# Statistical analysis of experimental data Variable distributions 

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Lecture 11
December 21, 2023

## Statistical analysis of experimental data

## Variable distributions

(1) Variable distributions
(2) Normalization of the distribution
(3) Unbinned likelihood
(4) Hypothesis Testing
(5) Homework

## Non-linear fit procedure

## Iterative procedure

We start from some "initial guess" of parameter values $\mathbf{a}_{\mathbf{0}}$.
Assuming small variations of the model parameters, $\mathbf{a}=\mathbf{a}_{\mathbf{0}}+\delta \mathbf{a}$, we can expand $\chi^{2}$ in a series:

$$
\chi^{2}(\mathbf{a})=\chi^{2}\left(\mathbf{a}_{\mathbf{0}}\right)-2 \mathbf{b} \cdot\left(\mathbf{a}-\mathbf{a}_{0}\right)+\ldots
$$

where $\mathbf{b}$ is the negative gradient of $\chi^{2}$ :

$$
\mathbf{b}=-\frac{1}{2} \nabla \chi^{2}\left(\mathbf{a}_{\mathbf{0}}\right) \quad b_{j}=-\frac{1}{2} \frac{\partial \chi^{2}}{\partial a_{j}}=\sum_{i=1}^{N} \frac{y_{i}-\mu_{i}}{\sigma_{i}^{2}} \cdot \frac{\partial \mu_{i}}{\partial a_{j}}
$$

Vector $\mathbf{b}$ defines the direction of steepest $\chi^{2}$ descent.
One of the possible procedures is to make a step in this direction:

$$
\mathbf{a}_{1}=\mathbf{a}_{0}+\varepsilon \mathbf{b}
$$

with small $\varepsilon>0$ and then repeat the whole procedure...

## Non-linear fit procedure

## Iterative procedure

We can try to be "smarter". Expanding $\chi^{2}$ to quadratic term:

$$
\chi^{2}(\mathbf{a})=\chi^{2}\left(\mathbf{a}_{0}\right)-2 \mathbf{b} \cdot\left(\mathbf{a}-\mathbf{a}_{0}\right)+\left(\mathbf{a}-\mathbf{a}_{0}\right)^{\top} \mathbb{A}\left(\mathbf{a}-\mathbf{a}_{0}\right)+\ldots
$$

where $\mathbb{A}$ is the so called Hessian matrix of second derivatives:

$$
\mathbb{A}_{j k}=\left.\frac{1}{2} \frac{\partial^{2} \chi^{2}}{\partial a_{j} \partial a_{k}}\right|_{\mathbf{a}=\mathbf{a}_{0}} \approx \sum_{i=1}^{N} \frac{1}{\sigma_{i}^{2}} \cdot \frac{\partial \mu_{i}}{\partial a_{j}} \cdot \frac{\partial \mu_{i}}{\partial a_{k}} \quad\left(\text { neglecting } \frac{\partial^{2} \mu_{i}}{\partial a_{j} \partial a_{k}}\right)
$$

In this approximation, we can calculate the expected position of the $\chi^{2}$ minimum:

$$
\begin{aligned}
\nabla \chi^{2}(\mathbf{a}) & =-2 \mathbf{b}+2 \mathbb{A}\left(\mathbf{a}-\mathbf{a}_{\mathbf{0}}\right)=0 \\
& \Rightarrow \mathbf{a}_{1}=\mathbf{a}_{0}+\mathbb{A}^{-1} \mathbf{b}
\end{aligned}
$$

and we can try to "jump" directly to the minimum...

## Non-linear fit procedure

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& \Rightarrow \mathbf{a}_{\mathbf{1}}=\mathbf{a}_{\mathbf{0}}+(\mathbb{A}+\lambda \cdot \mathbb{I})^{-1} \mathbf{b}
\end{aligned}
$$

or interpolate between "safe" and "fast" approach...

## Constrained fit

## Method of Lagrange Multipliers

The method, invented by J.L.Lagrange in 1788, applies to general minimization problem with additional constraints imposed.

Problem of finding minimum of $\chi^{2}(\mathbf{a})$ with constraints $w_{k}(\mathbf{a})=0$ is equivalent to finding a stationary point (point with all first derivatives at zero) of the Lagrange function:

$$
\mathcal{L}(\mathbf{a}, \boldsymbol{\lambda})=\chi^{2}(\mathbf{a})+\sum_{k} 2 \lambda_{k} w_{k}(\mathbf{a})
$$

where we introduce additional $K$ parameters $\lambda_{k}$ - Lagrange multipliers
Our problem is now reduced to finding parameters a and $\boldsymbol{\lambda}$ fulfilling

$$
\frac{\partial \mathcal{L}}{\partial a_{j}}=0 \quad \text { and } \quad \frac{\partial \mathcal{L}}{\partial \lambda_{k}}=0
$$

(without any additional constraints)

## Constrained fit

## Method of Lagrange Multipliers

We can write these equations the matrix form:

$$
\begin{gathered}
\left(\begin{array}{c|c}
\mathbb{A}^{2} & \mathbb{D} \\
\hline \mathbb{D}^{\top} & 0
\end{array}\right) \cdot\binom{\mathbf{a}}{\overline{\boldsymbol{\lambda}}}=\binom{\mathbf{b}}{\overline{\mathbf{c}}} \\
\text { where: } \mathbb{A}_{j k}=\sum_{i=1}^{N} \frac{f_{j}\left(x_{i}\right) f_{k}\left(x_{i}\right)}{\sigma_{i}^{2}}, \mathbb{D}_{j k}=d_{k, j} \quad \text { and } \quad b_{j}=\sum_{i=1}^{N} \frac{f_{j}\left(x_{i}\right) y_{i}}{\sigma_{i}^{2}}
\end{gathered}
$$ and the problem can be solved by inverting matrix $\tilde{\mathbb{A}}$.

