Statistical Methods in Particle Physics



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How to communicate the statistical uncertainty of a measurement

Interval estimation

- The standard deviation as statistical error
- Classical confidence intervals
 - Exact method
 - For a parameter with a Gaussian distributed estimator
 - For the mean of a Poisson distribution
 - Approximate method with maximum likelihood and chi2
- Limits near a physical boundary

Discussion:

Statistical and systematic errors



We have seen methods for estimating properties of probability density functions (pdf's) and ways to obtain the variance of the estimators.

Suppose the result of an experiment is an estimate of a certain parameter:

n observations of random variable x

Hypothesis for the pdf $f(x;\theta)$, true θ unknown parameter

From $\mathbf{x}_1, ..., \mathbf{x}_n$ build the function $\hat{\theta}(\mathbf{x}_1, ..., \mathbf{x}_n)$ e.g. max. likelihood

 \rightarrow Determine the estimator $\,\hat{\theta}_{\rm obs}({\rm value\ actually\ observed})$ and its standard deviation $\,\hat{\sigma}_{\hat{\theta}}$

The variance (or equivalently its square root, the standard deviation) of the estimator is a measure of how widely the estimates would be distributed if the experiment were to be repeated many times with the same number of observations per experiment

Standard deviation $\sigma \rightarrow$ statistical uncertainty or standard error

In reporting the measurement of θ as:

$$\hat{\theta}_{\mathrm{obs}} \pm \hat{\sigma}_{\hat{ heta}}$$

one means that repeated estimates all based on n observations of x would be distributed according to a pdf $g(\hat{\theta})$ centered around some true value θ and true standard deviation, which are estimated to be

$$\hat{ heta}_{_{obs}}$$
 and $\hat{\sigma}_{_{\hat{ heta}}}$

- For most practical estimators, the sample pdf g becomes approximately Gaussian in the large sample limit
- If more than one parameter is estimated, the pdf becomes a multidimensional Gaussian characterized by a covariance matrix V
- The standard deviation, and in case the covariance matrix, tell everything how repeated estimates would be distributed





If the form of the estimator pdf $g(\hat{\theta})$ is not Gaussian, then the 'standard deviation' definition of statistical error bars does not hold!

In such cases, one usually reports **confidence intervals**, an interval reflecting the statistical uncertainty of the parameter (it is an alternative, often equivalent, method)

 \rightarrow quantitative statement about the fraction of times that such an interval would contain the true value of the parameter in a large number of repeated experiments



Confidence intervals should:

- communicate objectively the result of the experiment;
- have a given probability of containing the true parameter;
- provide information needed to draw conclusions about the parameter possibly incorporating stated prior beliefs.

Very often they lead to asymmetric errors

Special case: estimate limits of parameters near a physically excluded region (e.g. an observed event rate consistent with zero)

Consider the estimator $\hat{\theta}$ for a parameter θ , and an estimate $\hat{\theta}_{obs}$ The sampling distribution for θ is $g(\hat{\theta}; \theta)$

By means of e.g. an analytical calculation or a Monte Carlo study, one knows g, which contains the true value θ as parameter.

That is, the real value of θ is not known, but for a given value of θ , one knows what the pdf of $\hat{\theta}$ would be Depends on true θ , which remains unknown !! For one given value of θ , we have:



Frequentist confidence interval

From $g(\hat{\theta}; \theta)$ one can determine the value u_{α} such that there is a fixed probability α to observe $\hat{\theta} \ge u_{\alpha}$:

$$\alpha = \mathsf{P}(\hat{\theta} \ge \mathsf{u}_{\alpha}(\theta))$$
$$= \int_{\mathsf{u}_{\alpha}(\theta)}^{\infty} \mathsf{g}(\hat{\theta};\theta) \, \mathsf{d}\hat{\theta}$$
$$= \mathsf{1} - \mathsf{G}(\mathsf{u}_{\alpha}(\theta);\theta)$$



 $g(\hat{\theta};\theta)$

0.5

And the value v_{β} such that there is the probability β to observe $\hat{\theta} \leq v_{\beta}$: $\beta = P(\hat{\theta} \leq v_{\beta}(\theta)) = \int_{-\infty}^{v_{\beta}(\theta)} g(\hat{\theta};\theta) d\hat{\theta} = G(v_{\beta}(\theta);\theta)$

