Statistics for Data Science 24-25

Notes

University of Pisa

M.Sc. in Data Science and Business Informatics

Contents

1 Probability

Probability (on a finite sample space)

A probability function P on a finite sample space assigns to each event $A \in \Omega$ a number $P(A) \in [0, 1]$ such that

- $P(\Omega) = 1$;
- $P(A \cup B) = P(A) + P(B)$ if A and B are disjoint.

$P(A)$ is called probability that event A occurs.

Probability (on an infinite sample space)

A probability function P on an infinite sample space assigns to each event $A \in \Omega$ a number $P(A)$ such that

- $P(\Omega) = 1$;
- $P(A_1 \cup A_2 \cup A_3 \cup \dots) = P(A_1) + P(A_2) + P(A_3) + \dots$ if $A_1, A_2, A_3, \dots$ are disjoint.

Properties:

- $P(A^c) = 1 - P(A)$
- $P(\emptyset) = 0$
- $P(A \cup B) = P(A) + P(B) - P(A \cap B)$
- $A \subseteq B \implies P(A) \leq P(B)$

Conditional probability

The conditional probability of A given C is given by

$$P(A|C) = \frac{P(A \cap C)}{P(C)}$$

provided $P(C) > 0$ (it is otherwise undefined).

A consequence of this definition is the **multiplication rule**: $P(A \cap C) = P(A|C) \cdot P(C) = P(C|A) \cdot P(A)$.

Law of total probability

Let $C_1, C_2, \dots, C_n$ be a partition of Ω (i.e., they are disjoint and their union is Ω). Then, given any event $A \in \Omega$, its probability can be computed as

$$P(A) = P(A|C_1) \cdot P(C_1) + P(A|C_2) \cdot P(C_2) + \dots + P(A|C_n) \cdot P(C_n)$$

Bayes' rule

Let $C_1, C_2, \ldots, C_n$ be a partition of Ω and A be an event in Ω. Then, the probability of C_i given A is given by

$$P(C_i|A) = \frac{P(A|C_i) \cdot P(C_i)}{P(A|C_1) \cdot P(C_1) + P(A|C_2) \cdot P(C_2) + \cdots + P(A|C_n) \cdot P(C_n)}$$

Two events A and B are **independent** if $P(B) = 0$, or:

- $P(A \cap B) = P(A) \cdot P(B)$, or, equivalently,
- $P(A|B) = P(A)$.

If A and B are independent, also any combination of their complements is independent.
In general, events $A_1, A_2, \ldots, A_n$ are independent if for any subset $I \subseteq \{1, 2, \ldots, n\}$:

$$P\left(\bigcap_{i \in I} A_i\right) = \prod_{i \in I} P(A_i)$$

This means that any possible subset of events in the collection is independent (since pairwise independence among individual events is not enough).

Two events A and B are **conditionally independent** given and event C ($P(C) > 0$) if $P(B|C) = 0$, or $P(A|B \cap C) = P(A|C)$. Since conditional probability is a probability, the definition is identical to the one above but conditioned on C.

2 Random variables

A **discrete random variable** takes a finite number of values, or a countably infinite number of values. Each discrete r.v. is described by a probability mass function and a cumumlative distribution function.

Probability mass function (PMF)

The PMF p of a discrete random variable X is a function $p : \mathbb{R} \to [0, 1]$, defined by

$$p(a) = P(X = a) \text{ for } -\infty < a < \infty$$

A **continuous random variable** takes any value in a continuous range (finite or infinite). Each continuous r.v. is described by a probability density function and a cumulative distribution function.

Probability density function (PDF)

A random variable X is countinuous if for some function $f : \mathbb{R} \to \mathbb{R}$ and any numbers a, b, with $a < b$,

$$P(a \leq X \leq b) = \int_a^b f(x)dx$$

where $f(x) \geq 0$ for all x and $\int_{-\infty}^{\infty} f(x)dx = 1$. f is called probability density function (PDF) of X.

Cumulative distribution function (CDF)

The CDF of a discrete random variable X is a function $F : \mathbb{R} \to [0, 1]$, defined by

$$F(a) = P(X \leq a) = \sum_{x \leq a} p(x) \quad \text{for } -\infty < a < \infty$$

The CDF of a continuous random variable X is a function $F : \mathbb{R} \to [0, 1]$, defined by

$$F(a) = P(X \leq a) = \int_{-\infty}^{a} f(x)dx \quad \text{for } -\infty < a < \infty$$

The **complementary cumulative distribution function** (CCDF) of a random variable is defined as $1 - F(a) = P(X > a)$.

Given two discrete random variables, we can define their **joint probability mass function** $p : \mathbb{R}^2 \in [0, 1]$, defined as

$$p(a, b) = P(X = a, Y = b) \text{ for } -\infty < a, b < \infty$$

For continuous random variables, we can similarly define the **joint probability density function** $f : \mathbb{R}^2 \to \mathbb{R}$, defined as

$$P(a_1 \leq X \leq b_1, a_2 \leq Y \leq b_2) = \int_{a_1}^{b_1} \int_{a_2}^{b_2} f(x, y)\ dy\ dx$$

The **joint cummulative distribution function** is defined as $F(a, b) = P(X \leq a, Y \leq b)$. For discrete random variables, this is calculated as

$$F(a, b) = P(X \leq a, Y \leq b) = \sum_{x \leq a} \sum_{y \leq b} p(x, y)$$

For continuous random variables, this is calculated as

$$F(a, b) = P(X \leq a, Y \leq b) = \int_{-\infty}^{a} \int_{-\infty}^{b} f(x, y)\ dy\ dx$$

The **marginal PMF** of a discrete r.v. X is

$$p_X(a) = P(X = a) = \sum_y p(a, y)$$

while the **marginal PDF** of a continuous r.v. X is

$$f_X(a) = \int_{-\infty}^{\infty} f(a, y)\ dy$$

In both cases, the **marginal distribution function** of X is

$$F_X(a) = P(X \leq a) = \lim_{b \to \infty} F_{XY}(a, b)$$

Conditional distribution of random variables

Let X and Y be two random variables, and P_{XY} their joint distribution. The conditional distribution of X given $Y \in B$, where $P(Y \in B) > 0$, is defined as

$$F_{X|Y \in B}(a) = P_{X|Y}(X \leq a | Y \in B) = \frac{P_{XY}(X \leq A, Y \in B)}{P_Y(Y \in B)}$$

Two random variables X and Y are **independent** ($X \perp\!\!\!\perp Y$) if

- $P_{X|Y}(X \leq a | Y \leq b) = P_X(X \leq a)$ for $a \in \mathbb{R}$, and for all b such that $P_Y(Y \leq b) > 0$, or, equivalently,
- $p_{XY}(x, y) = p_X(x) \cdot p_Y(y)$ (if discrete) or $f_{XY}(x, y) = f_X(x) \cdot f_Y(y)$ (if continuous).

Two random variables X and Y are said **identically distributed** ($X \sim Y$) if $F_X = F_Y$, i.e., $F_X(a) = F_Y(a)$ for $a \in \mathbb{R}$. If two random variables are both independent and identically distributed, they are said to be **independent and identically distributed** (i.i.d.).

Quantiles (percentiles)

Let X be a continuous random variable, and let p be a number in the interval $[0, 1]$. The p^{th} quantile (or $100p^{th}$ percentile) of the distribution of X is the smallest number q_p such that

$$F(q_p) = P(X \leq q_p) = p$$

The **median** of a distribution is the 50^{th} percentile. The **interquartile range** (IQR) is the difference between the 75^{th} and the 25^{th} percentiles. A more general definition, which holds also for discrete random variables, is

$$q_p = \inf_x \{P(X \leq x) \geq p\}$$

3 Probability distributions

3.1 Discrete distributions

Uniform distribution — $X \sim U(m, M)$

Models some experiment with $M - m + 1$ outcomes with the same probability of occurring. A random variable has uniform distribution if its PMF is given by

$$p(a) = P(X = a) = \frac{1}{M - m + 1} \qquad \text{for } a = m, m+1, \ldots, M$$

$$F(a) = \frac{\lfloor a \rfloor - m + 1}{M - m + 1} \qquad \text{for } m \leq a \leq M$$

$$\mathbb{E}[X] = \frac{m + M}{2} \qquad Var(X) = \frac{(M - m + 1)^2 - 1}{12}$$

Bernoulli distribution — $X \sim Ber(p)$

Models an experiment with two outcomes, success and failure, with probability $0 \leq p \leq 1$ of success. A random variable has the Bernoulli distribution if its PMF is given by

$$p(a) = P(X = a) = p^a (1 - p)^{1-a} \qquad \text{for } a = 0, 1$$

$$\mathbb{E}[X] = p \qquad Var(X) = p(1 - p)$$

Binomial distribution — $X \sim Bin(n, p)$

Models the number of successes in a sequence of n independent Bernoulli trials, each with probability $0 \leq p \leq 1$ of success. A random variable has the Binomial distribution if its PMF is given by

$$p(a) = P(X = a) = \binom{n}{a} p^a (1 - p)^{n-a} \qquad \text{for } a = 0, 1, \ldots, n$$

The sum of n independent Bernoulli r.v.s with parameter p is a Binomial r.v. with parameters n and p:

$$X = \sum_{i}^{n} X_i \sim Bin(n, p) \qquad \text{where } X_1, X_2, \ldots, X_n \sim Ber(p)$$

$$\mathbb{E}[X] = n \cdot p \qquad Var(X) = n \cdot p(1 - p)$$

Benford's law $X \sim Ben$

Models the distribution of the leading digits in many real-life numerical datasets. A random variable has the Benford's law distribution if its PMF is given by

$$p(a) = P(X = a) = \log_{10}(1 + \frac{1}{a}) - \log_{10}(1 + \frac{1}{a+1}) \qquad \text{for } a = 1, 2, \ldots, 9$$

Geometric distribution $X \sim Geo(p)$

Models the number of attempts needed to get the first success in a sequence of independent Bernoulli trials, each with probability $0 \leq p \leq 1$ of success. A random variable has the Geometric distribution if its PMF is given by

$$p(a) = P(X = a) = (1-p)^{a-1}p \qquad \text{for } a = 1, 2, \ldots$$

$$F(a) = 1 - (1-p)^a \qquad \text{for } a = 1, 2, \ldots$$

Given an infinite sequence of independent Bernoulli r.v.s with parameter p, the minimum number of trials needed to get a success is a Geometric r.v. with parameter p:

$$X = \min\{i : X_i = 1\} \sim Geo(p) \qquad \text{where } X_1, X_2, \cdots \sim Ber(p)$$

$$\mathbb{E}[X] = \frac{1}{p} \qquad Var(X) = \frac{1-p}{p^2}$$

Negative binomial (Pascal) distribution $X \sim NBin(n, p)$

Models the number of failures before the n-th success in a sequence of independent Bernoulli trials, each with probability $0 \leq p \leq 1$ of success. A random variable has the Negative binomial distribution if its PMF is given by

$$p(a) = P(X = a) = \binom{a+n-1}{a} p^n (1-p)^a \qquad \text{for } a = 0, 1, \ldots$$

Given n i.i.d. Geometric r.v.s, we can obtain a Negative binomial r.v. with parameters n and p as follows:

$$X = \sum_{i}^{n} X_i - n \sim NBin(n, p) \qquad \text{where } X_1, X_2, \ldots, X_n \sim Geo(p)$$

$$\mathbb{E}[X] = \frac{n \cdot p}{(1-p)} \qquad Var(X) = n\frac{1-p}{p^2}$$

Poisson distribution $X \sim Poi(\mu)$

Models the number of events occurring within some time interval, knowing the average rate of occurrence in that interval is μ. A random variable has the Poisson distribution if its PMF is given by

$$p(a) = P(X = a) = \frac{\mu^a}{a!}e^{-\mu} \qquad \text{for } a = 0, 1, 2, \ldots$$

The Poisson distribution can be approximated from the Binomial distribution:

$$Bin(n, p) \xrightarrow[n\to\infty]{} Poi(p \cdot n)$$

The approximation works for an experiment with an infinite number of Bernoulli trials, making it so that the mean rate of success is $\mu = p \cdot n$.

$$\mathbb{E}[X] = \mu \qquad Var(X) = \mu$$

Categorical distribution $X \sim Cat(\vec{p})$

A generalization of the Bernoulli distribution to 3 or more possible outcomes, each with its own probability of occurring. A random variable has the Categorical distribution if its PMF is given by

$$p(i) = P(X = i) = p_i \qquad i = 1, 2, \ldots, n_C - 1$$

The parameter $\vec{p}$ is a vector of probabilities, such that $\sum_i p_i = 1$.

Multinomial distribution $X \sim Mult(n, \vec{p})$

A generalization of the Binomial distribution to 3 or more possible outcomes, each with its own probability of occurring. A random variable has the Multinomial distribution if its PMF is given by

$$p(i_0, i_1, \ldots, i_{n_C-1}) = P(X = (i_0, i_1, \ldots, i_{n_C-1})) = \frac{n!}{i_0! \ldots i_{n_C-1}!} p_0^{i_0} p_1^{i_1} \ldots p_{n_C-1}^{i_{n_C-1}}$$

The sum of n independent Categorical r.v.s with parameter $\vec{p}$ is a Multinomial r.v. with parameters n and $\vec{p}$:

$$X = \sum_i^n X_i \sim Mult(n, \vec{p}) \qquad \text{where } X_1, X_2, \ldots, X_n \sim Cat(\vec{p})$$

3.2 Continuous distributions

Uniform distribution $X \sim U(\alpha, \beta)$

Models some experiment with arbitrary outcomes in the interval $[\alpha, \beta]$. A random variable has the Uniform distribution if its PDF is given by

$$f(x) = \frac{1}{\beta - \alpha} \qquad \text{for } \alpha \leq x \leq \beta$$

$$F(x) = \frac{x - \alpha}{\beta - \alpha} \qquad \text{for } \alpha \leq x \leq \beta$$

$$\mathbb{E}[X] = \frac{\alpha + \beta}{2} \qquad Var(X) = \frac{(\beta - \alpha)^2}{12}$$

Exponential distribution $X \sim Exp(\lambda)$

Models the time between subsequent events in a Poisson point process, with average rate of occurrence λ. A random variable has the Exponential distribution if its PDF is given by

$$f(x) = \lambda e^{-\lambda x} \qquad \text{for } x \geq 0$$

$$F(x) = 1 - e^{\lambda x}$$

$$\mathbb{E}[X] = \frac{1}{\lambda} \qquad Var(X) = \frac{1}{\lambda^2}$$

Normal (Gaussian) distribution $X \sim \mathcal{N}(\mu, \sigma^2)$

A random variable has a Normal distribution if its PDF is given by

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}(\frac{x-\mu}{\sigma})^2} \qquad \text{for } -\infty < x < \infty$$

The standard Normal distribution has $\mu = 0$ and $\sigma = 1$.
The Normal distribution can be approximated from the Binomial distribution:

$$Bin(n, p) \approx N(n \cdot p, n \cdot p(1 - p)) \qquad \text{for } n \to \infty \text{ and } 0 \ll p \ll 1$$

There is no closed form of the CDF of the Normal distribution, but any variable can be turned into a standard Normal variable and its probability can be estimated using the right tail probability table of $N(0, 1)$.

$$\mathbb{E}[X] = \mu \qquad Var(X) = \sigma^2$$

Erlang distribution $X \sim Erl(n, \lambda)$

Models the time until n events occur in a Poisson point process, with average rate of occurrence λ. A random variable has the Erlang distribution if its PDF is given by

$$f(x) = \frac{\lambda(\lambda x)^{n-1} e^{\lambda x}}{\Gamma(\alpha)} \qquad \text{for } x \geq 0$$

$\Gamma(\alpha) = (\alpha - 1)!$ is called Gamma function, and is a normalization factor ensuring that the integral of the PDF is equal to 1.

$$\mathbb{E}[X] = \frac{n}{\lambda} \qquad Var(X) = \frac{n}{\lambda^2}$$

Gamma distribution $X \sim Gam(\alpha, \lambda)$

Models the time until α quantities of something occur in a Poisson point process, with average rate of occurrence λ. It is a generalization of the Erlang distributions that also allows the first parameter to be any postive real number instead of a positive integer. A random variable has the Gamma distribution if its PDF is given by

$$f(x) = \frac{\lambda(\lambda x)^{\alpha-1} e^{\lambda x}}{\Gamma(\alpha)} \qquad \text{for } x \geq 0$$

The sum of n i.i.d. Exponential r.v.s. with parameter λ is Gamma distributed, with parameters n and λ:

$$X = \sum_{i}^{n} X_i \sim Gam(n, \lambda) \qquad \text{where } X_1, X_2, \ldots, X_n \sim Exp(\lambda)$$

$$\mathbb{E}[X] = \frac{n}{\lambda} \qquad Var(X) = \frac{n}{\lambda^2}$$

Cauchy distribution $X \sim Cau(\alpha, \beta)$

A random variable has the Cauchy distribution if its PDF is given by

$$f(x) = \frac{\beta}{\pi(\beta^2 + (x - \alpha)^2)} \qquad \text{for } -\infty < x < \infty$$

A special case of the Cauchy distribution is the standard Cauchy distribution, with $\alpha = 0$ and $\beta = 1$. This distribution is also the same as the ratio between two standard Normal r.v.s.

$$\mathbb{E}[X] = \text{undefined} \qquad Var(X) = \text{undefined}$$

4 Expectation

The expectation (or expected value, mean, center of gravity) of a random variable is a number that summarizes the most central value in that variable's distribution.

Expectation

The expectation of a discrete random variable X is calculated as

$$\mathbb{E}[X] = \sum_i x_i \cdot P(X = x_i) = \sum_i x_i \cdot p(x_i)$$

The expectation of a continuous random variable X is calculated as

$$\mathbb{E}[X] = \int_{-\infty}^{\infty} x \cdot f(x) dx$$

Expected value may be infinite or not exist for certain distributions. Consider the case of a continuous random variable. Its expected value, which is calculated as an integral I over $(-\infty, \infty)$ can be split into two terms, $I = I^- + I^+$, defined as follows:

$$I^- = \int_{-\infty}^{0} x \cdot f(x)$$

$$I^+ = \int_{0}^{\infty} x \cdot f(x)$$

Since $f(x)$ cannot take negative values, I^- is negative, and I^+ is positive. If I^- and I^+ are both finite, then the expected value exists and is finite. If one of them is infinite, the expected value is infinite. If both are infinite, the expected value does not exist. This can be generalized to discrete random variables, where the expectation is expressed as a sum instead of an integral (but can still similarly diverge or converge).

An example of distribution for which the expected value does not exist is the Cauchy distribution. An example of distribution for which the expected value is infinite is the Pareto distribution.

Change of variable formula (a.k.a. law of the unconscious/lazy statistician)

Let X be a random variable, and $g : \mathbb{R} \to \mathbb{R}$ be a function. If X is discrete, then

$$\mathbb{E}[g(X)] = \sum_i g(x_i) \cdot P(X = x_i)$$

If X is continuous, then

$$\mathbb{E}[g(X)] = \int_{-\infty}^{\infty} g(x) \cdot f(x)\ dx$$

Change of units theorem (for the expectation)

$\mathbb{E}[rX + s] = r\mathbb{E}[X] + s$

The expected value is **linear**. This means that $\mathbb{E}[aX + bY + c] = a\mathbb{E}[X] + b\mathbb{E}[Y] + c$ for any constants a, b, c. More in general, $\mathbb{E}[a_0 + \sum_i^n a_i \cdot X_i] = a_0 + \sum_i^n a_i \mathbb{E}[X_i]$

Jensen's inequality

Let g be a convex function, and let X be a random variable. Then

$$\mathbb{E}[g(X)] \geq g(\mathbb{E}[X])$$

If g is concave, the inequality is reversed. If g is linear, the inequality becomes an equality.