Covariance matrix for a can be extracted as:
(seems to work for linear problems)

$$
\left(\mathbb{C}_{\mathbf{a}}\right)_{i j}=\left(\tilde{\mathbb{A}}^{-1}\right)_{i j} \quad i, j=1 \ldots M
$$

## Including systematic effects

## General procedure

General procedure for including systematic uncertainties in the analysis is to consider corresponding systematic shifts as additional model parameters

$$
\begin{aligned}
\mu_{i} & =\mu\left(x_{i} ; \mathbf{a}, \mathbf{s}\right)=\mu\left(x_{i} ; \mathbf{a}^{\prime}\right) \\
\chi^{2}(\mathbf{a}, \mathbf{s}) & =\sum_{i=1}^{N} \frac{\left(y_{i}-\mu\left(x_{i}, \mathbf{a}, \mathbf{s}\right)\right)^{2}}{\sigma_{i}^{2}}+\sum_{k=1}^{K} \frac{\left(s_{k}-s_{0, k}\right)^{2}}{\sigma_{s_{k}}^{2}} \\
\chi^{2}\left(\mathbf{a}^{\prime}\right) & =\sum_{i=1}^{N} \frac{\left(y_{i}-\mu\left(x_{i}, \mathbf{a}^{\prime}\right)\right)^{2}}{\sigma_{i}^{2}}+\sum_{k=1}^{K} \delta_{k}^{2} \quad \delta_{k}=\frac{s_{k}-s_{0, k}}{\sigma_{s_{k}}}
\end{aligned}
$$

If systematic parameters are not independent (are correlated)

$$
\chi^{2}\left(\mathbf{a}^{\prime}\right)=\sum_{i=1}^{N} \frac{\left(y_{i}-\mu\left(x_{i}, \mathbf{a}^{\prime}\right)\right)^{2}}{\sigma_{i}^{2}}+\sum_{k, j}\left(s_{k}-s_{0, k}\right)\left(s_{j}-s_{0, j}\right)\left(\mathbb{C}_{\mathbf{s}}\right)_{j, k}^{-1}
$$

## Including systematic effects

## General procedure

$\chi^{2}$ minimization procedure is basically unchanged, only the additional terms (systematic constrains) need to be included in calculations (as for the parameter constraints).
Negative gradient of $\chi^{2} \quad$ uncorrelated systematics

$$
b_{j}=-\frac{1}{2} \frac{\partial \chi^{2}}{\partial a_{j}^{\prime}}=\sum_{i=1}^{N} \frac{y_{i}-\mu_{i}}{\sigma_{i}^{2}} \cdot \frac{\partial \mu_{i}}{\partial a_{j}^{\prime}}-\frac{s_{j}-s_{0, j}}{\sigma_{s_{j}}^{2}}
$$

Hessian matrix of second derivatives:

$$
\mathbb{A}_{j k}=\frac{1}{2} \frac{\partial^{2} \chi^{2}}{\partial a_{j}^{\prime} \partial a_{k}^{\prime}}=\sum_{i=1}^{N} \frac{1}{\sigma_{i}^{2}} \cdot \frac{\partial \mu_{i}}{\partial a_{j}^{\prime}} \cdot \frac{\partial \mu_{i}}{\partial a_{k}^{\prime}}+\frac{\delta_{j k}}{\sigma_{s_{k}}^{2}}
$$

where systematic shifts $\mathbf{s}$ are assumed to go first in a' (for proper indexing)

## Including systematic effects

## General procedure

$\chi^{2}$ minimization procedure is basically unchanged, only the additional terms (systematic constrains) need to be included in calculations (as for the parameter constraints).
Negative gradient of $\chi^{2} \quad$ general case

$$
b_{j}=-\frac{1}{2} \frac{\partial \chi^{2}}{\partial a_{j}^{\prime}}=\sum_{i=1}^{N} \frac{y_{i}-\mu_{i}}{\sigma_{i}^{2}} \cdot \frac{\partial \mu_{i}}{\partial a_{j}^{\prime}}-\sum_{k}\left(s_{k}-s_{0, k}\right)\left(\mathbb{C}_{\mathbf{s}}\right)_{j, k}^{-1}
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Hessian matrix of second derivatives:

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$$

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## Statistical analysis of experimental data

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## Variable distributions

## Problem

So far, we have considered sets of independent measurements of a random variable $Y$, which could depend on some controlled variable $X$ (and a number of model parameters a), assuming measurement fluctuations are described by Gaussian pdf.


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## Variable distributions

## Problem

However, the problem frequently met (in high energy physics experiments in particular) is that we want to extract model parameters not from the fit of $Y(X)$ dependence, but just from the distribution of the measured $X$ values. Results are often presented in a form of a histogram:


Example simulation of P3 experiment results (Advanced Physics Laboratory)

## Variable distributions

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Example simulation of P3 experiment results (Advanced Physics Laboratory)

## Variable distributions

## Problem

We can consider number of events in each bin of the histogram, $n_{i}$, as an independent measurement depending on the controlled variable $x_{i}$. The only problem we have, to use the $\chi^{2}$ minimization procedure, is to attribute measurement uncertainties to measured numbers of events.

Simple guess: assume $\sigma_{n_{i}}=\sqrt{n_{i}}$ works very well for large $n_{i}$


## Variable distributions

## Problem

We can consider number of events in each bin of the histogram, $n_{i}$, as an independent measurement depending on the controlled variable $x_{i}$. The only problem we have, to use the $\chi^{2}$ minimization procedure, is to attribute measurement uncertainties to measured numbers of events.

