

# Frequentist statistics

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# Introduce:

## 1. Parameter estimation

(1) The method of maximum likelihood

(2) The method of least squares

## 2. Confidence intervals

## 3. Confidence level upper limit

# Fundamental concepts

Consider an experiment whose outcome is characterized by one or more data values, which we can write as a vector  $\mathbf{x}$ . A *hypothesis*  $H$  is a statement about the probability for the data, often written  $P(\mathbf{x}|H)$ . (We will usually use a capital letter for a probability and lower case for a probability density. Often the term p.d.f. is used loosely to refer to either a probability or a probability density.) This could, for example, define completely the p.d.f. for the data (a *simple* hypothesis), or it could specify only the functional form of the p.d.f., with the values of one or more parameters not determined (a *composite* hypothesis).

If the probability  $P(\mathbf{x}|H)$  for data  $\mathbf{x}$  is regarded as a function of the hypothesis  $H$ , then it is called the *likelihood* of  $H$ , usually written  $L(H)$ . Often the hypothesis is characterized by one or more parameters  $\theta$ , in which case  $L(\theta) = P(\mathbf{x}|\theta)$  is called the *likelihood function*.

## Parameter estimation

(a) consistency, (b) bias, (c) efficiency

(a) An estimator is said to be consistent if the estimate  $\hat{\theta}$  converges in probability to the true value  $\theta$  as the amount of data increases. This property is so important that it is possessed by all commonly used estimators.

(b) The bias,  $b = E[\hat{\theta}] - \theta$ , is the difference between the expectation value of the estimator and the true value of the parameter. When  $b = 0$ , the estimator is said to be unbiased. The bias depends on the chosen metric, i.e., if  $\hat{\theta}$  is an unbiased estimator of  $\theta$ , then  $\hat{\theta}^2$  is not in general an unbiased estimator for  $\theta^2$ .

(c).Efficiency is the ratio of the minimum possible variance for any estimator of  $\theta$  to the variance  $V[\hat{\theta}]$  of the estimator  $\hat{\theta}$ .

## The method of maximum likelihood :

Suppose we have a set of measured quantities  $\mathbf{x}$  and the likelihood  $L(\boldsymbol{\theta}) = P(\mathbf{x}|\boldsymbol{\theta})$  for a set of parameters  $\boldsymbol{\theta} = (\theta_1, \dots, \theta_N)$ . The *maximum likelihood* (ML) estimators for  $\boldsymbol{\theta}$  are defined as the values that give the maximum of  $L$ . Because of the properties of the logarithm, it is usually easier to work with  $\ln L$ , and since both are maximized for the same parameter values  $\boldsymbol{\theta}$ , the ML estimators can be found by solving the *likelihood equations*,

$$\frac{\partial \ln L}{\partial \theta_i} = 0, \quad i = 1, \dots, N. \quad (39.9)$$

Often the solution must be found numerically. Maximum likelihood estimators are important because they are unbiased and efficient asymptotically (*i.e.*, for large data samples), under quite general conditions, and the method has a wide range of applicability.

$$L(\boldsymbol{\theta}) = \prod_{i=1}^n f(x_i; \boldsymbol{\theta}). \quad (39.10)$$

In this case the number of events  $n$  is regarded as fixed. If however the probability to observe  $n$  events itself depends on the parameters  $\boldsymbol{\theta}$ , then this dependence should be included in the likelihood. For example, if  $n$  follows a Poisson distribution with mean  $\mu$  and the independent  $x$  values all follow  $f(x; \boldsymbol{\theta})$ , then the likelihood becomes

$$L(\boldsymbol{\theta}) = \frac{\mu^n}{n!} e^{-\mu} \prod_{i=1}^n f(x_i; \boldsymbol{\theta}). \quad (39.11)$$

## The method of least squares :

The *method of least squares* (LS) coincides with the method of maximum likelihood in the following special case. Consider a set of  $N$  independent measurements  $y_i$  at known points  $x_i$ . The measurement  $y_i$  is assumed to be Gaussian distributed with mean  $\mu(x_i; \boldsymbol{\theta})$  and known variance  $\sigma_i^2$ . The goal is to construct estimators for the unknown parameters  $\boldsymbol{\theta}$ . The log-likelihood function contains the sum of squares

$$\chi^2(\boldsymbol{\theta}) = -2 \ln L(\boldsymbol{\theta}) + \text{constant} = \sum_{i=1}^N \frac{(y_i - \mu(x_i; \boldsymbol{\theta}))^2}{\sigma_i^2} . \quad (39.19)$$

The parameter values that maximize  $L$  are the same as those which minimize  $\chi^2$ .