Two-dimensional change of variable formula

Let X and Y be random variables, and let $g : \mathbb{R}^2 \to \mathbb{R}$ be a function. If X and Y are discrete, Then

$$\mathbb{E}[g(X, Y)] = \sum_i \sum_j g(a_i, b_i) P(X = a_i, Y = b_j)$$

If X and Y are continuous, then

$$\mathbb{E}[g(X, Y)] = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} g(x, y) f(x, y) \, dxdy$$

where $f(x, y)$ is their joint PDF.

If two variables are independent, then $\mathbb{E}[XY] = \mathbb{E}[X] \cdot \mathbb{E}Y$. This holds for any set of independent random variables. More in general, given $X_1, X_2, \ldots, X_n$ independent random variables, and let $h_i : \mathbb{R} \to \mathbb{R}$ be a function; define the random variable $Y = h_i(X_i)$. Then, $Y_1, Y_2, \ldots, Y_n$ are also independent.
If we take two random variables, $X \perp\!\!\!\perp Y$ such that $Y > 0$, we have $\mathbb{E}[X/Y] \geq \mathbb{E}[X]/\mathbb{E}[Y]$. Let $g(y) = \frac{1}{y}$, the inequality follows from Jensen's inequality and the linearity of expectation.

Conditional expectation

$$\mathbb{E}[X|Y = b] = \sum_i a_i p(a_i|b) \qquad \mathbb{E}[X|Y = y] = \int_{-\infty}^{\infty} x f(x|y) \, dx$$

Also, the following theorem holds.

Law of iterated/total expectation

$$\mathbb{E}_Y[\mathbb{E}[X|Y]] = \mathbb{E}[X]$$

Proof:

$$\mathbb{E}_Y[\mathbb{E}[X|Y]] = \sum_j \sum_i a_i p_{X|Y}(a_i|b_j) \cdot p_Y(b_j) = \sum_j \sum_i a_i p_{X,Y}(a_i, b_j) = \sum_i a_i p_X(a_i) = \mathbb{E}[X]$$

5 Variance

The variance of a random variable is a measure of how much the values of that variable spread around the mean. A low variance means that most values are close to the mean, while a high variance means that the values are more spread out.

Variance

The variance of a random variable X is defined as

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

Often, the **standard deviation** ($\sigma = \sqrt{Var(X)}$) is used instead. This is because the variance is in squared units, so the standard deviation is on the same scale as the expectation and is easier to interpret.

Just like expectation, variance may be infinite or not exist. Variance does not exist if the expectation does not exist, but there may be distributions where the expectation exists while the variance does not: an example of such distribution are the Power Laws.

Change of units theorem (for the variance)

$Var(rX + s) = r^2 Var(X)$

The variance is **not linear**. This means that $Var(aX + bY + c) \neq aVar(X) + bVar(Y) + c$ in general. However, if X and Y are independent, then $Var(X + Y) = Var(X) + Var(Y)$.

6 Covariance

Covariance

The covariance of two random variables X and Y is the number:

$$Cov(X, Y) = \mathbb{E}[(X - \mathbb{E}[X])(Y - \mathbb{E}[Y])] = \mathbb{E}[XY] - \mathbb{E}[X]\mathbb{E}[Y]$$

Given two random variables X and Y, the variance of their sum is:

$$Var(X+Y) = Var(X) + Var(Y) + 2Cov(X,Y)$$

If the random variables are independent, their covariance is 0 (and so the variance of the sum is the sum of the variances).
Given X and Y two random variables, and $r, s, t, u \in \mathbb{R}$, then

$$Cov(rX+s, tY+u) = rtCov(X,Y)$$

Hence, $Var(rX+sY+t) = r^2Var(X) + s^2Var(X) + 2rsCov(X,Y)$.

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7 Power laws and Zipf's law

Power laws are a family of "scale free" distributions. Most distributions have a typical size or scale, so they have some value around which measurements are centered. In contrast, power laws vary over a very large range where it's not possible to identify a typical value around which the distribution peaks.

Power law distribution $X \sim Pow(x_{min}, \alpha)$

A random variable has the power law distribution if for some $\alpha > 1$ its PDF is given by

$$f(x) = C \cdot x^{-\alpha} \qquad x \geq x_{min}$$

C is called **intercept**, while α is called **exponent**. If the function is expressed in logarithmic scale, we have

$$\log(f(x)) = -\alpha \cdot \log(x) + \log(C)$$

i.e., there is a linear relationship between $\log(f(x))$ and $\log(x)$. Graphically, this means that the distribution is a straight line in a log-log plot. The reason parameter x_{min} is included is to specify what is the exact lower bound after which a distribution shows a power law behaviour.

Being scale-free, we can identify some constant b such that $p(bx) = g(b)p(x)$, meaning that even if we multiply the variable by this scaling factor, the form of the distribution remains the same. In this case, we write

$$p(bx) = b^{-\alpha}C \cdot x^{-\alpha}.$$

Notice how the value of the intercept is not specified in the definition above. This is because after fixing x_{min} and α, C is uniquely determined by the condition that the integral of the PDF over the entire range must be 1:

$$1 = \int_{x_{min}}^{\infty} C \cdot x^{-\alpha}\, dx = \frac{C}{-\alpha+1}[x^{-\alpha+1}]_{x_{min}}^{\infty} = \frac{C}{\alpha-1}x_{min}^{-\alpha+1} \iff \boxed{C = \frac{(\alpha-1)}{x_{min}^{-\alpha+1}}}$$

This integral is finite only if $\alpha > 1$. If $\alpha < 1$, then it simply diverges. If $\alpha = 1$, the denominator becomes 0, and the integral is not defined. By substituting this value in the formula of the PDF, we get

$$f(x) = \frac{\alpha - 1}{x_{min}} \left(\frac{x}{x_{min}} \right)^{-\alpha}.$$

Using the same calculations we can find a closed formula for the CCDF:

$$P(X > x) = \int_x^{\infty} C \cdot x^{-\alpha} \, dx = \frac{C}{-\alpha + 1} [x^{-\alpha+1}]_{x_{min}}^{\infty} = \frac{C}{\alpha - 1} x^{-\alpha+1}.$$

Since we calculated C we can substitute it back in the formula to get

$$P(X > x) = \left(\frac{x}{x_{min}} \right)^{-\alpha+1}$$

Both the PDF and the CCDF have the same form, but with a different exponent. The CCDF also looks linear when plotted in a log-log scale. As for the expectation, we have

$$\mathbb{E}[X] = \int_{x_{min}}^{\infty} x \cdot C \cdot x^{-\alpha} \, dx = C \int_{x_{min}}^{\infty} x^{alpha+1} \, dx = \frac{C}{-\alpha + 2} \left[x^{-\alpha+2} \right]_{x_{min}}^{\infty} = \frac{C}{\alpha - 2} x_{min}^{-\alpha+2}.$$

Similarly to the calculations done to find C, we can observe how this integral is finite only for $\alpha > 2$: if $\alpha < 2$, the integral diverges, while if $\alpha = 2$, the denominator becomes 0 and the integral is not defined. Substituting the value of C back in the formula, we get

$$\mathbb{E}[X] = \frac{\alpha - 1}{\alpha - 2} x_{min}$$

Also for the variance, it is finite only for $\alpha > 3$.

Pareto distribution $X \sim Par(x_{min}, \beta)$

A random variable has the Pareto distribution if for some $\beta > 0$ its density function is given by

$$f(x) = C \cdot x^{-(\beta+1)} \qquad x \geq x_{min}$$

A Pareto distribution is actually just a power law, but expressed differently:
$Par(x_{min}, \beta) = Pow(x_{min}, \beta + 1)$.

Discrete power law distribution $X \sim Pow(\alpha, k_{min})$

A random variable has the discrete power law distribution if for some $\alpha > 1$ its PMF is given by

$$p(k) = C \cdot k^{-\alpha} \qquad k = k_{min}, k_{min} + 1, \ldots$$

Since the sum of probabilities must be 1, C is determined as

$$C = \frac{1}{sum_{k=k_{min}}^{\infty} k^{-\alpha}} = \frac{1}{\zeta(\alpha, k_{min})}$$

$\zeta(\alpha, k_{min})$ is the **Hurwitz zeta function**. A special case of it is the **Riemann zeta function**, which is $\zeta(\alpha) = \zeta(\alpha, 1)$

When we are studying a data sample and want to check if it follows a power law, we can plot the frequency of its values in log-log scale and verify if the points are aligned in a straight line. However, since the values in the tail are rarer, the data sample will have few of them. The resulting plot will likely present a lot of noise around the tail of the distribution, and it may not be obvious whether it is a power law or some similar distribution (such as exponential or log-normal). To fix this issue, we can follow two approaches:

- We estimate and plot the CCDF in log-log scale. As mentioned above, the CCDF of a power law also appears linear when plotted this way, with the advantage of being much more stable in the tail.
- We construct an histogram using logarithmic binning. This means that the bins are not equally spaced, but they grow exponentially. For example, the first bin goes from 1 to 10, the second from 10 to 100, the third from 100 to 1000, and so on. Since bins aggregate values, the effect of noise is reduced.

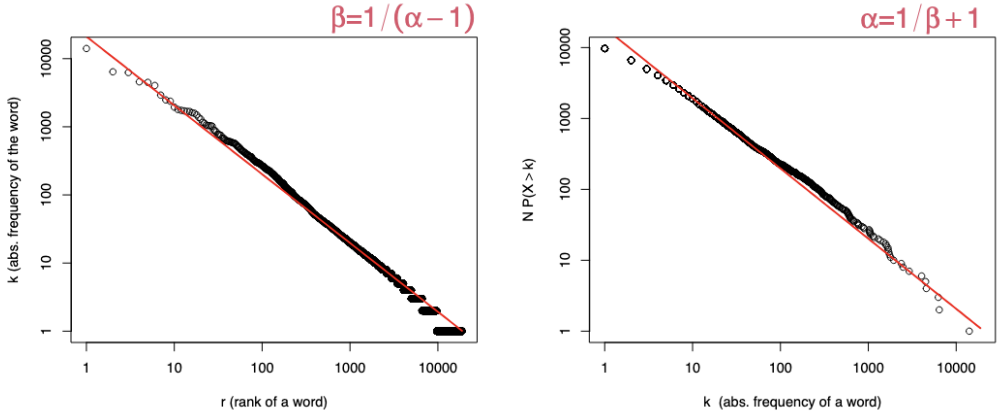
Zipf's law distribution $X \sim Zipf(\alpha)$

A random variable has the Zipf's law distribution if for some $\alpha > 1$ its PMF is given by

$$p(r) = C \cdot r^{-\alpha} \qquad r = 1, 2, \ldots, N$$

In a Zipf's law distribution, probabilities are assigned to the **ranks** of events; the higher the rank (i.e. closer to 1), the higher the probability. This is different than a power law distribution, where probabilities directly depend on the frequencies. For example: a discrete power law may model the probability of a word with a certain number of accurrences in a text, while Zipf's law may model the probability of a word with a certain rank in a list of words sorted by frequency.

We can try to convert a power-law into a Zipf's law and vice-versa. By comparing the PMF of a Zipf's law and the CCDF of a power law, they have the same form, and are actually representing the same information but with the axes inverted:



The rank r of a word with frequency k is equal to the number of words with frequency larger than k plus 1. In other words, $r = 1 + N \cdot P(X > k)$. If $X \sim Pow(1, \alpha)$, then $r = 1 + N \cdot P(X > k) \propto k^{-(\alpha-1)}$. By inverting, we get that $k \propto r^{-\frac{1}{\alpha-1}}$, i.e., the frequencies are Zipf's law distributed with parameter $\frac{1}{\alpha-1}$.

$$X \sim Pow(1, \alpha) \iff R \sim Zipf\left(\frac{1}{\alpha - 1}\right)$$

(R is a r.v. that models the ranks).
For this distribution, C is calculated as

$$C = \frac{1}{\sum_{r=1}^{N} r^{-\alpha}} = \frac{1}{\zeta(\alpha) - \zeta(\alpha, N+1)}$$

8 Computations with random variables

Consider a random variable X with a given distribution. Let $Y = g(X)$ be another random variable obtained as a function of the first. Then, the following theorems hold:

- If X is a discrete random variable, the PMF of $Y = g(X)$ is

$$P_Y(Y = y) = \sum_{g(x)=y} P_X(X = x) = \sum_{x \in g^{-1}(y)} P_X(X = x)$$

- If X is a continuous random variable, the CDF and PDF of $Y = g(X)$ when g is invertible is

$$F_y(y) = F_X(g^{-1}(y)) \qquad f_Y(y) = f_X(g^{-1}(y)) \left|\frac{dg^{-1}(y)}{dy}\right|$$

Change of units transformation

Let X be a continuous random variable. If we change units to $Y = rX + s$ for $r, s \in \mathbb{R}, r > 0$ then

$$F_Y(y) = F_X\left(\frac{y-s}{r}\right) \qquad f_Y(y) = \frac{1}{r} f_X\left(\frac{y-s}{r}\right)$$

Convolution of random variables

Let X adn Y be two independent random variables. If they are discrete with PMFs $p_X(x)$ and $p_Y(y)$, then the PMF of $Z = X + Y$ is

$$p_Z(z) = \sum_y p_X(c - x) \cdot p_Y(y)$$

If X and Y are continuous with PDFs $f_X(x)$ and $f_Y(y)$, then the PDF of $Z = X + Y$ is

$$f_Z(z) = \int_{-\infty}^{\infty} f_X(c - x) \cdot f_Y(y)\, dx$$

Maximum of random variables

Let $X_1, X_2, \ldots, X_n$ be n independent random variables with the same distribution function F, and let $Z = \max\{X_1, X_2, \ldots, X_n\}$. Then

$$F_Z(a) = (F(a))^n.$$

This is because $F_Z(a) = P(Z \leq a) = \prod_i^n P(X_i \leq a) = P(X_1 \leq a) \cdot P(X_2 \leq a) \cdot \ldots \cdot P(X_n \leq a) = (F(a))^n$.

Minimum of random variables

Let $X_1, X_2, \ldots, X_n$ be n independent random variables with the same distribution function F, and let $Z = \min\{X_1, X_2, \ldots, X_n\}$. Then

$$F_Z(a) = 1 - (1 - F(a))^n.$$

This is because $F_Z(a) = P(Z \leq a) = 1 - \prod_i^n P(X_i > a) = 1 - (1 - F(a))^n$.

Product of independent random variables

Let X and Y be two independent continuous random variables with PDFs f_X and f_Y. Then the PDF of $Z = XY$ is

$$f_Z(z) = \int_{-\infty}^{\infty} f_Y\left(\frac{z}{x}\right) f_X(x) \frac{1}{|x|}\, dx \qquad -\infty < z < \infty$$

Quotient of independent random variables

Let X and Y be two independent continuous random variables with PDFs f_X and f_Y. Then the PDF of $Z = X/Y$ is

$$f_Z(z) = \int_{-\infty}^{\infty} f_X(zx) f_Y(x) |x|\, dx \qquad -\infty < z < \infty$$

Propagation of independence

Let $X_1, X_2, \ldots, X_n$ be independent random variables. For each i, let $h_i : \mathbb{R} \to \mathbb{R}$ be a function, and define the r.v.s

$$Y_i = h_i(X_i)$$

Then $Y_1, Y_2, \ldots, Y_n$ are also independent.

9 Moments

Moment

Let X be a continuous random variable with PDF $f(x)$. The k^{th} moment of X (if it exists) is

$$\mathbb{E}[X^k] = \int_{-\infty}^{\infty} x^k \cdot f(x)\, dx$$

Th expected value of a random variable is its first moment.

Central moment

Let X be a continuous random variable with PDF $f(x)$. The k^{th} central moment of X (if it exists) is

$$\mu_k = \mathbb{E}[(X-\mu)^k] = \int_{-\infty}^{\infty} (x-\mu)^k f(x)\, dx$$

The variance of a random variable is its second central moment.
Another related concept is the k^{th} standardized moment, which is the k^{th} central moment divided by the standard deviation raised to the k^{th} power:

$$\tilde{\mu}_k = \frac{\mu_k}{\sigma^k} = \mathbb{E}\left[\left(\frac{X-\mu}{\sigma}\right)^k\right]$$

- $\tilde{\mu}_1 = 0$ (since $\mathbb{E}[X-\mu] = 0$ for any random variable);
- $\tilde{\mu}_2 = 1$ (since $\mathbb{E}[(X-\mu)^2] = \sigma^2$);
- $\tilde{\mu}_3$ is called **skewness** and measures the magnitude and direction of the asymmetry of the distribution. If it is 0, the distribution is symmetric, and mean, median, and mode coincide. If it is positive, the distribution is **right-skewed** (the mean is greater than mode and median), while if it is negative, the distribution is **left-skewed** (the mean is less than mode and median).

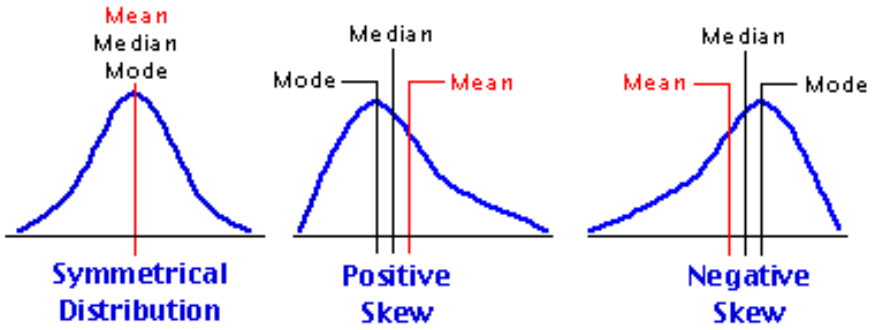


Figure 1: Skewness of distributions.

- $\tilde{\mu}_4$ is called **kurtosis** and measures the dispersion of the random variable around the values $\mu+\sigma$ and $\mu-\sigma$. Specifically, the kurtosis of a distribution is compared to that of a Normal distribution, which is always 3. Then, if the kurtosis is equal to 3, the distribuion is **mesokurtic** (similar to a Normal); if it is greater than 3, it is **leptokurtic** (the tails are fatter, while the middle is thinner); if it is less than 3, it is **platykurtic** (the tails are thinner, but the middle is larger).

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10 Distances between distributions

Distances and metrics

A distance over a set $\mathcal{A}$ is a function $d : \mathcal{A} \times \mathcal{A} \to \mathbb{R}$ such that:

- $d(x, y) \geq 0$ (non-negativity)
- $d(x, y) = 0$ iff $x = y$ (identity of indiscernibles)
- $d(x, y) = d(y, x)$ (symmetry)

Also, d is a metric if it also satisfies the triangle inequality: $d(x, z) \leq d(x, y) + d(y, z)$.

Distances and metrics over probability distributions are used to measure how far apart two distributions are. Calculating distances is very useful in statistics and machine learning: for example, after a dataset has been split into training and test sets, we can compare the distribution of the two to make sure they are similar (or, alternatively, to make sure they are different and study how well the model generalizes). This section will overview the most common distances used in statistics.

Total Variation (TV) distance

$$d_{TV}(X, Y) = \frac{1}{2} \sum_i |p_X(a_i) - p_y(a_i)| \qquad \text{(discrete case)}$$

$$d_{TV}(X, Y) = \frac{1}{2} \int |f_X(x) - f_Y(x)| dx \qquad \text{(continuous case)}$$

Kolmogorov-Smirnof (KS) distance

$$d_{KS}(X, Y) = \sup_x |F_X(x) - F_Y(x)|$$

Both are metrics. They have no closed forms, but they can be approximated from samples of the distributions.

Shannon's information entropy (H)

$$H(X) = \mathbb{E}[-\log(p(X))] = -\sum_i p(a_i)\log(p(a_i)) \qquad \text{(discrete case)}$$

$$H(X) = \mathbb{E}[-\log(f(X))] = -\int_{-\infty}^{\infty} f(x)\log(f(x))dx \qquad \text{(continuous case)}$$

Entropy measures the average level of information (or "surprise", "uncertainty") of a random variable. Information is inversely proportional to probability: the more unlikely an event is, the more information it carries. So, for example, a random variable that only takes a single value has zero entropy, because there is no uncertainty about its value. In contrast, a random variable that takes many values with equal probability has high entropy, because there is a lot of uncertainty about its value.

