarrow Definition I/5.1.9) $p(y|m_1), \dots, p(y|m_M)$ and prior probabilities (\rightarrow Definition I/5.1.3) $p(m_1), \dots, p(m_M)$. Then, the conditional probability (\rightarrow Definition I/1.3.4) of model m_i , given the data y , is called the posterior probability (\rightarrow Definition I/5.1.7) 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.

Metadata: ID: D87 | shortcut: pmp | author: JoramSoch | date: 2020-07-28, 03:30.

3.4.2 Derivation

Theorem: Let there be a set of generative models (\rightarrow Definition I/5.1.1) m_1, \dots, m_M with model evidences (\rightarrow Definition I/5.1.9) $p(y|m_1), \dots, p(y|m_M)$ and prior probabilities (\rightarrow Definition I/5.1.3) $p(m_1), \dots, p(m_M)$. Then, the posterior probability (\rightarrow Definition 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 Proof I/5.3.1), the posterior model probability (\rightarrow Definition 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 Definition 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 Definition I/1.3.4), we have

$$p(m_i|y) = \frac{p(y|m_i) p(m_i)}{\sum_{j=1}^M p(y|m_j) p(m_j)}. \quad (4)$$

Sources:

- original work

Metadata: ID: P139 | shortcut: pmp-der | author: JoramSoch | date: 2020-07-28, 03:58.

3.4.3 Calculation from Bayes factors

Theorem: Let m_0, m_1, \dots, m_M be $M + 1$ statistical models with model evidences (\rightarrow Definition IV/3.1.3) $p(y|m_0), p(y|m_1), \dots, p(y|m_M)$. Then, the posterior model probabilities (\rightarrow Definition 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 Definition IV/3.3.1) comparing model m_i with m_0 and α_i is the prior (\rightarrow Definition I/5.1.3) odds ratio (\rightarrow Definition “odds”) of model m_i against m_0 .

Proof: Define the Bayes factor (\rightarrow Definition 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 of m_i against m_0

$$\alpha_i = \frac{p(m_i)}{p(m_0)}. \quad (3)$$

The posterior model probability (\rightarrow Proof 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.

Metadata: ID: P74 | shortcut: pmp-bf | author: JoramSoch | date: 2020-03-03, 13:13.

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 Definition 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 Definition I/5.1.3), the posterior model probability (\rightarrow Definition 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 Proof I/5.3.2), the posterior odds ratio (\rightarrow Definition “odds”) 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 Definition I/5.1.3), the prior odds ratio (\rightarrow Definition “odds”) 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 Definition 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 Definition 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 Definition 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 Definition 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.

Metadata: ID: P73 | shortcut: pmp-lbf | author: JoramSoch | date: 2020-03-03, 12:27.

3.4.5 Calculation from log model evidences

Theorem: Let m_1, \dots, m_M be M statistical models with log model evidences (\rightarrow Definition IV/3.1.3) $\text{LME}(m_1), \dots, \text{LME}(m_M)$. Then, the posterior model probabilities (\rightarrow Definition 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 Definition I/5.1.3) model probabilities.

Proof: The posterior model probability (\rightarrow Proof 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 Definition 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.

Metadata: ID: P66 | shortcut: pmp-lme | author: JoramSoch | date: 2020-02-27, 21:33.

3.5 Bayesian model averaging

3.5.1 Definition

Definition: Let m_1, \dots, m_M be M statistical models (\rightarrow Definition I/5.1.4) with posterior model probabilities (\rightarrow Definition IV/3.4.1) $p(m_1|y), \dots, p(m_M|y)$ and posterior distributions (\rightarrow Definition I/5.1.7) $p(\theta|y, m_1), \dots, p(\theta|y, m_M)$. Then, Bayesian model averaging (BMA) consists in finding the marginal (\rightarrow Definition I/1.5.3) posterior (\rightarrow Definition I/5.1.7) density (\rightarrow Definition I/1.6.6), conditional (\rightarrow Definition I/1.3.4) on the measured data y , but unconditional (\rightarrow Definition 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.

Metadata: ID: D89 | shortcut: bma | author: JoramSoch | date: 2020-08-03, 21:34.

