Statistical analysis of experimental data
Least-squares method

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Lecture 08

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Least-squares method

Maximum Likelihood Method

The product:

$$L = \prod_{j=1}^{N} f(\mathbf{x}^{(j)}; \boldsymbol{\lambda})$$

is called a likelihood function.

The most commonly used approach to parameter estimation is the maximum likelihood approach: as the best estimate of the parameter set $\boldsymbol{\lambda}$ we choose the parameter values for which the likelihood function has a (global) maximum.

Frequently used is also log-likelihood function

$$\ell = \ln L = \sum_{j=1}^{N} \ln f(\mathbf{x}^{(j)}; \boldsymbol{\lambda})$$

we can look for maximum value of ℓ or minimum of $-2\,\ell = -2\ln L$

Multiple parameter estimate

Likelihood function (and log-likelihood) can depend on multiple parameters:

$$\boldsymbol{\lambda} = (\lambda_1 \ldots \lambda_p) \qquad L = \prod_{j=1}^{N} f(\mathbf{x}^{(j)}; \boldsymbol{\lambda}) \qquad \ell = \sum_{j=1}^{N} \ln f(\mathbf{x}^{(j)}; \boldsymbol{\lambda})$$

Best estimate of $\boldsymbol{\lambda}$, for given set of experimental results $\mathbf{x}^{(j)}$, corresponds to maximum of the likelihood function, which can be found by solving a system of equations:

$$\left.\frac{\partial \ell}{\partial \lambda_i}\right|_{i=1 \ldots p} = 0$$

The Likelihood Principle

G. Bohm and G. Zech

Given a p.d.f. $f(\mathbf{x}; \boldsymbol{\lambda})$ containing an unknown parameters of interest $\boldsymbol{\lambda}$ and observations $\mathbf{x}^{(j)}$, all information relevant for the estimation of the parameters $\boldsymbol{\lambda}$ is contained in the likelihood function $L(\boldsymbol{\lambda}; \mathbf{x}) = \prod f(\mathbf{x}^{(j)}; \boldsymbol{\lambda})$.

Parameter covariance matrix

For the considered case of multivariate normal distribution, best parameter estimates $\hat{\boldsymbol{\lambda}}$ are given by the measured variable values $\mathbf{x}$.

Unlike parameters $\boldsymbol{\lambda}$, parameter estimates $\hat{\boldsymbol{\lambda}}$ are random variables (functions of $\mathbf{x}$) and so we can consider covariance matrix for $\hat{\boldsymbol{\lambda}}$:

$$\mathbb{C}_{\mathbf{x}} = \mathbb{C}_{\hat{\boldsymbol{\lambda}}} = \left(-\frac{\partial^2 \ell}{\partial \lambda_i \, \partial \lambda_j} \right)^{-1}$$

Knowing the likelihood function, we can not only estimate parameter values, but also extract uncertainties and correlations of these estimates!

Recipe for a parameter uncertainty

G. Bohm and G. Zech

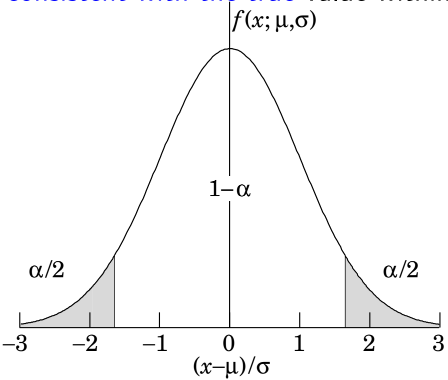
Standard error intervals of the extracted parameter are defined by the decrease of the log-likelihood function by 0.5 for one, by 2 for two and by 4.5 for three standard deviations.

Normal distribution

Meaning of σ is well defined for Gaussian distribution.

Probability for the experimental result to be consistent with the true value within $\pm N\,\sigma$:

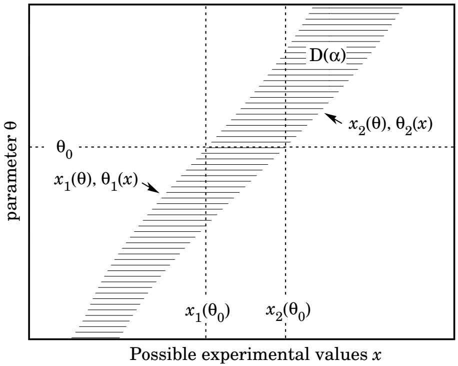
		$1-\alpha$	
$\pm 1\,\sigma$	$\Rightarrow$	68.27	%
$\pm 2\,\sigma$	$\Rightarrow$	95.45	%
$\pm 3\,\sigma$	$\Rightarrow$	99.73	%
$\pm 4\,\sigma$	$\Rightarrow$	99.9937	%
$\pm 5\,\sigma$	$\Rightarrow$	99.999943	%



There is a non-zero chance for deviation grater than 5σ, but it is extremely small

Frequentist confidence intervals

General procedure



- calculate limits of probability intervals for x, $x_1(\theta)$ and $x_2(\theta)$, for different values of θ
- calculated intervals define the "accepted region" in (θ, x)
- confidence interval for θ is defined by drawing line $x = x_m$ in the accepted region

$\Rightarrow$ limit on θ for given x_m, $\theta_1(x_m)$, corresponds to limit on x for given θ: $x_m = x_1(\theta_1)$.

R.L. Workman et al. (Particle Data Group), Prog. Theor. Exp. Phys. 2022, 083C01 (2022), PDG web page

Example procedure

Bayes theorem can be applied to the case of counting experiment (without background):

$$\mathcal{P}(\mu; n_m) \;=\; \frac{P(n_m;\mu)}{\int d\mu' \; P(n_m;\mu')} \cdot \mathcal{P}(\mu)$$

Integral in the denominator is equal to 1 (Gamma distribution).
Assuming flat "prior distribution" for μ (no earlier constraints) we get:

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

Upper limit on the expected number of events can be then calculated as:

$$\int_0^{\mu_{ul}} d\mu \;\; \mathcal{P}(\mu; n_m) \;=\; 1-\alpha$$

Surprisingly, the numerical result is the same as for Frequentist approach...

Solution

We still want to start from constructing the probability intervals in random variable x (or n) for given hypothesis μ.

Let $\mu_{best}(x)$ be the parameter value best describing measurement x (maximum likelihood).

How consistent is the considered parameter value μ with our measurement (described by μ_{best}) can be described by likelihood ratio:

$$R(x;\mu) \;=\; \frac{P(x;\mu)}{P(x;\mu_{best}(x))} \;\leq 1$$

We can now create the probability interval for x, $[x_1, x_2]$, by selecting values with highest R, up to given CL:

$$\int_{x_1}^{x_2} dx\, P(x;\mu) \;=\; 1-\alpha \quad \text{and} \quad \forall_{x \notin [x_1,x_2]}\; R(x) < R(x_1) = R(x_2)$$

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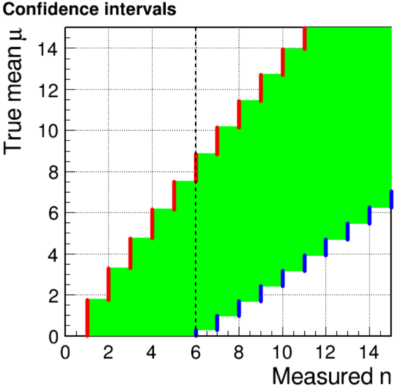
Example

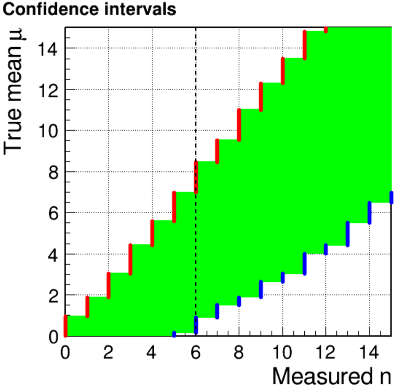
G.J.Feldman, R.D.Cousins, arXiv:physics/9711021

Calculations of 90% CL interval for counting experiment (Poisson variable) in the presence of known mean background $\mu_{bg} = 3.0$

Central 90% CL intervals



Unified 90% CL intervals



Least-squares method

Maximum Likelihood Method

see lectures 05 and 06

Let us consider N independent measurements of variable Y. Assuming measurement fluctuations are described by Gaussian pdf, the likelihood function is:

$$L = \prod_{i=1}^{N} G(y_i; \mu_i, \sigma_i) = \prod_{i=1}^{N} \frac{1}{\sigma_i \sqrt{2\pi}} \exp\left(-\frac{1}{2} \frac{(y_i - \mu_i)^2}{\sigma_i^2} \right)$$

Log-likelihood:

assuming σ_i are known

$$\ell = -\frac{1}{2} \sum \frac{(y_i - \mu_i)^2}{\sigma_i^2} + \text{const}$$

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Log-likelihood:

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We can define

$$\chi^2 = -2\,\ell = -2 \ln L = \sum_{i=1}^{N} \frac{(y_i - \mu_i)^2}{\sigma_i^2}$$

Maximum of (log-)likelihood function corresponds to minimum of χ^2

N=2

Let us introduce "shift" variables:

$$z_i = \frac{y_i - \mu_i}{\sigma_i}$$

which are (by construction) described by Gaussian pdf with $\mu = 0,\ \sigma = 1$.

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and then change variables to polar coordinates see lecture 04

$$f(r_z, \phi_z) = \frac{1}{2\pi} r_z \exp\left(-\frac{1}{2} r_z^2\right)$$

N=2

Integrating over ϕ_z and changing variable to r_z^2

$$f(r_z^2) = \frac{1}{2}\exp\left(-\frac{1}{2}r_z^2\right)$$

Distribution is exponential, corresponds to decay time distribution for $\tau = 2$...

N=2

Integrating over ϕ_z and changing variable to $r_z^2 = \chi^2$

$$f(\chi^2) = \frac{1}{2} \exp\left(-\frac{1}{2}\chi^2\right)$$

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Even N case

Sum of $n = N/2$ numbers from exponential distribution, is distributed according to Gamma distribution with $k = n = N/2$, $\lambda = 1/\tau = 1/2$ lecture 03

$$f(\chi^2) \;=\; \frac{1}{\Gamma(k)}\,(\chi^2)^{k-1}\,\lambda^k\,e^{-\lambda\chi^2}$$

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$$f(\chi^2) = \frac{1}{\Gamma(\frac{N}{2})} \left(\frac{1}{2}\right)^{\frac{N}{2}} (\chi^2)^{\frac{N}{2}-1} e^{-\chi^2/2}$$

The formula (as one can expect) works also for odd N...

