PHYS-F-482: Advance techniques in experimental physics

Theory of Estimators

Juan A. Aguilar

Table of Content

Parameter estimation

The parameters of a distribution are constants that characterize their shape:

$$f(x;\theta) = \frac{1}{\theta}\exp^{-\frac{x}{\theta}}$$

where x is a r.v. and θ is a *parameter*.

Suppose we have a sample of observed values $\vec{x} = (x_1, x_2, \dots)$ following the $f(x;\theta)$ distribution. We want to some function of the data $\vec{x}$ that **estimates** the value of the parameter θ.

$$\hat{\theta}(\vec{x})$$

We put a *hat* to say that this is an estimator. We sometimes called *estimator* to the function, and *estimate* to the value that comes out with particular data set.

Properties of Estimators

Estimates of $\hat{\theta}(\vec{x})$ depend on the r.v. $\vec{x}$, therefore, estiamtes are also r.v. and they follow an specific *pdf* $g(\hat{\theta};\theta)$ that generally depends on the true value θ:

- The **bias** of an estimator is defined as: $b = E[\hat{\theta}] - \theta$
  - Average repeated measurements should tend to 0 bias
- The **variance** is $V[\hat{\theta}] = E[\hat{\theta}^2] - (E[\hat{\theta}])^2$
  - Small variance

Properties of Estimators

Another measure of the quality of an estimator is called the *MSE* (Mean Squared error):

$$MSE = E[(\hat{\theta} - \theta)^2] = E[(\hat{\theta} - E[\hat{\theta}])^2] + (E[\hat{\theta} - \theta])^2 = V[\hat{\theta}] - b^2$$

👉 Small bias and variance are in general conflicting criteria. An estimator is called optimal if its bias is 0 and the variance minimal.

Example of estimator I

- Parameter: $\mu = E[x]$
- Estimator: $\hat{\mu} = \frac{1}{n}\sum_{i=1}^{n} x_i \equiv \bar{x}$

> **Bias**: $b = E[\hat{\mu}] - \mu = \frac{1}{n}E[x_1 + x_2 + \ldots + x_n] - \mu = \frac{1}{n}E[n\mu] - \mu = 0$
>
> **Variance**:
> $V[\hat{\mu}] = V[\frac{1}{n}x_1 + \ldots + \frac{1}{n}x_n] = \frac{1}{n^2}(V[x_1] + \ldots + V[x_n]) = \frac{1}{n^2}(n\sigma^2) = \frac{\sigma^2}{n}$

Example of estimator II

- Parameter: $\sigma^2 = V[x]$
- Estimator: $\hat{\sigma}^2 = \frac{1}{(n-1)} \sum_{i=1}^{n} (x_i - \bar{x})^2 \equiv s^2$

> **Bias**: $E[\hat{\sigma}^2] - \sigma^2 = 0$ (the factor $n-1$ makes it possible)
>
> **Variance**: $V[\hat{\sigma}^2] = \frac{1}{n}(\mu_4 - \frac{n-3}{n-1}\mu_2)$, where $\mu_k = \int (x-\mu)^k f(x) \mathrm{d}x$

The Likelihood Function

Suppose a set of measurements x_i each independent and identically distributed (i.i.d) ie, each follows a probability distribution $f(x;\vec{\theta})$ that depends on a set parameter $\vec{\theta}$.

If we evaluate the function with the data obtained and regard it as a function of the parameters $\vec{\theta}$ this is called the **likelihood funcion**:

$$\mathcal{L}(\vec{\theta}) = f(\vec{x};\vec{\theta}) = \prod_{i=1}^{n} f(x_i;\vec{\theta})$$

where x_i are constants

The Maximum Likelihood Method

The likelihood function is a function of $\vec{\theta}$ if we choose a θ close to the true value, it is expected that the probabilities are high. So we define the maximum likelihood (ML) estimators to be the parameters that maximize the likelihood. If the likelihood function is differentiable the estiamtors are given by:

$$\frac{\partial \mathcal{L}}{\partial \theta_i} = 0$$

ML method: Example I

Consider the decay time of a particle, which is given by the exponential *pdf* $f(t;\tau) = \frac{1}{\tau}e^{-t/\tau}$ where τ is the lifetime of the particle.
Imagine we have a set of measurements for different decays $t_1, \ldots, t_n$, the likelihood would be:

$$\mathcal{L}(\tau) = \prod_{i=1}^{n} \frac{1}{\tau} e^{-\frac{t_i}{\tau}}$$

The value of τ for which $\mathcal{L}(\tau)$ is maximum also gives the maximum value of its logarithm (the log-likelihood function):

$$\log \mathcal{L}(\tau) = \sum_{i=1}^{n} \log \frac{1}{\tau} e^{-\frac{t_i}{\tau}} = \sum_{i=1}^{n} \left(\log \frac{1}{n} - \frac{t_i}{\tau} \right)$$