Simple guess: assume $\sigma_{n_{i}}=\sqrt{n_{i}}$ results become biased when $n_{i}$ small, problem with $n_{i}=0$


## Variable distributions

## Least-squares fit

Considered approach was proposed by K.Pearson in 1900:

$$
\chi^{2}=\sum_{i=1}^{N_{b i n}} \frac{\left(n_{i}-\mu_{i}\right)^{2}}{n_{i}}
$$

when we use the property of the Poisson distribution $\mathbb{V}\left(n_{i}\right)=\mathbb{E}\left(n_{i}\right)=\mu_{i}$

## Variable distributions

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$$

when we use the property of the Poisson distribution $\mathbb{V}\left(n_{i}\right)=\mathbb{E}\left(n_{i}\right)=\mu_{i}$ Unfortunately, the result of the minimization turns out to be biased!
Let us assume that the model expectations can be presented as

$$
\mu_{i}=N f_{i}
$$

where $f_{i}$ represents the probability density (properly normalized)
From minimization condition, $\frac{\partial \chi^{2}}{\partial \mathrm{a}}=0$, biased estimate of $N$ is obtained:

$$
\hat{N}=N-\chi_{\min }^{2}
$$

## Variable distributions

## Example

It can be easily demonstrated for the flat distribution

$$
\mu_{i} \equiv \mu \Rightarrow \chi^{2}=\sum_{i=1}^{N_{b i n}} \frac{\left(n_{i}-\mu\right)^{2}}{n_{i}}=\sum_{i=1}^{N_{b i n}}\left(n_{i}-2 \mu+\frac{\mu^{2}}{n_{i}}\right)
$$

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$$

we then obtain:

$$
0=\frac{\partial \chi^{2}}{\partial \mu}=-2 N_{b i n}+2 \mu \sum_{i=1}^{N_{b i n}} \frac{1}{n_{i}}
$$

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we then obtain:

$$
\begin{aligned}
0 & =\frac{\partial \chi^{2}}{\partial \mu}=-2 N_{b i n}+2 \mu \sum_{i=1}^{N_{b i n}} \frac{1}{n_{i}} \\
& \Rightarrow \hat{\mu}=\left(\frac{1}{N_{b i n}} \sum_{i=1}^{N_{b i n}} \frac{1}{n_{i}}\right)^{-1}
\end{aligned}
$$

which is harmonic mean of $n_{i}$ ( not equal to the expected arithmetic mean)

## Variable distributions

## Least-squares fit

Alternative approach was proposed by J.Neyman in 1949:

$$
\chi^{2}=\sum_{i=1}^{N_{b i n}} \frac{\left(n_{i}-\mu_{i}\right)^{2}}{\mu_{i}}
$$

when we try to use "true" uncertainty in the denominator...

## Variable distributions

## Least-squares fit

Alternative approach was proposed by J.Neyman in 1949:

$$
\chi^{2}=\sum_{i=1}^{N_{b i n}} \frac{\left(n_{i}-\mu_{i}\right)^{2}}{\mu_{i}}
$$

when we try to use "true" uncertainty in the denominator...
Unfortunately, this approach also turns out to be biased!
Higher $\mu_{i}$ values are "preferred", as they result in smaller $\chi^{2}$ contribution (for given difference).
Estimate of $N$ obtained from minimization condition, $\frac{\partial \chi^{2}}{\partial \mathbf{a}}=0$ :

$$
\hat{N}=N+\frac{1}{2} \chi_{\min }^{2}
$$

## Variable distributions

## Example

Let as consider flat probability distribution again

$$
\mu_{i} \equiv \mu \Rightarrow \chi^{2}=\sum_{i=1}^{N_{\text {bin }}} \frac{\left(n_{i}-\mu\right)^{2}}{\mu}=\sum_{i=1}^{N_{\text {bin }}}\left(\frac{n_{i}^{2}}{\mu}-2 n_{i}+\mu\right)
$$

## Variable distributions

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$$

we then obtain:

$$
0=\frac{\partial \chi^{2}}{\partial \mu}=-\sum_{i=1}^{N_{b i n}} \frac{n_{i}^{2}}{\mu^{2}}+N_{b i n}
$$

## Variable distributions

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0 & =\frac{\partial \chi^{2}}{\partial \mu}=-\sum_{i=1}^{N_{b i n}} \frac{n_{i}^{2}}{\mu^{2}}+N_{b i n} \\
& \Rightarrow \quad \hat{\mu}^{2}
\end{aligned}=\frac{1}{N_{b i n}} \sum_{i=1}^{N_{b i n}} n_{i}^{2}, ~ l
$$

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$$
\begin{aligned}
& 0=\frac{\partial \chi^{2}}{\partial \mu}=-\sum_{i=1}^{N_{b i n}} \frac{n_{i}^{2}}{\mu^{2}}+N_{b i n} \\
& \Rightarrow \quad \hat{\mu}^{2}=\frac{1}{N_{b i n}} \sum_{i=1}^{N_{b i n}} n_{i}^{2} \\
& \left\langle\hat{\mu}^{2}\right\rangle=\left\langle n^{2}\right\rangle=\langle n\rangle^{2}+\left\langle(n-\langle n\rangle)^{2}\right\rangle=\mu^{2}+\mu
\end{aligned}
$$

which shows that the method results in biased (too high) value of $\hat{\mu}$

## Variable distributions

## Maximum Likelihood

The $\chi^{2}$ method, while giving (almost) correct results for large $n_{i}$ is clearly not suitable to fit variable distributions when $n_{i}$ can be small.

Solution is to use general Maximum Likelihood Method, look for parameter values for which the likelihood function has a (global) maximum.

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Solution is to use general Maximum Likelihood Method, look for parameter values for which the likelihood function has a (global) maximum.

We have $N_{b i n}$ independent measurements and each is described by the Poisson probability distribution. So the likelihood function is:

$$
L=\prod_{i=1}^{N_{\text {bin }}} P\left(n_{i} ; \mu_{i}\right)=\prod_{i=1}^{N_{\text {bin }}} \frac{\mu_{i}^{n_{i}} e^{-\mu_{i}}}{n!}
$$

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$$

Log-likelihood:

$$
\ell=\sum\left(n_{i} \ln \mu_{i}-\mu_{i}\right)-\sum \ln n_{i}!
$$

were the last term can be neglected in minimization (constant)

## Variable distributions

## Example

For our example of flat distribution, $\mu_{i} \equiv \mu$

$$
\begin{aligned}
L & =\prod_{i=1}^{N_{b_{b} n}} \frac{\mu^{n_{i}} e^{-\mu}}{n!} \\
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\ell & =\ln \mu \sum n_{i}-N \mu-\sum \ln n! \\
\frac{\partial \ell}{\partial \mu} & =\frac{1}{\mu} \sum n_{i}-N=0 \\
\Rightarrow \mu & =\frac{1}{N} \sum n_{i}
\end{aligned}
$$

we obtain an unbiased estimate of the expected value.