3.5.2 Derivation

Theorem: Let m_1, \dots, m_M be M statistical models (\rightarrow Definition I/5.1.4) with posterior model probabilities (\rightarrow Definition IV/3.4.1) $p(m_1|y), \dots, p(m_M|y)$ and posterior distributions (\rightarrow Definition I/5.1.7) $p(\theta|y, m_1), \dots, p(\theta|y, m_M)$. Then, the marginal (\rightarrow Definition I/1.5.3) posterior (\rightarrow Definition I/5.1.7) density (\rightarrow Definition I/1.6.6), conditional (\rightarrow Definition I/1.3.4) on the measured data y , but unconditional (\rightarrow Definition 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 Definition I/1.3.3), the probability distribution of the shared parameters θ conditional (\rightarrow Definition I/1.3.4) on the measured data y can be obtained by marginalizing (\rightarrow Definition I/1.3.3) over the discrete random variable (\rightarrow Definition 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 Definition 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 Definition I/5.1.7) of the i -th model and $p(m_i|y)$ happens to be the posterior probability (\rightarrow Definition IV/3.4.1) of the i -th model.

Sources:

- original work

Metadata: ID: P143 | shortcut: bma-der | author: JoramSoch | date: 2020-08-03, 22:05.

3.5.3 Calculation from log model evidences

Theorem: Let m_1, \dots, m_M be M statistical models (\rightarrow Definition I/5.1.4) describing the same measured data y with log model evidences (\rightarrow Definition IV/3.1.3) $\text{LME}(m_1), \dots, \text{LME}(m_M)$ and shared model parameters θ . Then, Bayesian model averaging (\rightarrow Definition 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 Definition I/1.3.3), the probability of the shared parameters θ conditional on the measured data y can be obtained (\rightarrow Proof 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 Definition IV/3.4.1) of the i -th model. One can express posterior model probabilities in terms of log model evidences (\rightarrow Proof 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.

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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	291
P2	mlr-ols	Ordinary least squares for multiple linear regression	JoramSoch	2019-09-27	445
P3	lme-anc	Partition of the log model evidence into accuracy and complexity	JoramSoch	2019-09-27	571
P4	bayes-th	Bayes' theorem	JoramSoch	2019-09-27	142
P5	mse-bnv	Partition of the mean squared error into bias and variance	JoramSoch	2019-11-27	121
P6	ng-kl	Kullback-Leibler divergence for the normal-gamma distribution	JoramSoch	2019-12-06	308
P7	glm-mle	Maximum likelihood estimation for the general linear model	JoramSoch	2019-12-06	490
P8	rsq-der	Derivation of R^2 and adjusted R^2	JoramSoch	2019-12-06	557
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P10	blr-post	Posterior distribution for Bayesian linear regression	JoramSoch	2020-01-03	477
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P130	var-add	Additivity of the variance for independent random variables	JoramSoch	2020-07-07	63
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P138	mean-lotus	Law of the unconscious statistician	JoramSoch	2020-07-22	55
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P142	duni-qf	Quantile function of the discrete uniform distribution	JoramSoch	2020-07-28	150
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P168	wald-mgf	Moment-generating function of the Wald distribution	tomfaulkenberry	2020-09-13	270
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P194	gam-qf	Quantile function of the gamma distribution	JoramSoch	2020-11-19	227
P195	beta-cdf	Cumulative distribution function of the beta distribution	JoramSoch	2020-11-19	265
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P197	chi2-pdf	Probability density function of the chi-squared distribution	JoramSoch	2020-11-25	256
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P199	dent-inv	Invariance of the differential entropy under addition of a constant	JoramSoch	2020-12-02	98