Let X be a discrete random variable with a finite domain of n elements. Per corollary of Jensen's inequality, since $log(x)$ is a concave function, we have:

$$H(X) = \mathbb{E}[-\log(p(X))] = \mathbb{E}\left[\log\left(\frac{1}{p(X)}\right)\right] \leq \log\left(\mathbb{E}\left[\frac{1}{p(X)}\right]\right)$$

Then, by change of variable:

$$\mathbb{E}\left[\frac{1}{p(X)}\right] = \sum_i \frac{p(a_i)}{p(a_i)} = n$$

So we can derive the following bound for the entropy:

$$H(X) \leq \log(n)$$

Cross entropy (H)

$$H(X;Y) = \mathbb{E}_X[-\log p_Y(Y)] = -\sum_i p_X(a_i)\log(p_Y(a_i)) \qquad \text{(discrete case)}$$

$$H(X;Y) = \mathbb{E}_X[-\log f_Y(Y)] = -\int_{-\infty}^{\infty} f_X(x)\log(f_Y(x))dx \qquad \text{(continuous case)}$$

Cross entropy measures the number of bits needed to encode values from X using a code based on Y. If the two have exactly the same distribution, the cross entropy is minimal: it is exactly equal to the entropy of X. The more the two are different, the more extra bits will be needed to encode the differences between the two.

Joint entropy (H)

$$H(X,Y) = \mathbb{E}[-\log(p(X,Y))] = -\sum_{i,j} p(a_i,a_j)\log(p(a_i,a_j)) \qquad \text{(discrete case)}$$

$$H(X,Y) = \mathbb{E}[-\log(f(X,Y))] = -\int_{-\infty}^{\infty} f(x,y)\log(f(x,y))dxdy \qquad \text{(continuous case)}$$

Joint entropy is simply the entropy of the joint distribution of two random variables X and Y. If the two are independent, then $p_{XY}(x,y) = p_X(x) \cdot p_Y(y)$ (and similarly for PDFs), so the above sum/integral can be split, making it so that $H(X,Y) = H(X) + H(Y)$.

Kullback-Leibler (KL) divergence

$$D_{KL}(X||Y) = \sum_i P_X(a_i)\log\left(\frac{p_X(a_i)}{p_y(a_i)}\right) = H(X;Y) - H(X) \qquad \text{(discrete case)}$$

$$D_{KL}(X||Y) = \int_{-\infty}^{\infty} f_X(x)\log\left(\frac{f_X(x)}{f_Y(x)}\right)dx = H(X;Y) - H(X) \qquad \text{(continuous case)}$$

KL divergence is also sometimes called relative entropy of X w.r.t. Y; it measures how well the distribution of the model Y can reconstruct the distribution of the data X. Since it can be expressed in terms of cross-entropy and entropy, it is easy to see that

- It is always non-negative, since the cross-entropy between two distributions can only be greater than or equal to the entropy of one of them.
- It is exactly 0 if the two distributions are the same.
- It is asymmetric.

Note that since it is not symmetric, it is not an actual distance.

Mutual information

Discrete case:

$$I(X,Y) = D_{KL}(p_{XY}||p_X p_Y) = \sum_{i,j} p_{XY}(a_i, a_j) \log\left(\frac{p_{XY}(a_i, a_j)}{p_X(a_i)p_y(a_j)}\right) =$$

$$= H(X) + H(Y) - H(X;Y)$$

Continuous case:

$$I(X,Y) = D_{KL}(f_{XY}||f_X f_Y) = \int_{-\infty}^{\infty} f_{XY}(x,y) \log\left(\frac{f_{XY}(x,y)}{f_X(x)f_Y(y)}\right) dxdy =$$

$$= H(X) + H(Y) - H(X;Y)$$

Mutual information measures how dependent the two distributions are. It quantifies how much the product of the marginals can reconstruct the joint distribution.

- It is always non-negative, since the sum of the individual entropies is always greater than or equal to the joint entropy.
- It is exactly 0 if $X \perp\!\!\!\perp Y$.
- It is symmetric.

In some cases, it may be useful to have a normalized measure of dependence. The **normalized mutual information** is defined as:

$$NMI(X,Y) = \frac{I(X,Y)}{\min\{H(X), H(Y)\}} \in [0,1]$$

Suppose we have an unknown variable X, and we observe a noisy function of it, called Y. Let $Z = f(Y)$, i.e., a processing of the noisy observations. Intuitively, Z cannot contain more information about X than Y does. This is known as the **data processing inequality**:

$$I(X,Y) \geq I(X,Z)$$

If they happen to be equal, and Z is a summary of Y, then Z is a sufficient statistic for X: it means that we can reconstruct X from Z with the same accuracy as from Y.

Earth mover's distance (Wasserstein metric)

$$EMD(X,Y) = \frac{\sum_{i,j} F_{i,j} \cdot |a_i - a_j|}{\sum_{i,j} F_{i,j}}$$

Earth's mover distance measures the minimum cost required to transform one distribution into another; the F in the formulas is the **flow** which minimizes the numerator (the cost). In practice, for pairs of univariate random vairables X and Y, is is calculated as follows:

$$EMD(X,Y) = \sum_i |F_X(a_i) - F_Y(a_i)| \qquad \text{(discrete case)}$$

$$EMD(X,Y) = \int_{-\infty}^{\infty} |F_X(x) - F_Y(x)|\, dx \qquad \text{(continuous case)}$$

For empirical distributions, assuming the samples are sorted in increasing order:

$$EMD(X,Y) = \frac{1}{n}\sum_i |x_i - y_i|$$

11 The law of large numbers

For many experiments that concern natural phenomena, different executions of the same experiment will likely yield different results. The variation in the outcome is due to randomness caused by uncontrollable factors. To mitigate the effect of this randomness, the same experiment can be repeated a number of times and the **average** of the results is studied instead. Formally, given $X_1, X_2, \ldots, X_n$ independent random variables, their average is

$$\bar{X}_n = \frac{X_1 + X_2 + \ldots + X_n}{n}$$

Expected value and variance of an average

If $\bar{X}_n$ is the average of n independent random variables with the same expectation μ and variance σ^2, then

$$\mathbb{E}[\bar{X}_n] = \mu \qquad Var(\bar{X}_n) = \frac{\sigma^2}{n}$$

The random variables do not need to be identically distributed. Note that the variance is inversely proportional to the number of random variables contributing to the average: the more variables we have, the more stable the average becomes.

Markov's inequality

Let $X \geq 0$ be a random variable, and let $a > 0$. Then

$$P(X \geq a) \leq \frac{\mathbb{E}[X]}{a}$$

Corollary: Assume $X \geq 0$, $\mathbb{E}[X] > 0$ and $k > 0$. Then

$$P(X \geq k\mathbb{E}[X]) \leq \frac{1}{k}$$

The proof is as follows: let $\mathbb{1}_{X \geq \alpha}$ be an indicator variable that is 1 if $X \geq \alpha$ and 0 otherwise. Then

$$\alpha \mathbb{1}_{X \geq \alpha} \leq X$$

$$\mathbb{E}[\alpha \mathbb{1}_{X \geq \alpha}] \leq \mathbb{E}[X]$$

$$\alpha P(X \geq \alpha) \leq \mathbb{E}[X]$$

$$P(X \geq \alpha) \leq \frac{\mathbb{E}[X]}{\alpha}$$

Chebyshev's inequality

Let X be a random variable, and $a > 0$. Then

$$P(|X - \mathbb{E}[X]| \geq a) \leq \frac{Var(X)}{a^2}$$

This inequality claims that most of the probability mass of a random variable is within a few standard deviations from the expected value. It is a consequence of Markov's inequality:

$$P(|X - \mathbb{E}[X]| \geq a) = P((X - \mathbb{E}[X])^2 \geq a^2) \leq \frac{\mathbb{E}[(X - \mathbb{E}[X])^2]}{a^2} = \frac{Var(X)}{a^2}$$

Now, we can apply Chebyshev's inequality to the average of n independent random variables, obtaining the following result:

The (weak) law of large numbers

Let $\bar{X}_n$ be the average of n independent random variables with the same expectation μ and variance σ^2. Then, for any $\varepsilon > 0$,

$$\lim_{n \to \infty} P(|\bar{X}_n - \mu| > \varepsilon) = 0$$

This law confirms what we previously observed with the variance of the average. As n goes to infinity, the probability that the value of the average significantly deviates from its expectation (that is also the same of the individual random variables in the average) becomes zero. This also holds if σ^2 is infinite, as long as the individual random variables have finite expectation.

The consequence of the law of large numbers is that by calculating the average of a reasonably large enough set of random variables we can recover not only the mean and the stardard deviation, but pretty much any feature of the distribution of the random variables. Next up are two application examples.

Recovering the probability of an event Assume we want to know the probability that the outcome of some experiment falls within a certain range, i.e., $p = P(a \leq X \leq b)$. We run n independent

measurements of this same experiment, and we model those results with the r.v.s $X_1, X_2, \ldots, X_n$. Then, we can define an indicator variable for each X_i:

$$Y_i = \mathbb{1}_{a \leq X_i \leq b} = \begin{cases} 1 & \text{if } a \leq X_i \leq b \\ 0 & \text{otherwise} \end{cases}$$

The Y_i are also independent (per the propagation of independence seen previously). Since Y_i is an indicator variable, we know that

$$\mathbb{E}[Y_i] = p = P(a \leq X_i \leq b) \qquad\qquad Var(Y_i) = p(1-p)$$

Let $\bar{Y}_n$ be the average of the indicator variables. By the law of large numbers:

$$\lim_{n \to \infty} P(|\bar{Y}_n - p| > \varepsilon) = 0$$

Informally, this means that if we perform the experiment n times, count the amount of times the outcome falls within the range $[a, b]$, and divide by n, we get an estimate of the real probability of that event. The larger n is, the better the estimate becomes.

Estimating conditional probability We want to estimate the conditional probability for two random variables: $p = P(C = c|A = a) = P(A = a, C = c)/P(A = a) = p_{ac}/p_a$. We run n independent measurements of the experiment, modeling each result as a pair (A_i, C_i). We define indicator variables as the example above:

$$Y_i = \mathbb{1}_{A_i = a \wedge C_i = c} = \begin{cases} 1 & \text{if } A_i = a \wedge C_i = c \\ 0 & \text{otherwise} \end{cases}$$

$$Z_i = \mathbb{1}_{A_i = a} = \begin{cases} 1 & \text{if } A_i = a \\ 0 & \text{otherwise} \end{cases}$$

By applying the (strong) law of large numbers, we get that

$$\lim_{n \to \infty} P(\bar{Y}_n = p_{ac}) = 1$$

$$\lim_{n \to \infty} P(\bar{Z}_n = p_a) = 1$$

The two limits can be condensed in a ratio to estimate the conditional probability:

$$\lim_{n \to \infty} P(\frac{\bar{Y}_n}{\bar{Z}_n} = \frac{p_{ac}}{p_a}) = 1$$

Hoeffding bound

If $\bar{X}_n$ is the average of n independent random variables with the same expectation μ and $P(a \leq X_i \leq b) = 1$, then for any $\varepsilon > 0$:

$$P(|\bar{X}_n - \mu| \geq \varepsilon) \leq 2e^{-2n\varepsilon^2/(b-a)^2}$$

This offers a tight bound on the probability that the average deviates from its expectation by an arbitrarily small amount, but requires that the random variables have a bounded support.

12 The central limit theorem

The central limit theorem

Let $X_1, X_2, \ldots, X_n$ ne any sequence of i.i.d. random variables with the same expectation μ and finite positive vairance σ^2. For $n \geq 1$, let Z_n be defined by

$$Z_n = \sqrt{n}\frac{\bar{X}_n - \mu}{\sigma}$$

Then, for any number a

$$\lim_{n\to\infty} F_{Z_n}(a) = \Phi(a)$$

where Φ is the distribution function of the $\mathcal{N}(0,1)$ distribution.

This theorem states that if we take the average of n random variables, remove its expectation, and divide by its standard deviation, the result is a random variable that converges to a standard normal distribution as n goes to infinity. But, in practice, how large should n be? A famous rule of thumb is to use $n \geq 30$ to get a good approximation, but it is mostly just a myth; the optimal value of n depends on the distribution of the random variables.

13 Summaries

Summaries are used to represent and describe the information contained in datasets. They csan be graphical summaries, which visually represent the data, or numerical summaries, which give a description of the data in terms of numbers.

13.1 Graphical summaries

Empirical CDF A random variable is completely characterized by its CDF. We can approximate the CDF with the empirical cumulative distribution function, which is defined as

$$F_n(x) = \frac{|\{i : [1,n] | x_i \leq x\}|}{n}$$

where the x_i are the observations in the dataset. The **Glivenko-Cantelli theorem** states that the empirical CDF converges to the true CDF as n goes to infinity:

$$P(\lim_{n\to\infty} \sup_x |F(x) - F_n(x)| = 0) = 1$$

This approximation can be plugged into different formulas to estimate other quantities, such as the mean or the variance.

Bar plots and histograms A bar plot is used for discrete data. It provides a frequency count for the values in the dataset, and approximates the PMF (as a consequence of the law of large numbers, as seen in a previous example):

$$P(X = a) \approx \frac{|\{i|x_i = a\}|}{n}$$

A histogram is used for continuous data. It provides frequency counts for ranges of values (instead of individual ones). The support of the random variable is first split into m intervals called **bins** (which can all have the same width or different widths), and the number of occurrences belonging to each bin is counted and normalized:

$$A_i = \frac{|\{j \in [1, n]|x_j \in B_j\}|}{n} \approx P(X \in B_i)$$

The bins can be plotted as rectangles so that their area is proportional to A_i; after fixing their width b_i, the height is found as $H_i = A_i/b_i$.

Bin width can be chosen in different ways, producing different results. It is common to choose the same width for all bins, such that, for a total number of bins m, the interval corresponding to the i^{th} bin is

$$B_i = (r + (i-1)b, r + i * b)$$

where r is the minimum value taken by the random variable, and b is the bin width. The optimal width can be found using **Mean Integrated Squared Error** (**MISE**):

$$MISE = \mathbb{E}\left[\int (\hat{f}(t) - f(t))^2 \, dt\right] = \int \int (\hat{f}(t) - f(t))^2 f(x_1) \dots f(x_n) \, dt dx_1 \dots dx_n$$

where $\hat{f}$ is the density estimation of the real PDF f. The minimum of the MISE for Normal distributions is represented by **Scott's normal reference rule**:

$$b = 3.49 \cdot s \cdot n^{-1/3}$$

wher s is the sample standard deviation.
Other options are:

- **Freedman-Diaconis' choice**:

  $$b = 2 \cdot \text{IQR} \cdot n^{-1/3}$$

  This choice is more robust to outliers than the previous.

- **Variable bin width** (such as logarithmic binning as seen in power-law distributions).

- **Fixing the number of bins, and derivaring the width from it**. Some common strategies are:

  $$m = \lceil \frac{\max x_i - \min x_i}{b} \rceil$$

  $$m = \lceil \sqrt{n} \rceil$$

  $$m = \lceil \log_2 n \rceil + 1 \text{ (Sturges' rule)}$$

  The latter assumes normal distribution for the true density. This distribution can be approximated by a $Bin(n, 0.5)$ distribution, so the absolute frequency of the i^{th} bin is $\binom{m-1}{i}$. The total frequency is $n = \sum_{i=0}^{m-1} \binom{m-1}{i} = 2^{m-1}$, from which m is derived.

Kernel density estimation A big disadvantage of histograms is that the result strictly depends on the number of bins/bin width chosen to visualize the data. Kernel density estimation is another popular method to summarize distributions which is not as sensitive to the choice of parameters.

The idea behind this method is to mix kernel functions (which can take different forms, see Fig 2) centered in each observation in the dataset. Since data is assumed to be of continuous nature, the presence of a certain value in the dataset also contributes to the density of the values around it. The kernel function models the way this density is distributed around that single observation, and by mixing together all the kernels, the result should be a good approximation of the true density.

- Epanechnikov $\frac{3}{4}(1-t^2)$ for $-1 \leq t \leq 1$
- Triweight $\frac{35}{32}(1-t^2)^3$ for $-1 \leq t \leq 1$
- Normal $\frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}t^2}$ for $-\infty < t < \infty$

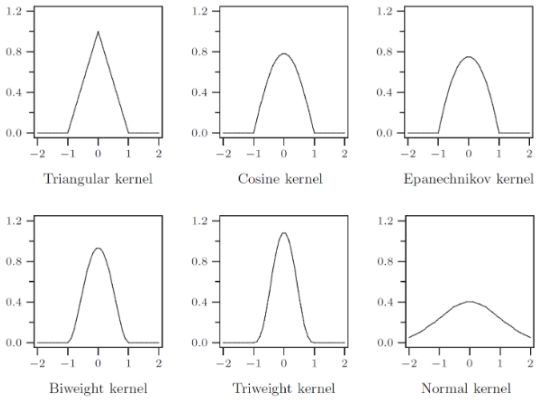

Figure 2: Examples of common kernels used in KDE.

Kernel

A kernel is a function $K : \mathbb{R} \to \mathbb{R}$ such that

- K is a probability density: $K(t) \geq 0$ and $\int_{-\infty}^{\infty} K(t)\, dt = 1$
- K is symmetric: $K(-t) = K(t)$
- $K(t) = 0$ for $|t| > 1$ (i.e., support is $[-1, 1]$)

The last requirement is not strictly necessary, actually; for example, the Normal kernel has unbounded support.

Each kernel function is characterized by a center (the observation), and a **bandwidth** h, which is a scaling factor over the support of the kernel from $[-1, 1]$ to $[-h, h]$. In other words, the badwidth determines how tall-thin or short-wide the kernel is around its center. We can then write

$$X \sim K(t) \implies h \cdot X + x_i \sim \frac{1}{h} K\left(\frac{t - x_i}{h}\right)$$

because of the change-of-units transformation formulas. The final kernel density estimate is the result of the **mixture** of all the scaled and shifted kernel densities:

$$f_{n,h}(t) = \frac{1}{nh} \sum_{i=1}^{n} K\left(\frac{t - x_i}{h}\right)$$

The $1/n$ in the formula is a normalization factor that ensures the density integrates to 1.

The choice of kernel is not critical to the final result; different kernels behave similarly. The key parameter is the bandwidth h. Also for KDE, MISE can be used to find the optimal value. Assuming the true density is Normal, the MISE is minimized for

$$h = \left(\frac{4}{3}\right)^{1/5} \cdot s \cdot n^{-1/5}$$

For other distributions, the optimal bandwidth can be found using plug-in selectors or cross validation selectors.

Another issue that may arise is when the support of the random variable is bounded. If KDE is used as is, the result will present density event corresponding to values that are not possible. To avoid this, boundary correction techniques are used; some examples are

- Kernel truncation and renormalization (forced truncation of the kernel outside the support);
- Linear combination kernel;
- Beta boundary kernels;
- Reflective kernels.

13.2 Numerical summaries

Sample summaries Summaries of the empirical data can be used to estimate summaries of the true distribution. The following are some common ones:

- **Sample mean**:
$$\bar{x} = \frac{x_1 + \ldots + x_n}{n}$$
- **Median**: Let $x_1, x_2, \ldots, x_n$ be the data in the sample, sorted.
$$Med(x_1, \ldots, x_n) = \begin{cases} x_{n/2} & \text{if } n \text{ is odd} \\ \frac{x_{n/2} + x_{n/2+1}}{2} & \text{if } n \text{ is even} \end{cases}$$
The median of a distriution corresponds to the 0.5^{th} quantile.
- **Sample variance and standard deviation**:
$$s_n^2 = \frac{\sum_i^n (x_i - \bar{x_n})^2}{n-1} \qquad\qquad s_n = \sqrt{s_n^2}$$
- **Median of absolute deviations**:
$$MAD(x_1, \ldots, x_n) = Med(|x_1 - Med(x_1, \ldots, x_n)|, \ldots, |x_n - Med(x_1, \ldots, x_n|))$$
If the distribution is symmetric, the MAD is exactly equal to the difference between the 0.75^{th} and 0.5^{th} quantiles.