## Variable distributions

## Maximum Likelihood fit

In the Maximum Likelihood approach, we can use all methods introduced for $\chi^{2}$ minimization, one only needs to make substitution

$$
\chi^{2}(\mathbf{x} ; \mathbf{a}) \quad \longrightarrow \quad-2 \ell(\mathbf{x} ; \mathbf{a})
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In the general fit approach:

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\mathbf{b}=-\frac{1}{2} \nabla \chi^{2}(\mathbf{a}) \quad \longrightarrow \quad \mathbf{b}=\nabla \ell(\mathbf{a}) \quad \text { or } \quad b_{j}=\frac{\partial \ell}{\partial a_{j}}
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\end{array}
$$

These derivatives can be directly calculated for the Poisson distribution:

$$
b_{j}=\sum_{i=1}^{N_{b i n}}\left(\frac{n_{i}}{\mu_{i}}-1\right) \frac{\partial \mu_{i}}{\partial a_{j}} \quad \text { and } \quad \mathbb{A}_{j k}=\sum_{i=1}^{N_{b i n}} \frac{n_{i}}{\mu_{i}^{2}} \frac{\partial \mu_{i}}{\partial a_{j}} \frac{\partial \mu_{i}}{\partial a_{k}}
$$

## Variable distributions

## Maximum Likelihood fit example

Iterative $\chi^{2}$ fit, using (modified) Pearson approach $\left(\sigma_{n_{i}}=\sqrt{n_{i}+1}\right)$


## Variable distributions

## Maximum Likelihood fit example

Iterative Maximum Log-Likelihood fit

$\mathrm{N}=10000$
Higher background level estimate in likelihood fit (underestimated in $\chi^{2}$ fit)

## Variable distributions

## Maximum Likelihood fit example

Iterative $\chi^{2}$ fit, using (modified) Pearson approach $\left(\sigma_{n_{i}}=\sqrt{n_{i}+1}\right)$


## Variable distributions

## Maximum Likelihood fit example

Iterative Maximum Log-Likelihood fit


Difference between two methods becomes significant for small $n_{i}$

## Variable distributions

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Iterative $\chi^{2}$ fit, using (modified) Pearson approach $\left(\sigma_{n_{i}}=\sqrt{n_{i}+1}\right)$


Difference between two methods becomes significant for small $n_{i}$

## Variable distributions

## Maximum Likelihood fit example

Iterative Maximum Log-Likelihood fit

$\mathrm{N}=100$
Difference between two methods becomes significant for small $n_{i}$

## Statistical analysis of experimental data

Variable distributions

(1) Variable distributions
(2) Normalization of the distribution
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## Normalization of the distribution

## Free normalization

It is quite often the case that normalization of our data sample (total number of registered events) is one of the (unknown) parameters of our model. We can then present model expectations as

$$
\mu_{i}\left(\mathbf{a}^{\prime}\right)=A f_{i}(\mathbf{a})
$$

where $f_{i}(\mathbf{a})$ is the probability density depending on model parameters a

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where $f_{i}(\mathbf{a})$ is the probability density depending on model parameters a
We can try to maximize log-likelihood with respect to $A$ :

$$
\ell=\sum\left(n_{i} \ln A+n_{i} \ln f_{i}-A f_{i}\right)-\sum \ln n_{i}!
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$$

where $f_{i}(\mathbf{a})$ is the probability density depending on model parameters a
We can try to maximize log-likelihood with respect to $A$ :

$$
\begin{aligned}
\ell & =\sum\left(n_{i} \ln A+n_{i} \ln f_{i}-A f_{i}\right)-\sum \ln n_{i}! \\
\frac{\partial \ell}{\partial A} & =\sum\left(\frac{n_{i}}{A}-f_{i}\right) \Rightarrow A=\frac{\sum n_{i}}{\sum f_{i}}
\end{aligned}
$$

which corresponds to the normalization condition: $\sum \mu_{i}=\sum n_{i}$

## Normalization of the distribution

## Normalization fit

If we do not care for normalization (and its uncertainty) and only want to consider shape of the distribution, we can reduce number of model parameters by including normalization condition in the definition of the model function:

$$
\mu_{i}(\mathbf{a})=\frac{\sum_{j=1}^{N_{b i n}} n_{j}}{\sum_{k=1}^{N_{b i n}} f_{k}} f_{i}(\mathbf{a})
$$

## Normalization of the distribution

## Normalization fit

If we do not care for normalization (and its uncertainty) and only want to consider shape of the distribution, we can reduce number of model parameters by including normalization condition in the definition of the model function:

$$
\mu_{i}(\mathbf{a})=\frac{\sum_{j=1}^{N_{\text {bin }}} n_{j}}{\sum_{k=1}^{N_{b i n}} f_{k}} f_{i}(\mathbf{a})
$$

If normalization is not correlated with other model parameters, derivatives of the normalization term can be neglected in the fit. If there are correlations, uncertainties on model parameters can be underestimated...