ML method: Example I

Finding the maximum $\frac{\partial \log \mathcal{L}(\tau)}{\partial \tau} = 0$ gives:

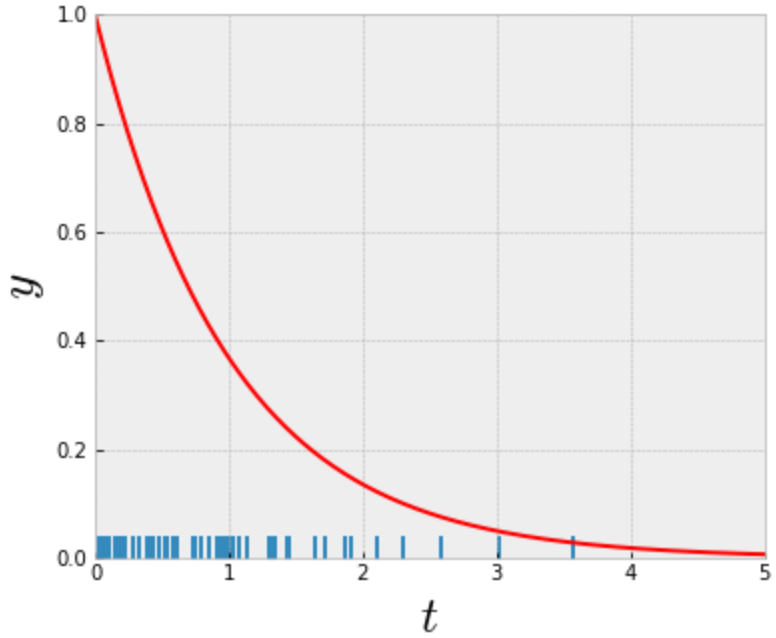
$$\hat{\tau} = \frac{1}{n} \sum_{i=1}^{n} t_i$$

```
%matplotlib inline
import numpy as np
import scipy as sp
from scipy import special
from scipy.stats import expon

import matplotlib.pylab as plt

from IPython.display import Markdown
```

ML method: Example I

```
def exp(x, tau):
    return 1/tau * np.exp(x/tau)
tau  = 1.

x = np.linspace(0, 10, 1000)
y = exp(x, tau)

nevents = 50
data = np.random.exponential(tau, nevents)

fig, ax = plt.subplots(figsize=(8,6))
ax.scatter(data, np.zeros(nevents), s = 500, marker = '|')
ax.plot(x, expon(0,tau).pdf(x), lw=2, color="red")
ax.set_xlim(0,5)
ax.set_ylim(0,1)
```

ML method: Example I




```
tau_estimate =  1./nevents * np.sum(data)
```

Best estimate is $\hat{\tau} = 1.01$

ML method: Example II

Let's consider the case of a gaussian distribution:

$$f(x;\mu,\sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-(x-\mu)^2/2\sigma^2}$$

If we have $x_1, \ldots, x_n$ independent randon variables that follow the gaussian distribution,the log-likelihood is given by:

$$\log \mathcal{L}(\mu,\sigma^2) = \sum_{i=1}^{n} \log f(x_i;\mu,\sigma^2) = \sum_{i=1} \left(\log \frac{1}{\sqrt{2\pi}} + \frac{1}{2} \log \frac{1}{\sigma^2} - \frac{(x_i-\mu)^2}{2\sigma^2} \right)$$

ML method: Example II

Calculating the derivatives for μ and σ^2 we have:

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

and

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

ML method: Example II

- The estimator for μ is unbiased, but we find that $E[\hat{\sigma^2}] = \frac{n-1}{n}\sigma^2$, so the ML estiamtor for σ^2 has a bias, that disappears when $n \to \infty$.
- To have an unbiased estimator we can use:

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

Variance of Estimators

Once we have defined the estimators, we want to report its *statistical error*. I.e., how widely the estimate will distribute if we repeat the measurement many times. We are going to see 4 methods:

1. Analytical (when possible)
2. Monte Carlo method
3. Using the information inequality
4. Graphical Method

Variance of Estimators: Analytical

In some cases we can calculate the variance analytically. For example for the exponential distribution.