P200	dent-add	Addition of the differential entropy upon multiplication with a constant	JoramSoch	2020-12-02	99
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P203	ug-lme	Log model evidence for the univariate Gaussian	JoramSoch	2021-03-03	351
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P210	ugkv-ztestp	Paired z-test for dependent observations	JoramSoch	2021-03-24	359
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P213	ugkv-lme	Log model evidence for the univariate Gaussian with known variance	JoramSoch	2021-03-24	365
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P223	ug-mle	Maximum likelihood estimation for the univariate Gaussian	JoramSoch	2021-04-16	340
P224	poissexp-mle	Maximum likelihood estimation for the Poisson distribution with exposure values	JoramSoch	2021-04-16	532
P225	poiss-prior	Conjugate prior distribution for Poisson-distributed data	JoramSoch	2020-04-21	527
P226	poiss-post	Posterior distribution for Poisson-distributed data	JoramSoch	2020-04-21	528
P227	poiss-lme	Log model evidence for Poisson-distributed data	JoramSoch	2020-04-21	530
P228	beta-mean	Mean of the beta distribution	JoramSoch	2021-04-29	266
P229	beta-var	Variance of the beta distribution	JoramSoch	2021-04-29	267
P230	poiss-var	Variance of the Poisson distribution	JoramSoch	2021-04-29	169
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P238	ng-dent	Differential entropy of the normal-gamma distribution	JoramSoch	2021-07-08	307
P239	gam-dent	Differential entropy of the gamma distribution	JoramSoch	2021-07-14	233
P240	ug-anc	Accuracy and complexity for the univariate Gaussian	JoramSoch	2021-07-14	354
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P242	prob-exc	Probability under mutual exclusivity	JoramSoch	2021-07-23	10
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P245	prob-comp	Probability of the complement	JoramSoch	2021-07-30	13
P246	prob-range	Range of probability	JoramSoch	2021-07-30	13
P247	prob-add	Addition law of probability	JoramSoch	2021-07-30	14
P248	prob-tot	Law of total probability	JoramSoch	2021-08-08	15
P249	prob-exh	Probability of exhaustive events	JoramSoch	2021-08-08	16
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P253	pmf-invft	Probability mass function of an invertible function of a random vector	JoramSoch	2021-08-30	22
P254	pdf-invft	Probability density function of an invertible function of a continuous random vector	JoramSoch	2021-08-30	26
P255	pdf-linfct	Probability density function of a linear function of a continuous random vector	JoramSoch	2021-08-30	28
P256	cdf-sumind	Cumulative distribution function of a sum of independent random variables	JoramSoch	2021-08-30	30
P257	pmf-sumind	Probability mass function of a sum of independent discrete random variables	JoramSoch	2021-08-30	20
P258	pdf-sumind	Probability density function of a sum of independent discrete random variables	JoramSoch	2021-08-30	23
P259	cf-fct	Characteristic function of a function of a random variable	JoramSoch	2021-09-22	38
P260	mgf-fct	Moment-generating function of a function of a random variable	JoramSoch	2021-09-22	39
P261	dent-addvec	Addition of the differential entropy upon multiplication with invertible matrix	JoramSoch	2021-10-07	100
P262	dent-noninv	Non-invariance of the differential entropy under change of variables	JoramSoch	2021-10-07	102
P263	t-pdf	Probability density function of the t-distribution	JoramSoch	2021-10-12	220
P264	f-pdf	Probability density function of the F-distribution	JoramSoch	2021-10-12	259
P265	tglm-dist	Distribution of the transformed general linear model	JoramSoch	2021-10-21	493
P266	tglm-para	Equivalence of parameter estimates from the transformed general linear model	JoramSoch	2021-10-21	494
P267	iglm-dist	Distribution of the inverse general linear model	JoramSoch	2021-10-21	495

P268	iglm-blue	Best linear unbiased estimator for the inverse general linear model	JoramSoch	2021-10-21	496
P269	cfm-para	Parameters of the corresponding forward model	JoramSoch	2021-10-21	498
P270	cfm-exist	Existence of a corresponding forward model	JoramSoch	2021-10-21	499
P271	slr-ols	Ordinary least squares for simple linear regression	JoramSoch	2021-10-27	409
P272	slr-olsmean	Expectation of parameter estimates for simple linear regression	JoramSoch	2021-10-27	414
P273	slr-olsvar	Variance of parameter estimates for simple linear regression	JoramSoch	2021-10-27	416
P274	slr-meancent	Effects of mean-centering on parameter estimates for simple linear regression	JoramSoch	2021-10-27	421
P275	slr-comp	The regression line goes through the center of mass point	JoramSoch	2021-10-27	423
P276	slr-ressum	The sum of residuals is zero in simple linear regression	JoramSoch	2021-10-27	437
P277	slr-rescorr	The residuals and the covariate are uncorrelated in simple linear regression	JoramSoch	2021-10-27	438
P278	slr-resvar	Relationship between residual variance and sample variance in simple linear regression	JoramSoch	2021-10-27	439
P279	slr-corr	Relationship between correlation coefficient and slope estimate in simple linear regression	JoramSoch	2021-10-27	441
P280	slr-rsq	Relationship between coefficient of determination and correlation coefficient in simple linear regression	JoramSoch	2021-10-27	442
P281	slr-mlr	Simple linear regression is a special case of multiple linear regression	JoramSoch	2021-11-09	408
P282	slr-olsdist	Distribution of parameter estimates for simple linear regression	JoramSoch	2021-11-09	419
P283	slr-proj	Projection of a data point to the regression line	JoramSoch	2021-11-09	424