G: cumulative distribution of g

Confidence belt





As long as $u_{\alpha}(\theta)$ and $v_{\beta}(\theta)$ are monotonically increasing functions of θ (they should be, if $\hat{\theta}$ is to be a good estimator of θ), then one can determine the inverse functions:

$$\mathbf{a}(\hat{\theta}) = \mathbf{u}_{\alpha}^{-1}(\hat{\theta}) \qquad \mathbf{b}(\hat{\theta}) = \mathbf{v}_{\beta}^{-1}(\hat{\theta})$$

Then:

$$\begin{split} \hat{\theta} &\geq \mathsf{u}_{\alpha}(\theta) &\Rightarrow \mathsf{a}(\hat{\theta}) &\geq \theta \\ \hat{\theta} &\leq \mathsf{v}_{\beta}(\theta) &\Rightarrow \mathsf{b}(\hat{\theta}) &\leq \theta \end{split}$$

Therefore:

$$P(a(\hat{\theta}) \ge \theta) = \alpha$$

$$P(b(\hat{\theta}) \le \theta) = \beta$$

$$P(a(\hat{\theta}) \le \theta \le b(\hat{\theta})) = 1 - \alpha - \beta$$

g(ê;9)

0.5

For the value of the estimator

Confidence belt

find the points where that intersects the confidence belt

this determines the points a and b

The interval [a,b] is called a **confidence interval at a confidence level** (or coverage probability) of $1 - \alpha - \beta$







Confidence interval

The interval [a,b] is called a **confidence interval at a confidence level** of $1 - \alpha - \beta$

Means that:

If the experiment were repeated many times, the interval [a,b] would include the true value of the parameter θ in a fraction $1 - \alpha - \beta$ of the experiments

Also: $1 - \alpha - \beta$ is the probability for the interval to cover the true value of the parameter

Quote as: $\hat{\theta}_{-c}^{+d}$ where $c = \hat{\theta} - a$, $d = b - \hat{\theta}$





One-sided and central confidence intervals



One often chooses α = β = γ/2 giving a so-called central confidence interval with probability 1 – γ

A central confidence interval does not necessarily mean that a and b are equidistant from the estimated $\hat{\theta}$, but only that the probabilities α and β are equal

In high energy physics, the error convention is to take the 68.3% central confidence interval (see later)

• Sometimes ONLY specify α OR β

\rightarrow one-sided confidence interval or limit

That is, the value a represents a lower limit on the parameter θ such that $a \le \theta$ with the probability $1 - \alpha$

Similarly, b represents an upper limit on θ such that $P(\theta \le b) = 1 - \beta$

Usually we do not construct confidence belts, but solve:

$$\alpha = \int_{u_{\alpha}(\theta)}^{\infty} g(\hat{\theta};\theta) d\hat{\theta} = \int_{\hat{\theta}_{obs}}^{\infty} g(\hat{\theta};a) d\hat{\theta}$$
$$\beta = \int_{-\infty}^{v_{\beta}(\theta)} g(\hat{\theta};\theta) d\hat{\theta} = \int_{-\infty}^{\hat{\theta}_{obs}} g(\hat{\theta};b) d\hat{\theta}$$





Confidence intervals for a parameter θ can be found by defining a **test** of the hypothesized value θ (do this for all θ):

- Specify values of the data that are 'disfavoured' by θ (critical region) such that:
 - P(data in critical region) $\leq \gamma$

for a specified γ , e.g. 0.05 or 0.1

 Invert the test to define a confidence interval as: set of θ values that would NOT be rejected in a test of size γ (the confidence level is 1-γ)

The interval will cover the true value of θ with probability $\ge 1 - \gamma$. Equivalent to a confidence belt construction. The confidence belt is acceptance region of a test Equivalently we can consider a significance test for each hypothesized value of θ , resulting in a p-value, p_{θ}

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If p_{\theta} < \gamma, then reject \theta
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The confidence interval at $CL = 1 - \gamma$ consists of those values of θ which are not rejected !