N=1

Bonamente

One can consider moment generating function (see lecture 04) for distribution of $u = z^2 = \chi^2$:

N=1 Bonamente

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$$M_1(t) \;=\; \mathbb{E}(e^{tu}) \;=\; \int_{-\infty}^{+\infty} dz\; f(z)\; e^{tz^2}$$

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$$= \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{\frac{1}{2} - t}} \sqrt{\pi} = \frac{1}{\sqrt{1 - 2t}}$$

Arbitrary N

Bonamente

Considered random variables z_i are independent, and $\chi^2 = \sum z_i^2$. Moment generating function for χ^2 distribution is thus given by:

$$M_N(t) = \prod_{i=1}^{N} M_1(t) = \left(\frac{1}{1-2t}\right)^{N/2}$$

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We can compare it with the moment generating functions for Gamma pdf

$$M_G(t) \;=\; \mathbb{E}(e^{tx}) \;=\; \int_0^{+\infty} dx\, \frac{1}{\Gamma(k)} x^{k-1}\, \lambda^k\, e^{-\lambda x}\, e^{tx}$$

$$= \frac{\lambda^k}{\Gamma(k)} \int_0^{+\infty} dx\; x^{k-1}\, e^{-x(\lambda - t)}$$

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χ^2 distribution

We conclude that distribution of χ^2 is described by Gamma pdf with:

$$k = \frac{N}{2} \quad \text{and} \quad \lambda = \frac{1}{2}$$

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Properties of the χ^2 distribution (see lecture 03)

$$\langle \chi^2 \rangle = \frac{k}{\lambda} = N$$

$$\mathbb{V}(\chi^2) = \frac{k}{\lambda^2} = 2N$$

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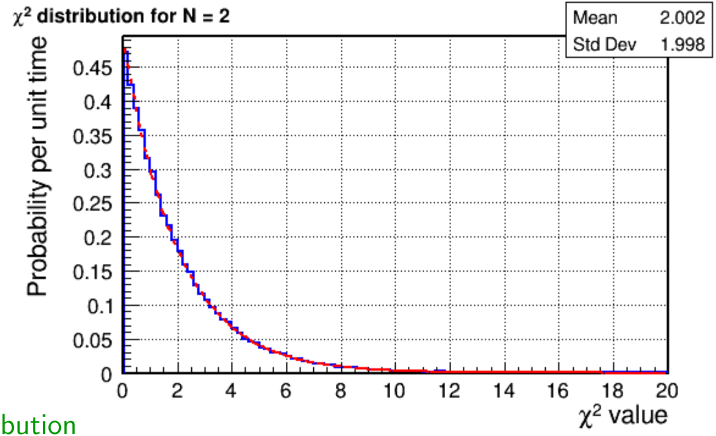
$$\sqrt{\mathbb{V}(\chi^2)} = \sigma_{\chi^2} = \sqrt{2N}$$

For small N, value of χ^2 is a subject to large fluctuations...

χ^2 distribution

08_chi2.ipynb Open in Colab

Results of the Monte Carlo sample generation (compared with predictions)



Exponential distribution

χ^2 distribution

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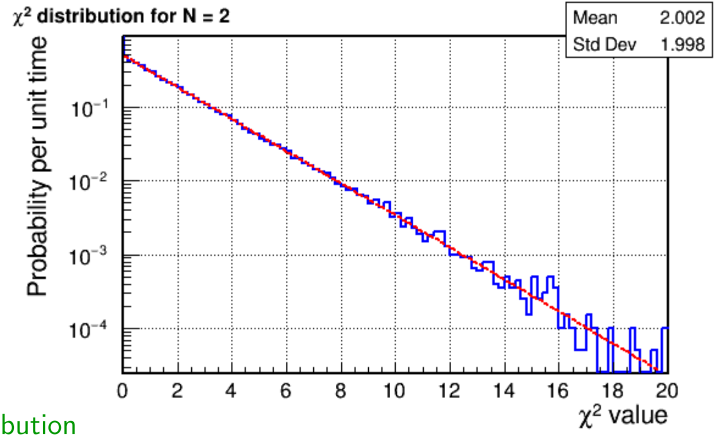

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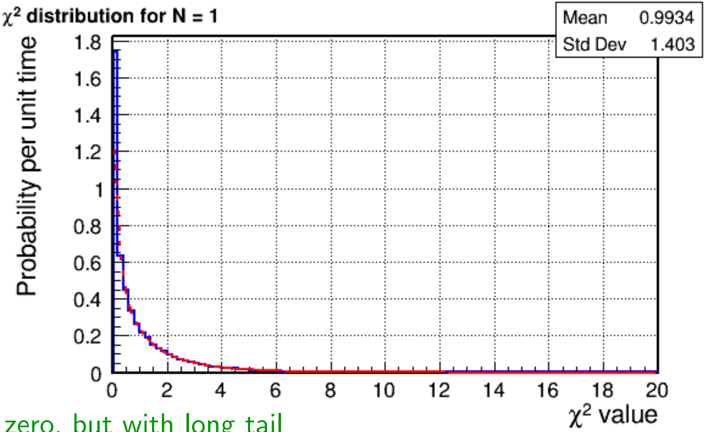

Sharply peaked at zero, but with long tail

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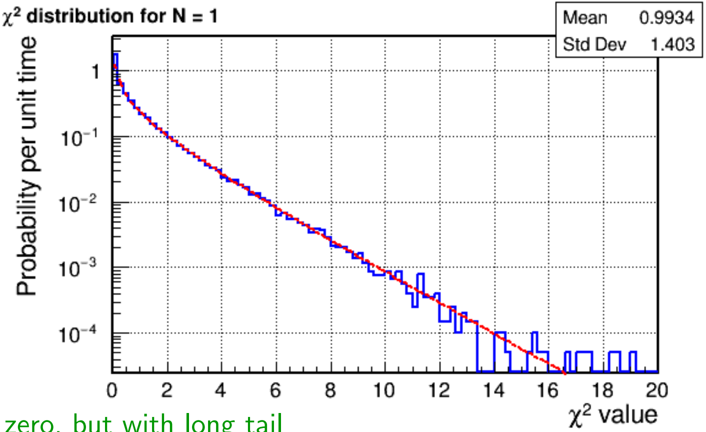

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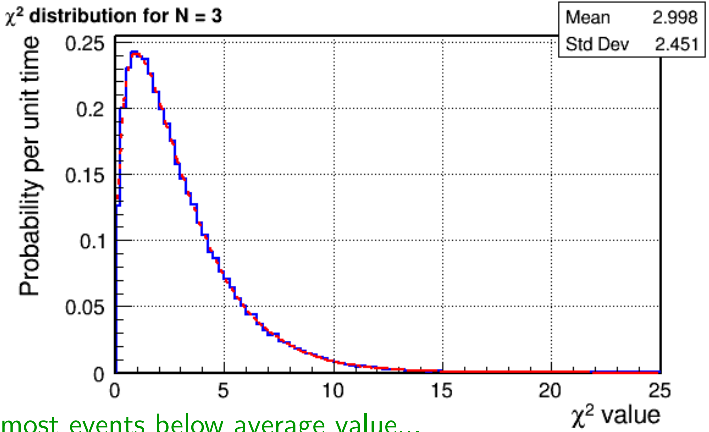

Very asymmetric, most events below average value...

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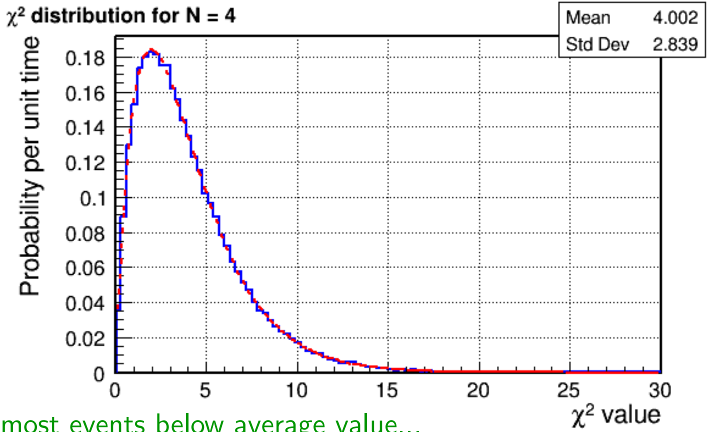

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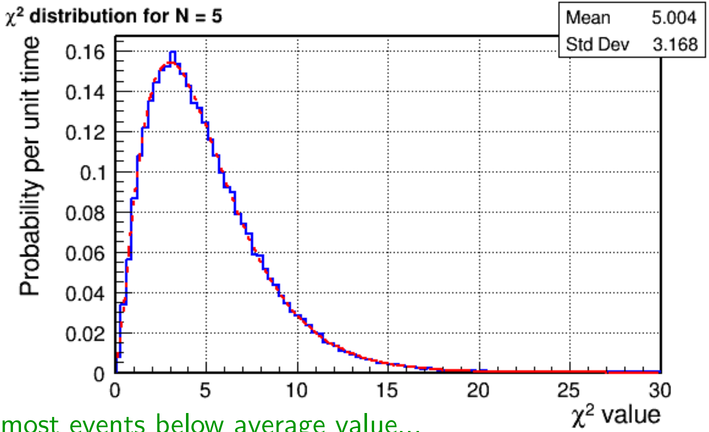

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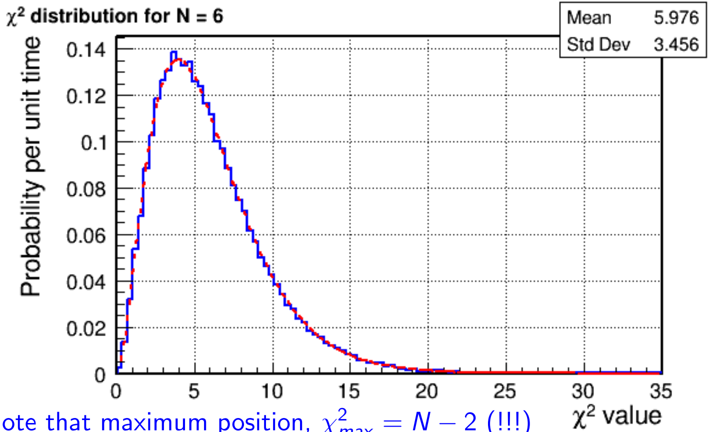

It is interesting to note that maximum position, $\chi^2_{max} = N - 2$ (!!!)