P284	slr-sss	Sums of squares for simple linear regression	JoramSoch	2021-11-09	425
P285	slr-mat	Transformation matrices for simple linear regression	JoramSoch	2021-11-09	427
P286	slr-wls	Weighted least squares for simple linear regression	JoramSoch	2021-11-16	430
P287	slr-mle	Maximum likelihood estimation for simple linear regression	JoramSoch	2021-11-16	433
P288	slr-ols2	Ordinary least squares for simple linear regression	JoramSoch	2021-11-16	412
P289	slr-wls2	Weighted least squares for simple linear regression	JoramSoch	2021-11-16	432
P290	slr-mle2	Maximum likelihood estimation for simple linear regression	JoramSoch	2021-11-16	436
P291	mean-tot	Law of total expectation	JoramSoch	2021-11-26	54
P292	var-tot	Law of total variance	JoramSoch	2021-11-26	64
P293	cov-tot	Law of total covariance	JoramSoch	2021-11-26	70
P294	dir-kl	Kullback-Leibler divergence for the Dirichlet distribution	JoramSoch	2021-12-02	316
P295	wish-kl	Kullback-Leibler divergence for the Wishart distribution	JoramSoch	2021-12-02	332
P296	matn-kl	Kullback-Leibler divergence for the matrix-normal distribution	JoramSoch	2021-12-02	325
P297	matn-samp	Sampling from the matrix-normal distribution	JoramSoch	2021-12-07	331
P298	mean-tr	Expected value of the trace of a matrix	JoramSoch	2021-12-07	51
P299	corr-z	Correlation coefficient in terms of standard scores	JoramSoch	2021-12-14	81
P300	corr-range	Correlation always falls between -1 and +1	JoramSoch	2021-12-14	79
P301	bern-var	Variance of the Bernoulli distribution	JoramSoch	2022-01-20	153
P302	bin-var	Variance of the binomial distribution	JoramSoch	2022-01-20	158

P303	bern-varrange	Range of the variance of the Bernoulli distribution	JoramSoch	2022-01-27	154
P304	bin-varrange	Range of the variance of the binomial distribution	JoramSoch	2022-01-27	159
P305	mlr-mll	Maximum log-likelihood for multiple linear regression	JoramSoch	2022-02-04	470
P306	lognorm-med	Median of the log-normal distribution	majapavlo	2022-02-07	251
P307	mlr-aic	Akaike information criterion for multiple linear regression	JoramSoch	2022-02-11	473
P308	mlr-bic	Bayesian information criterion for multiple linear regression	JoramSoch	2022-02-11	473
P309	mlr-aicc	Corrected Akaike information criterion for multiple linear regression	JoramSoch	2022-02-11	474
P310	lognorm-pdf	Probability density function of the log-normal distribution	majapavlo	2022-02-13	246
P311	lognorm-mode	Mode of the log-normal distribution	majapavlo	2022-02-13	251
P312	mlr-dev	Deviance for multiple linear regression	JoramSoch	2022-03-01	471
P313	blr-dic	Deviance information criterion for multiple linear regression	JoramSoch	2022-03-01	481
P314	lme-pnp	Log model evidence in terms of prior and posterior distribution	JoramSoch	2022-03-11	571
P315	aicc-mll	Corrected Akaike information criterion in terms of maximum log-likelihood	JoramSoch	2022-03-11	564
P316	aicc-aic	Corrected Akaike information criterion converges to uncorrected Akaike information criterion when infinite data are available	JoramSoch	2022-03-18	564
P317	mle-bias	Maximum likelihood estimation can result in biased estimates	JoramSoch	2022-03-18	126
P318	pval-h0	The p-value follows a uniform distribution under the null hypothesis	JoramSoch	2022-03-18	133
P319	prob-exh2	Probability of exhaustive events	JoramSoch	2022-03-27	16