## Normalization of the distribution

## Normalization fit example

Example of the likelihood fit including normalization condition


Results agree perfectly with the previous fit (with normalization as parameter)

## Normalization of the distribution

## Normalization constrain

It can also be the case that the normalization of data is known from theory or independent measurement (eg. luminosity). Let us assume it is known with relative uncertainty $\Delta$. We can write the log-likelihood as:

$$
\ell=\sum\left(n_{i} \ln s+n_{i} \ln \mu_{i}-s \mu_{i}\right)-\frac{1}{2} \frac{(s-1)^{2}}{\Delta^{2}}
$$

where $s$ is the factor scaling the nominal model expectations $\left(s_{0}=1\right)$

## Normalization of the distribution

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$$

where $s$ is the factor scaling the nominal model expectations $\left(s_{0}=1\right)$
We could use general approach to systematic effects, as described before. However, in case of the normalization systematics, the problem factorizes. We can extract $s$ from derivative:

$$
\frac{\partial \ell}{\partial s}=\frac{1}{s} \sum n_{i}-\sum \mu_{i}-\frac{s-1}{\Delta^{2}}=0
$$

## Normalization of the distribution

## Normalization constrain

To simplify this formula, let us introduce normalization shift, $s=1+\delta$.

$$
\sum n_{i}-(1+\delta) \sum \mu_{i}-\delta(1+\delta) \frac{1}{\Delta^{2}}=0
$$

If we now assume that normalization variation is small, $\delta \ll 1, \delta^{2} \ll \delta$

$$
\sum n_{i}-\sum \mu_{i}=\delta\left(\sum \mu_{i}+\frac{1}{\Delta^{2}}\right)
$$

## Normalization of the distribution

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$$
\begin{aligned}
& \sum n_{i}-\sum \mu_{i}=\delta\left(\sum \mu_{i}+\frac{1}{\Delta^{2}}\right) \\
\delta= & \frac{\sum n_{i}-\sum \mu_{i}}{\sum \mu_{i}+\frac{1}{\Delta^{2}}}
\end{aligned}
$$

## Normalization of the distribution

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If we now assume that normalization variation is small, $\delta \ll 1, \delta^{2} \ll \delta$

$$
\begin{aligned}
& \sum n_{i}-\sum \mu_{i} \\
&=\delta\left(\sum \mu_{i}+\frac{1}{\Delta^{2}}\right) \\
& \delta=\frac{\sum n_{i}-\sum \mu_{i}}{\sum \mu_{i}+\frac{1}{\Delta^{2}}} \Rightarrow s=1+\delta=\frac{\sum n_{i}+\frac{1}{\Delta^{2}}}{\sum \mu_{i}+\frac{1}{\Delta^{2}}}
\end{aligned}
$$

This constraint can be included in the model definition as well!
For $\Delta \rightarrow 0$ normalization becomes fixed $(s \equiv 1)$
For $\Delta \rightarrow \infty$ we reproduce "free normalization" result...

## Normalization of the distribution

## Normalization constrain

Normalization constrain can also be considered in the $\chi^{2}$ minimization:

$$
\chi^{2}=\sum_{i=1}^{N_{\text {bin }}} \frac{\left(n_{i}-s \mu_{i}\right)^{2}}{\sigma_{n_{i}}^{2}}+\frac{(s-1)^{2}}{\Delta^{2}}
$$

## Normalization of the distribution

## Normalization constrain

Normalization constrain can also be considered in the $\chi^{2}$ minimization:

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\begin{aligned}
\chi^{2} & =\sum_{i=1}^{N_{\text {bin }}} \frac{\left(n_{i}-s \mu_{i}\right)^{2}}{\sigma_{n_{i}}^{2}}+\frac{(s-1)^{2}}{\Delta^{2}} \\
\frac{\partial \chi^{2}}{\partial s} & =2 s \sum \frac{\mu_{i}^{2}}{\sigma_{n_{i}}^{2}}-2 \sum \frac{n_{i} \mu_{i}}{\sigma_{n_{i}}^{2}}+\frac{2(s-1)}{\Delta^{2}}=0
\end{aligned}
$$

## Normalization of the distribution

## Normalization constrain

Normalization constrain can also be considered in the $\chi^{2}$ minimization:

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& s\left(\sum \frac{\mu_{i}^{2}}{\sigma_{n_{i}}^{2}}+\frac{1}{\Delta^{2}}\right)=\sum \frac{n_{i} \mu_{i}}{\sigma_{n_{i}}^{2}}+\frac{1}{\Delta^{2}}
\end{aligned}
$$

## Normalization of the distribution

## Normalization constrain

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$$
\begin{gathered}
\chi^{2}=\sum_{i=1}^{N_{b i n}} \frac{\left(n_{i}-s \mu_{i}\right)^{2}}{\sigma_{n_{i}}^{2}}+\frac{(s-1)^{2}}{\Delta^{2}} \\
\frac{\partial \chi^{2}}{\partial s}=2 s \sum \frac{\mu_{i}^{2}}{\sigma_{n_{i}}^{2}}-2 \sum \frac{n_{i} \mu_{i}}{\sigma_{n_{i}}^{2}}+\frac{2(s-1)}{\Delta^{2}}=0 \\
s\left(\sum \frac{\mu_{i}^{2}}{\sigma_{n_{i}}^{2}}+\frac{1}{\Delta^{2}}\right)=\sum \frac{n_{i} \mu_{i}}{\sigma_{n_{i}}^{2}}+\frac{1}{\Delta^{2}} \\
s=\frac{\sum \frac{n_{i} \mu_{i}}{\sigma_{n_{i}}^{2}}+\frac{1}{\Delta^{2}}}{\sum \frac{\mu_{i}^{2}}{\sigma_{n_{i}}^{2}}+\frac{1}{\Delta^{2}}}
\end{gathered}
$$

which reduces to the previous result, if we assume $\sigma_{n_{i}}^{2}=\mu_{i}$

## Statistical analysis of experimental data

Variable distributions

(1) Variable distributions
(2) Normalization of the distribution
(3) Unbinned likelihood
(4) Hypothesis Testing
(5) Homework

## Unbinned likelihood

## Problem

When defining parameters of the histogram, which will be used to extract parameters of the variable distribution, we have to be very careful!

Example histogram from P3 exercise (real data), time bin $\Delta t=84 \mathrm{~ns}$


## Unbinned likelihood

## Problem

When defining parameters of the histogram, which will be used to extract parameters of the variable distribution, we have to be very careful!

Example histogram from P3 exercise (real data), time bin $\Delta t=100 \mathrm{~ns}$


## Unbinned likelihood

## Unbinned likelihood

We do need the histogram to visualize our data. But we do not need it to extract parameters of the distribution. We can do it directly from the data.