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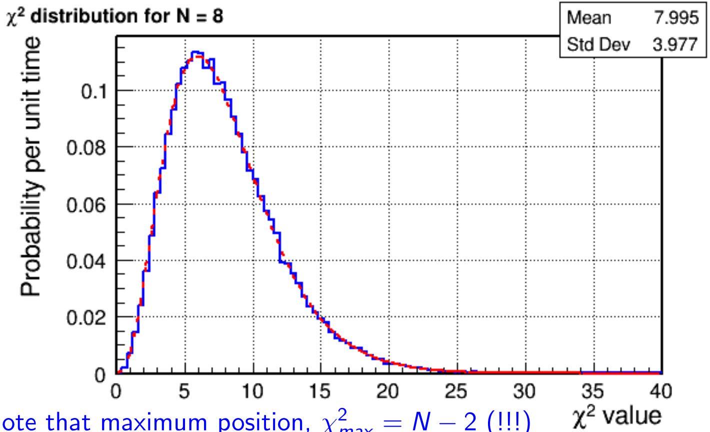

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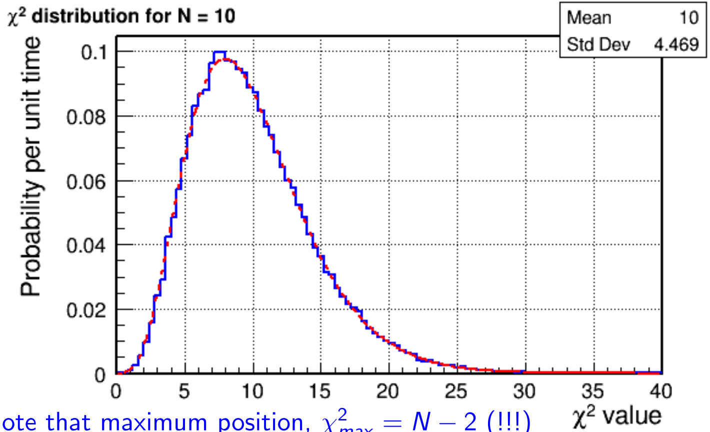

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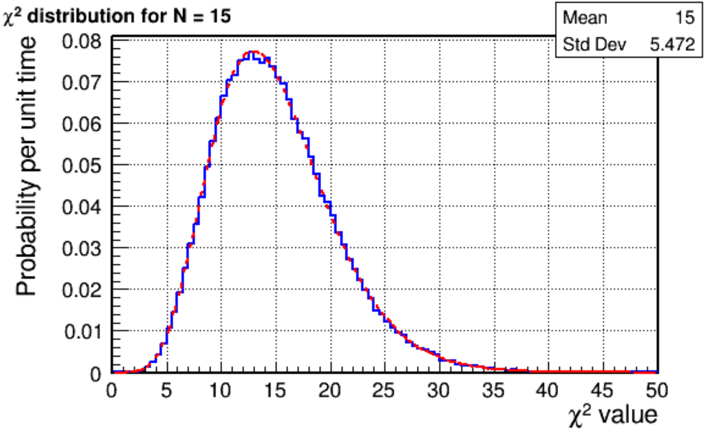

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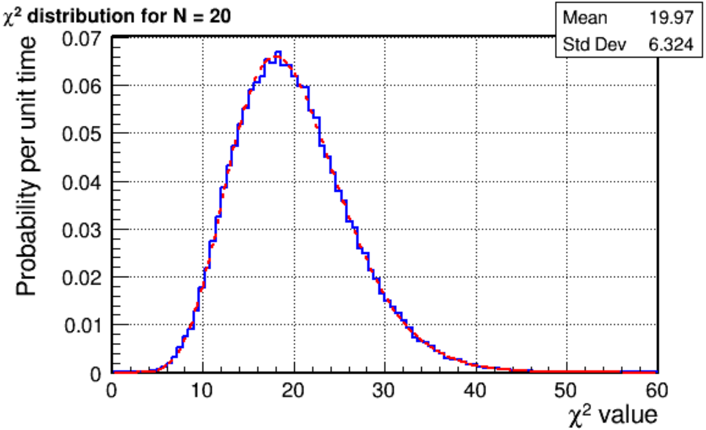

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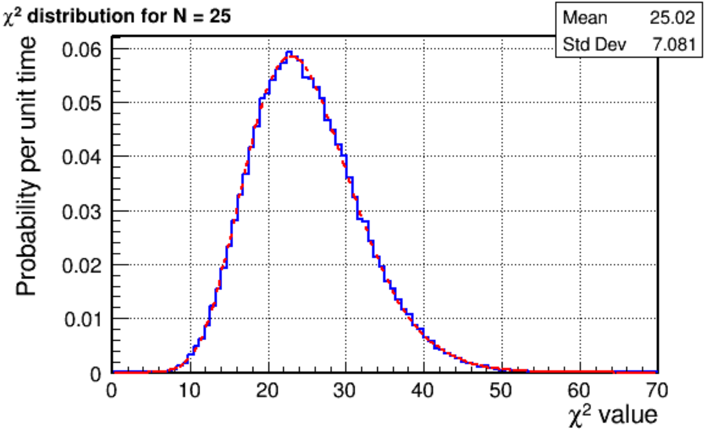

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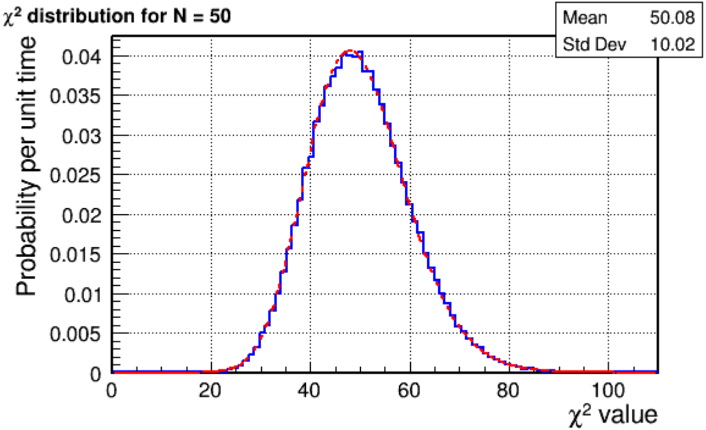

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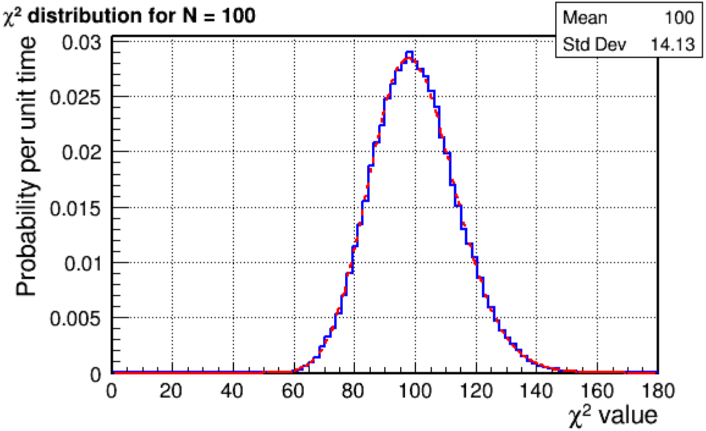

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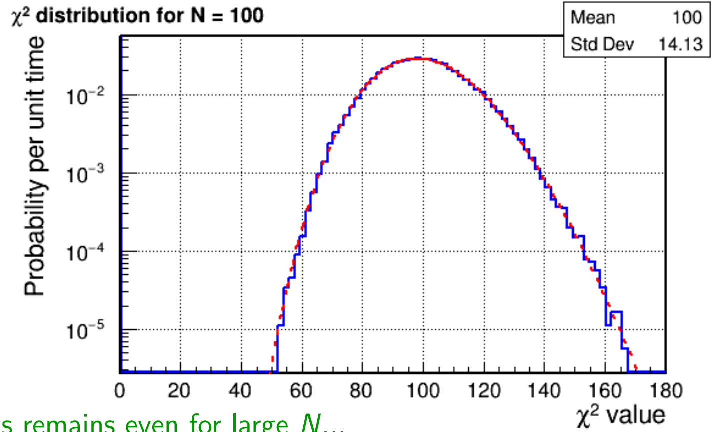

Asymmetry in tails remains even for large N...

Reduced χ^2

When discussing consistency of large data samples it is often convenient to use value of "reduced χ^2":

$$\chi^2_{red} = \frac{\chi^2}{N}$$

Distribution of χ^2_{red} is again described by the Gamma pdf with

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Properties of the distribution:

$$\langle \chi^2_{red} \rangle = 1 \qquad \mathbb{V}(\chi^2_{red}) = \sigma^2_{\chi^2_{red}} = \frac{2}{N}$$

Number of degrees of freedom

So far, we have only considered an ideal case, where both the expected values $\boldsymbol{\mu}$ and measurement uncertainties $\boldsymbol{\sigma}$ are known.

However, it is quite a common situation, when the expected value is extracted from the data:

$$\tilde{\chi}^2 = \sum_{i=1}^{N} \frac{(y_i - \bar{y})^2}{\sigma^2}$$

where we assume uniform uncertainties for simplicity.

What is the expected distribution for $\tilde{\chi}^2$?

Mean value corresponds to maximum likelihood $\Rightarrow$ $\tilde{\chi}^2 \leq \chi^2$

Number of degrees of freedom

We already know (lecture 04) that unbiased variance estimate for N measurements is

$$s^2 = \frac{1}{N-1} \sum_i (y_i - \bar{y})^2$$

so one can conclude:

$$\langle \tilde{\chi}^2 \rangle = N - 1$$

but this does not give us full information about the distribution...

Number of degrees of freedom

We already know (lecture 04) that unbiased variance estimate for N measurements is

$$s^2 = \frac{1}{N-1} \sum_i (y_i - \bar{y})^2$$

so one can conclude:

$$\langle \tilde{\chi}^2 \rangle = N - 1$$

but this does not give us full information about the distribution...

Simple variable transformation can be used: (Brandt)

$$x_k = \frac{1}{\sqrt{k(k+1)}} (y_1 + \ldots + y_k \; - \; y_{k+1}) \qquad k = 1 \ldots N-1$$

$$x_N = \sqrt{N} \cdot \bar{y}$$

One can verify that this is an orthogonal transformation...