P320	slr-olscorr	Parameter estimates for simple linear regression are uncorrelated after mean-centering	JoramSoch	2022-04-14	421
P321	norm-probstd	Probability of normal random variable being within standard deviations from its mean	JoramSoch	2022-05-08	202
P322	mult-cov	Covariance matrix of the multinomial distribution	adkipnis	2022-05-11	175
P323	nw-pdf	Probability density function of the normal-Wishart distribution	JoramSoch	2022-05-14	335
P324	ng-nw	Normal-gamma distribution is a special case of normal-Wishart distribution	JoramSoch	2022-05-20	302
P325	lognorm-cdf	Cumulative distribution function of the log-normal distribution	majapavlo	2022-06-29	247
P326	lognorm-qf	Quantile function of the log-normal distribution	majapavlo	2022-07-09	248
P327	nw-mean	Mean of the normal-Wishart distribution	JoramSoch	2022-07-14	336
P328	gam-wish	Gamma distribution is a special case of Wishart distribution	JoramSoch	2022-07-14	225
P329	mlr-glm	Multiple linear regression is a special case of the general linear model	JoramSoch	2022-07-21	444
P330	mvn-matn	Multivariate normal distribution is a special case of matrix-normal distribution	JoramSoch	2022-07-31	284
P331	norm-mvn	Normal distribution is a special case of multivariate normal distribution	JoramSoch	2022-08-19	194
P332	t-mvt	t-distribution is a special case of multivariate t-distribution	JoramSoch	2022-08-25	219
P333	mvt-pdf	Probability density function of the multivariate t-distribution	JoramSoch	2022-09-02	299
P334	bern-ent	Entropy of the Bernoulli distribution	JoramSoch	2022-09-02	155
P335	bin-ent	Entropy of the binomial distribution	JoramSoch	2022-09-02	160
P336	cat-ent	Entropy of the categorical distribution	JoramSoch	2022-09-09	173

P337	mult-ent	Entropy of the multinomial distribution	JoramSoch	2022-09-09	176
P338	cat-cov	Covariance matrix of the categorical distribution	JoramSoch	2022-09-09	172
P339	mvn-mean	Mean of the multivariate normal distribution	JoramSoch	2022-09-15	285
P340	mvn-cov	Covariance matrix of the multivariate normal distribution	JoramSoch	2022-09-15	286
P341	matn-mean	Mean of the matrix-normal distribution	JoramSoch	2022-09-15	323
P342	matn-cov	Covariance matrices of the matrix-normal distribution	JoramSoch	2022-09-15	323
P343	matn-marg	Marginal distributions for the matrix-normal distribution	JoramSoch	2022-09-15	328
P344	matn-dent	Differential entropy for the matrix-normal distribution	JoramSoch	2022-09-22	324
P345	ng-cov	Covariance and variance of the normal-gamma distribution	JoramSoch	2022-09-22	305
P346	ng-samp	Sampling from the normal-gamma distribution	JoramSoch	2022-09-22	314
P347	covmat-inv	Invariance of the covariance matrix under addition of constant vector	JoramSoch	2022-09-22	74
P348	covmat-scal	Scaling of the covariance matrix upon multiplication with constant matrix	JoramSoch	2022-09-22	74
P349	covmat-sum	Covariance matrix of the sum of two random vectors	JoramSoch	2022-09-26	75
P350	covmat-symm	Symmetry of the covariance matrix	JoramSoch	2022-09-26	72
P351	covmat-psd	Positive semi-definiteness of the covariance matrix	JoramSoch	2022-09-26	73
P352	cov-var	Self-covariance equals variance	JoramSoch	2022-09-26	68
P353	cov-symm	Symmetry of the covariance	JoramSoch	2022-09-26	68
P354	lognorm-mean	Mean of the log-normal distribution	majapavlo	2022-10-02	249
P355	lognorm-var	Variance of the log-normal distribution	majapavlo	2022-10-02	253