Likelihood of our data set can be calculated from single events:

$$
\begin{aligned}
L & =\prod_{i=1}^{N} f\left(x_{i} ; \mathbf{a}\right) \\
\text { or } \quad \ell & =\sum_{i=1}^{N} \ln f\left(x_{i} ; \mathbf{a}\right)
\end{aligned}
$$

when the sum runs over all collected events.
We can then fit parameters by looking for maximum of (log-)likelihood...
We look at the shape of the distribution only (normalization fixed)!

## Unbinned likelihood

## Example

Very simple example is the decay time measurement.
Let us assume that we measured decay times, $t_{i}$, of N identical particles. We know the probability distribution function:

$$
f(t)=\frac{1}{\tau} e^{-\frac{t}{\tau}}
$$

where the mean lifetime, $\tau$, is the only parameter.
We can write the formula for log-likelihood

$$
\ell=\sum_{i=1}^{N} \ln f\left(t_{i} ; \tau\right)=\sum_{i=1}^{N}\left(-\ln \tau-\frac{t_{i}}{\tau}\right)
$$

## Unbinned likelihood

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\begin{aligned}
\ell & =\sum_{i=1}^{N} \ln f\left(t_{i} ; \tau\right) \\
\frac{\partial \ell}{\partial \tau}=-\frac{N}{\tau}+\frac{1}{\tau^{2}} \sum_{i=1}^{N} t_{i} & =0
\end{aligned}
$$

## Unbinned likelihood

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$$
\begin{aligned}
\ell=\sum_{i=1}^{N} \ln f\left(t_{i} ; \tau\right) & =\sum_{i=1}^{N}\left(-\ln \tau-\frac{t_{i}}{\tau}\right) \\
\frac{\partial \ell}{\partial \tau}=-\frac{N}{\tau}+\frac{1}{\tau^{2}} \sum_{i=1}^{N} t_{i} & =0 \quad \Rightarrow \quad \tau=\frac{1}{N} \sum_{i=1}^{N} t_{i}
\end{aligned}
$$

## Unbinned likelihood

## General case

As before, we can use all methods introduced for $\chi^{2}$ minimization with proper substitution

$$
\chi^{2}(\mathbf{x} ; \mathbf{a}) \quad \longrightarrow \quad-2 \ell(\mathbf{x} ; \mathbf{a})
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## Unbinned likelihood

## General case

As before, we can use all methods introduced for $\chi^{2}$ minimization with proper substitution

$$
\chi^{2}(\mathbf{x} ; \mathbf{a}) \quad \longrightarrow \quad-2 \ell(\mathbf{x} ; \mathbf{a})
$$

In the general unbinned log-likelihood fit:

$$
f_{i}=f\left(x_{i}\right)
$$

$$
\begin{aligned}
b_{j} & =\frac{\partial \ell}{\partial a_{j}}=\sum_{i=1}^{N} \frac{1}{f_{i}} \frac{\partial f_{i}}{\partial a_{j}} \\
\mathbb{A}_{j k} & =-\frac{\partial^{2} \ell}{\partial a_{j} \partial a_{k}}=\sum_{i=1}^{N} \frac{1}{f_{i}^{2}} \frac{\partial \mu_{i}}{\partial a_{j}} \frac{\partial \mu_{i}}{\partial a_{k}}
\end{aligned}
$$

## Variable distributions

## Unbinned likelihood fit example

Iterative binned log-likelihood fit for comparison

Binned LL fit Npar = 3 LL =224.99/17 $\quad \tau=\mathbf{2 . 0 3 9} \pm \mathbf{0 . 3 6 2}$

$N=100$

## Variable distributions

## Unbinned likelihood fit example

Iterative unbinned log-likelihood fit

$\mathrm{N}=100$
Higher precision of the lifetime estimate!

## Variable distributions

## Unbinned likelihood fit example

Iterative unbinned log-likelihood fit

$\mathrm{N}=100$
Higher precision of the lifetime estimate! More details "visible" ...

## Unbinned likelihood

## Extended Maximum Likelihood

"Standard" (unbinned) maximum likelihood fit is sensitive only to the shape of the probability distribution (normalized by definition).

However, we can extend the likelihood definition to take possible normalization fluctuations into account:

$$
L\left(x_{i} ; \mu, \mathbf{a}\right)=\frac{\mu^{N} e^{-\mu}}{N!} \prod_{i=1}^{N} f\left(x_{i} ; \mathbf{a}\right)
$$

where $\mu$ is the now the expected total number of observed events.

$$
\ell\left(x_{i} ; \mu, \mathbf{a}\right)=N \ln \mu-\mu+\sum_{i=1}^{N} \ln f\left(x_{i} ; \mathbf{a}\right)+\text { const }
$$

## Unbinned likelihood

## Extended Maximum Likelihood

When $\mu$ is independent of $\mathbf{a}$, maximum of the (extended) likelihood corresponds to

$$
\mu=N
$$

and we reproduce our previous result.

## Unbinned likelihood

## Extended Maximum Likelihood

When $\mu$ is independent of $\mathbf{a}$, maximum of the (extended) likelihood corresponds to

$$
\mu=N
$$

and we reproduce our previous result.
However, we need to use the extended approach, if the total expected number of events depends on the model parameters

$$
\mu \quad \rightarrow \mu(\mathbf{a})
$$

and so it is related to the shape of the distribution.
If this is the case, extended approach is also required to get a correct estimate of the parameter uncertainties.

## Statistical analysis of experimental data

Variable distributions

(1) Variable distributions
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## Hypothesis Testing

## Problem

So far, we focused on the problem of extracting model parameters from the collected data sample. We used maximum likelihood approach (or $\chi^{2}$ minimization, which is a special case).

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However, what we often want to do is to "make choice", discriminate between two (or more) hypothesis based on the collected data.

We already addressed this problem (partially) when discussing limits (lecture 07) and consistency of the fit (lecture 08).