- We found the estimator as: $\hat{\tau} = \frac{1}{n}\sum_{i=1}^{n} t_i$
- Variance is defined as: $V[\hat{\tau}] = E[\hat{\tau^2}] - (E[\hat{\tau}])^2$

$$= \int \dots \int \left(\frac{1}{n}\sum_{i=1}^{n} t_i\right)^2 \frac{1}{\tau}e^{-t_1/\tau} \dots \frac{1}{\tau}e^{-t_n/\tau} \mathrm{d}t_1 \dots \mathrm{d}t_n - \left(\int \dots \int \left(\frac{1}{n}\sum_{i=1}^{n} t_i\right) \frac{1}{\tau}e^{-t_1/\tau} \dots \frac{1}{\tau}e^{-t_n/\tau} \mathrm{d}t_1 \dots \mathrm{d}t_n\right)^2$$

$$= \frac{\tau^2}{n}$$

- Note that the variance depends on τ the **true value**. In practice we take $\hat{\tau}$ as the value for the variance. In our example with 50 events we have:
  $\hat{\sigma}_{\hat{\tau}} = \sqrt{V[\hat{\tau}]} = \sqrt{\hat{\tau}^2/n} = 0.15$

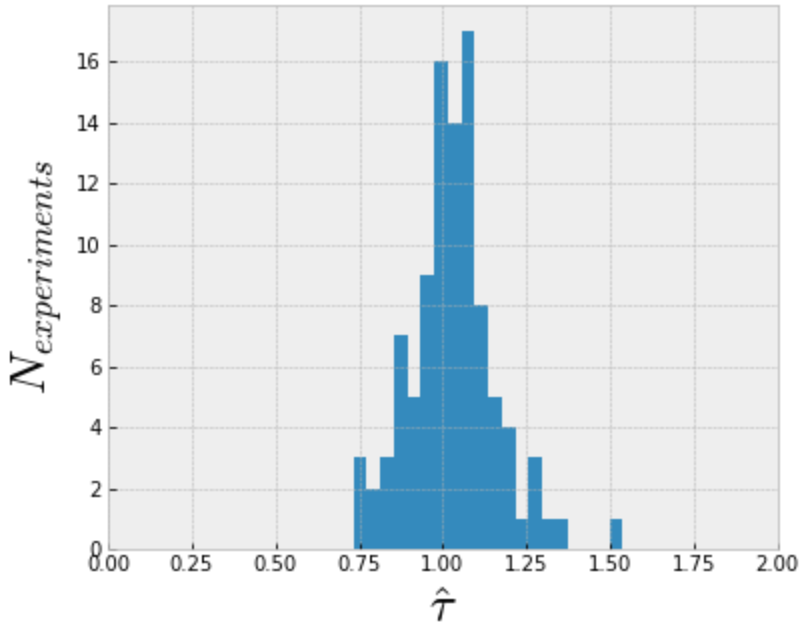
Variance of Estimators: Monte Carlo

In several cases, we cannot calcualte the variance analytically. In those cases we can use a Monte Carlo method:

```
nexperiments = 100
tau_estimates = []
for i in range(0, nexperiments):
   data = np.random.exponential(tau_estimate, nevents)tau_estimates.append(1./nevents * np.sum(data))
```

👉 Note that we used $\hat{\tau}$ to generate the pseudo-samples since we don't have access to the true τ.

Variance of Estimators: Monte Carlo



We obtained a standard deviation of $\hat{\sigma}_{\hat{\tau}} = 0.14$.