P356	beta-chi2	Relationship between chi-squared distribution and beta distribution	JoramSoch	2022-10-07	261
P357	betabin-mome	Method of moments for beta-binomial data	JoramSoch	2022-10-07	545
P358	bin-margcond	Marginal distribution of a conditional binomial distribution	JoramSoch	2022-10-07	161
P359	mean-prodsqr	Square of expectation of product is less than or equal to product of expectation of squares	JoramSoch	2022-10-11	53
P360	pgf-mean	Probability-generating function is expectation of function of random variable	JoramSoch	2022-10-11	42
P361	pgf-zero	Value of the probability-generating function for argument zero	JoramSoch	2022-10-11	42
P362	pgf-one	Value of the probability-generating function for argument one	JoramSoch	2022-10-11	43
P363	bin-pgf	Probability-generating function of the binomial distribution	JoramSoch	2022-10-11	157
P364	betabin-pmf	Probability mass function of the beta-binomial distribution	JoramSoch	2022-10-20	164
P365	betabin-pmfitogf	Expression of the probability mass function of the beta-binomial distribution using only the gamma function	JoramSoch	2022-10-20	165
P366	betabin-cdf	Cumulative distribution function of the beta-binomial distribution	JoramSoch	2022-10-22	166
P367	me-der	Derivation of the model evidence	JoramSoch	2022-10-20	569
P368	fe-der	Derivation of the family evidence	JoramSoch	2022-10-20	575
P369	anova1-ols	Ordinary least squares for one-way analysis of variance	JoramSoch	2022-11-06	377
P370	anova1-f	F-test for main effect in one-way analysis of variance	JoramSoch	2022-11-06	379
P371	anova2-ols	Ordinary least squares for two-way analysis of variance	JoramSoch	2022-11-06	388
P372	anova2-fme	F-test for main effect in two-way analysis of variance	JoramSoch	2022-11-10	400

P373	anova2-fia	F-test for interaction in two-way analysis of variance	JoramSoch	2022-11-11	403
P374	anova2-fgm	F-test for grand mean in two-way analysis of variance	JoramSoch	2022-11-11	404
P375	anova1-repara	Reparametrization for one-way analysis of variance	JoramSoch	2022-11-15	384
P376	anova1-pss	Partition of sums of squares in one-way analysis of variance	JoramSoch	2022-11-15	378
P377	anova1-fols	F-statistic in terms of ordinary least squares estimates in one-way analysis of variance	JoramSoch	2022-11-15	383
P378	anova2-cochran	Application of Cochran's theorem to two-way analysis of variance	JoramSoch	2022-11-16	394
P379	anova2-pss	Partition of sums of squares in two-way analysis of variance	JoramSoch	2022-11-16	392
P380	anova2-fols	F-statistics in terms of ordinary least squares estimates in two-way analysis of variance	JoramSoch	2022-11-16	406
P381	bin-mle	Maximum likelihood estimation for binomial observations	JoramSoch	2022-11-23	507
P382	bin-mll	Maximum log-likelihood for binomial observations	JoramSoch	2022-11-24	508
P383	bin-lbf	Log Bayes factor for binomial observations	JoramSoch	2022-11-25	513
P384	bin-pp	Posterior probability of the alternative model for binomial observations	JoramSoch	2022-11-26	514
P385	mult-mle	Maximum likelihood estimation for multinomial observations	JoramSoch	2022-12-02	516
P386	mult-mll	Maximum log-likelihood for multinomial observations	JoramSoch	2022-12-02	516
P387	mult-lbf	Log Bayes factor for multinomial observations	JoramSoch	2022-12-02	522
P388	mult-pp	Posterior probability of the alternative model for multinomial observations	JoramSoch	2022-12-02	524

P389	mlr-wlsdist	Distributions of estimated parameters, fitted signal and residuals in multiple linear regression upon weighted least squares	JoramSoch	2022-12-13	456
P390	mlr-rssdist	Distribution of residual sum of squares in multiple linear regression with weighted least squares	JoramSoch	2022-12-13	457
P391	mlr-t	t-test for multiple linear regression using contrast-based inference	JoramSoch	2022-12-13	463
P392	mlr-f	F-test for multiple linear regression using contrast-based inference	JoramSoch	2022-12-13	465
P393	mlr-ind	Independence of estimated parameters and residuals in multiple linear regression	JoramSoch	2022-12-13	453
P394	mvn-indprod	Independence of products of multivariate normal random vector	JoramSoch	2022-12-13	298
P395	mvn-chi2	Relationship between multivariate normal distribution and chi-squared distribution	JoramSoch	2022-12-20	283
P396	cuni-var	Variance of the continuous uniform distribution	JoramSoch	2022-12-20	184
P397	cuni-dent	Differential entropy of the continuous uniform distribution	JoramSoch	2022-12-20	185
P398	resvar-biasp	Maximum likelihood estimator of variance in multiple linear regression is biased	JoramSoch	2022-12-21	554
P399	mlr-symm	Projection matrix and residual-forming matrix are symmetric	JoramSoch	2022-12-22	451
P400	mlr-olsdist	Distributions of estimated parameters, fitted signal and residuals in multiple linear regression upon ordinary least squares	JoramSoch	2022-12-23	454
P401	exp-var	Variance of the exponential distribution	majapavlo	2023-01-23	242
P402	exg-pdf	Probability density function of the ex-Gaussian distribution	tomfaulkenberry	2023-04-18	274
P403	exp-mgf	Moment-generating function of the exponential distribution	tomfaulkenberry	2023-04-19	236