E.g. un upper limit on θ is the greatest value for which $p_{\theta} \ge \gamma$

In practice find by setting $p_{\theta} = \gamma$ and solve for θ

 $g(\hat{\theta};\theta)$

0.5

NOTE !!! the interval is random, the true θ is an unknown constant Often report interval [a,b] as

$$\hat{\theta}_{-c}^{+d}$$
 where $c = \hat{\theta} - a$, $d = b - \hat{\theta}$
ERROR BARS

So, what does $\hat{\theta} = 80.25^{+0.31}_{-0.25}$ mean?

- It does NOT mean: $P(80.00 < \theta < 80.56) = 1 \alpha \beta$
- But rather: repeat the experiment many times with the same sample size, construct interval according to the same prescription each time, in 1 – α – β of experiments, interval will cover θ

In the frequency interpretation, the true parameter θ is not a random variable and is assumed to not fluctuate from experiment to experiment. In this sense the probability that θ is in the confidence interval is either 0 or 1, but we do not know which. The interval itself, however is subject to fluctuations since it is constructed from the data.

 $g(\hat{\theta};\theta)$

0.5

Consider a Gaussian distributed estimator:

$$g(\hat{\theta};\theta) = \frac{1}{\sqrt{2\pi\sigma_{\hat{\theta}}^2}} \exp\left(\frac{-(\hat{\theta}-\theta)^2}{2\sigma_{\hat{\theta}}^2}\right)$$

with mean θ and standard deviation $\sigma_{\hat{\theta}}$ It has the cumulative distribution of $\hat{\theta}$:

$$G(\hat{\theta};\theta,\sigma_{\hat{\theta}}) = \int_{-\infty}^{\hat{\theta}} \frac{1}{\sqrt{2\pi\sigma_{\hat{\theta}}^{2}}} \exp\left(\frac{-(\hat{\theta}'-\theta)^{2}}{2\sigma_{\hat{\theta}}^{2}}\right) d\hat{\theta}'$$

This is a commonly occurring situation since, according to the **central limit theorem**, any estimator that is a linear function of a sum of random variables becomes Gaussian in the large sample limit.

 $\begin{array}{c}
\left(\widehat{\mathbf{e}}\right) \\
\left(\widehat{\mathbf{e}$

To find the confidence interval for θ , solve for a and b:

$$\alpha = 1 - G(\hat{\theta}_{obs}; a, \sigma_{\hat{\theta}}) = 1 - \Phi \left(\frac{\hat{\theta}_{obs} - a}{\sigma_{\hat{\theta}}} \right)$$
$$\beta = G(\hat{\theta}_{obs}; b, \sigma_{\hat{\theta}}) = \Phi \left(\frac{\hat{\theta}_{obs} - b}{\sigma_{\hat{\theta}}} \right)$$

where G is the cumulative distribution for $\hat{\theta}$ and

 $\Phi(\mathbf{x}) = \int_{-\infty}^{\mathbf{x}} \frac{1}{\sqrt{2\pi}} e^{-\mathbf{x}'^{2}/2} d\mathbf{x}' \text{ is the cumulative for the standard} Gaussian}$

Confidence interval for Gaussian



Solving for a and b:

$$\mathbf{a} = \hat{\theta}_{obs} - \sigma_{\hat{\theta}} \Phi^{-1}(1 - \alpha)$$
$$\mathbf{b} = \hat{\theta}_{obs} + \sigma_{\hat{\theta}} \Phi^{-1}(1 - \beta)$$

Φ⁻¹ = quantile of standard Gaussian (inverse of cumulative distribution, use ROOT)

$$\rightarrow \Phi^{-1}(1-\alpha), \Phi^{-1}(1-\beta)$$
 give how many standard deviations a and b are from $\hat{\theta}$

Quantiles of the standard Gaussian

When we have a Gaussian estimator, to have a central confidence interval or a one-sided limit, we need to know the quantiles shown here:



 $g(\hat{\theta};\theta)$

0.5

 $\begin{array}{c} \widehat{\Phi} \\ \widehat{\Phi} \\ \widehat{\Phi} \\ \widehat{\Phi} \\ \widehat{\Phi} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ \end{array} \right)$

Typically, take a round number for the quantile (NUMBER OF SIGMAS !!!)