Variance of Estimators: The Rao-Cramer-Frechet Limit

The *information inequality* (RCF) sets a lower bound on the variance of any estimator:

$$V[\hat{\theta}] \geq \frac{\left(1 + \frac{\partial b}{\partial \theta}\right)^2}{E\left[-\frac{\partial^2 \log \mathcal{L}}{\partial \theta^2}\right]}$$

This is the **Minimum Variance Bound**, where b is the bias ($b = E[\hat{\theta} - \theta]$). For unbiased estimatos we have the Cramer-Rao bound:

$$V[\hat{\theta}] \geq \frac{1}{E\left[-\frac{\partial^2 \log \mathcal{L}}{\partial \theta^2}\right]} = \frac{1}{\mathcal{I}(\theta)}$$

where $\mathcal{I}(\theta) = -E\left[\frac{\partial^2 \log \mathcal{L}}{\partial \theta^2}\right]$ is the **Fisher information**.

Variance of Estimators: The Rao-Cramer-Frechet Limit

For the case of more parameters $\vec{\theta} = (\theta_1, \ldots \theta_n)$, the covariance matrix of their estimators, V_{ij} is given by:

$$(V^{-1})_{ij} = E\left[-\frac{\partial^2 \log \mathcal{L}}{\partial\theta_i \partial\theta_j}\right]$$

It is impractical, in many instances, to calculate the RCF bound instead we can estimate it as:

$$\widehat{(V^{-1})}_{ij} = -\frac{\partial^2 \log \mathcal{L}}{\partial\theta_i \partial\theta_j}\bigg|_{\vec{\theta}=\hat{\vec{\theta}}}$$

and for one parameter:

$$\widehat{\sigma^2_{\hat{\theta}}} = \left(-1 \Big/ \frac{\partial^2 \log \mathcal{L}}{\partial\theta^2}\right)\bigg|_{\theta=\hat{\theta}}$$

Variance of Estimators: The Graphic Method

The graphic method is consists on evaluating the shape of the likelihood around its minuma (we saw this in BAC3 labs). For that we can expand in as Taylor expansion:

$$\log \mathcal{L}(\theta) = \log \mathcal{L}(\hat{\theta}) + \left[\frac{\partial \log \mathcal{L}}{\partial \theta}\right]_{\theta=\hat{\theta}} (\theta - \hat{\theta}) + \frac{1}{2}\left[\frac{\partial^2 \log \mathcal{L}}{\partial \theta^2}\right]_{\theta=\hat{\theta}} (\theta - \hat{\theta})^2 + \dots$$

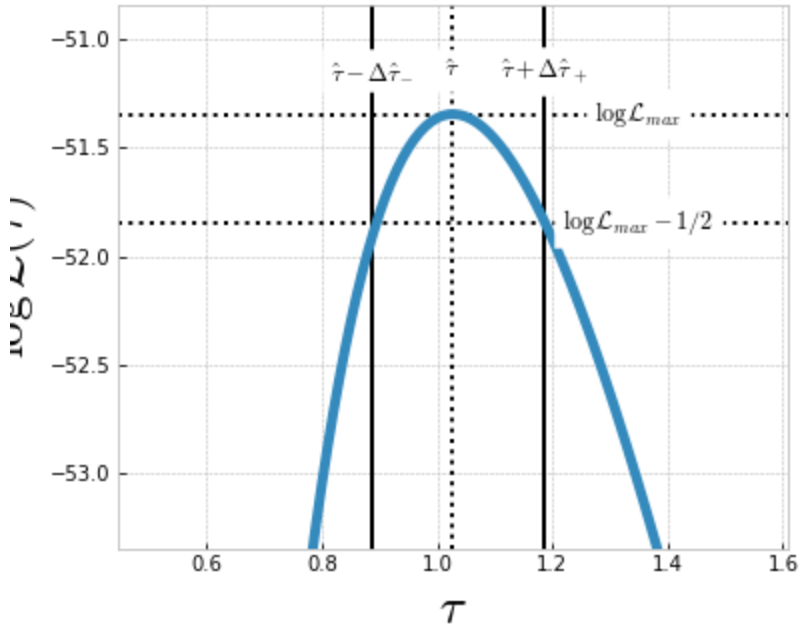
By definition $\log \mathcal{L}(\hat{\theta}) = \log \mathcal{L}_{max}$. Also the first derivative is 0, since it's evaluted at its maximum so:

$$\log \mathcal{L}(\theta) = \log \mathcal{L}_{max} - \frac{(\theta - \hat{\theta})^2}{2\widehat{\sigma^2_{\hat{\theta}}}}$$

or

$$\log \mathcal{L}(\theta \pm \widehat{\sigma_{\hat{\theta}}}) = \log \mathcal{L}_{max} - \frac{1}{2}$$