P404	exg-mgf	Moment-generating function of the ex-Gaussian distribution	tomfaulkenberry	2023-04-19	276
P405	exg-mean	Mean of the ex-Gaussian distribution	tomfaulkenberry	2023-04-19	277
P406	exg-var	Variance of the ex-Gaussian distribution	tomfaulkenberry	2023-04-19	278
P407	skew-mean	Partition of skewness into expected values	tomfaulkenberry	2023-04-20	65
P408	exg-skew	Skewness of the ex-Gaussian distribution	tomfaulkenberry	2023-04-21	280
P409	exp-skew	Skewness of the exponential distribution	tomfaulkenberry	2023-04-24	243
P410	duni-ent	Entropy of the discrete uniform distribution	JoramSoch	2023-08-11	151

2 Definition by Number

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D1	mvn	Multivariate normal distribution	JoramSoch	2020-01-22	283
D2	mgf	Moment-generating function	JoramSoch	2020-01-22	38
D3	cuni	Continuous uniform distribution	JoramSoch	2020-01-27	179
D4	norm	Normal distribution	JoramSoch	2020-01-27	186
D5	ng	Normal-gamma distribution	JoramSoch	2020-01-27	301
D6	matn	Matrix-normal distribution	JoramSoch	2020-01-27	321
D7	gam	Gamma distribution	JoramSoch	2020-02-08	222
D8	exp	Exponential distribution	JoramSoch	2020-02-08	235
D9	pmf	Probability mass function	JoramSoch	2020-02-13	19
D10	pdf	Probability density function	JoramSoch	2020-02-13	22
D11	mean	Expected value	JoramSoch	2020-02-13	44
D12	var	Variance	JoramSoch	2020-02-13	58
D13	cdf	Cumulative distribution function	JoramSoch	2020-02-17	29
D14	qf	Quantile function	JoramSoch	2020-02-17	36
D15	ent	Shannon entropy	JoramSoch	2020-02-19	91
D16	dent	Differential entropy	JoramSoch	2020-02-19	97
D17	ent-cond	Conditional entropy	JoramSoch	2020-02-19	93
D18	ent-joint	Joint entropy	JoramSoch	2020-02-19	93
D19	mi	Mutual information	JoramSoch	2020-02-19	108
D19	mi	Mutual information	JoramSoch	2020-02-19	108
D20	resvar	Residual variance	JoramSoch	2020-02-25	552
D21	rsq	Coefficient of determination	JoramSoch	2020-02-25	557
D22	snr	Signal-to-noise ratio	JoramSoch	2020-02-25	560
D23	aic	Akaike information criterion	JoramSoch	2020-02-25	563
D24	bic	Bayesian information criterion	JoramSoch	2020-02-25	565
D25	dic	Deviance information criterion	JoramSoch	2020-02-25	567
D26	lme	Log model evidence	JoramSoch	2020-02-25	570
D27	gm	Generative model	JoramSoch	2020-03-03	135