## Hypothesis Testing

## Problem

So far, we focused on the problem of extracting model parameters from the collected data sample. We used maximum likelihood approach (or $\chi^{2}$ minimization, which is a special case).

However, what we often want to do is to "make choice", discriminate between two (or more) hypothesis based on the collected data.

We already addressed this problem (partially) when discussing limits (lecture 07) and consistency of the fit (lecture 08).

The general formulation of the problem:
how to discriminate between two model hypothesis $H_{0}$ and $H_{1}$ based on the collected data $D$ ?
Common case:
$H_{0}$ - Standard Model is valid, $H_{1}-\mathrm{SM}+$ additional BSM contribution
$D$ - the whole collected data sample, subset, or a single measurement

## Hypothesis Testing

## Example

We can consider measurement of $X$, where exponential decrease is expected in the SM and BSM signal is expected to be visible as a peak

Distribution of generated measurements


This is a case with very clear separation...

## Hypothesis Testing

## Example

We can consider measurement of $X$, where exponential decrease is expected in the SM and BSM signal is expected to be visible as a peak

Distribution of generated measurements


More difficult when the two distributions overlap

## Hypothesis Testing

## Example

We can consider measurement of $X$, where exponential decrease is expected in the SM and BSM signal is expected to be visible as a peak

Distribution of generated measurements


More difficult when the two distributions overlap and statistics is small...

## Hypothesis Testing

## Neyman-Pearson Lemma

According to Neymann and Pearson, the optimal, "most powerful" method to discriminate between the two hypothesis is to look at likelihood ratio

$$
Q(D)=\frac{L\left(D \mid H_{1}\right)}{L\left(D \mid H_{0}\right)}
$$

When considering single measurements, making a cut on $Q(x)$ is the optimal way to classify events. By using likelihood ratio, multi-dimensional measurements (whole events) are also presented as single number...

## Hypothesis Testing

## Neyman-Pearson Lemma

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When considering single measurements, making a cut on $Q(x)$ is the optimal way to classify events. By using likelihood ratio, multi-dimensional measurements (whole events) are also presented as single number...

When we consider the whole sample of collected data, value of $Q(D)$ is the best discriminant between the two hypothesis.

Still, one needs to compare the value of $Q(D)$ resulting from the measurement, with the expected $Q$ distributions for the two hypothesis.

## Hypothesis Testing

## $C L_{s}$ method

This method was introduced at the end of LEP running, when some hints for Higgs boson production were observed


## Hypothesis Testing

## $\mathrm{CL}_{\mathrm{s}}$ method

The two hypothesis we consider in this case:
$H_{0}$ - Standard Model without Higgs contribution - "background" only (b)
$H_{1}-\mathrm{SM}$ with Higgs contribution - "signal+background" (s+b) where we can consider different masses of the Higgs, $\mathrm{m}_{H}$

## Hypothesis Testing

## $\mathrm{CL}_{\mathrm{s}}$ method

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$H_{1}-\mathrm{SM}$ with Higgs contribution - "signal+background" (s+b) where we can consider different masses of the Higgs, $\mathrm{m}_{H}$

Instead of using $Q$, it is more convenient to use

$$
q=-2 \ln Q=-2 \ell\left(D \mid H_{1}\right)+2 \ell\left(D \mid H_{0}\right)=\chi^{2}\left(D \mid H_{1}\right)-\chi^{2}\left(D \mid H_{0}\right)
$$

where:

- positive $q$ values are expected for data looking more like background only $\left(H_{0}\right)$
- negative $q$ values indicate that data are better described by signal+background $\left(H_{1}\right)$


## Hypothesis Testing

## $\mathrm{CL}_{\mathrm{s}}$ method

Value of $q$ from LEP, $q_{d a t}$, was compared with distribution obtained with multiple Monte Carlo experiments for $m_{H}=115.6 \mathrm{GeV}$.


## Hypothesis Testing

## $C L_{s}$ method

Value of $q$ from LEP, $q_{d a t}$, was compared with distribution obtained with multiple Monte Carlo experiments for $m_{H}=115.6 \mathrm{GeV}$.


We can define

$$
C L_{s+b}=\int_{q_{d a t}}^{+\infty} d q f^{H 1}(q)
$$

$\Leftarrow$ indicated as blue area

## Hypothesis Testing

## $C L_{s}$ method

Value of $q$ from LEP, $q_{d a t}$, was compared with distribution obtained with multiple Monte Carlo experiments for $m_{H}=115.6 \mathrm{GeV}$.

$\Leftarrow$ indicated as red is $1-C L_{b}$
$\Leftarrow$ indicated as blue area and compare it with

$$
C L_{b}=\int_{q_{d a t}}^{+\infty} d q f^{H 0}(q)
$$

## Hypothesis Testing

## $\mathrm{CL}_{\mathrm{s}}$ method

Measured and expected $q$（for two hypothesis）as a function of the assumed Higgs mass．


Looks like we exclude $H_{0}$ up to mass $\sim 118 \mathrm{GeV}$（Frequentist 97．5\％CL）

## Hypothesis Testing

## $\mathrm{CL}_{\mathrm{s}}$ method

Measured and expected $q$ (for two hypothesis) as a function of the assumed Higgs mass.


Looks like we exclude $H_{0}$ up to mass $\sim 118 \mathrm{GeV}$ (Frequentist 97.5\%CL) But there is almost no difference between expectations for $H_{1}$ and $H_{0}$ ?!

## Hypothesis Testing

## $\mathrm{CL}_{\text {s }}$ method



With tight event selection, LEP experiments observed 4 candidate events with reconstructed mass, $m_{H}^{\text {rec }}>109 \mathrm{GeV}$.