Order statistics Let $x_1, x_2, \ldots, x_n$ be the ordered sequence of values in a sample. $x_{\langle i \rangle}$ is the i^{th} order statistic. Order statistics are used to calculate empirical quantiles. Formally, the p^{th} quantile is the value q_p such that $q_p = \inf_x\{P(X \leq x) \geq p\} = \inf_x\{F(x) \geq p\}$ (to be read as: "the smallest number x such that the probability of X being less or equal than x is greater or equal than p"). To find the empirical quantiles, we use the empirical approximation of the CDF in place of the true CDF:

$$q_p = \inf_x\{F_n(x) \geq p\} = \inf_x\left\{\frac{|\{i|x_i \leq x\}|}{n} \geq p\right\}$$

There are actually many ways to find the quantiles of a distribution. In `R`, there are 9 variants. The default one is type 7:

$$p = \frac{i-1}{n-1} \implies q_p = x_{\langle p\cdot(n-1)+1\rangle}$$

Another common choice is type 6:

$$p = \frac{i}{n+1} \implies q_p = x_{\langle p\cdot(n+1)\rangle}$$

The difference between the methods is irrelevant for big enough datasets.

What if the supposed index of the quantile is not an integer? In this case, the quantile is approximated using linear interpolation. Let $k = \lfloor p\cdot(n+1)\rfloor$ (or whatever other formula is used by the chosen method). Then,

$$q_p = x_{\langle k\rangle} + \alpha \cdot (x_{\langle k+1\rangle} - x_{\langle k\rangle})$$

where $\alpha = p \cdot (n+1) - k$, i.e., the decimal part of the index.

Association and correlation **Association** measures how much information one variable provides on another. If two variables are independent, they are not associated. Association is maximum when one variable is a (invertible) function of the other. **Correlation** measures the presence and strenght of an increasing/decreasing trend between two variables. If two variables are independent, their correlation is always 0, but the opposite is not always true.

Correlation

Let X and Y be two random variables. The correlation coefficient ρ is defined to be 0 if $Var(X) = 0$ or $Var(Y) = 0$, and otherwise as

$$\rho = \frac{Cov(X,Y)}{\sqrt{Var(X)\cdot Var(Y)}} \tag{1}$$

Some common correlation coefficients are:

- **Pearson's r**: it is obtained by substituting the sample covariance and the sample standard deviations of the random variables in the formula above:

  $$s_{xy} = \frac{\sum_{i=1}^{n}(x_i - \bar{x})\cdot(y_i - \bar{y})}{n-1} \qquad r = \frac{s_{xy}}{s_x \cdot s_y}$$

  It is bounded in the interval $[-1, 1]$. The computational cost to calculate it is $O(n)$. A limitation of Pearson's r is that it can only detect linear relationships between random variables, and it can only be used when the variables are continuous.

- **Spearman's ρ**: this coefficient is calculated as the correlation between ranks of the observations. Let $rank(x)$ be the ranks of the values of the variable x. Then, Spearman's ρ is calculated as

$$\rho = r(rank(x), rank(y)) = 1 - \frac{6 \sum_{i=1}^{n} (rank(x)_i - rank(y)_i)^2}{n \cdot (n^2 - 1)}$$

  This coefficient assesses monotonic relationships of any kind (both linear and non-linear). The computational cost to calculate it is $O(n \cdot \log n)$, since it requires a sorting of the data to compute the ranks. It can be used when both variables are ordinal, continuous, or when one is ordinal and the other is continuous.

- **Kendall's τ**: this coefficient compares the sign of the differences between successive pairs of observations. It is calculated as

$$\tau_a = \frac{2 \sum_{i<j} sign(x_i - x_j) \cdot sign(y_i - y_j)}{n \cdot (n - 1)}$$

  It calculates the fraction of concordant pairs minus discordant pairs of values between the two variables, and it is bounded in the interval $[-1, 1]$. The computational cost to calculate it is $O(n^2)$. There is a variant, τ_b, which also takes into account the possibility of ties; instead of dividing by $n \cdot (n - 1)$, it counts how many pairs do not present a tie in x or y. It can be used when both variables are ordinal, or when one is ordinal and the other is continuous.

- **Somer's D**: this coefficient is used when one variable is continuous and the other is binary. It can be seen as an asymmetric version of Kendall's τ:

$$D = \frac{\tau_{xy}}{\tau yy} = \frac{\sum_{i<j} sign(x_i - x_j) \cdot sign(y_i - y_j)}{\sum_{i<j} sign(y_i - y_j)^2} \tag{2}$$

  It calculates the fraction of concordant pairs minus discordant pairs over the number of unequal pairs of values in y. An example application can be seen with probabilistic classifiers: x is the confidence prediction of an example being positive, y is the true class, and D is the Gini index of the classifier.

- **Thiel's U**: it is used when both variables are nominal. It can be calculated in a symmetric and an asymmetric way:

$$U_{sym} = \frac{2 \cdot I(X, Y)}{H(X) + H(Y)} \qquad\qquad U_{asym} = \frac{I(X, Y)}{H(X)}$$

  where $I(X, Y)$ is the mutual information between X and Y, and $H(X), H(Y)$ are the entropies of the two random variables. The asymmetrical version, specifically, indicates what fraction of X can be predicted by Y.

14 Estimators

A dataset is a st of repeated measurements of a specific phenomenon which we want to understand better. The phenomenon can be modeled using some probability distribuion, so the dataset (which is the realization of a random sample from that distribution) can be used to approximate its parameters.

Random sample

A random sample is a collection of i.i.d. random variables $X_1, X_2, \ldots, X_n \sim F(\alpha)$, where $F()$ is the distribution and α its parameter(s).

A classic example is the approximation of the speed of light by physicist A. A. Michelson, done in 1879. His dataset of measurements consisted of 100 different measurements, each which was in itself th average of repeated measurements on several variables (e.g., distance between the tools used). At the end, his estimate was off by about 150 km/s, likely due to him missing some source of error despite his meticulousness; still, he had the intuition of using the average of a dataset to estimate the parameter of a distribution (in this case, the one that describes the speed of light).

Estimand and estimate

An estimand θ is an unknown parameter of a distribution $F()$.
An estimate t of θ is a value that is obtained as a function $h()$ over a dataset:

$$t = h(x_1, \ldots, x_n) \tag{3}$$

Statistics and estimator

A statistics is a function $h(X_1, \ldots, X_n)$ of random variables.
An estimator of a parameter θ is a statistics $T_n = h(X_1, \ldots, X_n)$ intended to provide information about θ.

Using the speed of light example, we can model is as follows: the dataset of measurements is the realization of a random sample of random variables. Each random variable is defined as:

$$X_i = c + \epsilon_i$$

where c is the speed of light, and ϵ_i is a measurement error, assumed to be normally distributed with mean 0 ad variance σ^2. The **estimand** is the expected value of one of these variables: $\theta = \mathbb{E}[X_i]$. We can define an **estimator** as the average of the sample:

$$T_n = \bar{X}_n = \sum_{i=1}^{n} \frac{X_1 + X_2, \ldots, +X_n}{n}$$

Finally, the **estimate** is the actual value we get by plugging the values collected in the dataset to the estimator.

Unbiased estimator

An estimator $T_n = h(X_1, \ldots, X_n)$ of a parameter θ is unbiased if

$$\mathbb{E}[T_n] = \theta$$

If $\mathbb{E}[T_n] - \theta \neq 0$, the estimator is biased.

Bias, if present, can be either positive or negative. An estimator may be **asymptotically unbiased** if it its unbiased as the sample size n approaches infinity:

$$\lim_{n \to \infty} \mathbb{E}[T_n] = \theta$$

Sometimes, the estimator is indicated with the same symbol as the estimand, but with a hat on top: $\hat{\theta}$ (e.g., $\hat{\mu}$ is an estimator for the mean, $\hat{sigma}$ is an estimator for the standard deviation).

Bias can be thought of as a measure of how well the estimator can approsimate the parameter of interest. If it is unbiased, it means it has the capacity to estimate the parameter correctly. Estimators are also characterized by their variance. **Variance** is a measure of how much the estimate can sway from the true value of the parameter, regardless of bias. An estimator can have low bias, but high variance, meaning that it can approximate the parameter, but the response is not necessarily reliable. When the same estimand has multiple unbiased estimators, variance is a measure of their efficiency. Let T_1 and T_2 be unbiased estimators of θ; T_1 is **more efficient** than T_1 if $Var(T_2) < Var(T_1)$. The **relative efficiency** of T_2 w.r.t. T_1 is $Var(T_1)/Var(T_2)$. The standard deviation of the estimator is called **standard error** (**SE**).

Unbiased estimators for expectation and variance

Let $X_1, X_2, \ldots, X_n$ be a random sample from a distribution with finite expectation μ and finite variance σ. Then

$$\bar{X}_n = \frac{X_1 + X_2 + \ldots + X_n}{n}$$

is an unbiased estimator for μ, and

$$S^2 = \frac{1}{n-1} \sum_{i=1}^{n} (X_i - \bar{X}_n)^2$$

is an unbiased estimator for σ^2.

We've already seen how the expected value of the mean is also the mean of the distribution. Also, per the central limit theorem, the variance of the mean goes to 0 as n goes to infinity.

Why is the estimator of the variance divided by $n-1$ instead of n? This is called Bessel's correction, and it is used to make sure the estimator is unbiased. The proof is explained below. First, for any random variable X_i, the following hold true:

(1) $\mathbb{E}[X_i - \bar{X}_n] = \mathbb{E}[X_i] - \mathbb{E}[\bar{X}_n] = \mu - \mu = 0$

(2) $Var(X_i - \bar{X}_n) = \mathbb{E}[(X_i - \bar{X}_n)^2] - E[X_i - \bar{X}_n]^2 = \mathbb{E}[(X_i - \bar{X}_n)^2] = \sigma^2$

X_i and $\bar{X}_n$ are not independent, because the latter is a function of the former. However, we can split the mean, removing X_i from it, getting two independent terms:

$$X_i - \bar{X}_n = X_i - \frac{1}{n}\sum_{j=1}^{n} X_j = X_i - \frac{1}{n}X_i - \frac{1}{n}\sum_{j=1, j\neq i} X_j = \frac{n-1}{n}X_i - \frac{1}{n}\sum_{j=1, j\neq i} X_j$$

We can now easily calculate the variance, since it is the sum of the variances of the two terms:

$$Var(X_i - \bar{X}_n) = Var\left(\frac{n-1}{n}X_i - \frac{1}{n}\sum_{j=1, j\neq i} X_j\right) = Var\left(\frac{n-1}{n}X_i\right) + Var\left(\frac{1}{n}\sum_{j=1, j\neq i} X_j\right) =$$

$$= \frac{(n-1)^2}{n^2}\sigma^2 - \frac{1}{n^2}(n-1)\sigma^2 = \frac{n-1}{n}\sigma^2$$

Finally, we apply the above calculations to find the expected value of the estimator for the variance:

$$\mathbb{E}[S_n^2] = \mathbb{E}\left[\frac{1}{n-1}\sum_{i=1}^{n}(X_i - \bar{X}_n)^2\right] = \frac{1}{n-1}\sum_{i=1}^{n}\mathbb{E}[(X_i - \bar{X}_n)^2] =$$

$$= \frac{1}{n-1}\sum_{i=1}^{n} Var(X_i - \bar{X}_n) = \frac{1}{n-1}n\frac{n-1}{n}\sigma^2 = \sigma^2$$

Additionally,

$$Var(S_n)^2 = \frac{1}{n}(\mu_4 - \frac{n-3}{n-1}\sigma^4)$$

which goes to 0 as n goes to infinity.
Intuitively, the need for this correction can be explained by the fact that the X_i and the mean $\bar{X}_n$ are not independent; if we know $n-1$ random variables and the mean, we can always deduce the n^{th} random variable. In this sense, the estimator has $n-1$ **degrees of freedom**: in general, the degrees of freedom of any estimator is the number of observations minus the number of parameters already estimated.

What about the standard deviation? Unfortunately, the square root of the estimator of the variance is not an unbiased estimator for the standard deviation. By Jensen's inequality, since the square root is a concave function, we have:

$$\mathbb{E}[\sqrt{S_n^2}] = \mathbb{E}[S_n] < \sqrt{\mathbb{E}[S_n^2]} = \sigma$$

This is true for most estimators: if T is unbiased for θ, $g(T)$ is not necessarily unbiased for $g(\theta)$; the only exception is when $g()$ is a linear transformation (since by Jensen's inequality the strict equality holds). A non-parametric unbiased estimator for the standard deviation does not exist: we need to know the distribution to estimate it unbiasedly.

Unbiased estimator for the median

Let $X_1, \ldots, X_n$ be a random sample from a distribution with PDF $f(x)$. Let $m = F^{-1}(0.5)$ be the true median of the distribution. Let

$$T = Med(X_1, \ldots, X_n).$$

Then

$$T \sim \mathcal{N}\left(m, \frac{1}{4nf(m)^2}\right) \quad \text{as} \quad n \to \infty$$

and T is an unbiased estimator for the median as n goes to infinity.

Unbiased estimator for quantiles

Let $X_1, \ldots, X_n$ be a random sample from a distribution with PDF $f(x)$. Let q_p the the true p^{th} quantile of the distribution. Let

$$T = q_{X_1,\ldots,X_n}(p)$$

Then

$$T \sim \mathcal{N}\left(q_p, \frac{p(1-p)}{nf(q_p)^2}\right) \quad \text{as} \quad n \to \infty$$

and T is an unbiased estimator for the p^{th} quantile as n goes to infinity.

Unbiased estimator for the Median of Absolute Deviations (MAD)

Let $X_1, \ldots, X_n$ be a random sample from a distribution. Let Md be the true median of absolute deviations of the distribution. Let

$$T = MAD(X_1, \ldots, X_n) = Med(|X_1 - Med(X_1, \ldots, X_n)|, \ldots, |X_n - Med(X_1, \ldots, X_n)|)$$

Then

$$T \sim \mathcal{N}\left(Md, \frac{\sigma_1^2}{n}\right)$$

(where σ_1^2 is defined in terms of Md, median, and CDF of the distribution) and T is an unbiased estimator for the MAD as n goes to infinity.

All the above estimators are found by applying the corresponding version of the central limit theorem (CLT for medians, CLT for quantiles, CLT for MAD).

For correlation, the various coefficients seen in the previous section are estimators of the true correlation coefficient between two random variables. Pearson's r is an estimator for ρ, but the distribution of r is highly skewed. To fix this issue, the **Fisher transformation** can be applied, defined as follows: $FisherZ(r) = \frac{1}{2}\log\frac{1+r}{1-r}$. The distribution of the Fisher-transformed coefficient is approximately

normal:

$$FisherZ(r) \sim \mathcal{N}\left(FisherZ(\rho), \frac{1}{n-3}\right)$$

Hence, if we apply the inverse transformation to its expected value we get

$$FisherZ^{-1}(\mathbb{E}[FisherZ(r)]) = \rho$$

This is also true for Spearman's ρ, sicne it is a special case of Pearson's r.
For Kendall's τ_a, we have, for $n > 10$, that

$$\tau_a(X, Y) \sim \mathcal{N}\left(\theta, \frac{2(2n+5)}{9n(n-1)}\right)$$

where $\theta = \mathbb{E}_{X_1, X_2 \sim F_X, Y_1, Y_2 \sim F_Y}[sign(X_1 - X_2) \cdot sign(Y_1 - Y_2)]$. Hence τ_a is an unbiased estimator for θ.

Mean Squared Error (MSE)

The Mean Squared Error of an estimator T for a parameter θ is defined as

$$MSE(T) = \mathbb{E}[(T - \theta)^2]$$

The MSE can be used to compare different estimators by considering both their bias and variance. The lower the MSE, the better the estimator. The MSE can be decomposed into the sum of the variance and the square of the bias:

$$MSE(T) = \mathbb{E}[(T - \mathbb{E}[T] + \mathbb{E}[T] - \theta)^2] =$$

$$= \mathbb{E}[(T - \mathbb{E}[T])^2] + (\mathbb{E}[T] - \theta)^2 + 2\underbrace{\mathbb{E}[T - \mathbb{E}[T]]}_{(this\ is\ 0)}(E[T] - \theta) = Var(T) + Bias(T)^2$$

A biased estimator with low variance may be better than an unbiased estimator with high variance, since the latter may have a higher MSE.

Consistent estimator

An estimator T_n is a squared error consistent estimator if

$$\lim_{n \to \infty} MSE(T_n) = 0$$

A consistent estimator has both bias and variance go to 0 as n goes to 0. For example, $\bar{X}_n$ is a squared error consistent estimator of μ.

Minimum Variance Unbiased Estimator (MVUE)

An unbiased estimator T_n of θ is a Minimum Variance Unbiased Estimator if

$$Var(T_n) \leq Var(S_n)$$

for all unbiased estimators S_n of θ.

As a corollary, if T_n is a MVUE, then $MSE(T_n) \leq MSE(S_n)$. $\bar{X}_n$ is also a MVUE of μ when the random sample is normally distributed with parameters μ and σ^2.

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15 Maximum Likelihood Estimation

The previous sections showed different ways to derive parameter estimators using the "plug-in method": knowing a sample, we use a formula of random variables, substitute the empirical data, and obtain an estimate. This section will introduce a more general parametric principle to derive estimators, called **Maximum Likelihood Estimation** (**MLE**). The maximum likelihood principle states: "Given a dataset, choose the parameter(s) of interest that maximize the likelihood of observing that dataset".

Likelihood, Log-likelihood

Let $x_1, \ldots, x_n$ be a dataset, realization of a random sample $X_1, \ldots, X_n$, where the PMF/PDF of X_i is $f_\theta()$, parametric on θ. The likelihood function is defined as

$$L(\theta) = \prod_{i=1}^{n} f_\theta(x_i)$$

and the log likelihood function is defined as

$$\ell(\theta) = \log L(\theta) = \sum_{i=1}^{n} \log f_\theta(x_i)$$

The goal of MLE is to find the parameter value(s) that maximize the likelihood of the data. Since finding the maximum (in practice, derivating) a product is difficult, the logarithm of it is used instead, since it is a monotonic function (so the maximum remains the same) and the original likelihood can be converted to a sum of terms. Another issue to consider when using products is that when it is computed, the result can become very small, leading to numerical instability.

Maximum Likelihood estimates

The maximum likelihood estimates of θ is the value $t = \arg\max_\theta L(\theta) = \arg\max_\theta \ell(\theta)$. The statistics over the random sample

$$\hat{\theta}_{ML} = \arg\max_\theta L(\theta) = \arg\max_\theta \ell(\theta)$$

is called maximum likelihood estimator for θ.

Often, loss functions are used to evaluate the quality of the estimator. Some examples are:

- **Negative log-likelihood**: $nLL(\theta) = -\ell(\theta)$
- **Akaike Information Criterion** (**AIC**): $AIC = 2|\theta| - 2\ell(\theta)$. This function balances model fit (in the second term) with model simplicity (in the first term).

- **Bayesian Information Criterion** (**BIC**): $BIC = |\theta| \log(\theta) - 2\ell(\theta)$. It has a stronger penalty for model complexity compared to AIC.

The last two can be used to compare models with different number of parameters since they consider complexity as well as fit.

MLE estimators can be biased, but under mild assumptions, they are always asymtotically unbiased, and (also asymptotically) they always have the smallest variance among unbiased estimators. Additionally, if $\hat{\theta}$ is the MLE estimator of θ and $g()$ is an invertible function, $g(\hat{\theta})$ is the MLE estimator of $g(\theta)$.

