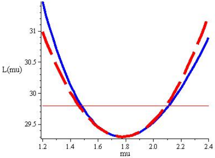
Parameter Estimation Part A

The Likelihood Method



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Parameter estimation

Common task

- Determine from measurements with uncertainties the best values of (physical) parameters
- Estimation is a mathematical procedure (!)
- Any parameter makes sense **only** within a model
- The model is encoded in the pdf of the parameters
- Wrong models deliver wrong answers!
- Uncertainties must be known: Variances and Covariances
- Distinguish between:
  - Statistical uncertainties
  - Systematic uncertainties

Parameter estimation

Fundamental properties of estimators

Estimators can be characterized as *good* or *bad*

The characterization classes are:

- Consistency: the true value and the estimated value are equivalent

$$\lim_{n \to \infty} \hat{a} = a$$

- Bias: the expectation value is equivalent to true value

$$\langle \hat{a} \rangle = a$$

- Efficiency: small variance

The inherent accuracy of an estimator is limited!

Consistency

- Parameters are estimated from limited samples
- Any sample exhibits statistical fluctuations
- For large samples, the effect of fluctuations lessens
- If the difference between the true value and the estimated value vanishes, the estimator is **consistent**

Formal definition

An estimator is consistent, if it tends to the true value as the number of data tends to infinity:

$$\lim_{n\to\infty} \hat{a} = a$$

Bias

- For finite amounts of data the estimated parameter is unlikely to have the true value
- A good estimator has the equal chances of over- and underestimation of the true value
- Such an estimator is unbiased
- This can be expressed in terms of the expectation value of the estimator

Formal definition

An estimator is unbiased, if its expectation value is the same as the true value:

$$\langle \hat{a} \rangle = a$$

Efficiency

- The estimated value depends on the given data sample
- The fluctuations of the sample influence the estimator
- An efficient estimator exhibits a small fluctuation or spread
- The spread is measured in terms of the variance of the estimator

Formal definition

An estimator is efficient if its variance is small.

Minimum Variance Bound

(Without proof) There is a lower bound on the variance of an estimator!

- There are different names for this:
  Cramér-Rao bound (or inequality), Fréchet inequality, MVB, CRLB
- It uses the (in the simple/unbiased form) the Likelihood function $\mathcal{L}$:

$$\sigma_{\hat{a}}^2 \leq \frac{1}{\langle (d\mathcal{L}/da)^2 \rangle}$$

- An estimator is efficient, if its variance is equal to the MVB

Characterization of Maximum Likelihood

Most important parameter estimation method

- Maximum Likelihood estimators are (usually) consistent
- Maximum Likelihood are biased (!) for small N
  for large N it becomes unbiased
- It is usually the optimal estimation in terms of the Minimum Variance Bound

Warning

- Maximum Likelihood is (usually) consistent, but biased!
- Maximum Likelihood estimators invariant under parameter transformations!:

$$\widehat{f(a)} = f(\hat{a}) \qquad e.g. : \widehat{\sigma^2} = (\hat{\sigma})^2$$

Bias example

Consider a symmetric pdf around a_0, let $\hat{a}$ be an unbiased estimator

Equal chances that $\hat{a}$ is either 10% too large or too small

- Equally possible:

$$\hat{a} = 1.1a_0 \qquad \hat{a} = 0.9a_0$$

- Now consider (non-linear) transformation $y : x \to x^2$, then

$$\hat{a}^2 = 1.21a_0^2 \qquad \hat{a}^2 = 0.81a_0^2$$

- Probability content doesn't change, equal chances that $\hat{a}^2$ is 21% larger or 19% smaller than a_0^2
- In short: the pdf becomes asymmetric and therefore biased

The maximum Likelihood method

Requirements

- Data, e.g. n measurements x_i
- A model, e.g. a pdf $f(x;a)$
- The function has to be normalized for all a:

$$\int f(x;a)dx = 1$$

The formula

Maximize the product of all functions at the given measurements:

$$\mathcal{L}(\vec{x};a) = f(x_1;a)\cdot f(x_2;a)...f(x_n;a) = \prod_i^n f(x_i;a)$$

to obtain the best estimator for the parameter(s).