$\operatorname{central}$		one-sided		
$\Phi^{-1}(1 - \gamma/2)$	$1-\gamma$	$\Phi^{-1}(1-\alpha)$	$1 - \alpha$	
1	0.6827	1	0.8413	
2	0.9544	2	0.9772	
3	0.9973	3	0.9987	

Or a round number for the coverage probability:

ce	ntral	one-sided		
$1-\gamma$	$\Phi^{-1}(1-\gamma/2)$	$1 - \alpha$	$\Phi^{-1}(1-\alpha)$	
0.90	1.645	0.90	1.282	
0.95	1.960	0.95	1.645	
0.99	2.576	0.99	2.326	



For the conventional 68.3% central confidence interval, one has: $\alpha = \beta = \gamma/2$ With $\Phi^{-1}(\gamma - \gamma/\gamma) = 1$

i.e. a 1 σ error bar.

This results in the simple prescription:

$$[\mathsf{a},\mathsf{b}] = [\hat{\theta}_{\mathsf{obs}} - \sigma_{\hat{\theta}}, \hat{\theta}_{\mathsf{obs}} + \sigma_{\hat{\theta}}]$$

The final result of the measurement of θ is then simply reported as:

$$\hat{ heta}_{ ext{obs}} \pm \sigma_{\hat{ heta}}$$



Suppose n is Poisson distributed, the estimator: $\hat{v} = n$

$$P(n;v) = \frac{v^n}{n!} e^{-v}$$
, $n = 0, 1, ...$

A single measurement gives $\hat{\nu}_{obs} = n_{obs} \rightarrow \text{construct}$ the confidence interval for ν

Minor problem: for fixed α , β , the confidence belt does not exist for all ν Just solve: $n_{obs}-1$

$$\alpha = P(\hat{\nu} \ge \hat{\nu}_{obs}; a) = 1 - \sum_{n=0}^{\infty} \frac{a^n}{n!} e^{-a}$$

$$\beta = P(\hat{\nu} \le \hat{\nu}_{obs}; b) = \sum_{n=0}^{n_{obs}} \frac{b^n}{n!} e^{-b}$$

for a and b



Use the trick:

$$\sum_{n=0}^{n_{obs}} \frac{\nu^{n}}{n!} e^{-\nu} = 1 - F_{\chi^{2}}(2\nu; n_{d} = 2(n_{obs} + 1))$$

where F_{χ^2} is the cumulative chi-square distribution for n_d degrees of freedom.

Find:

$$a = \frac{1}{2} F_{\chi^2}^{-1}(\alpha; n_d = 2n_{obs})$$

$$b = \frac{1}{2} F_{\chi^2}^{-1}(1 - \beta; n_d = 2(n_{obs} + 1))$$

where $F_{\chi^2}^{-1}$ is the quantile of the chi-square distribution



An important case: $n_{obs} = 0$

$$\beta = \sum_{n=0}^{0} \frac{b^n e^{-b}}{n!} = e^{-b} \rightarrow b = -\log\beta$$

Calculate an upper limit at confidence level $(1-\beta) = 95\%$

$$b = -\log(0.05) = 2.996 \approx 3$$

Useful table:

$n_{ m obs}$	lower limit a			upper limit b		
	$\alpha = 0.1$	$\alpha=0.05$	$\alpha = 0.01$	$\beta = 0.1$	$\beta=0.05$	$\beta=0.01$
0				2.30	3.00	4.61
1	0.105	0.051	0.010	3.89	4.74	6.64
2	0.532	0.355	0.149	5.32	6.30	8.41
3	1.10	0.818	0.436	6.68	7.75	10.04
4	1.74	1.37	0.823	7.99	9.15	11.60
5	2.43	1.97	1.28	9.27	10.51	13.11

Often the purpose of an experiment is to search for a new effect, the existence of which would imply that a certain parameter is not equal to zero. For example, the existence of the Higgs.

If the data yield a value of the parameter significantly different from zero, then the new effect has been **discovered**, and the parameter's value and a confidence interval to reflect its error are given as the result.