Number of degrees of freedom

If y_i are independent random variables with Gaussian pdf, so are x_i. Also:

$$\sum_{i=1}^{N} x_i^2 = \sum_{i=1}^{N} y_i^2$$

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We can now rewrite the formula for $\tilde{\chi}^2$ in the new basis:

$$\begin{aligned}\sigma^2 \cdot \tilde{\chi}^2 &= \sum_{i=1}^{N}(y_i - \bar{y})^2 = \sum_{i=1}^{N} y_i^2 - 2\bar{y}\sum_{i=1}^{N} y_i + N\bar{y}^2 \\ &= \sum_{i=1}^{N} y_i^2 - N\bar{y}^2\end{aligned}$$

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$\Rightarrow$ distribution of $\tilde{\chi}^2$ corresponds to that of χ^2 for $N_{df} = N - 1$ variables...

Least-squares method

Data consistency test

Value of χ^2 (or χ^2_{red}) can be used to verify the consistency of the given data set $\mathbf{y}$ (with uncertainties $\boldsymbol{\sigma}$) with the model predictions given by $\boldsymbol{\mu}$

We can try to test the theoretical model, verify our estimates of measurement uncertainties, or check the consistency of the experimental procedure...

If the model does not describe the data, higher χ^2 values are expected.

How to quantify the level of agreement?

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If the model does not describe the data, higher χ^2 values are expected.

How to quantify the level of agreement?

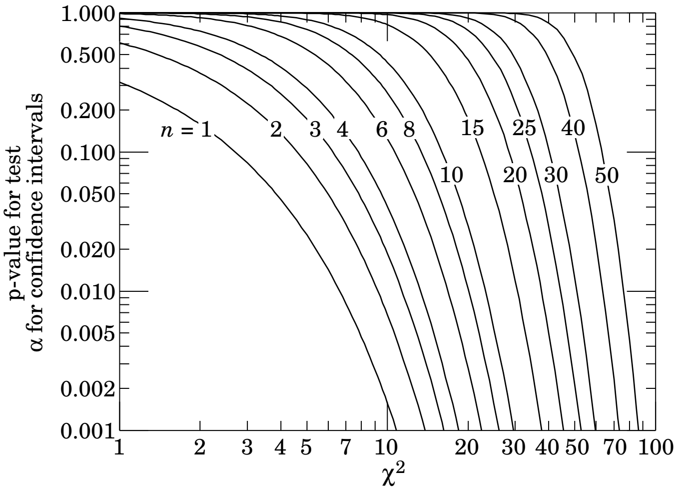
We can calculate the probability of obtaining given value of χ^2 or lower:

$$P(\chi^2) \;=\; \int_0^{\chi^2} d\chi^{2\prime}\, f(\chi^{2\prime})$$

given by the cumulative probability distribution. $1 - P(\chi^2)$ is sometimes referred to as p-value

Data consistency test

Plot of p-values
as a function of χ^2
for different N_{df}



(PDG)

Critical χ^2

The other approach is to define, for given probability P (confidence level) the critical value of χ^2, corresponding the the frequentist upper limit:

$$\int_0^{\chi^2_{crit}} d\chi^2 \, f(\chi^2) \; = \; P \qquad\qquad \int_{\chi^2_{crit}}^{+\infty} d\chi^2 \, f(\chi^2) \; = \; 1 - P \; = \; 1 - \alpha$$

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Very low P values ($P \ll 1$) are also not expected (not likely)!
If $\chi^2 \ll N$ (except for very small N), this usually indicates a problem:

- overestimated uncertainties of measurements (or correlations not properly included)
- hidden correlations between measurements (which we treat as independent variables)

Critical χ^2

Table of critical χ^2 values (Brand)

$$P = \int_0^{\chi_P^2} f(\chi^2; f)\,\mathrm{d}\chi^2$$

f	P 0.900	0.950	0.990	0.995	0.999
1	2.706	3.841	6.635	7.879	10.828
2	4.605	5.991	9.210	10.597	13.816
3	6.251	7.815	11.345	12.838	16.266
4	7.779	9.488	13.277	14.860	18.467
5	9.236	11.070	15.086	16.750	20.515
6	10.645	12.592	16.812	18.548	22.458
7	12.017	14.067	18.475	20.278	24.322
8	13.362	15.507	20.090	21.955	26.124
9	14.684	16.919	21.666	23.589	27.877
10	15.987	18.307	23.209	25.188	29.588

Critical χ^2

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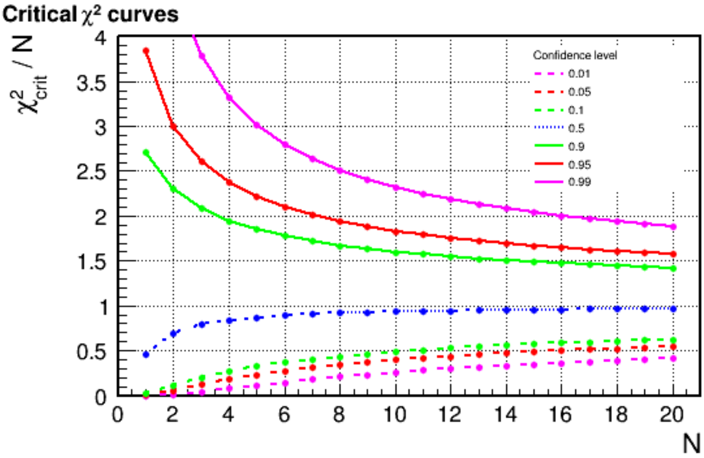
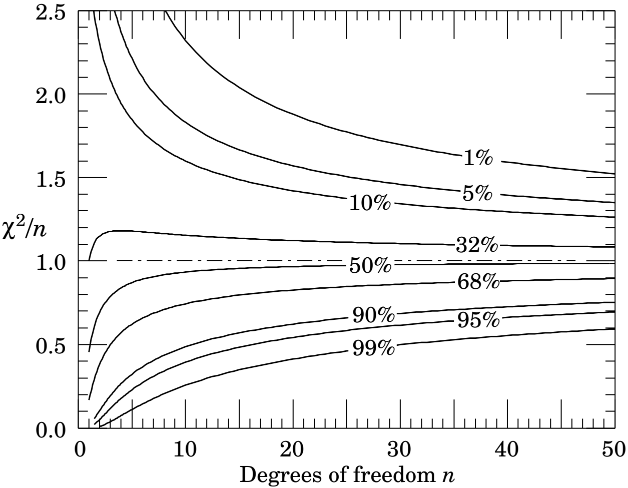
Plot of critical values for reduced χ^2



Critical χ^2

Plot of critical values
for reduced χ^2
(indicated is $p = 1 - P$)

(PDG)



Student's t Distribution

We can verify consistency of the series of measurements **x** with the true value μ by looking at the shift parameter for the mean

$$z = \frac{\bar{x} - \mu}{\sigma_{\bar{x}}}$$

where mean value $\bar{x}$ is the best estimate of μ assuming Gaussian pdf.

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If the measurement uncertainties are unknown, or not reliable, we can estimate the variance of the sample from the data itself (lecture 04)

$$s^2 = \frac{1}{N-1} \sum_i (x_i - \bar{x})^2$$

s^2 distribution corresponds to χ^2 distribution for $N-1$ degrees of freedom

Student's t Distribution

Consistency of our measurements **x** with the true value μ can be now described by

$$t = \frac{\bar{x} - \mu}{s/\sqrt{N}}$$

but the distribution of t is no longer Gaussian (due to s being a random variable as well).

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$$f(t; n) = \frac{1}{\sqrt{n\,\pi}} \frac{\Gamma(\frac{n+1}{2})}{\Gamma(\frac{n}{2})} \left(1 + \frac{t^2}{n}\right)^{-\frac{n+1}{2}}$$

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Distribution is symmetric and has a mean of zero, but larger tails than the Gaussian distribution, for small N in particular.

Student's t Distribution

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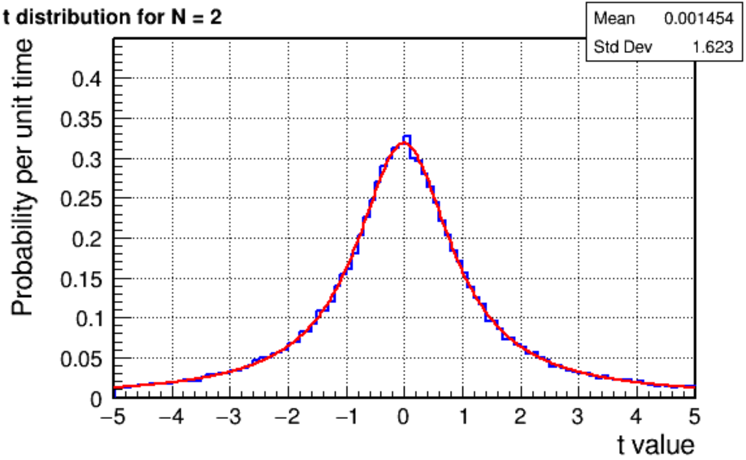

Shape of the t distribution for different numbers of measurements

$N_{df} = N - 1 = 1$

Student's t Distribution

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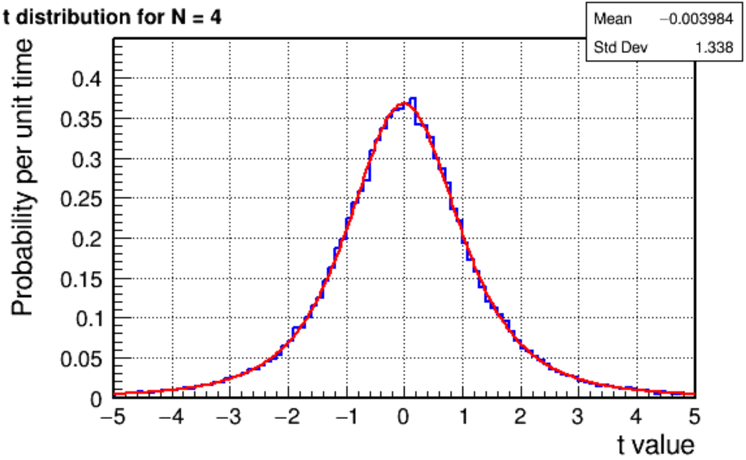