Variance of Estimators: The Graphic Method



In this case: $\Delta\hat{\tau}_+ = 0.16$ and $\Delta\hat{\tau}_- = 0.14 \rightarrow \hat{\sigma}_{\hat{\tau}} \approx 0.15$

Variance of Estimators: Gaussian approximation

The M.L. estimate, $\hat{\theta}$, depends on randomly distributed variables, $x_1, \ldots, x_n$, therefore it also a *random variable*. Since it depends on a large number of random variables, the **Central Limit Theorem** says that $\hat{\theta}$ should follow a gaussian distribution with the true, θ, as central value:

$$\mathcal{L}(\hat{\theta}) = \frac{1}{\sqrt{2\pi\sigma^2_{\hat{\theta}}}} e^{-\frac{1}{2}\frac{(\theta-\hat{\theta})^2}{\sigma^2_{\hat{\theta}}}}$$

or in $\log$:

$$\log \mathcal{L}(\hat{\theta}) = -\frac{1}{2}\frac{(\theta-\hat{\theta})^2}{\sigma^2_{\hat{\theta}}} - \frac{1}{2}\log(2\pi\sigma^2_{\hat{\theta}})$$

which is similar to the result we obteined with the Taylor expansion.

Variance of Estimators: Two correlated estimates

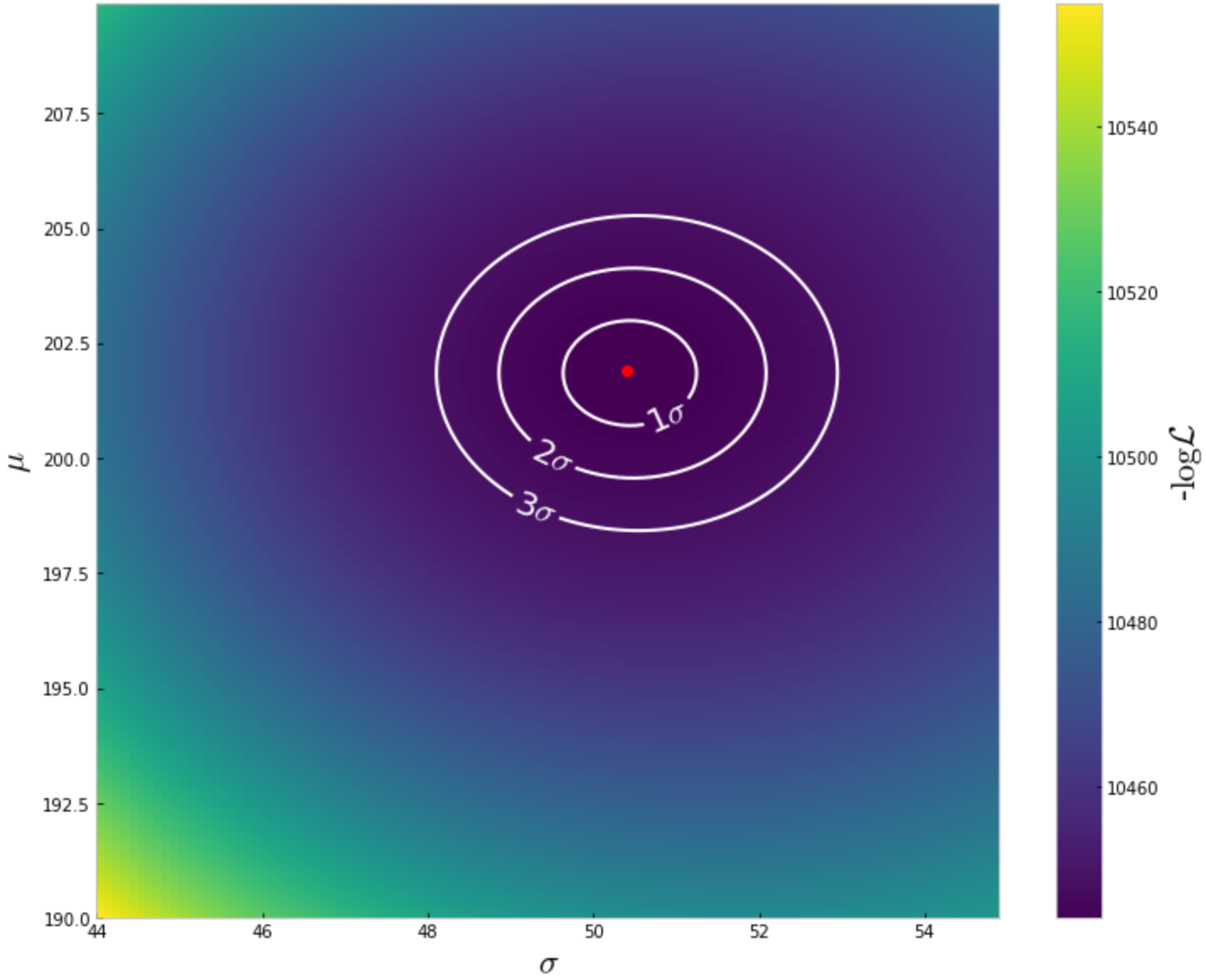
If we have different estimates, $\hat{\theta}_1, \hat{\theta}_2$ that are correlated. For large n, the likelihood takes the gaussian approximation:

$$\log \mathcal{L}(\hat{\theta}_1, \hat{\theta}_2) \approx \frac{1}{\sqrt{1-\rho^2}} \frac{1}{2\pi\sqrt{\sigma^2_{\hat{\theta}_1}\sigma^2_{\hat{\theta}_2}}} e^{-\frac{1}{2(1-\rho^2)}\frac{(\theta_1-\hat{\theta}_1)^2}{\sigma^2_{\hat{\theta}_1}}\frac{(\theta_2-\hat{\theta}_2)^2}{\sigma^2_{\hat{\theta}_2}} - 2\rho\frac{(\theta_1-\hat{\theta}_1)}{\sigma_{\hat{\theta}_1}}\frac{(\theta_2-\hat{\theta}_2)}{\sigma_{\hat{\theta}_1}}}$$

The $\log \mathcal{L}$ then takes a quadratic form near maximum which is a paraboloid centered at $\hat{\theta}_1, \hat{\theta}_2$ in the θ_1, θ_2 space.

Variance of Estimators: Two correlated estimates

The contour $\log \mathcal{L}(\hat{\theta}_1, \hat{\theta}_2) = \log \mathcal{L}_{max} - 1/2$ is an ellipse:



Variance of Estimators: Two correlated estimates

The angle of the ellipse, ϕ is given by:

$$\tan 2\phi = \frac{2\rho\hat{\sigma}_{\theta_1}\hat{\sigma}_{\theta_2}}{\hat{\sigma}^2_{\theta_1} - \hat{\sigma}^2_{\theta_1}}$$

Correlations between estimators result in an increase of their standard deviations.

Extended Maximum Likelihood Method

Sometimes the total number of events in a sample is a fixed number, sometimes, n is also a random variable.

> Example 1: For the muon life time, you can decide to run you experiment until you always get n number of triggers, since you only care about the Δt.
> Example 2: You look for a rare physics event (like a desintegration) and you measure the number of events n in fixed time window.

Extended Maximum Likelihood Method

In this cases, n will be often a Poisson random variable with mean ν. The results of an experiment will be: n, x_1, ... x_n.

The extended likelihood is defined as:

$$\mathcal{L}(n, \vec{\theta}) = \frac{\nu^n}{n!} e^{-\nu} \prod_{i=1}^{n} f(x_i; \vec{\theta})$$

We have now 2 options:

1. The expected number of events denpends on the unknown parameters $\vec{\theta}$, i.e. $\nu = \nu(\vec{\theta})$.
2. The two, ν and $\vec{\theta}$ are independent.

Extended Maximum Likelihood Method

Suppose theory gived $\nu = \nu(\vec{\theta})$ then the log-likelihood can be written as:

$$\log \mathcal{L}(\vec{\theta}) = -\nu(\vec{\theta}) + \sum_{i=1}^{n} \log(\nu(\vec{\theta}) f(x_i; \vec{\theta})) + C$$

> Example: A process where the number of events depends on the cross-section $\sigma(\vec{\theta})$ predicted as function of the parameters of the theory, $\vec{\theta}$ that also dictate the shape of the distribution of events x_i.