If, on the other hand, the data result in a fitted value of the parameter that is consistent with zero, then the result of the experiment is reported by giving an **upper limit** on the parameter (a similar situation occurs when absence of the new effect corresponds to a parameter being large or infinite; one then places a lower limit).

The procedure to set limits is very delicate and can present serious difficulties (estimators which can take on values in the excluded region, negative mass of a particle, negative number of events, etc).



Consider the case of finding $n = n_s + n_b$ events where

n_b events from known processes (background)

n_s events from a new process (signal)

are Poisson random variables with means s and b. Therefore $n = n_s + n_b$ is also Poisson distributed, with mean s+b Assume b is known.

Suppose we are searching for evidence of the signal process, but the number of events found is roughly equal to the expected number of background events, e.g. b = 4.6 and we observe $n_{obs} = 5$ events.

The evidence for the presence of signal events is not statistically significant

 \rightarrow set an upper limit on the parameter s



Find the hypothetical value of s such that there is a given small probability, say γ =0.05 to find as few events as we did or less:

$$\gamma = P(n \le n_{obs}; s, b) = \sum_{n=0}^{n_{obs}} \frac{(s+b)^n}{n!} e^{-(s+b)}$$

Solve numerically for $s = s_{up}$

This gives an upper limit on s at a confidence level of (1-γ)

Example (see page before): Suppose b = 0 and we find $n_{obs} = 0$. For $(1-\gamma) = 0.95$, $s_{up} \approx 3$ To solve for s_{lo} , s_{up} , we can exploit the relation to the χ^2 distribution (see page 22)

$$s_{lo} = \frac{1}{2} F_{\chi^2}^{-1}(\alpha; 2n) - b$$

$$s_{up} = \frac{1}{2} F_{\chi^2}^{-1}(1 - \beta; 2(n + 1)) - b$$

For low fluctuation of n, this can give negative result for s_{up} i.e. confidence interval is empty



 $g(\hat{\theta}; \theta)$

0.5



Suppose for example b = 2.5 and we observe n = 0. If we choose CL = 0.9, we find from the formula for s_{up} :

$$s_{up} = -0.197$$
 (CL = 0.90)

Physicist:

We already knew $s \ge 0$ before we started; cannot use negative upper limit to report a result!

Statistician:

The interval is designed to cover the true value only 90% of the time: This was clearly not one of those times.

Not uncommon dilemma when limit of parameter is close to a physical boundary!



In Bayesian statistics we need to start with "prior pdf" $\pi(\theta)$: this reflects the degree of belief about θ before doing the experiment

Bayes' theorem tells how our beliefs should be updated in light of the data x:

$$p(\theta|\mathbf{x}) = \frac{\mathsf{L}(\mathbf{x}|\theta) \ \pi(\theta)}{\int \mathsf{L}(\mathbf{x}|\theta') \ \pi(\theta') \ \mathsf{d}\theta'} \propto \mathsf{L}(\mathbf{x}|\theta) \ \pi(\theta)$$

We will integrate the posterior pdf $p(\theta|x)$ to give interval with any desired probability content.

E.g. for Poisson parameter: 95% CL upper limit from

$$0.95 = \int_{-\infty}^{s_{up}} p(s|n) ds$$

 $g(\hat{\theta};\theta)$

0.5



Include knowledge that $s \ge 0$, by setting prior $\pi(s) = 0$ for s < 0. Often try to reflect the 'prior ignorance' with e.g.

$$\pi(\mathbf{s}) = \begin{cases} 1, \ \mathbf{s} \ge 0\\ 0, \text{ otherwise} \end{cases}$$

Not normalized, but this is OK as long as L(s) dies off for large s.

Not invariant under change of parameter – if we had used instead a flat prior for, say, the mass of the Higgs boson, this would imply a non-flat prior for the expected number of Higgs events.

Does not really reflect a reasonable degree of belief, but often used as a point of reference,

Or viewed of as a recipe for producing an interval whose frequentist properties can be studies (coverage will depend on true s)

For special case b=0, Bayesian upper limit with flat prior numerically same as classical case (only a coincidence!)