D28	lf	Likelihood function	JoramSoch	2020-03-03	135
D28	lf	Likelihood function	JoramSoch	2020-03-03	135
D29	prior	Prior distribution	JoramSoch	2020-03-03	135
D30	fpm	Full probability model	JoramSoch	2020-03-03	136
D31	jl	Joint likelihood	JoramSoch	2020-03-03	136
D32	post	Posterior distribution	JoramSoch	2020-03-03	137
D33	ml	Marginal likelihood	JoramSoch	2020-03-03	138
D34	dent-cond	Conditional differential entropy	JoramSoch	2020-03-21	103
D35	dent-joint	Joint differential entropy	JoramSoch	2020-03-21	104
D36	mlr	Multiple linear regression	JoramSoch	2020-03-21	443
D37	tss	Total sum of squares	JoramSoch	2020-03-21	446
D38	ess	Explained sum of squares	JoramSoch	2020-03-21	447
D39	rss	Residual sum of squares	JoramSoch	2020-03-21	447
D40	glm	General linear model	JoramSoch	2020-03-21	488
D41	poiss-data	Poisson-distributed data	JoramSoch	2020-03-22	525
D42	poissexp	Poisson distribution with exposure values	JoramSoch	2020-03-22	532
D43	wish	Wishart distribution	JoramSoch	2020-03-22	331
D44	bern	Bernoulli distribution	JoramSoch	2020-03-22	151
D45	bin	Binomial distribution	JoramSoch	2020-03-22	155
D46	cat	Categorical distribution	JoramSoch	2020-03-22	171
D47	mult	Multinomial distribution	JoramSoch	2020-03-22	173
D48	prob	Probability	JoramSoch	2020-05-10	5
D49	prob-joint	Joint probability	JoramSoch	2020-05-10	6
D50	prob-marg	Law of marginal probability	JoramSoch	2020-05-10	6
D51	prob-cond	Law of conditional probability	JoramSoch	2020-05-10	6
D52	kl	Kullback-Leibler divergence	JoramSoch	2020-05-10	112
D53	beta	Beta distribution	JoramSoch	2020-05-10	261
D54	dir	Dirichlet distribution	JoramSoch	2020-05-10	315
D55	dist	Probability distribution	JoramSoch	2020-05-17	18
D56	dist-joint	Joint probability distribution	JoramSoch	2020-05-17	18

D57	dist-marg	Marginal probability distribution	JoramSoch	2020-05-17	18
D58	dist-cond	Conditional probability distribution	JoramSoch	2020-05-17	19
D59	llf	Log-likelihood function	JoramSoch	2020-05-17	125
D60	mle	Maximum likelihood estimation	JoramSoch	2020-05-15	125
D61	mll	Maximum log-likelihood	JoramSoch	2020-05-15	126
D62	poiss	Poisson distribution	JoramSoch	2020-05-25	167
D63	snorm	Standard normal distribution	JoramSoch	2020-05-26	187
D64	sgam	Standard gamma distribution	JoramSoch	2020-05-26	222
D65	rvar	Random variable	JoramSoch	2020-05-27	3
D66	rvec	Random vector	JoramSoch	2020-05-27	4
D67	rmat	Random matrix	JoramSoch	2020-05-27	4
D68	cgf	Cumulant-generating function	JoramSoch	2020-05-31	44
D69	pgf	Probability-generating function	JoramSoch	2020-05-31	41
D70	cov	Covariance	JoramSoch	2020-06-02	66
D71	corr	Correlation	JoramSoch	2020-06-02	79
D72	covmat	Covariance matrix	JoramSoch	2020-06-06	70
D73	corrmat	Correlation matrix	JoramSoch	2020-06-06	81
D74	precmat	Precision matrix	JoramSoch	2020-06-06	77
D75	ind	Statistical independence	JoramSoch	2020-06-06	7
D76	logreg	Logistic regression	JoramSoch	2020-06-28	548
D77	beta-data	Beta-distributed data	JoramSoch	2020-06-28	540
D78	bin-data	Binomial observations	JoramSoch	2020-07-07	507
D79	mult-data	Multinomial observations	JoramSoch	2020-07-07	515
D80	lfe	Log family evidence	JoramSoch	2020-07-13	576
D81	emat	Estimation matrix	JoramSoch	2020-07-22	449
D82	pmat	Projection matrix	JoramSoch	2020-07-22	449
D83	rformat	Residual-forming matrix	JoramSoch	2020-07-22	449
D84	lbf	Log Bayes factor	JoramSoch	2020-07-22	583
D85	ent-cross	Cross-entropy	JoramSoch	2020-07-28	94
D86	dent-cross	Differential cross-entropy	JoramSoch	2020-07-28	104

D87	pmp	Posterior model probability	JoramSoch	2020-07-28	585
D88	duni	Discrete uniform distribution	JoramSoch	2020-07-28	148
D89	bma	Bayesian model averaging	JoramSoch	2020-08-03	589
D90	mom	Moment	JoramSoch	2020-08-19	85
D91	fwhm	Full width at half maximum	JoramSoch	2020-08-19	84
D92	bf	Bayes factor	tomfaulkenberry	2020-08-26	578
D93	enclm	Encompassing model	tomfaulkenberry	2020-09-02	583
D94	std	Standard deviation	JoramSoch	2020-09-03	84
D95	wald	Wald distribution	tomfaulkenberry	2020-09-04	269
D96	const	Constant	JoramSoch	2020-09-09	4
D97	mom-raw	Raw moment	JoramSoch	2020-10-08	87
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