# Statistical analysis of experimental data
# **Least-squares method (2)**

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**Lecture 08**

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## Least-squares method (2)

1. Non-linear fit procedure
2. $F$-test
3. Constrained fit
4. Homework

# $\chi^2$ distribution

## Maximum Likelihood Method

see lectures 04 and 05

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 $\sigma_i$ are known

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

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 $\chi^2$

## $\chi^2$ distribution

We conclude that distribution of $\chi^2$ is described by Gamma pdf with:

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

Properties of the $\chi^2$ distribution (see lecture 02)

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

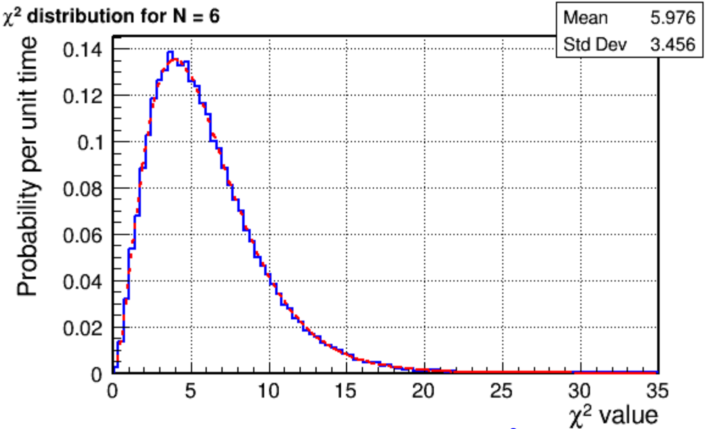
$$\mathbb{V}(\chi^2) = \frac{k}{\lambda^2} = 2N$$

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

For small N, value of $\chi^2$ is a subject to large fluctuations...

## $\chi^2$ distribution

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




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

## Reduced $\chi^2$

When discussing consistency of large data samples it is often convenient to use reduced $\chi^2$ value:

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

Distribution of $\chi^2_{red}$ is again described by Gamma pdf with

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

Properties of the distribution:

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

## General case

We introduced $\chi^2$ in a very general form:

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

where different $\mu_i$ and $\sigma_i$ are possible for each of N measurement $y_i$

It is quite often the case that values of $\mu_i$ 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 $\chi^2$ 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.

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 on given set of points $x_i$ should work best...

## Parameter fit

Bonamente

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

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

which can be rewritten as:

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

or in the matrix form:

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

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

## Parameter fit

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

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

This also gives us the estimate of parameter covariance matrix:

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

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...

## 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).

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

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...

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# Non-linear fit procedure

## General case

We consider $\chi^2$ in a general form:

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

where in general different $\sigma_i$ are allowed for each of N measurements $y_i$.

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Values of $\mu_i$ depend on some controlled variables $x_i$ and a set of model parameters **a**:

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

We look for the best estimate of **a**, which should correspond to the global minimum of $\chi^2(\mathbf{a})$ for given set of data points $(x_i, y_i)$.

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For linear problem, this minimum can be found directly... (lecture 07)

For non-linear problems, we need to use iterative procedures...

## Iterative procedure (Brandt)

We start from some "initial guess" of parameter values $\mathbf{a_0}$.

Assuming small variations of the model parameters, $\mathbf{a} = \mathbf{a_0} + \delta\mathbf{a}$, we can expand $\chi^2$ in a series:

$$\chi^2(\mathbf{a}) \;=\; \chi^2(\mathbf{a_0}) - \mathbf{b}\cdot(\mathbf{a} - \mathbf{a_0}) + \ldots$$

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

$$\mathbf{b} \;=\; -\nabla\,\chi^2(\mathbf{a_0}) \qquad\qquad b_j \;=\; -\frac{\partial\chi^2}{\partial a_j} \;=\; \sum_{i=1}^{N} \frac{2(y_i - \mu_i)}{\sigma_i^2}\cdot\frac{\partial\mu_i}{\partial a_j}$$

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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 (Brandt)

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

$$\chi^2(\mathbf{a}) = \chi^2(\mathbf{a_0}) - \mathbf{b}\cdot(\mathbf{a}-\mathbf{a_0}) + \frac{1}{2}(\mathbf{a}-\mathbf{a_0})^\mathsf{T}\mathbb{A}(\mathbf{a}-\mathbf{a_0}) + \ldots$$