Extended Maximum Likelihood Method

In case ν and $\vec{\theta}$ are independent we can find the estimator $\hat{\vec{\theta}}$ by maximizing ($\partial / \partial \vec{\theta}$):

$$\log \mathcal{L}(\vec{\theta}) = n \log \nu - \nu + \sum_{i=1}^{n} \log f(x_i; \vec{\theta}) + C$$

likewhise the estimator $\hat{\nu}$ can be find by maximizing over ν:

$$\frac{\partial \log \mathcal{L}(\vec{\theta})}{\partial \nu} = 0 = \frac{n}{\nu} - 1 \rightarrow \hat{\nu} = n$$

Extended Maximum Likelihood: Example

Let's assume a sample mixed with two types of events, a signal that follows a known distribution $f_s(x)$ and background events distributed as $f_b(x)$. We defined:

- signal fraction $= \theta$.
- expected number of events $= \nu$.
- observed number of events $= n$.
- expected number of signal events $\mu_s = \theta\nu$
- expected number of background events $\mu_b = (1-\theta)\nu$

The goal is to estimate μ_s and μ_b. The overall dsitribution of events can be defined as:

$$f(x;\mu_s,\mu_b) = \frac{\mu_s}{\mu_s+\mu_b} f_s(x) + \frac{\mu_b}{\mu_s+\mu_b} f_b(x)$$

Extended Maximum Likelihood: Example

The observed number of events will follow a Poisson distribution as:

$$P(n;\mu_s\mu_b) = \frac{(\mu_s+\mu_b)^n}{n!}e^{-(\mu_s+\mu_b)}$$

The likelihood can be written as:

$$\log\mathcal{L}(\mu_s,\mu_b) = -(\mu_s+\mu_b) + \sum_{i=1}^{n}\log[(\mu_s+\mu_b)f(x_i;\mu_s,\mu_b)]$$

which becomes:

$$\log\mathcal{L}(\mu_s,\mu_b) = -(\mu_s+\mu_b) + \sum_{i=1}^{n}\log[\mu_s f_s(x_i)+\mu_b f_b(x_i)]$$

Extended Maximum Likelihood: Example

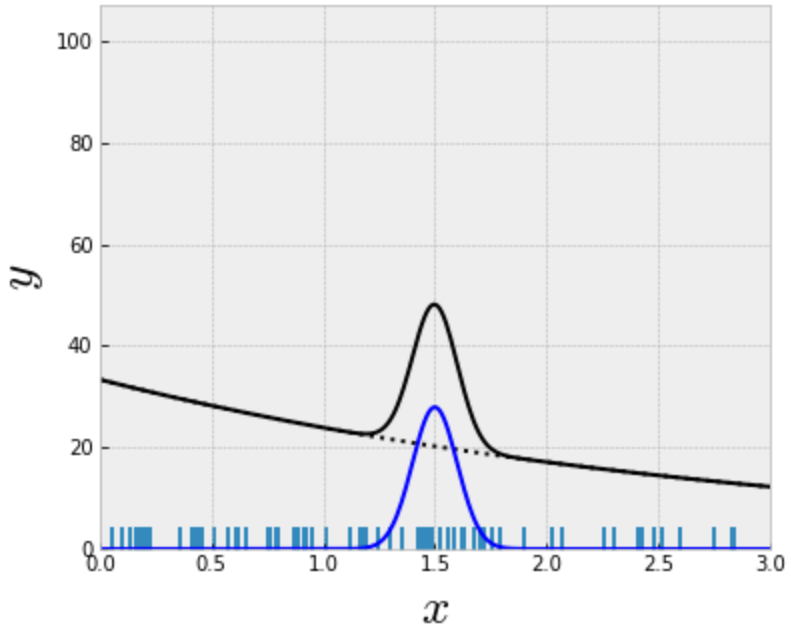
Let's generate a sample of with defined distributions for background and signal

```
tau = 3
bg_events = 100
background = np.random.exponential(tau, bg_events)
sig_events = 7
mu = 1.5
sigma = 0.1
signal = np.random.normal(mu, sigma, sig_events)

ntotal = bg_events + sig_events

from argparse import Namespace

truth = Namespace(mu_s = sig_events, mu_b = bg_events)

print (truth)
```

We have a true values $\mu_s = 7$ and $\mu_b = 100$.