Maximization

Finding the maximum is straightforward

- For a single parameter a

$$\frac{d\mathcal{L}(\vec{x};a)}{da} = 0$$

- For multiple parameters $\vec{a} = a_1, \ldots a_m$:

$$\frac{\partial\mathcal{L}(\vec{a})}{\partial a_k} = 0 \quad , \forall k = 1, \ldots, m$$

Log Likelihood

Different formulation

- Often: too much data to calculate $\mathcal{L}$ accurately
- Take logarithm of $\mathcal{L} \Longrightarrow \ln \mathcal{L}$
- Use negative value in order to use only one numerical routine for minimization (like for χ^2 minimization)

Formula

$$\ell(\vec{x}; a) = -\ln \mathcal{L}(\vec{x}; a)$$

General properties

Important reminder:

- One needs to know the underlying pdf
- Wrong pdf will yield a wrong or non-sensical result
- Always check the result:
  - Do the found parameters describe the data (at all!?)
  - Parameter at boundary of parameter space?
    This is always trouble
- There is **no** consistency check inherent to the method

Example: Likelihood estimation of mean I

Consider (once again) a radioactive source; n measurements are taken under the same conditions, counted are the number of decays r_i in a given, constant time interval

What's the mean number of decays?

- Naive (?): Simply take the arithmetic mean

$$\mu = \frac{1}{n} \sum_{i}^{n} r_i$$

- Wrong (!): Take the weighted mean
- Maximum Likelihood

Example: Likelihood estimation of mean II

Estimation via ML

r_i follows a Poisson distribution:

$$P(r_i;\mu) = \frac{\mu^{r_i} e^{-\mu}}{r_i!}$$

The Likelihood function is therefore

$$\mathcal{L}(\mu) = \prod_i^n P(r_i;\mu) = \prod_i^n \frac{\mu^{r_i} e^{-\mu}}{r_i!}$$

Negative logarithm:

$$\ell(\mu) = -\ln \mathcal{L}(\mu) = -\sum_i^n \ln \frac{\mu^{r_i} e^{-\mu}}{r_i!} = \sum_i^n (-r_i \ln \mu + \mu + \ln r_i!)$$

Example: Likelihood estimation of mean III

Estimation via ML

Differentiate for the parameter μ:

$$\frac{d}{d\mu}\ell(\mu) = \frac{d}{d\mu}\sum_i^n (-r_i \ln \mu + \mu + \ln r_i!) = \sum_i^n \left(-r_i \frac{1}{\mu} + 1\right)$$

set to zero:

$$0 = \sum_i^n \left(-r_i \frac{1}{\mu} + 1\right) = n - \frac{1}{\mu}\sum_i^n r_i$$

$$\implies \mu = \frac{1}{n}\sum_i^n r_i$$

This yields the same result as the naive expectation.

What is the uncertainty of the estimation?

Consider the following statements (without proof):

- In the limit of $n \to \infty$ the likelihood function $\mathcal{L}$ is approximately Gaussian,
- the mean μ of this distribution is the **true** mean value of the parameter and
- the variance goes to zero $\sigma \to 0$

(we will formalize this a little later.)

Intuitive explanation:

If you sample from a certain population that follows a certain distribution, the best estimator for a parameter is **itself** a random variable.

Now evolve the likelihood function around the best estimator.

Series evolution of the likelihood function

With

$$\frac{d}{da}\ell(a)\bigg|_{a=\hat{a}} = 0$$

this is

$$\ell(a) = \ell(\hat{a}) + \frac{1}{2}(a-\hat{a})^2 \left.\frac{d^2\ell(a)}{da^2}\right|_{a=\hat{a}} + \dots$$

For the likelihood function $\mathcal{L}$ this is

$$\mathcal{L} \approx const \cdot e^{-\frac{1}{2}\left\{(a-\hat{a})^2 \left.\frac{d^2\ell(a)}{da^2}\right|_{\hat{a}}\right\}}$$

From this expression the variance can be identified:

$$\sigma_a^2 = \left(\left.\frac{d^2\ell(a)}{da^2}\right|_{\hat{a}} \right)^{-1}$$

Continue example

What is the uncertainty of the estimation of the mean number of decays?

The best estimator was the arithmetic mean:

$$\mu = \frac{1}{n}\sum_{i}^{n} r_i$$

Now calculate the variance of μ, take the second derivative at $\mu = \hat{\mu}$:

$$\left.\frac{d^2\ell(\mu)}{d\mu^2}\right|_{\mu=\hat{\mu}} = \frac{1}{\hat{\mu}}\sum_{i}^{n} r_i = \frac{1}{\hat{\mu}^2}\hat{\mu}n = \frac{n}{\hat{\mu}} = \frac{1}{\sigma_\mu^2}$$

$$\Longrightarrow \sigma_\mu^2 = \frac{\hat{\mu}}{n}$$

If the true value μ is not known, then the variance is calculated from the best estimation.