Otherwise Bayesian limit is everywhere greater than classical ('conservative'). Never goes negative. Does not depend on b if n=0

Solve numerically to find limit s



Bayesian interval with flat prior for s





Recall the trick to estimate $\sigma_{\hat{\theta}}$ if $\ln L(\theta)$ is parabolic:

$$\ln L(\hat{\theta} \pm N \sigma_{\hat{\theta}}) = \ln L_{\max} - \frac{N^2}{2}$$

CLAIM: this still works even if In L is not parabolic, as an approximation for the confidence interval.

i.e. use

$$\ln L(\hat{\theta_{-c}^{+d}}) = \ln L_{max} - \frac{N^2}{2}$$
$$\chi^2(\hat{\theta_{-c}^{+d}}) = chi2_{min} + N^2$$

where N = $\Phi^{-1}(1 - \gamma/2)$

is the quantile of the standard Gaussian corresponding to the CL 1- γ . For example: N = 1 \rightarrow 1- γ = 0.683 Exponential example (see lecture 10): take interval where In L is within 1/2 of the maximum \rightarrow approximation of 68.3% confidence interval



 $g(\hat{\boldsymbol{\theta}};\boldsymbol{\theta})$

0.5

In many practical applications, estimators are Gaussian distributed (at least approximately). In this case the confidence interval can be determined easily.

Similarly is for estimators with a Poisson distribution.

But even in the other cases, a simple approximate technique can be applied using the likelihood function (or equivalently the function).

Statistical uncertainty or random error

Random errors are errors in measurement that lead to measurable values being inconsistent when repeated measures of a constant attribute or quantity are taken. The word random indicates that they are inherently unpredictable, and have null expected value, namely, they are scattered about the true value, and tend to have null arithmetic mean when a measurement is repeated several times with the same instrument. All measurements are prone to random error.

Random error is caused by unpredictable fluctuations in the readings of a measurement apparatus, or in the experimenter's interpretation of the instrumental reading; these fluctuations may be in part due to interference of the environment with the measurement process.

The concept of random error is closely related to the concept of precision. The higher the precision of a measurement instrument, the smaller the variability (standard deviation) of the fluctuations in its readings.

Systematic errors are biases in measurement which lead to the situation where the mean of many separate measurements differs significantly from the actual value of the measured attribute. All measurements are prone to systematic errors, often of several different types. Sources of systematic error may be:

- imperfect calibration of measurement instruments (zero error),
- changes in the environment which interfere with the measurement process and
- sometimes imperfect methods of observation can be either zero error or percentage error.

For example: consider an experimenter taking a reading of the time period of a pendulum swinging past a fiducial mark: If their stop-watch or timer starts with 1 second on the clock then all of their results will be off by 1 second (zero error). If the experimenter repeats this experiment twenty times (starting at 1 second each time), then there will be a percentage error in the calculated average of their results; the final result will be slightly larger than the true period. Distance measured by radar will be systematically overestimated if the slight slowing down of the waves in air is not accounted for. Incorrect zeroing of an instrument leading to a zero error is an example of systematic error in instrumentation.

Systematic errors may also be present in the result of an estimate based on a mathematical model or physical law. For instance, the estimated oscillation frequency of a pendulum will be systematically in error if slight movement of the support is not accounted for.

Systematic errors can be either constant, or be related (e.g. proportional or a percentage) to the actual value of the measured quantity, or even to the value of a different quantity (the reading of a ruler can be affected by environment temperature). When they are constant, they are simply due to incorrect zeroing of the instrument. When they are not constant, they can change sign. For instance, if a thermometer is affected by a proportional systematic error equal to 2% of the actual temperature, and the actual temperature is 200°, 0°, or -100° , the measured temperature will be 204° (systematic error = +4°), 0° (null systematic error) or -102° (systematic error = -2°), respectively. Thus, the temperature will be overestimated when it will be above zero, and underestimated when it will be below zero.

Constant systematic errors are very difficult to deal with, because their effects are only observable if they can be removed. Such errors cannot be removed by repeating measurements or averaging large numbers of results. A common method to remove systematic error is through calibration of the measurement instrument.

In a statistical context, the term systematic error usually arises where the sizes and directions of possible errors are unknown.