Extended Maximum Likelihood: Example

We can plot the sample and the distributions as:



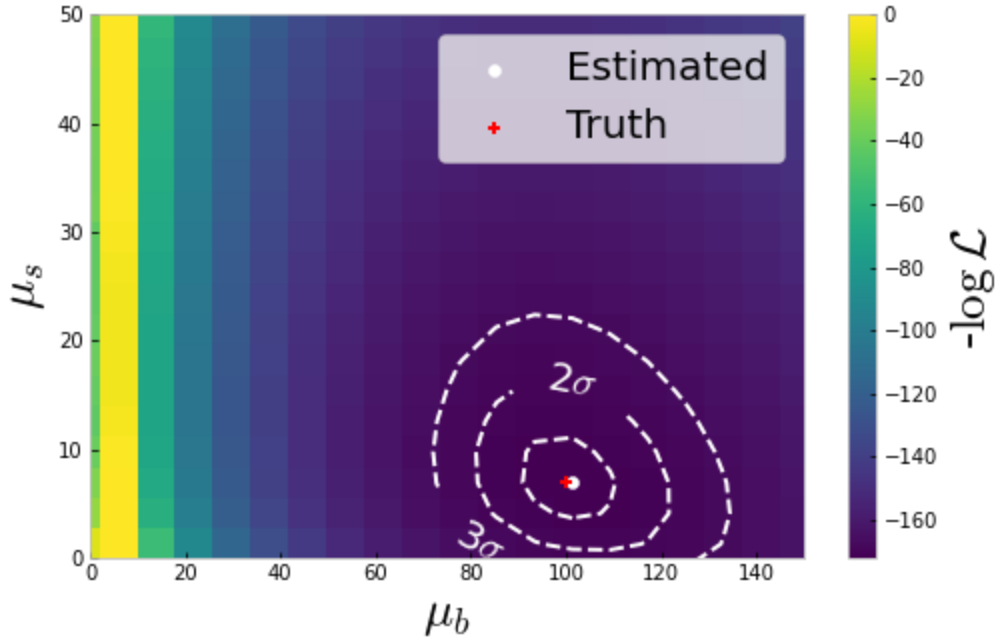
Extended Maximum Likelihood: Example

We can now define the $-\log \mathcal{L}$ and find its minima:

```
def likelihood(mu_s, mu_b):
    values = np.log(mu_s * norm(mu, sigma).pdf(sample) + mu_b * expon(0, tau).pdf(sample))
    return (mu_s + mu_b) - np.sum(values)
```

Extended Maximum Likelihood: Example

For one specific MC sample we find the best estimates:



$\hat{\mu}_s = 6.9, \hat{\mu}_b = 101.3$ with errors given by the countours.

Extended Maximum Likelihood: Example

- Sometimes a downgoing fluctuation of the background in the signal region can result in a *negative* signal estimate $\hat{\mu}_s$.
- We can let that happen as long as the total *pdf* $f(x; \hat{\mu}_s, \hat{\mu}_b) > 0$, i.e. remains positive everywhere.

Binned Maximum Likelihood

- When data is large, using the individual events might be very CPU consuming. In this case it is better to use histrograms.
- The number if events in the bin-i based on the unknown parameters, $\vec{\theta}$ is:

$$\nu(\vec{\theta})_i = n_{tot} \int_{x^i_{min}}^{x^i_{max}} f(x;\vec{\theta}) \mathrm{d}x$$

  where x^i_{min}, x^i_{max} are the limits of the bin.
- So we have a vector $\vec{\nu} = (\nu_1, \ldots \nu_N)$ of N bins of expected values per fin, plus a vector $\vec{n} = (n_1, \ldots n_N)$ of measured content per bin

Binned Maximum Likelihood II

- We can model data as a multinominal distribution:

$$f(\vec{n}, \vec{\nu}) = \frac{n_{tot}!}{n_1! \dots n_N!} \left(\frac{\nu_1}{n_{tot}} \right)^{n_1} \dots \left(\frac{\nu_N}{n_{tot}} \right)^{n_N}$$

- where the probability of falling in a bin is given by ν_i / n_{tot}.
- The log-likelihood is given by:

$$\log \mathcal{L}(\vec{\theta}) = \sum_{i=1}^{N} n_i \log \nu_i(\vec{\theta}) + C$$