Shape of the t distribution for different numbers of measurements

$$N_{df} = N - 1 = 3$$

Student's t Distribution

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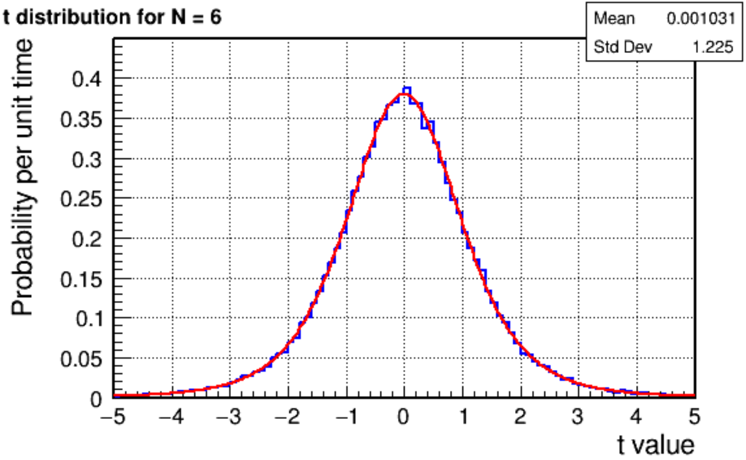

Shape of the t distribution for different numbers of measurements

$N_{df} = N - 1 = 5$

Student's t Distribution

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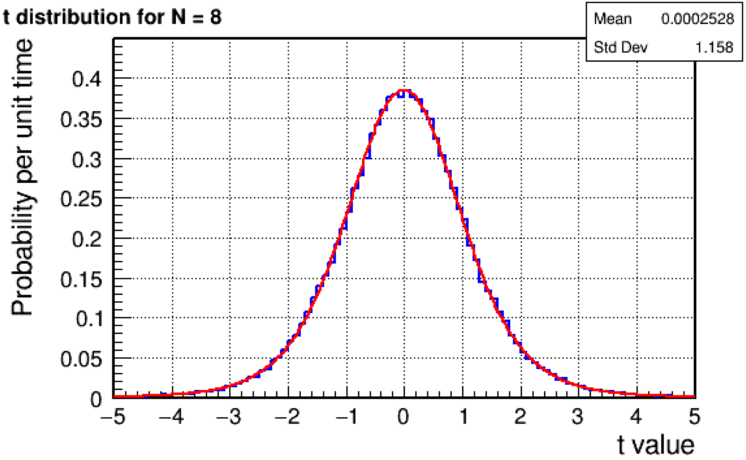

Shape of the t distribution for different numbers of measurements

$$N_{df} = N - 1 = 7$$

Student's t Distribution

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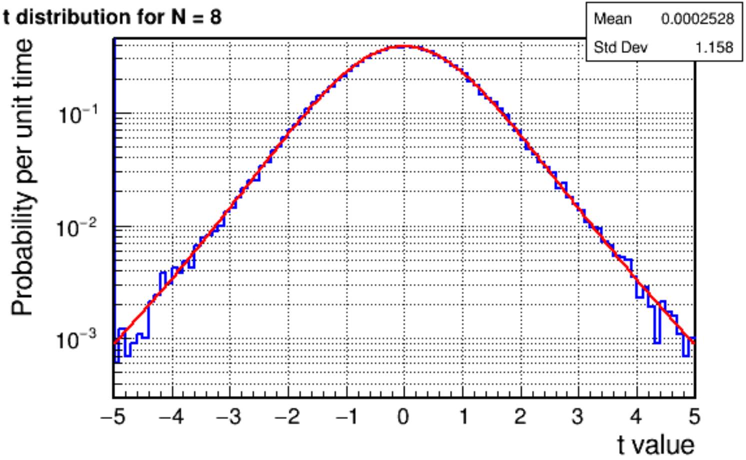

Shape of the t distribution for different numbers of measurements

$N_{df} = N - 1 = 7$

tails are clearly non-Gaussian...

Student's t Distribution

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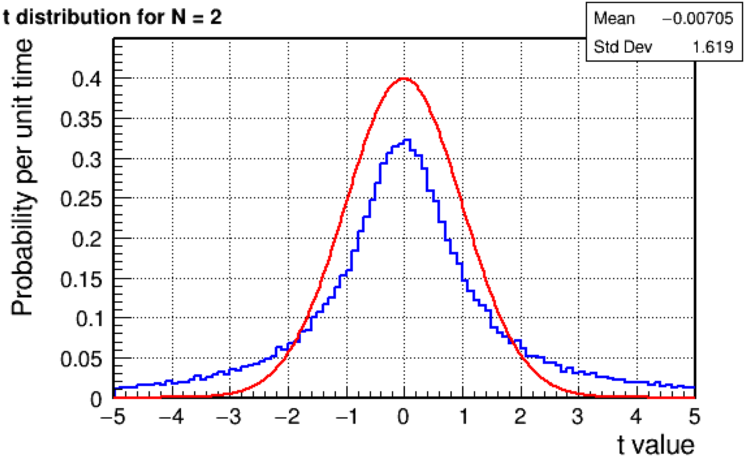

Shape of the t distribution compared with Gaussian distribution

$N_{df} = N - 1 = 1$

Student's t Distribution

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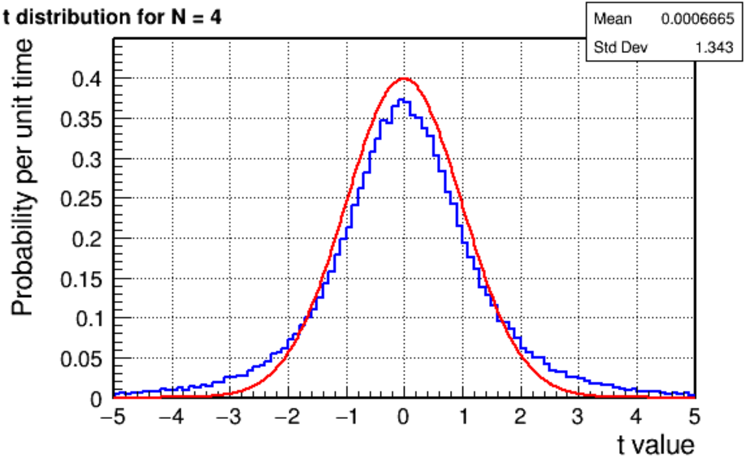

Shape of the t distribution compared with Gaussian distribution

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Student's t Distribution

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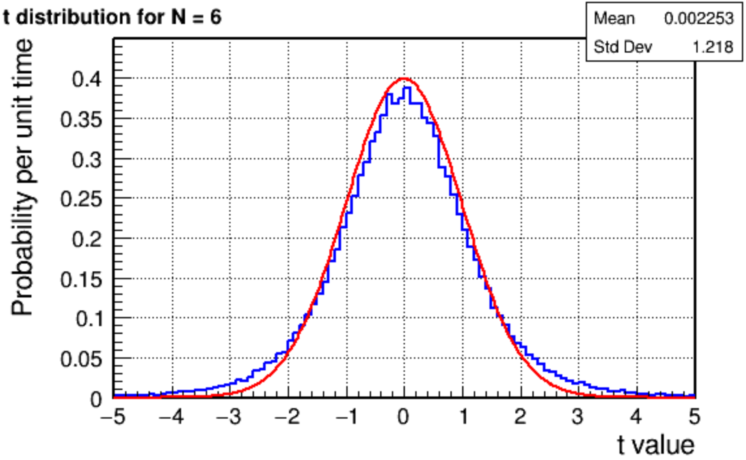

Shape of the t distribution compared with Gaussian distribution

$N_{df} = N - 1 = 5$

Student's t Distribution

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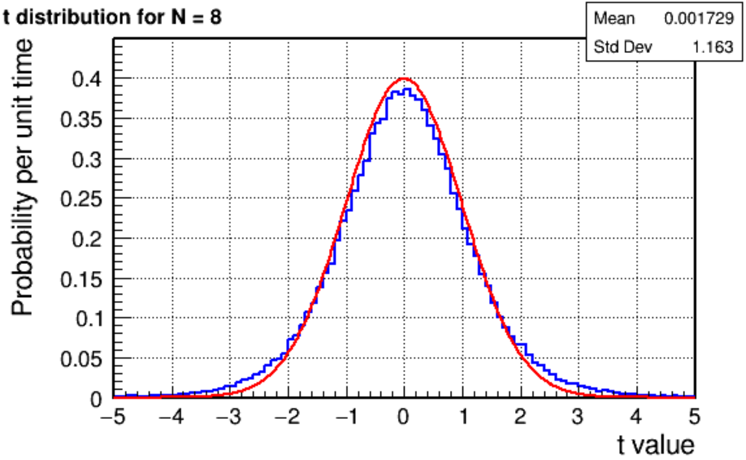

Shape of the t distribution compared with Gaussian distribution

$$N_{df} = N - 1 = 7$$

Student's t Distribution

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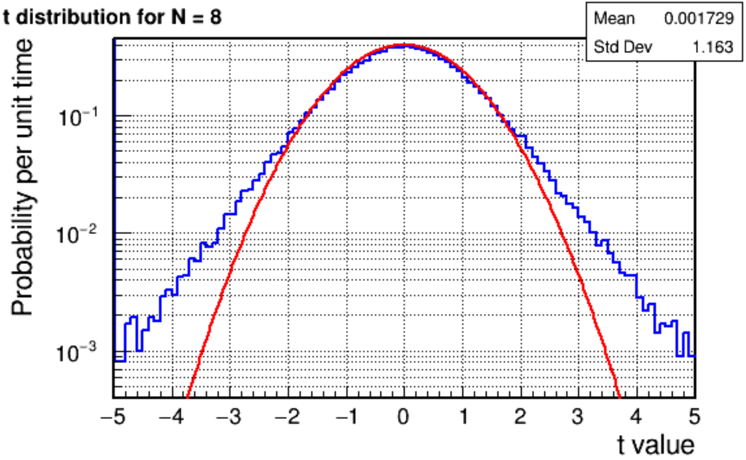

Shape of the t distribution compared with Gaussian distribution

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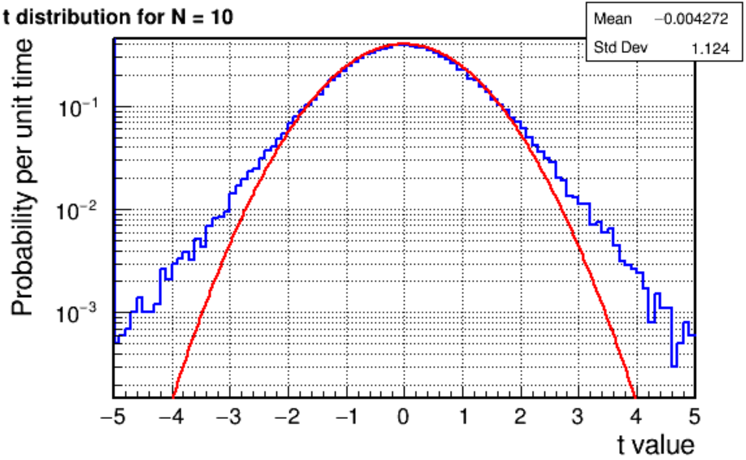

Shape of the t distribution compared with Gaussian distribution

Probability of large fluctuations still significantly enhanced!