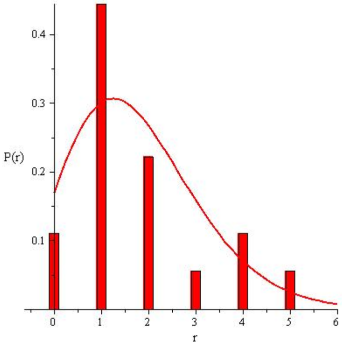
Numerical example

A set of rate measurements at fixed intervals of a radioactive source yielded

$$r_i = [1, 1, 5, 4, 2, 0, 3, 2, 4, 1, 2, 1, 1, 0, 1, 1, 2, 1]$$

Assume a Poisson distribution

Better check: histogram the values and compare it with a Poisson. The estimated, best value for the mean is $\mu = \frac{1}{n}\sum_i^n r_i = 1.78$ the estimated uncertainty from this is $\sigma_\mu = \sqrt{\mu/n} = 0.31$



Looks OK!

Uncertainty estimation: the parabolic approximation I

Often the likelihood function $\ell = -\ln \mathcal{L}$ can be approximated by a parabola in the direct vicinity of the minimum:

$$\ell(\mu) \approx \ell(\hat{\mu}) + \frac{1}{2}\frac{(\mu - \hat{\mu})^2}{\sigma_\mu^2}$$

From $\mu = \hat{\mu} + \sigma_\mu$ can be then deduced, that the standard deviation can be determined implicitly from the points of intersection of the parabola with the constant

$$\ell_{min} + \frac{1}{2}$$

Uncertainty estimation: the parabolic approximation II

In almost all cases, the second derivative of $\ell(a)$ can't be calculated (accurately) – how is the uncertainty determined then?
The relation still holds:

$$\ell(\hat{\mu} \pm \sigma_\mu) = \ell_{min} + \frac{1}{2}$$

- In the parabolic approximation is $\mathcal{L}(a) = e^{-\ell(a)}$ a Gaussian distribution around the *true* value $\hat{a}$
- What if the approximation is not very good?

Uncertainty estimation: general solution

If the symmetric Gauss function isn't a good description, asymmetric errors σ_l and σ_r can be derived from

$$\ell(\hat{\mu} - \sigma_l) = \ell(\hat{\mu} + \sigma_r) = \ell_{min} + \frac{1}{2}$$

- In principle it's always possible to transform the parameter a with $b(a)$, so that $\ell(b(a))$ becomes parabolic
- One doesn't even need to know the transformation, the probability content in an interval is always conserved!

$\Longrightarrow$ This interval always contains the central 68% probability.

The result can then be written as

$$\mu^{+\sigma_r}_{-\sigma_l}$$

Continue numerical example

- Estimated mean is $\mu = \frac{1}{n}\sum_i^n r_i = 1.78$
- In the parabolic approximation the uncertainty is $\sigma_\mu = \sqrt{\mu/n} = 0.31$
- For finding the *true* parameter uncertainty, solve the actual Likelihood function for the intersection points with $\ell_{min} + \frac{1}{2}$:

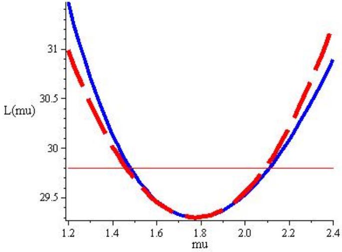
The result is

either

$$\mu = 1.78 \pm 0.31$$

or

$$\mu = 1.78^{+0.33}_{-0.30}$$



General expression for uncertainties

- The intervals that contain k standard deviations can be determined likewise:
$$\ell(\hat{a} - k\sigma_l) = \ell(\hat{a} + k\sigma_r) = \ell_{min} + \frac{k^2}{2}$$
- The amount of probability is the same as for the Gaussian distribution
- E.g. 2σ are in $\ell_{min} + 2$ and corresponds to 95% probability
  3σ are defined by $\ell_{min} + \frac{9}{2}$, corresponding to 99%, etc.

Binned Likelihood

The task

- J number of bins, each with n_j entries
- Fit pdf $f(x;a)$ to the number of entries in each bin
- Obtain the best value for a using the data

Consider the number of bin entries n_j as random variables

- Underlying pdf is Poisson with mean value μ_j:

$$P(n_j;\mu_j) = \frac{\mu_j^{n_j} e^{-\mu_j}}{n_j!}$$

- The mean value μ_j depends on the fit parameter a: $\mu_j(a)$
- The Poissonian describes the distribution of entries in each bin

Binned Likelihood II

How to obtain $\mu_j(a)$?