Cross entropy and negative log likelihood There is a connection between the cross entropy and the negative log likelihood functions. Assume we have the random variables X, Y with PMF p_x and p_y. The cross entropy of X with respect to Y is defined as

$$H(X;Y) = -\sum_i p_x(a_i) \log p_y(a_i).$$

The negative log-likelihood is

$$nLL(\theta) = -\sum_i \underbrace{\log(f_\theta(x_i))}_{This\ is\ \log p_y(a_i)} = H(X;Y)$$

where $X \sim F_n$ and $Y \sim F_\theta$. Minimizing the cross entropy (or the KL-divergence) between empirical and theoretical distributions is equivalent to maximizing the likelihood of the data.

Score function and Fisher Information The entropy of a random variable is the mean information carried by it. Then, the partial derivative (w.r.t. θ) of the logarithm of f_θ represents the change in information as θ varies. It turns out that

$$\mathbb{E}\left[\frac{\partial}{\partial\theta} \log f_\theta(X)\right] = 0$$

for any X. Instead of studying the expectation, we consider the variance. Formally, we define the score function and the Fisher information as follows:

Score function

The score function is the random variable

$$S(\theta) = \frac{\partial}{\partial\theta}\ell(\theta) = \sum_{i=1}^{n} \frac{\partial}{\partial\theta} \log f_\theta(X_i)$$

Fisher information

The Fisher information is the variance of th score function:

$$I(\theta) = Var(S(\theta)) = \mathbb{E}[S(\theta^2)]$$

The Fisher information measures the sensitivity of X with respect to θ. If small changes in θ cause large changes in the density function, the Fisher information is high: this means that the data provides information on the correct θ.

For unbiased estimators, the **Cramér-Rao bound** holds, stating that for any unbiased estimator T:

$$Var(T) \geq \frac{1}{I(\theta)}$$

An unbiased estimator for which the equality holds is a Minimum Variance Unbiased Estimator. The **absolute efficiency** of an estimator can be then calculated as

$$e(T) = \frac{1}{I(\theta) \cdot Var(T)} \in [0, 1]$$

Recall that a MLE estimator is always asymptotically unbiased and has asymptotic minimum variance. Also by Cramér-Rao, asymptotically we have that

$$se(\hat{\theta}_{ML}) = \sqrt{Var(\hat{\theta}_{ML})} = \frac{1}{\sqrt{n \cdot I(\theta)}}$$

where se is the standard error of the estimator.

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16 Regression

Regression analysis is a set of statistical processes used to estimate the relationship between one or more dependent variables, and one or more independent variables. This relationship may be linear or non-linear, and regression analysis can be used for both cases. This section will start with the simplest case (univariate simple linear regression), and gradually introduce more complex cases.

16.1 Simple linear regression

In a simple linear regression model for a bivariate dataset $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$, we assume the x_i are non-random, and the y_i are realizations of random variables Y_i satisfying the following equation:

$$Y_i = \alpha + \beta x_i + U_i \qquad\qquad i = 1, 2, \ldots, n$$

where $U_1, U_2, \ldots, U_n$ are independent random variables with 0 expectation and constant variance σ^2. The equalities above describe a regression line, $y = \alpha + \beta x$, where α is the **intercept**, and β is the **slope** of the line. x is called **independent** (or *explanatory*) variable, while y is the **dependent** (or *response*) variable. Since the U_i are independent, and each Y_i is a function of the respective U_i, the Y_i are also independent (per the propagation of indipendence rule). They are not identically distributed, however, since each Y_i depends on a different x_i. All the Y_i have the same variance σ^2 (same as the U_i). This property is called **homoscedasticity**.

Least Squares Estimation To estimate the values of α and β, an initial idea is to use MLE. However, MLE is a parametric method, meaning that we need to know the distribution of the U_i beforehand. The alternative is to use the **Least Squares** method: let

$$y_i - \alpha - \beta x_i$$

be the **residual** of the i^{th} observation, which is the realization of $U_i = Y_i - \alpha - \beta x_i$. The least squares method aims to minimize the sum of squares of residuals across all observations:

$$\hat{\alpha}, \hat{\beta} = \arg\min_{\alpha,\beta} S(\alpha, \beta) = \arg\min_{\alpha,\beta} \sum_{i=1}^{n} (y_i - \alpha - \beta x_i)^2$$

$S(\alpha, \beta)$ is called **Sum of Squares of Errors** (**SSE**) or Residual Sum of Squares (RSS). To minimize the function, we need to calculate the partial derivatives with respect to α and β, and set them to 0. The partial derivatives are:

$$\frac{\partial}{\partial \alpha} S(\alpha, \beta) = -2 \sum_{i=1}^{n} (y_i - \alpha - \beta x_i) \qquad \frac{\partial}{\partial \beta} S(\alpha, \beta) = -2 \sum_{i_1}^{n} x_i (y_i - \alpha - \beta x_i)$$

By setting both to 0, we get the estimates

$$\hat{\alpha} = \bar{y}_n - \hat{\beta} \bar{x}_n \qquad \hat{\beta} = \frac{n \sum_{i=1}^{n} x_i y_i - (\sum_{i=1}^{n} x_i)(\sum_{i=1}^{n} y_i)}{n \sum_{i=1}^{n} x_i^2 - (\sum_{i=1}^{n} x_i)^2}$$

The $\hat{y}_i = \hat{\alpha} + \hat{\beta} x_i$ are called **fitted values**. The difference between the fitted value and the observed value is called residual: $y_i - \hat{y}_i$.
An equivalent form of $\hat{\beta}$ is the following:

$$\hat{\beta} = \frac{\sum_{i=1}^{n} (x_i - \bar{x}_n)(y_i - \bar{y}_n)}{SXX} = r_{xy} \frac{s_y}{s_x}$$

where:

- $SXX = \sum_{i=1}^{n} (x_i - \bar{x}_n)^2$;
- r_{xy} is the Pearson's correlation coefficient between x and y;
- s_x and s_y are the sample standard deviations of x and y, respectively.

The line described by the equation $y = \hat{\alpha} + \hat{\beta} x$ always passes through the center of gravity $(\bar{x}_n, \bar{y}_n)$:

$$\hat{\alpha} = \bar{y}_n - \hat{\beta} \bar{x}_n \implies \hat{\alpha} + \hat{\beta} \bar{x}_n = \bar{y}_n - \hat{\beta} \bar{x}_n + \hat{\beta} \bar{x}_n = \bar{y}_n$$

Finally, we can define the estimator of the Y_i:

$$\hat{Y}_i = \hat{\alpha} + \hat{\beta} x_i$$

Unbiasedness of LS estimators Both LS estimators of slope and interept are unbiased, and the following is the proof. Starting with the estimator of $\hat{\beta}$, it can be rewritten as:

$$\hat{\beta} = \frac{\sum_{i=1}^{n}(x_i - \bar{x}_n)(Y_i - \bar{Y}_n)}{SXX} = \frac{\sum_{i=1}^{n}(x_i - \bar{x}_n)Y_i - \sum_{i_1}^{n}(x_i - \bar{x}_n)\bar{Y}_n}{SXX} = \frac{\sum_{i=1}^{n}(x_i - \bar{x}_n)Y_i}{SXX}$$

(this is because $\sum_{i=1}^{n}(x_i - \bar{x}_n) = 0$). We can now calculate its expectation, which is:

$$\mathbb{E}[\hat{\beta}] = \frac{\sum_{i=1}^{n}(x_i - \bar{x}_n)\mathbb{E}[Y_i]}{SXX} = \frac{\sum_{i=1}^{n}(x_i - \bar{x}_n)(\alpha + \beta x_i)}{SXX} =$$

$$\alpha \underbrace{\frac{\sum_{i=1}^{n}(x_i - \bar{x}_n)}{SXX}}_{\textit{this it 0 as above}} + \beta \frac{\sum_{i=1}^{n}(x_i - \bar{x}_n)x_i}{SXX} = \beta \frac{\sum_{i=1}^{n}(x_i - \bar{x}_n)x_i}{SXX} = \beta$$

Moreover, its variance is:

$$Var(\hat{\beta}) = \frac{\sum_{i=1}^{n}(x_i - \bar{x}_n)^2 Var(Y_i)}{SXX^2} = \sigma^2 \frac{\sum_{i=1}^{n}(x_i - \bar{x}_n)^2}{SXX^2} = \frac{\sigma^2}{SXX}$$

Now, we calculate the expectation of $\hat{\alpha}$:

$$\mathbb{E}[\hat{\alpha}] = \mathbb{E}[\bar{Y}_n] - \bar{x}_n\mathbb{E}[\hat{\beta}] = \frac{1}{n}\sum_{i=1}^{n}\mathbb{E}[Y_i] - \bar{x}_n\beta =$$

$$= \frac{1}{n}\sum_{i=1}^{n}(\alpha + \beta x_i) - \bar{x}_n\beta = \frac{n\alpha}{n} + \frac{\beta}{n}\sum_{i=1}^{n}x_i - \bar{x}_n\beta =$$

$$= \alpha + \bar{x}_n\beta - \bar{x}_n\beta = \alpha$$

Moreover, its variance is:

$$Var(\hat{\alpha}) = Var(\bar{Y}_n - \hat{\beta}\bar{x}_n) = Var(\bar{Y}_n) + \bar{x}_n^2 Var(\hat{\beta}) - 2Cov(\bar{Y}_n, \beta\bar{x}_n) =$$

$$= \frac{\sigma^2}{n} + \bar{x}_n^2\frac{\sigma^2}{SXX} - 2\bar{x}_n\underbrace{Cov(\bar{Y}_n, \hat{\beta})}_{\textit{this is 0}} = \sigma^2\left(\frac{1}{n} + \frac{\bar{x}_n^2}{SXX}\right)$$

Both variances of the two estimators use σ^2, which is unknown. We cannot estimate it using the unbiased estimator $\hat{\sigma}^2 = \sum_{i=1}^{n}(Y_i - \bar{Y}_n)^2/(n-1)$, because the Y_i all have a different expectation. In this case, an unbiased estimator for the variance is

$$\hat{\sigma}^2 = \frac{\sum_{i=1}^{n}(y_i - \hat{\alpha} - \hat{\beta}x_i)^2}{n-2}$$

Its square root, $\hat{\sigma}$, is called **residual standard error**. The standard errors of the coefficient estimators are defined as estimates of their respective standard deviations:

$$se(\hat{\alpha}) = \hat{\sigma}\sqrt{\left(\frac{1}{n} + \frac{\bar{x}_n^2}{SXX}\right)} \qquad\qquad se(\hat{\beta}) = \frac{\sigma}{\sqrt{SXX}}$$

A measure close to the residual standard error is the **Root Mean Squared Error**, defined as:

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{a} - \hat{\beta}x_i)^2}$$

The estimators of the Y_i are also unbiased:

$$\mathbb{E}[\hat{Y}_i] = \mathbb{E}[\hat{\alpha}] + \mathbb{E}[\hat{\beta}]x_i = \alpha + \beta x_i$$

Its variance is the same as the estimate for the variance of the Y_i. The prediction uncertainty at a x_i is reported as $\hat{y} \pm se(\hat{y})$. The standard error of the fitted value at x_0 is:

$$se(\hat{y}) = \hat{\sigma}\sqrt{\frac{1}{n} + \frac{(\bar{x}_n - x_0)^2}{SXX}}$$

LSE and MLE MLE and LSE are equivalent in a special case: when the U_i random variables are normally distributed with mean 0 and variance σ^2. The Y_i then are also normally distributed; specifically, $Y_i \sim \mathcal{N}(\alpha + \beta x_i, \sigma^2)$.
The log-likelihood function is:

$$\ell(\alpha, \beta) = \sum_{i=1}^{n} \log\left(\frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{y_i - \alpha - \beta x_i}{\sigma}\right)^2}\right) = -n\log(\sigma\sqrt{2\pi}) - \frac{1}{2}\left(\frac{\sum_{i=1}^{n}(y_i - \alpha - \beta x_i)}{\sigma}\right)^2$$

It turns out that $\arg\max_{\alpha,\beta} \ell(\alpha, \beta) = \hat{\alpha}, \hat{\beta}$ as found for LSE.

Total variability and R^2 The total variability of the observed data is calculated as the **Sum of Squares Total** (**SST**):

$$SST = \sum_{i=1}^{n}(y_i - \bar{y}_n)^2$$

It is the sum of the squared differences between each observation y_i and their mean.
The total variability of the fitted data is instead calculated as the **Sum of Squares of Regression** (**SSR**):

$$SSR = \sum_{i=1}^{n}(\hat{y}_i - \bar{\hat{y}}_n)^2$$

It is identical to the above, but uses the fitted values instead of those in the dataset.
The total variablity of the residuals, which is the unexplained variability, is calculatd as the aforementioned **Sum of Squares of Errors** (**SSE**):

$$SSE = \sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

The three quantities are related by the following equation:

$$SST = SSR + SSE$$

Also, $1 - SSE/SST$ (or SSR/SST) is the *fraction of explained variability over total variability.* We can now express the variances of the observations, of the residuals, and of the fitted values using the three quantities above:

$$\sigma_y^2 = \frac{\sum_{i=1}^{n}(y_i - \bar{y}_n)^2}{n-1} = \frac{SST}{n-1} \qquad \text{(Variance of the } y\text{)}$$

$$\sigma_{res}^2 = \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)}{n-1} = \frac{SSE}{n-1} \qquad \text{(Variance of the residuals)}$$

$$\sigma_{\hat{y}}^2 = \frac{\sum_{i=1}^{n}(\hat{y}_i - \bar{\hat{y}}_n)^2}{n-1} = \frac{SSR}{n-1} \qquad \text{(Variance of the fitted values)}$$

These quantities are used to define the **coefficient of determination** R^2:

$$R^2 = 1 - \frac{\sigma^2_{res}}{\sigma^2_y} = \frac{\sigma^2_{\hat{y}}}{\sigma^2_y}$$

It is a measure of how well the regression line fits the data. For simple linear regression, it is equal to the square of the Pearson's correlation coefficient between y and $\hat{y}$:

$$R^2 = r^2_{y\hat{y}} = \frac{[\sum_{i=1}^{n}(y_i - \bar{y}_n) \cdot (\hat{y}_i - \bar{\hat{y}}_n)]^2}{\sum_{i=1}^{n}(y_i - \bar{y}_n)^2 \cdot \sum_{i=1}^{n}(\hat{y}_i - \bar{\hat{y}}_n)^2}$$

When we take the adjusted sample variance of the residuals:

$$\hat{\sigma}^2_{res} = \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{n-2} = \frac{SSE}{n-2}$$

we can then define the **adjusted coefficient of determination** $adjR^2$:

$$adjR^2 = 1 - \frac{\hat{\sigma}^2_{res}}{\sigma^2_y} = 1 - \frac{SSE/(n-2)}{SST/(n-1)} = 1 - \frac{SSE}{SST} \cdot \frac{n-1}{n-2}$$

16.2 Weighted simple regression

Weighted simple regression is a variant of linear simple regression where each observation is associated to a weight w_i that indicates how important that observation is to the estimation of the regression line parameters. The error function that is maximized is

$$S(\alpha, \beta) = \sum_{i=1}^{n}(y_i - \alpha - \beta x_i)^2 w_i$$

For natural number weights, the resulting effect is the same as replicating the same observation w_i times.

16.3 Polynomial simple regression

Polynomial simple regression is another variant where the relationship between the indipendent and dependent variables is modeled as a polynomial of degree k. The error function is

$$S(\alpha, \beta) = \sum_{i=1}^{n}(y_i - \alpha - \beta x_i - \beta_2 x_i^2 - \ldots - \beta_k x_i^k)^2$$

It may suffer from collinearity (explained later).

16.4 Non-linear simple regression

Non-linear simple regression models the relationship between independent and dependent as:

$$Y_i = f(\alpha, \beta, x_i) + U_i$$

where $f()$ is a non-linear function. The error function to minimize is then

$$S(\alpha, \beta) = \sum_{i=1}^{n}(y_i - f(\alpha, \beta, x_i))^2$$

$\arg\min_{\alpha,\beta} S(\alpha,\beta)$ may not have a closed form, so numerical methods are used to find the minimum: a typical example of such method is gradient descent, which iteratively updates the parameters α and β in the direction of the negative gradient of the error function.
In some cases, the non-linear function can be transformed in an equivalent linear function. For example, recall the PDF of Power Laws: $f(\alpha,\beta,x_i) = \alpha x_i^{\beta}$. We can solve it by taking the logarithm of both sides: $\log Y_i = \log\alpha + \beta\log x_i + U_i$. After finding the LSE estimators of the parameters, $\log\hat{\alpha}$ and $\hat{beta}$, we can rewrite the equation:

$$Y_i = \hat{\alpha} x_i^{\hat{\beta}} e^{U_i}$$

Notice how in this example the error term becomes a multiplicative factor instead of an additive one.

16.5 Multiple linear regression

In multiple linear regression, the dataset of observations is multivariate, meaning that each observation is a vector of k independent variables and one dependent variable:

$$(x_1^1, x_1^2, \ldots, x_1^k, y_1), (x_2^1, x_2^2, \ldots, x_2^k, y_2), \ldots, (x_n^1, x_n^2, \ldots, x_n^k, y_n)$$

The relationship between the i^{th} dependent variable and the i^{th} observation is:

$$Y_i = \alpha + \beta_1 x_i^1 + \ldots + \beta_k x_i^k + U_i$$

Or, in vector terms:

$$Y_i = x_i \cdot \boldsymbol{\beta}^T + U_i \qquad \text{where } \beta = (\alpha, \beta_1, \ldots, \beta_k) \text{ and } x_i = (1, x_i^1, \ldots, x_i^k)$$

Using this vector notation, we can then express the model as:

$$\mathbf{Y} = \mathbf{X} \cdot \boldsymbol{\beta}^T + \mathbf{U}$$

$$\begin{pmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{pmatrix} = \begin{pmatrix} 1 & x_1^1 & x_1^2 & \ldots & x_1^k \\ 1 & x_2^1 & x_2^2 & \ldots & x_2^k \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_n^1 & x_n^2 & \ldots & x_n^k \end{pmatrix} \begin{pmatrix} \alpha \\ \beta_1 \\ \vdots \\ \beta_k \end{pmatrix} + \begin{pmatrix} U_1 \\ U_2 \\ \vdots \\ U_n \end{pmatrix}$$

Estimators for the parameters of the model are found through the same method as for simple linear regression, but here we can reformulate the sum of the squares of the residuals as the squared euclidean norm of the residuals:

$$\hat{\boldsymbol{\beta}} = \arg\min_{\beta} S(\beta) = \arg\min_{\beta} \sum_{i=1}^{n} (y_i - x_i \cdot \boldsymbol{\beta}^T)^2 = \arg\min_{\beta} ||\mathbf{y} - \mathbf{X} \cdot \beta^T||^2$$

And the solution is

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}^T \cdot \mathbf{X})^{-1} \cdot \mathbf{X}^T \cdot \mathbf{y}$$

Here α is treated as the first element of β. The element β_i can be interpreted as the change of the dependent variable Y for a unit change of the i^{th} independent variable, while keeping all the other independent variables constant. The estimator above is a MVUE.