Student's t Distribution

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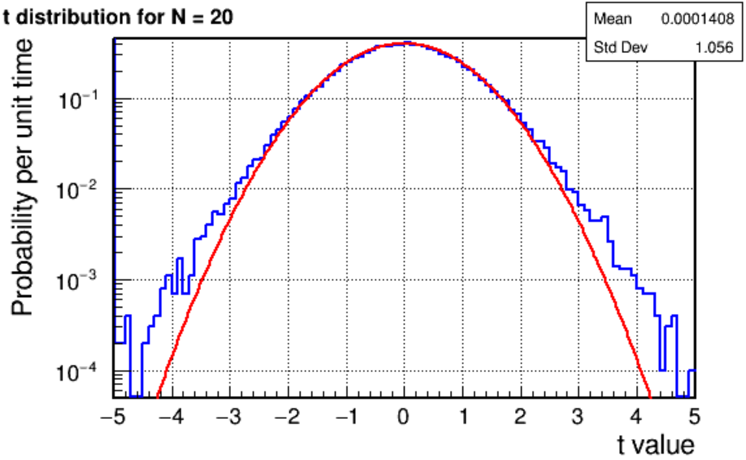

Shape of the t distribution compared with Gaussian distribution

Student's t Distribution

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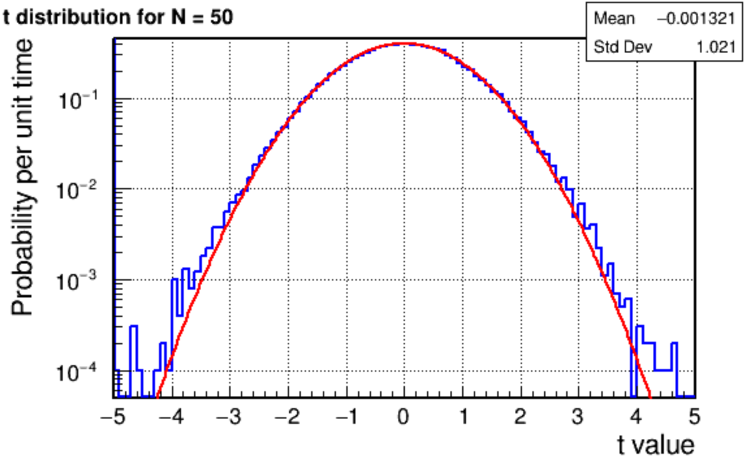

Shape of the t distribution compared with Gaussian distribution

Student's t Distribution

08_t-dist.ipynb

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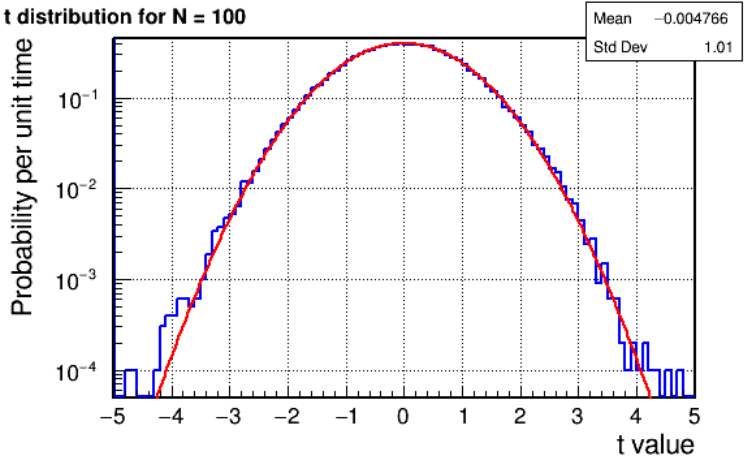


Shape of the t distribution compared with Gaussian distribution

Converges to the Gaussian distribution for large N

Student's t Distribution (Brandt)

"Critical values" of t for small numbers of degrees of freedom f

$$P = \int_{-\infty}^{t_P} f(t; f)\,\mathrm{d}t$$

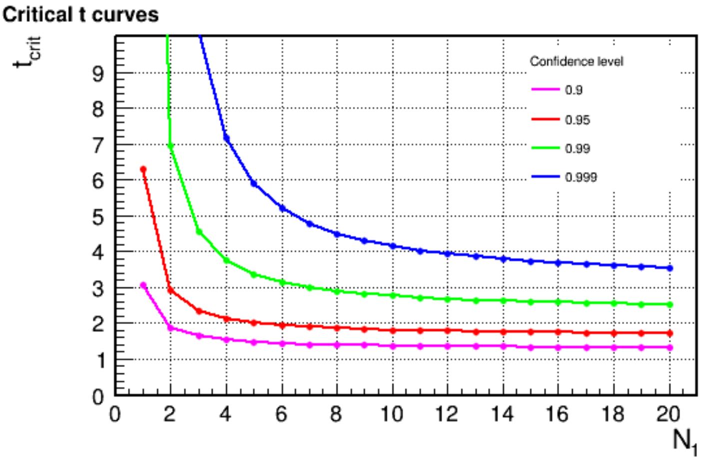
	P						
f	0.9000	0.9500	0.9750	0.9900	0.9950	0.9990	0.9995
1	3.078	6.314	12.706	31.821	63.657	318.309	636.619
2	1.886	2.920	4.303	6.965	9.925	22.327	31.599
3	1.638	2.353	3.182	4.541	5.841	10.215	12.924
4	1.533	2.132	2.776	3.747	4.604	7.173	8.610
5	1.476	2.015	2.571	3.365	4.032	5.893	6.869
6	1.440	1.943	2.447	3.143	3.707	5.208	5.959
7	1.415	1.895	2.365	2.998	3.499	4.785	5.408
8	1.397	1.860	2.306	2.896	3.355	4.501	5.041
9	1.383	1.833	2.262	2.821	3.250	4.297	4.781
10	1.372	1.812	2.228	2.764	3.169	4.144	4.587
11	1.363	1.796	2.201	2.718	3.106	4.025	4.437
12	1.356	1.782	2.179	2.681	3.055	3.930	4.318
13	1.350	1.771	2.160	2.650	3.012	3.852	4.221
14	1.345	1.761	2.145	2.624	2.977	3.787	4.140

Student's t Distribution

08_t-limit.ipynb Open in Colab

Plot of critical values for t

Large deviations much more probable for small N



Least-squares method

General case

We introduced χ^2 in a very general form:

$$\chi^2 = \sum_{i=1}^{N} \frac{(y_i - \mu_i)^2}{\sigma_i^2}$$

where different μ_i and σ_i are possible for each of N measurement y_i

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where different μ_i and σ_i are possible for each of N measurement y_i

It is quite often the case that values of μ_i depend on some controlled variables x_i and a smaller set of model parameters:

$$\mu_i = \mu(x_i; \mathbf{a})$$

we can then use the least-squares method to extract the best estimates of parameters **a** from the collected set of data points (x_i, y_i)

We can look for minimum of χ^2 using different numerical algorithms...

Linear case

The case which is particularly interesting is when the dependence is linear in parameters (!):

$$\mu(x; \mathbf{a}) \;=\; \sum_{k=1}^{M} a_k \, f_k(x)$$

where $f_k(x)$ is a set of functions with arbitrary analytical form.

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where $f_k(x)$ is a set of functions with arbitrary analytical form.

One of the examples is the polynomial series:

$$f_k(x) \;=\; x^k \qquad \Rightarrow \quad \mu(x;\mathbf{a}) \;=\; \sum_{k=1}^{M} a_k\, x^{k-1}$$

but any set of functions can be used, if they are not linearly dependent.
Functions ortogonal for a given set of points x_i should work best...

Parameter fit

Bonamente

Least-squares method is the special case of the maximum likelihood approach, when we can assume Gaussian pdf for measurements y_i.

As the best estimate of the parameter set **a** we choose the parameter values which correspond to the (global) χ^2 minimum ($\Rightarrow$ maximum of log-likelihood)

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To look for χ^2 maximum, we consider partial derivatives:

$$\frac{\partial \chi^2}{\partial a_l} = \frac{\partial}{\partial a_l} \sum_{i=1}^{N} \left(\frac{y_i - \sum_{k=1}^{M} a_k \, f_k(x)}{\sigma_i} \right)^2 = 0$$

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$$= -2 \sum_{i=1}^{N} \left(\frac{y_i - \sum_{k=1}^{M} a_k \; f_k(x)}{\sigma_i^2} \right) f_l(x_i)$$

Parameter fit

Bonamente

We obtain a set of M equations for M parameters a_i:

$$\sum_{i=1}^{N} \frac{f_l(x_i)}{\sigma_i^2} \left(y_i - \sum_{k=1}^{M} a_k \, f_k(x) \right) \;=\; 0 \qquad l = 1 \ldots M$$

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which can be rewritten as:

$$\sum_{k=1}^{M} \left(\sum_{i=1}^{N} \frac{f_l(x_i) \, f_k(x_i)}{\sigma_i^2} \right) a_k = \sum_{i=1}^{N} \frac{f_l(x_i) \, y_i}{\sigma_i^2}$$

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or in the matrix form:

$$\mathbb{A} \cdot \mathbf{a} \quad = \quad \mathbf{b}$$

where $\quad \mathbb{A}_{lk} \; = \; \sum_{i=1}^{N} \frac{f_l(x_i) \; f_k(x_i)}{\sigma_i^2} \quad$ and $\quad b_l \; = \; \sum_{i=1}^{N} \frac{f_l(x_i) \; y_i}{\sigma_i^2}$

Parameter fit

Solution of this set of equations can be obtained by inverting matrix $\mathbb{A}$

$$\mathbf{a} = \mathbb{A}^{-1} \cdot \mathbf{b}$$

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This also gives us the estimate of parameter covariance matrix:

$$\mathbb{C}_{\mathbf{a}} \; = \; \left(- \frac{\partial^2 \ell}{\partial a_l \, \partial a_k} \right)^{-1} = \left(\frac{1}{2} \frac{\partial^2 \chi^2}{\partial a_l \, \partial a_k} \right)^{-1} = \; \mathbb{A}^{-1}$$

Parameter fit

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$$\mathbf{a} \;=\; \mathbb{A}^{-1} \cdot \mathbf{b}$$

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One can write

$$\mathbb{C}_{\mathbf{a}} \;=\; \left(\sum_{i=1}^{N} \frac{f_l(x_i) \; f_k(x_i)}{\sigma_i^2} \right)^{-1}$$

Expected uncertainties of the extracted parameter values depend on the choice of measurement points x_i but, surprisingly, do not depend on the actual results y_i

$\Rightarrow$ very useful when planning the experiment...