- Get the probability "amount" by integrating the pdf $f(x;a)$ for the bin j

$$p_j = \int_{bin_j} f(x;a)dx$$

- This can be approximated (mean value theorem of integration), with x_c the bin center position and Δx the interval width

$$p_j \approx f(x_c;a)\Delta x$$

- The expected mean number of entries is obtained by multiplying with the total number of entries n, so

$$\mu_j(a) = np_j \approx nf(x_c;a)\Delta x$$

Binned Likelihood function

Master formula for binned Likelihood

$$F(a) = -\sum_j^J \ln\left(\frac{\mu_j^{n_j} e^{-\mu_j}}{n_j!}\right) = -\sum_j^J n_j \ln \mu_j + \sum_j^J \mu_j + \underbrace{\sum_j^J \ln(n_j!)}_{const}$$

- This is the formula to use for Poisson distributed variables (since it's unbiased)
- It's also valid if the n_j are small or even zero (!)
- The last term doesn't play any role in the minimization, since it's constant for given data
- It's directly related to the binned χ^2 formula (not shown here)

Multi-dimensional parameters

The generalization to more than parameter $\vec{a} = a_1, \ldots, a_m$ leads to the Likelihood function for n measurements:

$$\mathcal{L}(\vec{a}) = \prod_{i}^{n} f(x_i; \vec{a})$$

- The minimization procedure is the same
- What's with the uncertainties of the parameters? And Correlations?

Answer (as so often): evolve the Likelihood function in a Taylor series

Taylor series evolution of $\ell(\vec{a})$

Evolve $\ell(\vec{a}) = -\ln \mathcal{L}(\vec{a})$ around the true values $\hat{\vec{a}}$:

$$\begin{aligned}\ell(\vec{a}) &= \ell(\hat{\vec{a}}) + \frac{1}{2}\sum_i^n \sum_j^n (a_i - \hat{a}_i)(a_j - \hat{a}_j)\frac{\partial^2 \ell(\vec{a})}{\partial a_i \partial a_j} + \ldots \\ &= \ell(\hat{\vec{a}}) + \frac{1}{2}\sum_i^n \sum_j^n (a_i - \hat{a}_i)(a_j - \hat{a}_j) G_{ij} + \ldots\end{aligned}$$

The Likelihood function will become Gaussian for $n \to \infty$. Comparing

$$\mathcal{L}(\vec{a}) = e^{-\ell(\vec{a})}$$

yields the identification of the inverse covariance matrix

$$G = V^{-1}$$

with the Hesse Matrix $G_{ij} = \frac{\partial^2 \ell(\vec{a})}{\partial^2 \vec{a}}$

Probability contents

Also in the case of more than one dimension all results can be taken from the integrated Gaussian distribution.

- The 1σ contour is defined by $\ell(\vec{\hat{a}}) + \frac{1}{2}$
- The 2σ contour is defined by $\ell(\vec{\hat{a}}) + 2$
- etc.

The probability contents can be calculated with integrating the Gauss function.

Likelihood for two parameters

- The probability to find a pair within the 1σ contour is 39%
- In the parabolic approximation the contour is an ellipsis in the a_1, a_2 plane
- In the general case the curves are asymmetric but contain the same amount of probability

Uncertainty of parameters

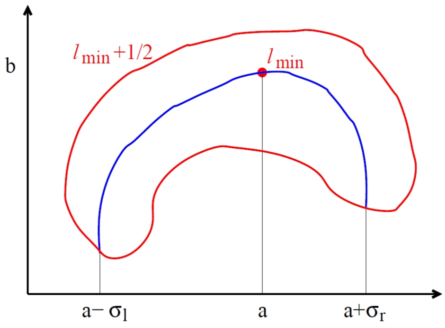
The uncertainty of a parameter is determined by minimizing w.r.t. all other parameters

The minimum of this function ℓ' serves as reference for ℓ_{min}

Example:

- This is the 1σ contour for two parameters a, b
- Parabolic approximation doesn't fit
- Still within contour area with 39% probability

Blue curve: to find uncertainty on a, $\ell(a, b)$ must be minimized w.r.t b for fixed value of a



Summary

- Parameter Estimation is a well defined mathematical procedure
- Presented method: Maximum Likelihood
- Uncertainties and Covariances are also extract-able
- No consistency check method – check plausibility of results
- Even more carefully check the pdfs/the model
- The results can still be ill-defined: crap in, crap out