16.6 Multivariate multiple linear regression

Multivariate multiple linear regression models the relationship between two or mode dependent variables and two or more independent variables. In vector notation, we can express the model as:

$$\mathbf{Y} = \mathbf{X} \cdot \boldsymbol{\beta}^T + \mathbf{U}$$

$$\begin{pmatrix} Y_1^1 & \dots & Y_1^m \\ Y_2^1 & \dots & Y_2^m \\ \vdots & \vdots & \vdots \\ Y_n^1 & \dots & Y_n^m \end{pmatrix} = \begin{pmatrix} 1 & x_1^1 & x_1^2 & \dots & x_1^k \\ 1 & x_2^1 & x_2^2 & \dots & x_2^k \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_n^1 & x_n^2 & \dots & x_n^k \end{pmatrix} \begin{pmatrix} \alpha^1 & \alpha^2 & \dots & \alpha^m \\ \beta_1^1 & \beta_1^2 & \dots & \beta_1^m \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \beta_k^1 & \beta_k^2 & \dots & \beta_k^m \end{pmatrix} + \begin{pmatrix} U_1^1 & U_1^2 & \dots & U_1^m \\ U_2^1 & U_2^2 & \dots & U_2^m \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ U_n^1 & U_n^2 & \dots & U_n^m \end{pmatrix}$$

The dataset contains n observations, each with k independent variables and m dependent variables. The resulting model is not simply a collection of m multiple linear regression models. The error terms in the same column of $\mathbf{U}$ are independent (like in single multiple linear regression), but the error terms in the same row may be correlated, so coefficients for different dependent variables may covary.

16.7 Issues with linear regression

Omitted variable bias Suppose the real model involves two independent variables, x and z:

$$Y_i = \alpha + \beta_1 x_i + \beta_2 z_i + U_i$$

with $\beta_2 \neq 0$, meaning that Y is determined by Z. We may omit this variable for a multitude of reasons: for example, we don't know the variable exists, or we're aware of it but we cannot collect data for it. In this case, we would fit a model of the form:

$$Y_i = \alpha + \beta_1 x_i + U_i'$$

where $U_i' = \beta_2 z_i + U_i$. Clearly, the expected value of this "new" error term is not 0: $\mathbb{E}[U_i'] = \mathbb{E}[\beta_2 z_i] + \mathbb{E}[U_i] = \beta_2 z_i \neq 0$. The consequence of this is that the estimator for β is biased:

$$\mathbb{E}[\hat{\beta}_1] = \beta_1 + \beta_2 \delta$$

i.e., it has a bias equal to the coefficient of the omitted variable, times the slope coefficient of the regression line of Z with respect to X: $Z_i = \gamma + \delta x_i + U_i''$. This slope is then

$$\delta = r_{xz} \frac{s_z}{s_x}$$

So, if the two are uncorrelated, the bias is 0. If they are correlated, the bias is non-zero, and may be positive or negative depending on the direction of the correlation. We can interpret this to say that if we omit an independent variable that is correlated with another, the coefficient of the included variable will "absorb" the effect of the omitted variable, proportionally to the correlation between the two.

Multi-collinearity Multi-collinearity is a phenomenon that occurs when two or more independent variables are highly correlated. Imagine our model is build using two independent variables, such that

$$Y_i = \alpha + \beta_1 x_i^1 + \beta_2 x_i^2 + U_i$$

It can be shown that for $j \in 1, 2$:

$$Var(\hat{\beta}_j) = \frac{1}{(1 - r^2)} \cdot \frac{\sigma^2}{SXX_j}$$

where r is the correlation between x^1 and x^2, σ^2 is the variance of the error term, and $SXX_j = \sum_{i=1}^{n}(x_i^j - \bar{x}_n^j)^2$. This means that the more the independent variables are correlated, the higher the variance of the estimator of the model parameters. In general, for more than two variables, the variance is

$$Var(\hat{\beta}_j) = \frac{1}{(1 - R_j^2)} \cdot \frac{\sigma^2}{SXX_j}$$

where R_j^2 is the coefficient of determination in the regression of x_j from all other x_i. The term $1/(1-R_j^2)$ is called **variance inflation factor**. If this factor is 1, it means x_j is not at all correlated with the other independent variables, and th variance of the estimator is the same as the one for simple linear regression. If the R_j^2 is 1, the VIF goes to infinity, so the variance of the estimator is also infinite.

Variable selection Recall that when the distribution of the error terms is $\mathcal{N}(0, \sigma^2)$, the distribution of the Y_i is also normal ($\mathcal{N}(x_i \cdot \beta), \sigma^2$), so LSE and MLE applied to find the estimators of slope and intercept are equivalent. The log-likelihood function is $\ell(\beta) = \sum_{i=1}^{n} \log(\phi(y_i))$. We can use the Akaike Information Criterion (AIC) to evaluate the goodness of the current model and choose which combination of variables produces the best result. The AIC balances model fit against simplicity, so minimizing it is equivalent to finding the simplest model that best fits the data. `stepAIC()` is an `R` function that performs this task. The pseudocode is as follows: The variant presented above is the

---

function STEPAIC($S = \{x^1, \ldots, x^k\}$)
  $b = AIC(S)$
  while S does not change **do**
    $x = \arg\min_{x \in S} AIC(S \backslash \{x\})$
    $v = AIC(S \backslash \{x\})$
    if $v < b$ **then**
      $S = S \backslash \{x\}$
      $b = v$
    end if
  end while
  return S
end function

"backward" selection method, which starts with a model that uses all variables and each iteration of the loop removes the one that produces the best improvement in AIC, until no more improvements can be found. The other variant, "forward", starts with an empty model and adds the variable that produces the least increase in AIC.

Overfitting If a linear model is trained as is, it may become too complex and fit the noise in the data instead of the trend. This phenomenon is called overfitting, and it can be mitigated using

regularization techniques that penalize model complexity. The most common techniques are Ridge Regression (Tikhonov regularization) and Lasso (Least Absolute Shrinkage and Selection Operator) Regression (L1 regularization). They can also be used together in penalized regression. All of them consist in adding one or more penalization terms to the SSE function. Below are the equations for each technique:

- **Ridge regression**:

$$S(\boldsymbol{\beta}) = \|\mathbf{y} - \mathbf{X} \cdot \boldsymbol{\beta}^T\|^2 + \lambda\|\boldsymbol{\beta}\|^2$$

  The penalty term depends on the square of the norm 2 of the coefficients vector. λ is a hyperparameter that controls how strong the penalization acts. The result of this regularization is that the coefficients of the independent variables are kept small, but not exactly 0 (so no vatiable is excluded from the model).

- **Lasso**:

$$S(\boldsymbol{\beta}) = \|\mathbf{y} - \mathbf{X} \cdot \boldsymbol{\beta}^T\|^2 + \lambda\|\boldsymbol{\beta}\|_1$$

  Similar to the one above, but the penalty term is calculated on the norm 1 of the coefficients vector. The result of this regularization is that variables with minor contribution to the model will have the corresponding coefficient set to 0, effectively removing them.

- **Penalized linear regression**:

$$S(\boldsymbol{\beta}) = \|\mathbf{y} - \mathbf{X} \cdot \boldsymbol{\beta}^T\|^2 + \lambda_1\|\boldsymbol{\beta}\|_1 + \lambda_2\|\boldsymbol{\beta}\|^2$$

  A simple combination of Ridge regression and Lasso.

---

17 Logistic regression

Consider a bivariate dataset $(x_1, y_1), \ldots, (x_n, y_n)$, where $y_i \in \{0, 1\}$, i.e., Y_i is a binary variable. The goal is to train a model that predicts to which class (negative = 0, positive = 1) an observation belongs to. If linear regression is used, the model performances will be poor, showing a low R^2. This is because the dependent variable is binary, so the trend is not linear. Instead of directly modeling the dependent variable using linear regression, we can instead use it to model the probability of the dependent variable being equal to 1. We can "transform" the original dataset into a new one where each distinct value of x is paired with the fraction of 1s found for that value:

$$D = (d_1, f_1), (d_2, f_2), \ldots, (d_m, f_m) \qquad \text{where } f_i = \frac{|\{j \in [1, n] : x_j = d_i \wedge y_j = 1\}|}{|\{j \in [1, n] : x_j = d_i\}|}$$

so the linear model can be applied to the new dataset D:

$$F_i = \alpha + \beta d_i + U_i$$

where $F_i = P(Y_i = 1)$.

Still, the model is not perfect, since the dependent variable is a probability, i.e., bounded between 0 and 1, while the linear regression model returns values in $\mathbb{R}$. Additionally, the relationship between the values of the independent variable(s) and their probability of belonging to the positive class is **sigmoidal** (S-shaped) and not linear. Rather than F_i, we model the **log odds** of F_i:

$$\mathit{logit}(F_i) = \alpha + \beta d_i + U_i$$

The **logit** and its inverse, the **logistic function**, are sigmoidal functions defined as:

$$\mathit{logit}(p) = \log\left(\frac{p}{1-p}\right) \qquad\qquad \mathit{inv.logit}(x) = \frac{e^x}{1+e^x} = \frac{1}{1+e^{-x}}$$

Since $F_i = P(Y_i = 1)$, and Y_i can take only values 1 with probability p_i or 0 with probability $1 - p_i$, the Y_i are Bernoulli distributed with parameter p_i, hence the error term U_i is not necessary. The probability p_i can be then retrieved by inverting the logit function:

$$p_i = \mathit{inv.logit}(\alpha + \beta x_i) = \frac{1}{1+e^{-(\alpha+\beta x_i)}}$$

Since the distribution is known, MLE can be used to estimate α and β, where the log likelihood function is:

$$\ell(\alpha, \beta) = \log\left(\prod_{i=1}^{n} p_i^{y_i}(1-p_i)^{(1-y_i)}\right) = \sum_{i=1}^{n}(y_i \log p_i + (1-y_i)\log(1-p_i)) =$$

$$\sum_{i=1}^{n}(y_i \log(\mathit{inv.logit}(\alpha+\beta x_i)) + (1-y_i)\log(1-\mathit{inv.logit}(\alpha+\beta x_i)))$$

Since $p_i/(1-p_i) = e^{\alpha+\beta x_i}$, e^β can be interpreted as the expected change in the odds of the data point belonging to the positive class for a unit change in x_i. When $x_i = 0$, then $e^\alpha/(1+e^\alpha)$ can be interpreted as the base probability of the data point belonging to the positive class.

Logistic regression, as well as linear regression, belongs to the family of **generalized linear models** (**GLM**), in which the outcome of the dependent variable is assumed to be generated by a particular distribution, and a link function is used to relate the mean of the distribution to the linear model. In the case of binary logistic regression, the distribution is Bernoulli and the link function is the logit function.

Logistic regression can also be regularized by adding penalty terms to the log likelihood. **Elastic net** regularization is a combination of L1 and L2 regularization, where the function to be minimized is:

$$-\ell(\boldsymbol{\beta}) + \lambda\left(\frac{1-\alpha}{2}\|\boldsymbol{\beta}\|^2 + \alpha\|\boldsymbol{\beta}\|_1\right)$$

where:

- $\alpha = 0$ is equivalent to Ridge regression (L2 regularization);
- $\alpha = 1$ is equivalent to Lasso regression (L1 regularization);
- $0 < \alpha < 1$ is a combination of both.

18 Statistical decision theory

Statistical decision theory is concerned with making decisions based on statistical knowledge. An example of a decision problem is the following: given a set of hypotheses, which one is the most probable given the observed data? We've already introduced Maximum Likelihood Estimation, which assumes a specific distribution and maximizes the likelihood function of the data with respect to the parameters of the distribution. This method is **frequentist**, in that it interprets probability as the frequency of a certain event occurring in a large number of trials. **Bayesian** methods, instead, interpret probability as a measure of belief, and require the prior distribution of the parameters to be estimated. A Bayesian method is **Maximum a Posteriori** (**MAP**), which finds the parameters that maximize the posterior probability of the parameters given the data:

$$\theta_{MAP} = \arg\max_{\theta} P(\theta|X_1 = x_1, \ldots, X_n = x_n) = \arg\max_{\theta} P(X_1 = x_1, \ldots, X_n = x_n|\theta)P(\theta)$$

MAP and MLE are equivalent when the prior distribution is uniform, since in that case the prior becomes a multiplicative constant and can be ignored.

18.1 Learning and prediction

The problem above is called **classification** (or **concept learning**) **problem**. Given:

- A dataset $X = (W, C)$, where W are the predictive features and C the class, with $sup(C) = \{0, 1, 2, \ldots, n_c - 1\}$;
- A training set of observations $x_1, \ldots, x_n$, with $x_i = (w_i, c_i)$ for $i = 1, \ldots, n$;
- Θ, the hypothesis space of functions that represent th joint density f_θ of W and C;

which $\theta \in \Theta$ is the most probable given the set of observations? With MLE, we write

$$\theta_{MLE} = \arg\min_{\theta} \sum_{i=1}^{n} -\ell(\theta) = \arg\min_{\theta} \sum_{i=1}^{n} -\log(f_\theta(x_i)) = \arg\max_{\theta} \sum_{i=1}^{n} -\log(f_\theta(w_i, c_i)) =$$

$$= \arg\min_{\theta} \sum_{i=1}^{n} -\log(f_\theta(c_i|w_i)f_\theta(w_i)) = \arg\min_{\theta} \sum_{i=1}^{n} -\log(f_\theta(c_i|w_i)) - \sum_{i=1}^{n} -\log(f_\theta(w_i)) =$$

$$= \arg\min_{\theta} \sum_{i=1}^{n} -\log(f_\theta(c_i|w_i))$$

The reason we can exclude $\log(f_\theta(w_i))$ from the function is because we assume the distribution of W is independent from that of θ, thus it is a constant with respect to θ. The function $f_\theta(c|w) = P(C = c|W = w, \theta)$ is called **probabilistic classifier** trained from $x_1, \ldots, x_n$.

Minimizing the MLE is, in fact, equivalent to minimizing the Kullback-Leibler divergence between the true distribution $f_{\theta_{TRUE}}$ and the estimated distribution f_θ:

$$\theta_{MLE} = \arg\min_{\theta} \sum_{i=1}^{n} -\log(f_\theta(c_i|w_i)) + \log(f_{\theta_{TRUE}}(c_i|w_i)) = \arg\min_{\theta} \frac{1}{n} \sum_{i=1}^{n} \log\left(\frac{f_{\theta_{TRUE}}(c_i|w_i)}{f_\theta(c_i|w_i)}\right)$$

(here we simply added and multiplied by constant terms). Then, by the law of large numbers, as n goes to infinity, this is equivalent to

$$\xrightarrow{n\to\infty}_{LLN} \arg\min_\theta \mathbb{E}_{(W,C)\sim f_{\theta_{TRUE}}}\left[\log\frac{f_{\theta_{TRUE}}(C|W)}{f_\theta(C|W)}\right] = \arg\min_\theta D_{KL}(\theta_{TRUE}||\theta) = \arg\min_\theta H(\theta_{TRUE};\theta)$$

Another problem of statistical decision theory is the **classification** (or **concept prediction**) **problem**. Given $\theta \in \Theta$ and $W = w$, what is the most probable class c? This is equivalent to finding

$$c = \arg\max_c P(C = c, W = w|\theta) =$$

$$= \arg\max_c P(C = c|W = w, \theta) \cdot P(W = w|\theta) = \arg\max_c f_\theta(c|w)$$

The best possible decision is the one obtained from the hypothesis called Bayes decision rule.

Bayes decision rule

Fix $\theta \in \Theta$. The Bayes decision rule is

$$y^*_\theta(w) = \arg\max_c f_\theta(c|w)$$

and for any decision rule $y^+_\theta : \mathbb{R}^{|W|} \to \{0, 1, \ldots, n_c - 1\}$:

$$P(y^*_\theta(W) \neq C) \leq P(y^+_\theta(W) \neq C)$$

The proof is as follows. We can write the probability of the Bayes decision rule being right using an indicator function:

$$P(y^*_\theta(W) = C) = \mathbb{E}[\mathbb{1}_{y^*_\theta(W)=C}] = \mathbb{E}[\mathbb{E}_C[\mathbb{1}_{y^*_\theta(W)=C}|W = w]]$$

Then we can compare the two probabilities:

$$\mathbb{E}[\mathbb{E}_C[\mathbb{1}_{y^*_\theta(W)=C}|W = w]] \geq \mathbb{E}[\mathbb{E}_C[\mathbb{1}_{y^+_\theta(W)=C}|W = W]] = \mathbb{E}[\mathbb{1}_{y^+_\theta(W)=C}] = P(y^+_\theta(W) = C)$$

Each decision rule corresponds to a **decision boundary**, which is the region $w \in \mathbb{R}^{|W|}$ such that $y^+_\theta(w)$ can admit as possible answers two or more classes. The decision boundary of the Bayes decision rule is the region of the feature space where there are multiple classes that correspond to the maximum posterior probability.

Assume we do not fit any parameter in the hypothesis. Which is, in general, the most probable class given only the predictive features w? A possible answer may be to find the most probable model with MAP, and use its prediction, i.e.,

$$c = \arg\max_c P(C = c|W = w, \theta_{MAP})$$

However, MAP finds the most probable model, not necessarily the best. Let's make an example. Let $\Theta = \{\theta_1, \theta_2, \theta_3\}$, and assume the posterior probabilities are:

- $P(\theta_1|x_1, \ldots, x_n) = 0.4$ and $f_{\theta_1}(1|w) = 1$,

- $P(\theta_2|x_1,\ldots,x_n) = P(\theta_3|x_1,\ldots,x_n) = 0.3$ and $f_{\theta_2}(0|w) = f_{\theta_3}(0|w) = 1$.

According to MAP, the most probable model is θ_1. Yet, class 0 has the largest probability over the hypothesis space, while the hypothesis that uses θ_1 always predicts class 1. The solution is to use the Bayes optimal prediction.

Bayes optimal prediction

Given a set of observations $x_1,\ldots,x_n$, the Bayes optimal prediction is

$$c = \arg\max_c \sum_{\theta\in\Theta} f_\theta(c|w)P(\theta|x_1,\ldots,x_n)$$

A **learner** is a computable function that maps a training set to a decision rule.

No-Free-Lunch theorem

Consider a binary classification problem, and a finite domain $dom(W) < \infty$. For any learner $\mathcal{A}$, there exists a distribution F with $(W,C) \sim F$ such that:

1. For at least $\frac{1}{7}$ of the training sets (realizations of F^n), with $n < |dom(W)|/2$, the decision rule y_θ^+ produced by $\mathcal{A}$ has an error of at least $\frac{1}{8}$:

$$P_F(y_\theta^+(W) \neq C) \geq \frac{1}{8}$$

2. There exists an error-free decision rule y_θ^* such that

$$P_F(y_\theta^*(W) \neq C) = 0.$$

This theorem states that there is no "universal learner", i.e., a learner that can always map a training set to a decision rule with 0 error.

18.2 Probabilistic classifiers

A **probabilistic classifier** is a function that maps each instance to the probability of belonging to each class:

$$f_\theta(c|w) \in [0,1] \qquad\qquad \sum_c f_\theta(c|w) = 1$$

The predicted class of an instance is the one that corresponds to the highest probability given that instance. The probability itself is a measure of the confidence of the classifier in its answer.
An **unnormalized classifier** is a function that maps each instance to a vector of real numbers:

$$f_\theta(c|w) \in \mathbb{R}$$

Each value in the vector represents the confidence of belonging to each class, but they are not actual probabilities. They can be normalized to obtain a probabilistic classifier using the **softmax function**:

$$softmax((v_0, v_1, \ldots, v_{n_c-1})) = \left(\frac{e^{v_0}}{\sum_i e^{v_i}}, \frac{e^{v_1}}{\sum_i e^{v_i}}, \ldots, \frac{e^{v_{n_c-1}}}{\sum_i e^{v_i}}\right)$$

In a binary classification problem, the softmax function can be expressed in terms of the sigmoid function:

$$softmax((0, v_1)) = (1 - z, z) \qquad \text{where } z = sigmoid(v_1) = \frac{1}{1 + e^{-v_1}}$$

Some useful properties of the softmax function are:

- It is invariant to the sum of a constant to all the elements of the vector:

$$softmax(v + c) = softmax(v)$$

- Its derivative is:

$$\frac{\partial}{\partial v} softmax(v) = softmax(v)(1 - softmax(v))$$

Normally, we're mostly interested in the probability of the positive class. We then use a **score function**, defined as

$$s_\theta(w) = f_\theta(1|w) = P(C = 1|W = w, \theta)$$

such that the confidence of the most probable class is

$$\max\{1 - s_\theta(w), s_\theta(w)\}$$

Using the score function, we can express the classifier with a single function:

$$f_\theta(c_i|w_i) = s_\theta(w_i)^{c_i}(1 - s_\theta(w_i))^{(1-c_i)}$$

Using this form of the classifier, MLE can be applied to find the parameters of the model. Maximizing the likelihood is equivalent to minimizing the **cross-entropy loss** (or **log-loss**):

$$\theta_{MLE} = \arg\min_\theta \sum_{i=1}^{n} -log(f_\theta(c_i|w_i)) = \arg\min_\theta \frac{1}{n} \sum_{i=1}^{n} -c_i \log(s_\theta(w_i)) - (1 - c_i) \log(1 - s_\theta(w_i))$$

$$\ell_\theta(c, w) = \begin{cases} -\log(s_\theta(w)) & \text{if } c = 1 \\ -\log(1 - s_\theta(w)) & \text{if } c = 0 \end{cases}$$

$$\text{Then: } \theta_{MLE} = \arg\min_\theta \frac{1}{n} \sum_{i=1}^{n} \ell_\theta(c_i, w_i)$$

Formally, this minimization is known as empirical risk minimization.