The minimum of the chi-square function in Equation (39.19) defines the least-squares estimators  $\hat{\boldsymbol{\theta}}$  for the more general case where the  $y_i$  are not Gaussian distributed as long as they are independent. If they are not independent but rather have a covariance matrix  $V_{ij} = \text{cov}[y_i, y_j]$ , then the LS estimators are determined by the minimum of

$$\chi^2(\boldsymbol{\theta}) = (\mathbf{y} - \boldsymbol{\mu}(\boldsymbol{\theta}))^T \mathbf{V}^{-1} (\mathbf{y} - \boldsymbol{\mu}(\boldsymbol{\theta})) , \quad (39.20)$$

## Frequentist confidence intervals :

Confidence intervals are constructed in order to have a coverage probability greater than or equal to a given confidence level, regardless of the true parameter's value.

confidence intervals are said to have a confidence level (CL) equal to  $1 - \alpha$ .

$$1 - \alpha = P(x_1(\theta) < x < x_2(\theta)) = P(\theta_2(x) < \theta < \theta_1(x)) . \quad (39.68)$$

In this probability statement,  $\theta_1(x)$  and  $\theta_2(x)$ , *i.e.*, the endpoints of the interval, are the random variables and  $\theta$  is an unknown constant. If the experiment were to be repeated a large number of times, the interval  $[\theta_1, \theta_2]$  would vary, covering the fixed value  $\theta$  in a fraction  $1 - \alpha$  of the experiments.

## Gaussian distributed measurements:

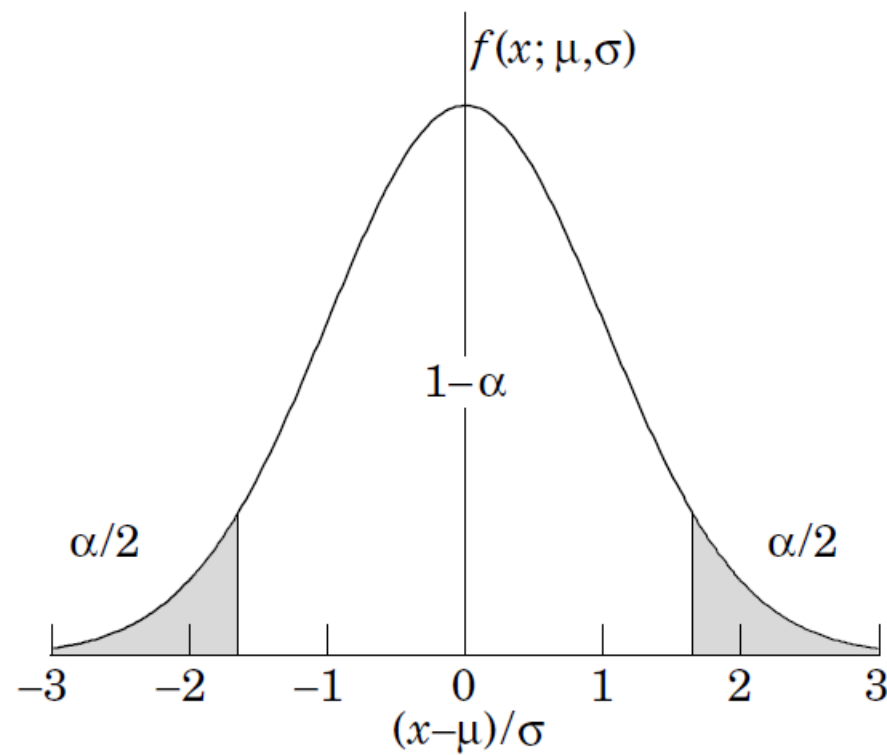
An important example of constructing a confidence interval is when the data consists of a single random variable  $x$  that follows a Gaussian distribution; this is often the case when  $x$  represents an estimator for a parameter and one has a sufficiently large data sample. If there is more than one parameter being estimated, the multivariate Gaussian is used. For the univariate case with known  $\sigma$ , the probability that the measured value  $x$  will fall within  $\pm\delta$  of the true value  $\mu$  is