Linear fit example

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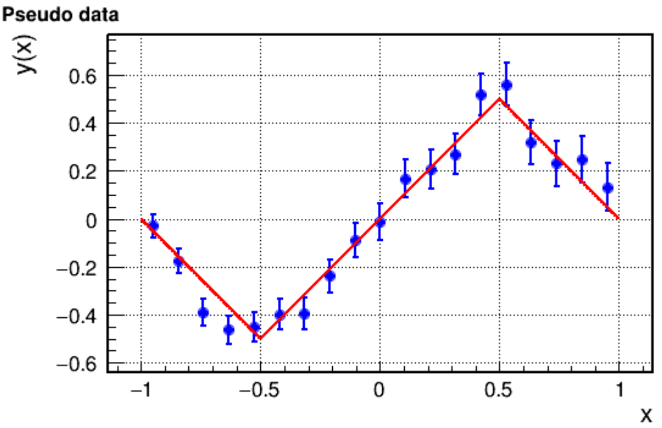
Fitting Fourier series to example data set

example model ⇒



Linear fit example

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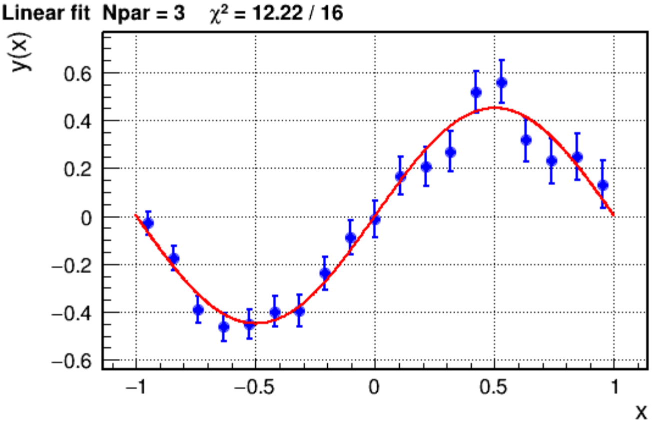
Fitting Fourier series to example data set

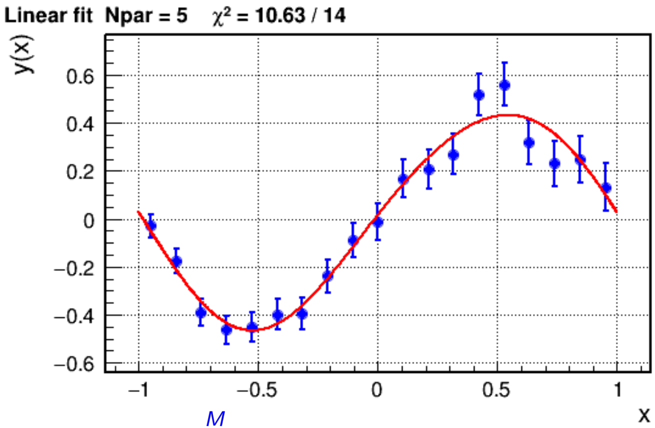


$$y(x) = a_0 + a_1 \sin(x) + a_2 \cos(x)$$

Linear fit example

08_fit1.ipynb Open in Colab

Fitting Fourier series to example data set



$$y(x) \quad = \quad a_0 + \sum_{n=1}^{M} a_{2n-1} \sin(nx) + a_{2n} \cos(nx) \qquad M = 2$$

Linear fit example

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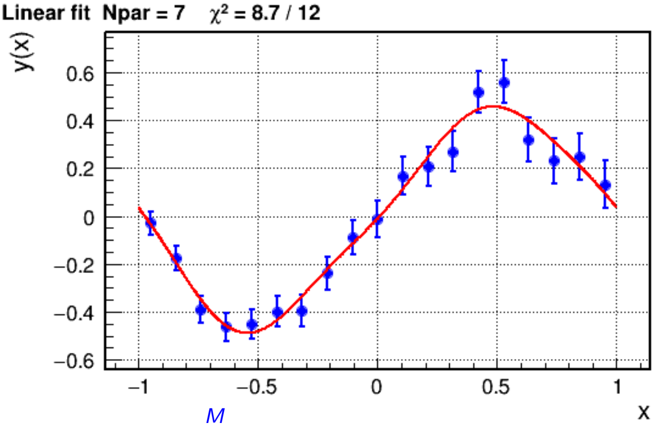
Fitting Fourier series to example data set

Probably optimal choice



$$y(x) = a_0 + \sum_{n=1}^{M} a_{2n-1} \sin(nx) + a_{2n} \cos(nx) \qquad M = 3$$

Linear fit example

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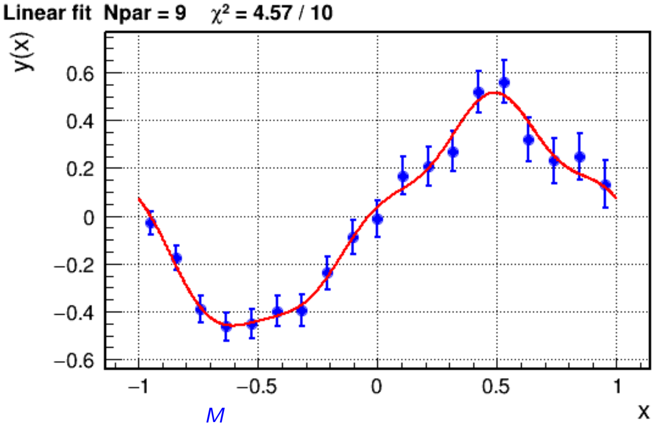
Fitting Fourier series to example data set

"Overtraining"



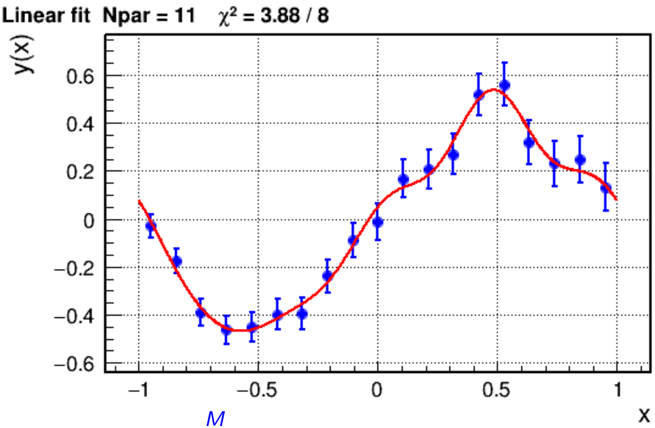
$$y(x) = a_0 + \sum_{n=1}^{M} a_{2n-1}\sin(nx) + a_{2n}\cos(nx) \qquad M = 4$$

Linear fit example

08_fit1.ipynb Open in Colab

Fitting Fourier series to example data set

"Overtraining"



$$y(x) = a_0 + \sum_{n=1}^{M} a_{2n-1}\sin(nx) + a_{2n}\cos(nx) \qquad M = 5$$

Linear fit example

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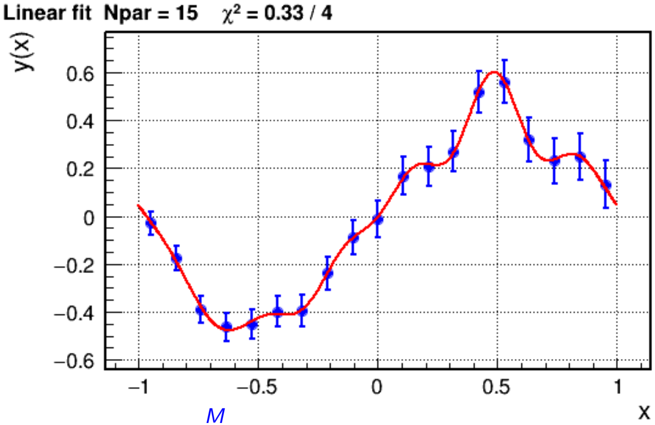
Fitting Fourier series to example data set

"Overtraining"



$$y(x) = a_0 + \sum_{n=1}^{M} a_{2n-1}\sin(nx) + a_{2n}\cos(nx) \qquad M = 6$$

Best fit choice?

If the functional dependence is not predicted by any theory/model, we can try to fit a polynomial or function series. When should we stop?

How can we recognize that we have too many parameters?
Beside looking at the P value corresponding to the obtained χ^2

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- Adding new parameter results in only moderate χ^2 decrease, $\mathcal{O}(1)$

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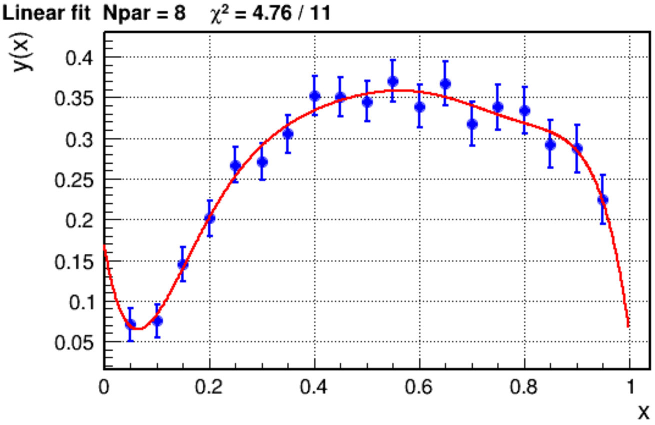
- Parameters become highly correlated
- Values and errors of the individual parameters increase
  differences of large contributions
- Additional parameters are consistent with zero
- Fit starts to follow fluctuations of the measurement results

Best fit choice?