Empirical risk minimization

Let $\ell : \{0, \ldots, n_c - 1\} \times \mathbb{R}^{|W|} \to \mathbb{R}_{\geq 0}$ be a loss function. Empirical risk minimization is the problem of finding the parameters θ that minimize the empirical risk, represented as the average of the loss function over the training set:

$$\theta_{ERM} = \arg\min_\theta \frac{1}{n} \sum_{i=1}^{n} \ell_\theta(c_i, w_i)$$

MLE with log-loss is a special case of ERM. There are various other loss functions that can be used; for example, the 0-1 loss function, which is defined as $\ell_\theta(c, w) = \mathbb{1}_{y_\theta^+(w) \neq c}$. However, this function is not convex, and not differentiable, making the corresponding optimization problem NP-hard. Other examples are the L_p error losses, which are defined as $\ell_\theta(c, w) = |s_\theta(w) - c|^p$. Common choices are

$$\ell_\theta(c, w) = |s_\theta(w) - c| \qquad \text{(Absolute error (L1) loss)}$$

$$\ell_\theta(c, w) = (s_\theta(w) - c)^2 \qquad \text{(Squared error (L2, Brier score) loss)}$$

When using the squared error loss, ERM is equivalent to minimizing the **mean squared error** (**MSE**), which is simply the average of the squared differences (L2 loss) between the predicted and actual values:

$$MSE = \frac{1}{n} \sum_{i=1}^{n} (s_\theta(w_i) - c_i)^2$$

For the law of large numbers, as n goes to infinity, the MSE converges exactly to the expected value of the squared error:

$$MSE \xrightarrow{n \to \infty}_{LLN} \mathbb{E}_{(W,C) \sim f_{\theta_{TRUE}}}[(s_\theta(W) - C)^2],$$

meaning that the MSE approximates the mean squared error over the whole population. MSE was already introduced in the context of estimators, but there the second term is a constant (the parameter to estimate). We can similarly decompose the MSE into the three terms that contribute to the error, assuming that $C = D + \epsilon$ with $\mathbb{E}[\epsilon] = 0$:

$$\mathbb{E}_{(W,C) \sim f_{\theta_{TRUE}}}[(s_\theta(W) - C)^2] = Var(s_\theta(W)) + \mathbb{E}[s_\theta(W) - C]^2 + Var(\epsilon)$$

The first term is the variance of the scores; it is minimized by a constant score, but this increases the bias. The second term is the squared bias; it is minimized by interpolating the training data, but this increases the variance. The third term is the irreducible error, inherent to the data.

Risk (Expected Prediction Error EPE)

The risk w.r.t. a loss function ℓ_θ is

$$R(\theta_{TRUE}, \theta) = \mathbb{E}_{(W,C) \sim f_{\theta_{TRUE}}}[\ell_\theta(C, W)]$$

Proper scoring rule

A loss function is a proper scoring rule if

$$\theta_{TRUE} = \arg\min_\theta R(\theta_{TRUE}, \theta)$$

Log-loss, squared error loss, and 0-1 loss are all proper scoring rules, while absolute error loss is not. Still, 0-1 loss is discountinuous. For proper scoring rules, the parameters found by ERM are

asymptotically unbiased: $\theta_{ERM} \xrightarrow{n\to\infty} \theta_{TRUE}$. For the log-loss, the risk is equivalent to the KL-divergence:

$$R(\theta_{TRUE}, \theta) = D_{KL}(\theta_{TRUE}||\theta) \geq 0$$

Risk is defined with respect to a specific true parameter set. The **maximum risk** is

$$\bar{R}(\theta) = \sup_{\theta} R(\theta_{TRUE}, \theta)$$

Minmax rule

A classifier $f_{\theta'}$ such that $\bar{R}(\theta) = \inf_\theta \bar{R}(\theta)$ is called a minmax rule.

In other words, a minmax rule is a classifier whose maximum risk is the minimum risk possible across all true parameters.

Bayes risk, Bayes rule

Let $f(\theta_{TRUE})$ be the prior of θ_{TRUE}. The Bayes risk is

$$r(\theta) = \int R(\theta_{TRUE}, \theta) f(\theta_{TRUE})\ d\theta_{TRUE}$$

A classifier $f_{\theta'}$ such that $r(\theta') = \inf_\theta r(\theta)$ is called a Bayes rule.

Best classifier for 0-1 loss Assume 0-1 risk is being used to evaluate the classifier. The risk is

$$\arg\min_{y_\theta^+} \mathbb{E}_{(W,C)\sim f_{\theta_{TRUE}}}[\mathbb{1}_{y_\theta^+(W)\neq C}]$$

Then, the binary class Bayes optimal classifier is

$$y^*_{\theta_{TRUE}}(w) = \begin{cases} 1 & \text{if } \eta(w) \geq 0.5 \\ 0 & \text{if } \eta(w) < 0.5 \end{cases}$$

$$\eta(w) = P_{\theta_{TRUE}}(C = 1|W = w)$$

We can compare the expected risk of the Bayes optimal classifier with that of a generic classifier y_θ^+, and prove that it is always smaller or equal than the latter:

$$\mathbb{E}_{(W,C)\sim f_{\theta_{TRUE}}}[\mathbb{1}_{y_\theta^+(W)\neq C}] \overset{\text{(Law of iter. exp.)}}{=} \mathbb{E}_W[\mathbb{E}_C[\mathbb{1}_{y_\theta^+(W)\neq C}|W]] =$$

$$= \mathbb{E}_W[P(C=1|W)\cdot\mathbb{1}_{y_\theta^+(W)\neq 1} + P(C=0|W)\cdot\mathbb{1}_{y_\theta^+(W)\neq 0}] =$$

$$= \mathbb{E}_W[\eta(W)\cdot\mathbb{1}_{y_\theta^+(W)=0} + (1-\eta(W))\cdot\mathbb{1}_{y_\theta^+(W)=1}] =$$

$$\geq \mathbb{E}_W[\min\{\eta(W), 1-\eta(W)\}] =$$

$$= \mathbb{E}_W[\eta(W)\cdot\mathbb{1}_{y^*_{\theta_{TRUE}}(W)=0} + (1-\eta(W))\cdot\mathbb{1}_{y^*_{\theta_{TRUE}}(W)=1}] =$$

$$= E_{(W,C)\sim f_{\theta_{TRUE}}}[\mathbb{1}_{y^*_{\theta_{TRUE}}(W)\neq C}]$$

It is important to note that the Bayes optimal classifier is only a theoretical concept, and cannot be built in practice since it would require us to know the function $\eta(W)$; that is, the real distribution of the data. Using the plug-in rule, we can approximate this function with the empirical distribution of the data to build a classifier:

$$\hat{\eta}(w) = f_\theta(c|w) = P_\theta(C=1|W=w)$$

Loss functions and margin Assume a classifier trained on a dataset with binary classes $C = \{-1, 1\}$, and which produces unnormalized scores via a function $s_\theta(w)$. The corresponding Bayes decision rule is

$$y^*_\theta = sign(s_\theta(w))$$

i.e., the classifier should return 1 when the score is positive, -1 when the score is negative. We can then define the **margin** for the dataset (w, c) as

$$m = c \cdot s_\theta(w)$$

The margin is positive if the prediction is correct (so if both c and $s_\theta(w)$ have the same sign), otherwise it is negative. Minimizing the loss is equivalent to maximizing the margin, because the more the classifier is correct, the larger is the margin. Loss functions themselves can be rewritten in terms of the margin m:

- **0-1 loss**: $\phi(m) = \mathbb{1}_{m\leq 0}$
- **Logistic log-loss**: $\phi(m) = \log_2(1 + e^{-m})$
- **Squared error loss**: $\phi(m) = (1-m)^2$
- **SVM/Hinge loss**: $\phi(m) = \max\{0, 1-m\}$
- **AdaBoost/Exponential loss**: $\phi(m) = e^{-m}$

Various methods exist for margin maximization for convex margin-based loss, which also provide bounds for 0-1 loss.

18.3 Rejection option

The output of a binary probabilistic classifier is the probability of belonging to the positive class. Based on that probability, we can assign a certain input to the negative or positive class with a given confidence; $s(w)$ for the positive class, $1 - s(w)$ for the negative class (where the score is normalized). Sometimes, the classifier may return a score that is very close to $1/2$, so it is not strongly in favor of one or the other class. It may be useful to introduce a reject option for the classifier, so that if the score falls within some distance to $1/2$ the classifier abstains from deciding at all. In real applications, a reject option can be used to highlight and understand cases where a classifier performs poorly, or when the decision to be taken is ethically or socially sensitive (e.g., credit scoring, disease prediction).

Formally, the Bayes optimal classifier with the reject option can be written as the following case-based function:

$$y^{*,d}_{\theta_{TRUE}}(w) = \begin{cases} 1 & \text{if } \eta(w) > 1 - d \\ 0 & \text{if } \eta(w) < d \\ abstain & \text{if } d \leq \min\{\eta(w), 1 - \eta(w)\} \end{cases}$$

where $d \in [0, 1/2]$ is the **reject cost**. It represents the upper bound on the misclassification error of the classifier, since when it does not abstain, then $d > \min\{\eta(w), 1-\eta(w)\} = P_{\theta_{TRUE}}(y^*_\theta(w) \neq c)$. Also, the following theorem holds:

$$\arg\min_{y^+_\theta} \mathbb{E}_{(W,C)\sim f_{\theta_{TRUE}}}[d \cdot \mathbb{1}_{y^+_\theta(W)=abstain} + \mathbb{1}_{y^+_\theta(W)\neq C, y^+_\theta(W)\neq abstain}] = y^{*,d}_{\theta_{TRUE}}$$

This theorem states that the Bayes optimal classifier with reject cost d is also the classifier that minimizes the risk (which considers both the cases in which the classifier makes a mistake, and those in which it rejects in instance).

A **selective binary classifier** is a pair (s_θ, g_θ), where $s_\theta()$ is a classifier, and $g : \mathbb{R}^{|W|} \to \{0, 1\}$ is a selection function, which returns 1 if the input instance can be confidently classified, or 0 if the instance must be rejected:

$$(s_\theta, g_\theta)(w) = \begin{cases} s_\theta(w) & \text{if } g_\theta(w) = 1 \\ abstain & \text{otherwise} \end{cases}$$

Coverage (support) and risk

The coverage of a selective classifier is

$$\phi(g_\theta) = \mathbb{E}_{(W,C)\sim f_{\theta_{TRUE}}}[g_\theta(W)]$$

which is the expected probability of the accepted region.
The risk with respect to a loss function ℓ_θ is

$$R(s_\theta, g_\theta) = \mathbb{E}_{(W,C)\sim f_{\theta_{TRUE}}}[\ell_\theta(C, W)]/\phi(g_\theta)$$

Coverage and risk of a selective classifier require the true distribution to be known. They can be estimated empirically:

$$\hat{\phi}(g_\theta) = \frac{\sum_{i=1}^{n} g_\theta(w_i)}{n} \qquad\qquad \hat{r}(s_\theta, g_\theta) = \frac{1}{n} \frac{\sum_{i=1}^{n} \ell_\theta(c_i, w_i) g_\theta(w_i)}{\hat{\phi}(g_\theta)}$$

The **selective classification problem** is to minimize the risk while guaranteeing a certain minimum coverage c:

$$\arg\min_\theta R(s_\theta, g_\theta), \text{such that } \phi(g_\theta) \geq c$$

A **soft selective binary classifier** is a variant of selective binary classifiers that is defined by the pair (s_θ, k_θ), where k_θ is a confidence function:

$$(s_\theta, g_\theta)(w) = \begin{cases} s_\theta(w) & \text{if } k_\theta(w) \geq \tau \\ \textit{abstain} & \text{otherwise} \end{cases}$$

where $\tau \in [1/2, 1]$. A good confidence function should rank instances based on descending loss: if $k(w) \leq k(w')$, then $\mathbb{E}[\ell_\theta(C, w)] \geq \mathbb{E}[\ell_\theta(C, w')]$.

The inherent trade-off between risk and coverage is summarized by the **risk-coverage curve**, which tracks how changes in coverage affect the overall risk of the classifier. If the coverage is high, the risk is also high, because we "admit" more classifications even when the confidence is low. If the coverage is low, the risk is also lower, because we only classify instances associated with a high confidence (so they are more likely to be correct).

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19 Confidence intervals

Previous sections focused on point estimates of the parameters of a distribution. This section will focus on confidence intervals, which are ranges of plausible values for the parameters of a distribution, as opposed to point estimates, which are single values. A confidence interval can be thought as a *interval* of values $[l, u]$ for which we can be *confident* the unknown parameters falls in with a specific probability, called confidence level.

Confidence intervals

Suppose a dataset $x_1, \ldots, x_n$ is given, modeled as a realization of random variables $X_1, \ldots, X_n$. Let θ be the parameter of interest, and $\gamma \in [0, 1]$. If there exist sample statistics $L_n = g(X_1, \ldots, X_n)$ and $U_n = h(X_1, \ldots, X_n)$ such that

$$P(L_n \leq \theta \leq U_n) = \gamma$$

for every value of θ, then

$$(l_n, u_n)$$

where $l_n = g(x_1, \ldots, x_n)$ and $u_n = h(x_1, \ldots, x_n)$ is called a $100\gamma\%$ confidence interval for θ. γ is called the confidence level.

Sometimes, the confidence interval is **conservative**, i.e., the interval is built from the fact that $P(L_n < \theta < U_n) \geq \gamma$. There is no way of knowing for certain if the interval is correct or not, only that the parameter is within that interval with a certain probability γ. While γ is called confidence level, $\alpha = 1 - \gamma$ is called **significance level**. So a 95% confidence interval corresponds to a significance level of 5%.

19.1 Confidence intervals for the mean

We can define some general methods for two cases, each with a number of subcases: normally distributed data with known or unknown variance, and general data with unknown variance.

19.1.1 Normal data

Critical values

The (right) critical value z_p of $Z \sim \mathcal{N}(0,1)$ is the number with right tail probability p:

$$P(Z \geq z_p) = p$$

For an $x > 0$, the right tail probability of a standard normal distribution $\Phi(x)$ is equal to $1 - \Phi(x)$: this value can be approximated by referencing a table of the standard normal distribution and interpolating between values as needed. If z_p is the right critical value, it is also the $(1-p)^{th}$ quantile of the standard normal distribution:

$$1 - \Phi(z_p) = p \implies \Phi(z_p) = 1 - p$$

By symmetry of the normal distribution:

$$1 - \Phi(z_p) = \Phi(-z_p) = p \implies z_{1-p} = -z_p$$

Known variance Given a dataset $x_1, \ldots, x_n$, realization of a random sample $X_1, \ldots, X_n$, with $X_i \sim (\mu, \sigma^2)$, we want to estimate μ with a confidence interval, knowing what σ^2 is. The average of the random sample $\bar{X}_n$ has distribution $\mathcal{N}(\mu, \sigma^2/n)$. We also know that, by the central limit theorem,

$$Z = \sqrt{n} \cdot \frac{\bar{X}_n - \mu}{\sigma} \sim \mathcal{N}(0,1)$$

We can exploit this fact to build the confidence interval with confidence level γ for μ. The confidence interval may be **two-sided**, **one-sided upper** or **one-sided lower**. The two-sided confidence interval is the most common, and is defined from:

$$P(c_l \leq Z \leq c_u) = \gamma \text{ or } P(Z \leq c_l) + P(Z \geq c_u) = 1 - \gamma = \alpha$$

$$P(Z \leq c_l) = P(Z \geq c_u) = \frac{\alpha}{2}$$

Since the distribution is symmetric, $c_u = -c_l = z_{\alpha/2}$. Then, to isolate the mean, we can write:

$$P(c_l \leq Z \leq c_u) = P(-z_{\alpha/2} \leq \sqrt{n} \cdot \frac{\bar{X}_n - \mu}{\sigma} \leq z_{\alpha/2}) =$$

$$= P(-z_{\alpha/2}\frac{\sigma}{\sqrt{n}} \leq \bar{X}_n - \mu \leq z_{\alpha/2}\frac{\sigma}{\sqrt{n}}) =$$

$$= P(\bar{X}_n - z_{\alpha/2}\frac{\sigma}{\sqrt{n}} \leq \mu \leq \bar{X}_n + z_{\alpha/2}\frac{\sigma}{\sqrt{n}}) = \gamma$$

Ergo, $(\bar{x}_n - z_{\alpha/2} \cdot \sigma/\sqrt{n}, \bar{x}_n + z_{\alpha/2} \cdot \sigma/\sqrt{n})$ is a $100\gamma\%$ confidence interval for μ.

To build a one-sided confidence interval, we apply the same idea. The left interval is defined from the fact that:

$$P(c_l \leq Z) = \gamma$$

so c_l is the critical value $z_\gamma = -z_{1-\gamma} = -z_\alpha$ of the standard normal distribution. Then, as above, we obtain the confidence interval:

$$P(c_l \leq Z) = P(\bar{X}_n - z_\alpha\frac{\sigma}{\sqrt{n}} \leq \mu) = \gamma$$

Then $(\bar{x}_n - z_\alpha \cdot \sigma/\sqrt{n}, \infty)$ is a $100\gamma\%$ confidence interval for μ. The right interval is defined from the fact that:

$$P(Z \leq c_u) = \gamma \text{ or } P(Z \geq c_u) = 1 - \gamma = \alpha$$

so c_u is the critical value z_α. Then, as above, we obtain the confidence interval $(-\infty, \bar{x}_n + z_\alpha \cdot \sigma/\sqrt{n})$.

Unknown variance The procedure is almost identical to that above, but we need to estimate the variance. We know that an unbiased estimator of the variance is:

$$S^2 = \frac{1}{n-1}\sum_{i=1}^{n}(X_i - \bar{X}_n)^2$$

and also S_n^2/n is an unbiased estimator of $Var(\bar{X}_n)$. The key difference is that the distribution of $T = \frac{\bar{X}_n - \mu}{S_n/\sqrt{n}}$ is not normal, but follows a Student's t-distribution with $n-1$ degrees of freedom.

Student's t-distribution $X \sim t(m)$

A continuous random variable has a t-distribution with parameter $m \geq 1$, where m is an integer, if its PDF is given by:

$$f(x) = k_m \left(1 + \frac{x^2}{m}\right)^{-\frac{m+1}{2}} \qquad \text{for } -\infty < x < \infty$$

where

$$k_m = \frac{\Gamma(\frac{m+1}{2})}{\left(\Gamma(\frac{m}{2})\sqrt{(m\pi)}\right)} .$$

This distribution is referred to as the t-distribution with m degrees of freedom.
For $m \to \infty$, the t-distribution converges to the standard normal distribution.

$$\mathbb{E}[X] = 0 \text{ for } m \geq 2 \qquad Var(X) = \frac{m}{m-2} \text{ for } m \geq 3$$

Critical values for the t-distribution are defined in the same way as for the normal distribution, and have the same properties.