$$1 - \alpha = \frac{1}{\sqrt{2\pi}\sigma} \int_{\mu-\delta}^{\mu+\delta} e^{-(x-\mu)^2/2\sigma^2} dx = \operatorname{erf}\left(\frac{\delta}{\sqrt{2}\sigma}\right) = 2\Phi\left(\frac{\delta}{\sigma}\right) - 1, \quad (39.70)$$

**Table 39.1:** Area of the tails  $\alpha$  outside  $\pm\delta$  from the mean of a Gaussian distribution.

$\alpha$	$\delta$	$\alpha$	$\delta$
0.3173	$1\sigma$	0.2	$1.28\sigma$
$4.55 \times 10^{-2}$	$2\sigma$	0.1	$1.64\sigma$
$2.7 \times 10^{-3}$	$3\sigma$	0.05	$1.96\sigma$
$6.3 \times 10^{-5}$	$4\sigma$	0.01	$2.58\sigma$
$5.7 \times 10^{-7}$	$5\sigma$	0.001	$3.29\sigma$
$2.0 \times 10^{-9}$	$6\sigma$	$10^{-4}$	$3.89\sigma$





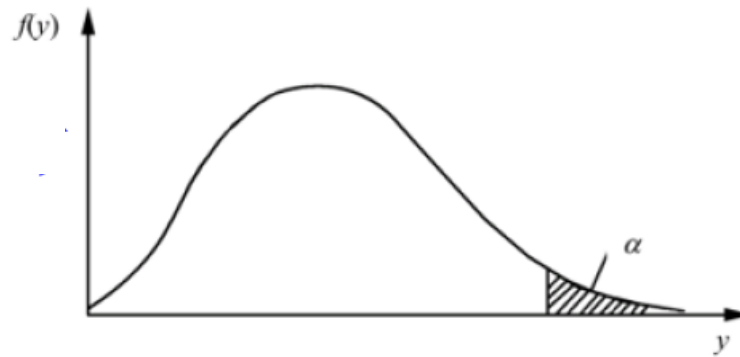
**Figure 39.4:** Illustration of a symmetric 90% confidence interval (unshaded) for a Gaussian-distributed measurement of a single quantity. Integrated probabilities, defined by  $\alpha = 0.1$ , are as shown.

The relation (39.70) can be re-expressed using the cumulative distribution function for the  $\chi^2$  distribution as

$$\alpha = 1 - F(\chi^2; n) , \quad (39.71)$$

for  $\chi^2 = (\delta/\sigma)^2$  and  $n = 1$  degree of freedom. This can be seen as the  $n = 1$  curve in

The upper  $\alpha$  percentage point of  $\chi^2(n)$  ( $0 < \alpha < 1$ ) *approximate* the upper  $\alpha$  percentage point of Gaussian distributed  $N(0,1)$ .



Confidence level upper limit:

In the limit case of subsample capacity  $n \rightarrow \infty$ , the likelihood estimation of the parameter  $\hat{\theta}$  obeys the Gaussian distribution with the mean value  $\theta$  and the variance as  $\sigma^2$ , so

$$r = 1 - \alpha = \frac{\int_{-\infty}^x L(x|\theta) d\theta}{\int_{-\infty}^{+\infty} L(x|\theta) d\theta}$$

If we want get the 95% confidence level upper limit, we can let  $r=95\%$ , and we can get the value  $x$ . The value  $x$  is our upper limit.

Thank you