## Hypothesis Testing

## $C L_{s}$ method

| $1-\alpha=90 \%$ |  |  | $1-\alpha=95 \%$ |  |
| ---: | :---: | ---: | :---: | ---: |
| $n$ | $\mu_{1}$ | $\mu_{2}$ | $\mu_{1}$ | $\mu_{2}$ |
| 0 | 0.00 | 2.44 | 0.00 | 3.09 |
| 1 | 0.11 | 4.36 | 0.05 | 5.14 |
| 2 | 0.53 | 5.91 | 0.36 | 6.72 |
| 3 | 1.10 | 7.42 | 0.82 | 8.25 |
| 4 | 1.47 | 8.60 | 1.37 | 9.76 |
| 5 | 1.84 | 9.99 | 1.84 | 11.26 |
| 6 | 2.21 | 11.47 | 2.21 | 12.75 |
| 7 | 3.56 | 12.53 | 2.58 | 13.81 |
| 8 | 3.96 | 13.99 | 2.94 | 15.29 |
| 9 | 4.36 | 15.30 | 4.36 | 16.77 |
| 10 | 5.50 | 16.50 | 4.75 | 17.82 |

With tight event selection，LEP experiments observed 4 candidate events with reconstructed mass，$m_{H}^{\text {rec }}>109 \mathrm{GeV}$ ．

Expectations of the background only hyposthesis，$b=1.2$ is below 95\％CL limit（both Cental and Unified，refer lecture 07）

Unified intervals（RPP）

## Hypothesis Testing

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Unified intervals (RPP)

With tight event selection, LEP experiments observed 4 candidate events with reconstructed mass, $m_{H}^{\text {rec }}>109 \mathrm{GeV}$.

Expectations of the background only hyposthesis, $b=1.2$ is below 95\% CL limit (both Cental and Unified, refer lecture 07)

Does it mean that we can exclude $H_{0}$ hypothesis (Standard Model predictions)?

All we can say is that
"probability of SM reproducing this data is below $5 \%$ "...

But we know that it can still be due to fluctuations...

## Hypothesis Testing

## $C L_{s}$ method

Experiments at LEP, running with energy up to $\sqrt{s}=210 \mathrm{GeV}$, could only observe Higgs bosons with mass of up to about 118 GeV (produced together with $Z$ boson: $e^{+} e^{-} \rightarrow Z H$ )

For higher masses, signal+background hypothesis $\left(H_{1}\right)$ becomes indistinguishable from background only one ( $H_{0}$ )

In strictly frequentiest approach we could exclude (on $95 \% \mathrm{CL}$ ) not only the SM, but also all Higgs scenarios $\left(H_{1}\right)$ with $m_{H}>118 \mathrm{GeV}$ !..

Frequentist approach gives us result which is correct (from statistical point of view) but not very useful for discriminating the two hypothesis! Too sensitive to background fluctuations...

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## $C L_{s}$ method

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Frequentist approach gives us result which is correct (from statistical point of view) but not very useful for discriminating the two hypothesis! Too sensitive to background fluctuations...

Solution is to look for confidence level of $H_{1}$ relative to $H_{0}$ :

$$
C L_{s}=\frac{C L_{s+b}}{C L_{b}}
$$

## Hypothesis Testing

## $\mathrm{CL}_{\mathrm{s}}$ method example

Counting experiment with expected background $\mu_{\text {bg }}=3$ and $N_{\text {obs }}=7$


Probability of background hypothesis to result in $N_{\text {obs }} \leq 7$ is $98.8 \%$
$\Rightarrow \mathrm{CL}_{\mathrm{s}}$ limit on number of signal events is $10.17 \quad(95 \% \mathrm{CL})$

## Hypothesis Testing

## $\mathrm{CL}_{\mathrm{s}}$ method example

Counting experiment with expected background $\mu_{\mathrm{bg}}=3$ and $N_{\text {obs }}=3$


Probability of background hypothesis to result in $N_{\text {obs }} \leq 3$ is $64.7 \%$
$\Rightarrow C L_{\text {s }}$ limit on number of signal events is $5.40 \quad(95 \% C L)$

## Hypothesis Testing

## $\mathrm{CL}_{\mathrm{s}}$ method example

Counting experiment with expected background $\mu_{\text {bg }}=3$ and $N_{\text {obs }}=1$


Probability of background hypothesis to result in $N_{\text {obs }} \leq 1$ is $19.9 \%$
$\Rightarrow C L_{\text {s }}$ limit on number of signal events is $3.64 \quad(95 \% C L)$

## Hypothesis Testing

## $\mathrm{CL}_{\mathrm{s}}$ method example

Counting experiment with expected background $\mu_{\mathrm{bg}}=3$ and $N_{\text {obs }}=0$


Probability of background hypothesis to result in $N_{\text {obs }}=0$ is $4.98 \%$
$\Rightarrow C L_{\text {s }}$ limit on number of signal events is $3.00 \quad(95 \% C L)$

## Hypothesis Testing

## $\mathrm{CL}_{\mathrm{s}}$ method

## Final Higgs limits from LEP

In the modified approach，we exclude （at $95 \% \mathrm{CL}$ ）all scenarios with

$$
C L_{s}<0.05
$$

This means that the probability of $H_{1}$ to reproduce the collected data is less than 5\％of the SM probability：

$$
P\left(q>q_{d a t} \mid H_{1}\right)<0.05 P\left(q>q_{d a t} \mid H_{0}\right)
$$



## Statistical analysis of experimental data

Variable distributions

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## Homework

## Homework

Solutions to be uploaded by January 18.
1000 events were collected in the muon lifetime measurement.
Distribution can be described by the formula:

$$
\frac{d N}{d t}=\frac{N_{\text {sig }}}{\tau} e^{-\frac{t}{\tau}}+\frac{d N_{b g}}{d t} \quad 0 \leq t \leq 15 \mu s
$$

with flat background level known to be $\frac{d N_{b g}}{d t}=10 \pm \Delta \mu \mathrm{s}^{-1}$
Estimate the dependence of the uncertainty on the muon lifetime, $\sigma_{\tau}$, obtained from the fit on the assumed background uncertainty $\Delta$.

Hint: consider the Hessian matrix of the fit

## Homework

## Homework

## Solutions to be uploaded by January 18.

Example data


## Homework

## Homework

## Solutions to be uploaded by January 18.

Example data