08_fit3.ipynb

Open in Colab

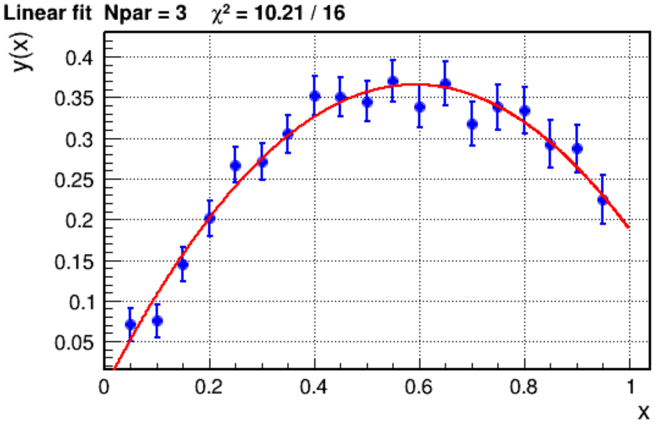
Example of fit with too high polynomial order



Best fit choice?

08_fit3.ipynb Open in Colab

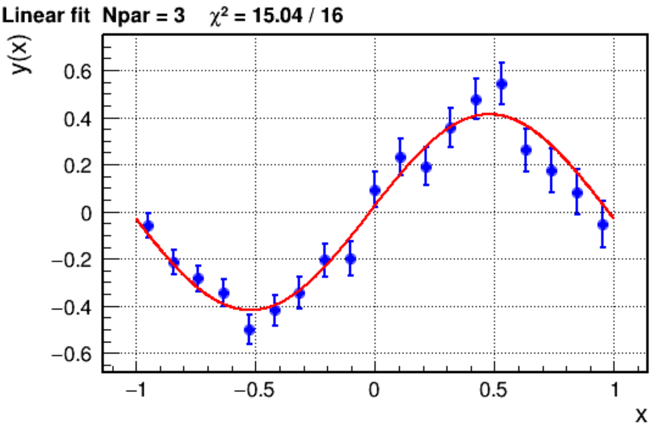
Example of fit with proper polynomial order



Learning on errors

08_fit4.ipynb Open in Colab

When "wrong" set of functions (highly correlated) is selected...



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Learning on errors

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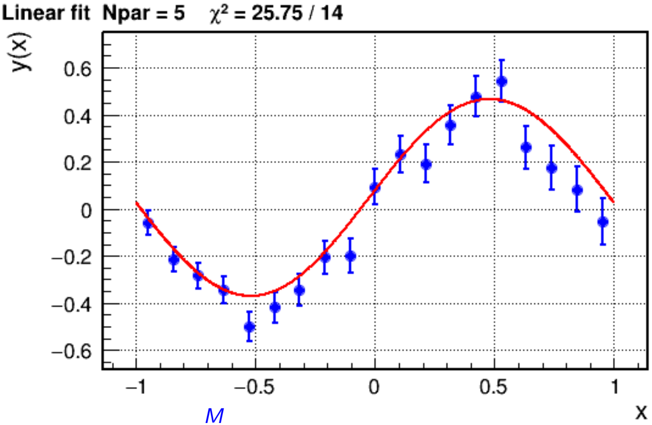

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Learning on errors

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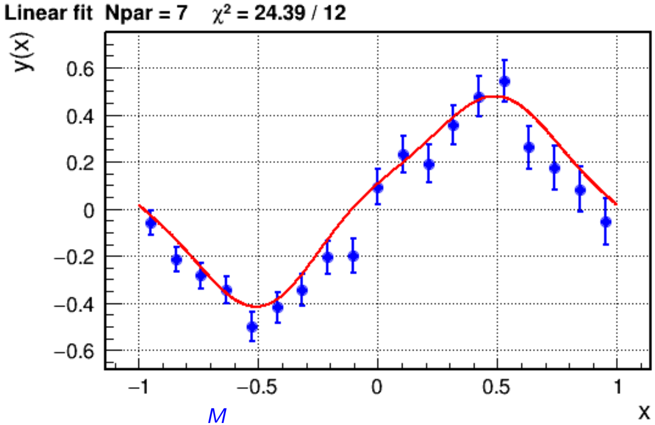

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Learning on errors

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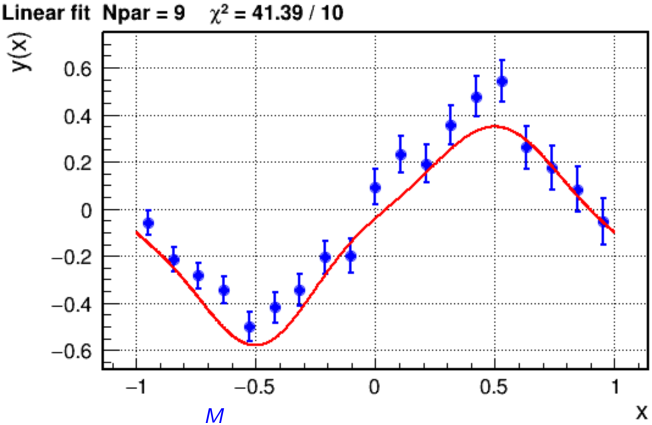
When “wrong” set of functions (highly correlated) is selected…

Poor numerical precision due to high correlations between parameters.



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Learning on errors

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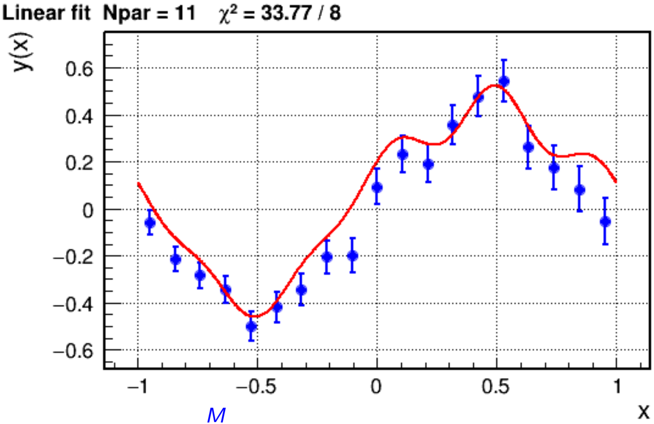
Poor numerical precision due to high correlations between parameters.

$\sin^2(x) + \cos^2(x) = 1$



$$y(x) = a_0 + \sum_{n=1}^{M} a_{2n-1} \sin^n(x) + a_{2n} \cos^n(x) \qquad M = 5$$

Polynomial fit example

For clarity of notation, it is convenient to change parameter numbering to $k,\ l = 0 \ldots M$ (for polynomial fit of order M, $M+1$ parameters).

$$\mathbb{A}_{l\,k} = \sum_{i=1}^{N} \frac{x_i^{(l+k)}}{\sigma_i^2} \quad \text{and} \quad b_l = \sum_{i=1}^{N} \frac{x_i^l\ y_i}{\sigma_i^2}$$

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For uniform uncertainties it is then:

$$\mathbb{A} = \frac{1}{\sigma^2} \sum_{i=1}^{N} \begin{pmatrix} 1 & x_i & \ldots & x_i^M \\ x_i & x_i^2 & \ldots & x_i^{M+1} \\ \vdots & & & \vdots \\ x_i^M & x_i^{M+1} & \ldots & x_i^{2M} \end{pmatrix} \qquad \mathbf{b} = \frac{1}{\sigma^2} \sum_{i=1}^{N} \begin{pmatrix} y_i \\ y_i\ x_i \\ \vdots \\ y_i\ x_i^M \end{pmatrix}$$

quite simple to implement...

Uncertainty estimate

The χ^2 value at the minimum can be then calculated as:

$$\tilde{\chi}^2 = (\mathbf{y} - \mu(\mathbf{x}; \mathbf{a}))^\intercal \, \mathbb{A} \, (\mathbf{y} - \mu(\mathbf{x}; \mathbf{a}))$$

Its distribution should correspond to the χ^2 distribution for $N_{df} = N - M$

Uncertainty estimate

The χ^2 value at the minimum can be then calculated as:

$$\tilde{\chi}^2 = (\mathbf{y} - \mu(\mathbf{x};\mathbf{a}))^\mathsf{T} \, \mathbb{A} \, (\mathbf{y} - \mu(\mathbf{x};\mathbf{a}))$$

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If uncertainty is the same for all measurements, the extracted parameter values are independent on it (!).

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Its distribution should correspond to the χ^2 distribution for $N_{df} = N - M$

If uncertainty is the same for all measurements, the extracted parameter values are independent on it (!). We can use the calculated value of $\tilde{\chi}^2$ to validate the model (test model hypothesis), but also to "correct" our uncertainties, if we consider them unreliable (or they are unknown):

$$\tilde{\sigma}^2 = \frac{\sigma^2 \, \tilde{\chi}^2}{N - M}$$

This is useful in particular when $\tilde{\chi}^2 \ll N_{df}$ (overestimated σ)
For $\tilde{\chi}^2 \gg N_{df}$ we need to consider the possibility that our model is wrong...

Multiple independent variables

The described approach works also for multi-dimensional dependencies!

For example, we can consider polynomial of order M in two coordinates:

$$\mu(x, z; \mathbf{a}) = \sum_{k=0}^{M} \sum_{l=0}^{M} a_{kl}\, x^k\, z^l$$

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All we need to do is to order the pairs of indexes, so that vector **a** is properly defined.
Example for $M = 1$ (2-D plane): $\mathbf{a} = (a_{00}, a_{10}, a_{01})$

$$\mathbb{A} = \frac{1}{\sigma^2} \sum_{i=1}^{N} \begin{pmatrix} 1 & x & z \\ x & x^2 & x\,z \\ z & x\,z & z^2 \end{pmatrix} \qquad \mathbf{b} = \frac{1}{\sigma^2} \sum_{i=1}^{N} \begin{pmatrix} y \\ y\,x \\ y\,z \end{pmatrix}$$

where measurement indexes $i = 1 \ldots N$ were skipped for variables x_i, y_i and z_i

Least-squares method

Homework

Solutions to be uploaded by December 14.

Download the set of data from the lecture home page.

Use linear regression method to fit polynomial dependence to the data.

Calculate p-value for the 2nd order polynomial (parabola) fit.

Find the order of polynomial, which is adequate for the description of the data and give arguments for your choice.