Critical value

The (right) critical value $t_{m,p}$ of $T \sim t(m)$ is the number with right tail probability p:

$$P(T \geq t_{m,p}) = p$$

The approach to to build the confidence interval is the same as above. The two-sided confidence interval is defined from:

$$P(\bar{X}_n - t_{n-1,\alpha/2}\frac{S_n}{\sqrt{n}} \leq \mu \leq \bar{X}_n + t_{n-1,\alpha/2}\frac{S_n}{\sqrt{n}}) = \gamma$$

such that $(\bar{x}_n - t_{n-1,\alpha/2} \cdot s_n/\sqrt{n}, \bar{x}_n + t_{n-1,\alpha/2} \cdot s_n/\sqrt{n})$ is a $100\gamma\%$ confidence interval for μ. The one-sided confidence intervals are defined from:

$$P(\bar{X}_n - t_{n-1,\alpha}\frac{S_n}{\sqrt{n}} \leq \mu) = \gamma$$

$$P(\mu \leq \bar{X}_n + t_{n-1,\alpha}\frac{S_n}{\sqrt{n}}) = \gamma$$

such that $(\bar{x}_n - t_{n-1,\alpha} \cdot s_n/\sqrt{n}, \infty)$ and $(-\infty, \bar{x}_n + t_{n-1,\alpha} \cdot s_n/\sqrt{n})$ are respectively left- and right-sided $100\gamma\%$ confidence intervals for μ.

19.1.2 General data

This method is used when the distribution of the data is not normal, and the variance is unknown. The variance can be estimated with the sample variance S^2. Then, for a variant of the central limit

theorem, for n that goes to infinity, the following holds:

$$T = \sqrt{n} \cdot \frac{\bar{X}_n - \mu}{S_n} \to \mathcal{N}(0,1)$$

So, if the sample size is large enough, we can approximate the distribution of T with a normal distribution, and use the same method for normal distribution with unknown variance. For example, the two-sided confidence interval is defined from:

$$P(\bar{X}_n - z_{\alpha/2}\frac{S_n}{\sqrt{n}} \leq \mu \leq \bar{X}_n + z_{\alpha/2}\frac{S_n}{\sqrt{n}}) \approx \gamma$$

such that $(\bar{x}_n - z_{\alpha/2} \cdot s_n/\sqrt{n}, \bar{x}_n + z_{\alpha/2} \cdot s_n/\sqrt{n})$ is a $100\gamma\%$ confidence interval for μ.

Determining the sample size If we fix the significance level α, the narrower the confidence interval, the better the estimate, since there is a smaller range of possible values for that parameter, lowering the variance of the estimate. Sometimes, confidence intervals are built by fixing some accuracy requirements, such as the maximum width w of the interval (i.e., find a $100\gamma\%$ C.I. (l_n, u_n) such that $u_n - l_n \leq w$). To satisfy the requirement, we need to find the optimal sample size n. Let's consider the case of normal data with known variance: the C.I. is estimated by $(l_n, u_n) = (\bar{X}_n - z_{\alpha/2} \cdot \sigma/\sqrt{n}, \bar{X}_n + z_{\alpha/2} \cdot \sigma/\sqrt{n})$. Then, the bound on the width of the interval is:

$$u_n - l_n = 2 \cdot z_{\alpha/2} \cdot \frac{\sigma}{\sqrt{n}} \leq w$$

$$n \geq \left(\frac{2 \cdot z_{\alpha/2} \cdot \sigma}{w}\right)^2$$

Wald confidence intervals The confidence intervals above can be generalized in the from

$$\theta \in \hat{\theta} \pm z_{\alpha/2} \cdot \frac{\sigma}{\sqrt{n}} \text{ or } \theta \in \hat{\theta} \pm t_{n-1,\alpha/2} \cdot \frac{S_n}{\sqrt{n}}$$

where $\hat{\theta}$ is the point estimate of the parameter θ. These intervals originate from the **Wald test statistics**, which is used to test the null hypothesis that the parameter θ is equal to a specific value θ_0 (hypothesis testing will be introduced later). The test statistic is defined as:

$$T = \frac{\hat{\theta} - \theta}{\sqrt{Var(\hat{\theta})}} = \frac{\hat{\theta} - \theta}{se(\hat{\theta})}$$

A limitation of this method is that it can only be applied to symmetric intervals, and it is not valid for small sample sizes (it follows an asymptotic distribution).

19.2 Confidence intervals for proportions

Proportions are ratios of counts, like classifier accuracy. Accuracy can also be used to estimate the mean of a Bernoulli distribution. Assume we have a dataset $x_1, \ldots, x_n$, realization of a random sample $X_1, \ldots, X_n \sim Ber(p)$. Then each $x_i = \mathbb{1}_{y_\theta^+(w_i)=c_i}$ is 1 if the classifier is correctly classifying w_i as c_i, and 0 otherwise. p is the unknown misclassification error of the classifier. Let $B = \sum_{i=1}^n X_i \sim Bin(n,p)$, and let $b = \sum_{i=1}^n x_i$ be the number of correct classifications. Depending on the sample size, two methods can be used:

- **Small sample size**: we build the exact confidence interval (l_B, u_B) such that:

$$l_B = \min_\theta \left\{ \sum_{x=B}^{n} \binom{n}{x} \theta^x (1-\theta)^{n-x} \geq \alpha/2 \right\} \qquad u_B = \max_\theta \left\{ \sum_{x=B}^{n} \binom{n}{x} \theta^x (1-\theta)^{n-x} \geq \alpha/2 \right\}$$

  The found l_B is the left critical value, the smallest value of θ for which $P(B \leq X) \geq \alpha/2$ for $X \sim Bin(n, \theta)$. Similarly, u_B is the right critical value, for which $P(B \geq X) \geq \alpha/2$. The interval (l_B, u_B) is a $100\gamma\%$ confidence interval for p.

- **Large sample size**: when n is large, the Binomial distribution can be approximated with a normal one. Let $B = \sum_{i=1}^{n} X_i \sim Bin(n, p)$ and $\bar{X}_n = B/n$. For the De Moivre-Laplace theorem, $B \sim Bin(n, p) \approx \mathcal{N}(np, np(1-p))$. Then, the average $\bar{X}_n$ is also normally distributed with the following parameters: $\bar{X}_n \sim \mathcal{N}(p, p(1-p)/n)$.

  The standard error of the average is

$$se(\bar{X}_n) = \sqrt{np(1-p)} \approx \sqrt{\bar{X}_n(1-\bar{X}_n)/n}$$

  The approximation is done because we do not know p. Exploiting the central limit theorem, the variable

$$T = \frac{(\bar{X}_n - p)}{se(\bar{X}_n)}$$

  is approximately normally distributed with mean 0 and variance 1, and we can use the methods for the normal distribution. The two-sided confidence interval is defined from:

$$P\left(\bar{X}_n - z_{\alpha/2} \sqrt{\frac{\bar{X}_n(1-\bar{X}_n)}{n}} \leq p \leq \bar{X}_n + z_{\alpha/2} \sqrt{\frac{\bar{X}_n(1-\bar{X}_n)}{n}} \right) = \gamma$$

  such that $(\bar{x}_n - z_{\alpha/2} \cdot \sqrt{\bar{x}_n(1-\bar{x}_n)/n}, \bar{x}_n + z_{\alpha/2} \cdot \sqrt{\bar{x}_n(1-\bar{x}_n)/n})$ is a $100\gamma\%$ confidence interval for p. This is also a Wald confidence interval, since it is determined from the point estimate of the mean. It has the same limitations as the Wald confidence intervals mentioned before.

19.3 Confidence intervals for simple linear regression

19.3.1 Regression coefficients

Simple linear regression models the relationship between the dependent vairable Y and the independent variable X as a linear function: $Y_i = \alpha + \beta x_i + U_i$, where $U_i \sim \mathcal{N}(0, \sigma^2)$. We also have $\hat{\beta} \sim \mathcal{N}(\beta, Var(\hat{\beta}))$, where $Var(\hat{\beta}) = \frac{\sigma^2}{SXX}$ is unknown. The Wald statistic is $t(n-2)$ distributed:

$$T = \frac{\hat{\beta} - \beta}{se(\hat{\beta})} \sim t(n-2)$$

We can then use T to isolate β and build the confidence interval. The critical values are estimated from the t-distribution with $n-2$ degrees of freedom.
The same procedure can be applied to get a confidence interval for the intercept α.

19.3.2 Fitted values

Also for the fitted values a Wald confidence interval can be built. The estimator of the fitted value y is $\hat{y} = \hat{\alpha} + \hat{\beta}x_0$ at x_0, with standard error:

$$se(\hat{y}) = \hat{\sigma}\sqrt{\frac{1}{n} + \frac{(\bar{x} - x_0)^2}{SXX}}$$

Then, the interval is in the form $y \in \hat{y} \pm t_{n-2,\alpha} se(\hat{y})$. This interval is for the *expected value* of Y at x_0, i.e., the average of the predicted values for that input.

Other than confidence intervals, we can also find **prediction intervals**, which predicts the specific predicted value of Y at x_0 and considers the error term as well. Let

$$\hat{V} = \hat{\alpha} + \hat{\beta}x_0 + U$$

be the estimator of the predicted value. Assuming the error term U is normally distributed, the variance of the predicted value is:

$$Var(\hat{V}) = \sigma^2 \left(1 + \frac{1}{n} + \frac{(\bar{x}_n - x_0)^2}{SXX}\right)$$

The prediction interval is $y \in \hat{y} \pm t_{n-2,\alpha} se(\hat{v})$. This interval lets us conclude that the specific predicted value of Y at x_0 is between $\hat{y} - t_{n-2,\alpha} se(\hat{v})$ and $\hat{y} + t_{n-2,\alpha} se(\hat{v})$.

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20 Bootstrap and resampling

20.1 Bootstrap

Bootstrapping is a statistical method used to estimate the distribution of estimators by resampling with replacement from the data. To illustrate the concept, we use a simple example. Let $X_1, \ldots, X_n \sim F$ be a random sample, where F is the unknown distribution of the population. We want to study the distributtion of some parameter of the distribution; let it be the mean. We can build an estimator to get a point estimate of that parameter from a specific dataset. For the mean, we already observed that the sample mean is an unbiased estimator for the population mean. If we have multiple datasets from the same population, each of them will give us a different sample mean; then, if we calculate the empirical distribution of the sample means, by the Glivenko-Cantelli theorem, it will converge to the real distribution of the sample means, which is the same as the distribution of the population mean. However, we usually have only one dataset.

Once we have a dataset, we can use it to both get a point estimate of the parameter of interest, and also to derive the empirical distribution $\hat{F}$ of the sample. This empirical distribution is then used to generate a number of **bootstrap samples** $x_1^*, \ldots, x_n^*$ using random sampling with replacement from the original dataset. For each bootstrap sample, we calculate the point estimate of the parameter of interest, and finally we determine the empirical distribution of it.

Bootstrap principle

Use the dataset $x_1, \ldots, x_n$ to compute an estimate $\hat{F}$ for the true distribution F. Replace the random sample $X_1, \ldots, X_n$ from F with a random sample $X_1^*, \ldots, X_n^*$ from $\hat{F}$. Approximate the probability distribution of $h(X_1, \ldots, X_n)$ by that of $h(X_1^*, \ldots, X_n^*)$.

20.1.1 Empirical bootstrap

Assuming we know absolutely nothing abount F, the empirical CDF is calculated as

$$\hat{F}(a) = F_n(a) = \frac{|\{i \in 1 \ldots n : x_i \leq a\}|}{n}$$

Often, the bootstrap approximation is better if we relate the estimator to the corresponding parameter, e.g., instead of approximating the distribution of the mean, we approximate that of $\Delta = \bar{X}_n - \mu$ by $\Delta^* = \bar{X}_n^* - \mu^*$, where μ^* is the sample mean $\bar{x}_n$ of the initial dataset. This is done to reduce the distance between the estimated distribution and the true distribution.
The realization of the difference Δ^* of a sample is $\delta^* = \bar{x}_n^* - \mu^* = \bar{x}_n^* - \bar{x}_n$. Then, since

$$\mathbb{E}[\Delta] = \mathbb{E}[\bar{X}_n] - \mu \approx \mathbb{E}[\Delta^*] \approx mean(\delta^*)$$

we can estimate the real mean by reversing the equality:

$$\hat{\mu} = \mathbb{E}[\bar{X}_n] - mean(\delta^*) \approx \bar{x}_n - mean(\delta^*)$$

Also, the standard error of the mean can be approximated from the standard deviation of the empirical distribution of δ^*:

$$se(\bar{X}_n) = \sqrt{Var(\bar{X}_n)} = \sqrt{Var(\bar{X}_n - \mu)} \approx \sqrt{Var(\bar{X}_n^* - \mu^*)} \approx sd(\delta^*)$$

Other than point estimates, we can establish confidence intervals for the parameters. Let $\delta = \bar{x}_n - \mu$ be the realization of Δ. Then a confidence interval for δ is $(q_{\alpha/2}, q_{1-\alpha/2})$, where the quantiles are calculated from the empirical distribution of δ^*. The confidence interval of the mean is

$$q_{\frac{\alpha}{2}} \leq \delta = \bar{x}_n - \mu \leq q_{\frac{1-\alpha}{2}} \implies \mu \in (\bar{x}_n - q_{\frac{1-\alpha}{2}}, \bar{x}_n - q_{\frac{\alpha}{2}})$$

`R` has a built-in method for bootstrap confidence intervals, `boot.ci`. It allows the user to choose the type of confidence interval, such as:

- `type='basic'`: $(q_{\alpha/2}, q_{1-\alpha/2})$. Same method as the one described above.
- `type='perc'`: $(q_{\alpha/2}, q_{1-\alpha/2})$. No shift. Quantiles are estimated from the empirical distribution of $\bar{x}_n$.
- `type='norm'`: $(\bar{x}_n - q_{1-\alpha/2}, \bar{x}_n - q_{\alpha/2})$. Quantiles are calculated over $\mathcal{N}(mean(\delta^*), Var(\delta^*))$ (i.e., the distribution of the deltas is assumed to be normal).

- `type='bca'`: "bias-corrected and acceleration" method. It corrects the skewness of the distribution to adjust the confidence interval (if it is positively skewed, the interval is shifted to the right; if it is negatively skewed, the interval is shifted to the left).
- `type='stud'`: $(\bar{x}_n - q_{1-\alpha/2}\frac{s_n}{\sqrt{n}}, \bar{x}_n - q_{\alpha/2}\frac{s_n}{\sqrt{n}})$. Quantiles are calculated over the t-distribution with $n-1$ degrees of freedom.

Until now only the mean was considered, but the bootstrap method can be applied to any estimator, such as the variance, or the linear regression coefficients. Bootstrap is generally good to estimate parameters which are not greatly perturbed by small perturbations of the data: it has issues with approximating extreme values, such as percentiles or the maximum/minimum of a distribution.

How many bootstrap samples? In order to get a good result, the sample size must be large enough. Let n be the size of the original sample of the data, the total number of distinct possible bootstrap samples is $\binom{2n-1}{n-1}$. A rule of thumb is to use $B = 1000$ bootstrap samples. An alternative is to use **Jackknife resampling**, which works by extracting n samples of size $n-1$ from the original dataset, such that sample i includes all the data points except the i^{th} one.

$$1 : x_2, x_3, x_4, \ldots, x_n$$

$$2 : x_1, x_3, x_4, \ldots, x_n$$

$$3 : x_1, x_2, x_4, \ldots, x_n$$

$$\vdots$$

$$n : x_1, x_2, x_3, \ldots, x_{n-1}$$

20.1.2 Parametric bootstrap

Let $X_1, \ldots, X_n \sim F(\gamma)$ be a random sample, with known family F but unknown parameter γ, and we are interested in approximating the distribution of some parameter θ. Given a dataset $x_1, \ldots, x_n$, we can derive an estimate $\hat{\gamma}$ of γ, such that $F(\hat{\gamma})$ is the empirical distribution of the sample. This distribution is then used to generate a number of bootstrap samples $x_1^*, \ldots, x_n^*$ (realizations of $X_1^*, \ldots, X_n^* \sim F(\hat{\gamma})$), and from each of them a point estimate of θ.

Parametric bootstrap is also often used to estimate the distribution of the difference between the sample parameter and the real one. For example, if we take the mean $\bar{X}_n$, we would estimate the distribution of $\Delta = \bar{X}_n - \mu$ by that of $\Delta^* = \bar{X}_n - \mu_{\hat{\theta}}$, i.e., we compute the expectation $\mu^* = \mu_{\hat{\theta}}$ of $F_{\hat{\theta}}$. Like empirical bootstrap, we can also calculate confidence intervals for the parameter of interest.

20.2 Resampling methods

This section describes how to use resampling methods to estimate the performance of a classifier. We introduced the concept of risk as a measure of how well a classifier preforms, as it is the expected value of the loss function given the data. There are a series of possible approaches to estimate the risk given a dataset:

- **Holdout method**: the dataset is split into training and test set. The decision rule is trained on the training set only, and the empirical risk is calculated on the test set.

$$\hat{r} = \frac{1}{n}\sum_{i=1}^{n} \ell_\theta(c_i, w_i) \qquad\qquad se = \sqrt{\frac{\hat{r}(1-\hat{r})}{n}}$$

  The biggest drawback of this method is that the result depends on how the data is split into train/test, and also the estimate has high variablity.

- **Random sampling**: holdout is repeated k times, and the average of the k estimates is taken as the final estimate.

$$\hat{r} = \frac{1}{k}\sum_{j=1}^{k} \hat{r}^j \qquad\qquad se = \sqrt{\frac{1}{k-1}\sum_{j=1}^{k}(\hat{r}^j - \hat{r})^2}$$

  The $\hat{r}_j$ term is the error calculated on the j^{th} holdout sample:

$$\hat{r}^j = \frac{1}{n_j}\sum_{i=1}^{n_j} \ell_\theta(c_i^j, w_i^j)$$

  Unfortunately, this method yields a wrong estimate, since the test sets (and as a consequence also the error estimates) are not independent.

- **k-fold cross-validation**: the empirical risk is averaged over k-fold splits of the dataset, guaranteeing that the test sets are independent.

$$\hat{r} = \frac{1}{k}\hat{r}^j \qquad\qquad se = \sqrt{\frac{1}{k-1}\sum_{j}(\hat{r}^j - \hat{r})^2}$$

  Here the error of a split is calculated as

$$\hat{r}^j = \frac{1}{n/k}\sum_{i=1}^{n/k} \ell_\theta(c_i^j, w_i^j)$$

  i.e., each test set has size n/k. This method has still the issue of the training sets across splits not being independent, which results in the error estimates also not being independent. Cross-validation estimates the average error across training sets.

  If the classifier is stable over the folds, then we can use $se = \sqrt{\frac{\hat{r}(1-\hat{r})}{n}}$. The estimation is similar to holdout, but all data instances are used. This is also the implementation in `R`.

  Setting $k = n$ results in what is called **leave-one-out cross-validation** (**LOOCV**).

- **.632 bootstrap algorithm**: this method combines bootstrap and cross-validation. The classifier is trained on bootstrap samples, and the empirical risk is estimated on a test set which corresponds to all the data points not included in the sample. For k bootstrap runs, the risk is estimated as

$$\hat{r} = \frac{1}{k}\sum_{j}(0.632\hat{r}^j + 0.368\hat{r}_{tr})$$

where $\hat{r}^j$ is the empirical risk on the j^{th} bootstrap sample, and $\hat{r}_{tr}$ is the empirical risk over the original dataset.

Bootstrap has low variance, but it is very biased. k-fold cross-validation has a low bias and variance can be controlled by choosing the number of folds.