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

$$\mathbb{A}_{jk} = \left.\frac{\partial^2\chi^2}{\partial a_j\,\partial a_k}\right|_{\mathbf{a}=\mathbf{a_0}}$$

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

$$\nabla \chi^2(\mathbf{a}) = -\mathbf{b} + \mathbb{A} (\mathbf{a} - \mathbf{a_0})$$

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$$\nabla\,\chi^2(\mathbf{a}) \;=\; -\,\mathbf{b} \,+\, \mathbb{A}\,(\mathbf{a}-\mathbf{a_0}) \;=\; 0$$

$$\Rightarrow\quad \mathbf{a_m} \;=\; \mathbf{a_0} \,+\, \mathbb{A}^{-1}\mathbf{b}$$

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

## Iterative procedure (Brandt)

Efficiency of the iterative procedure depends strongly on the model and the data used, but also on the initial choice of model parameters $\mathbf{a_0}$.

# Non-linear fit procedure

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If our "initial guess" is close to the true minimum, procedure based on Hessian matrix inversion is very efficient and converges fast.
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There are many different numerical algorithms for solving this problem, and there is no universal "best choice"...

One of the main problems in minimization is that finding the minimum does not guarantee that it is a global minimum...

## Marquardt Minimization (Brandt)

One of the popular approaches, combining the two previously discussed:

$$\mathbf{a_{i+1}} = \mathbf{a_i} + \varepsilon \mathbf{b} \qquad \mathbf{a_{i+1}} = \mathbf{a_i} + \mathbb{A}^{-1}\mathbf{b}$$

## Marquardt Minimization

(Brandt)

One of the popular approaches, combining the two previously discussed:

$$\mathbf{a_{i+1}} = \mathbf{a_i} + (\mathbb{A} + \lambda \cdot \mathbb{I})^{-1}\, \mathbf{b}$$

where $\lambda$ is an additional parameter determining the performance of the algorithm:

- for $\lambda \gg 1$ we make a small step along the gradient direction
  which corresponds to the gradient minimization with $\varepsilon \approx \frac{1}{\lambda}$
- for $\lambda \ll 1$ we try to "jump" directly to the minimum position
  Hessian matrix solution is reproduced for $\lambda \to 0$

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The key element proposed by D.W.Marquardt (1963) was to use variable $\lambda$ parameter, adjusting its value to the results of the previous step...

## Marquardt Minimization (Brandt)

The following algorithm can be used:

1. Take initial parameter values $\mathbf{a_0}$ resulting in $\chi^2$ value of $\chi^2_0$. Assume $\lambda_0 = 0.01$.

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3. Calculate new parameter vector:

$$\mathbf{a_{i+1}} = \mathbf{a_i} + (\mathbb{A} + \lambda_i \cdot \mathbb{I})^{-1} \mathbf{b}$$

and calculate the corresponding value of $\chi^2_{i+1}$

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and calculate the corresponding value of $\chi^2_{i+1}$
4. Compare with the previous iteration:
   - If $\chi^2_{i+1} < \chi^2_i$:
     $\Rightarrow$ accept the new parameter set and decrease $\lambda$ by factor 10
   - If $\chi^2_{i+1} \geq \chi^2_i$:
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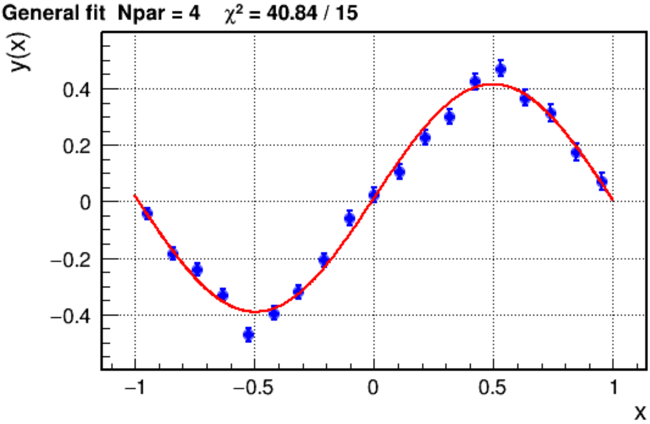
5. Iterate points 2–4 until required precision reached

## Marquardt Minimization example

Fitting Fourier series to example data set




$$y(x) \quad = \quad a_1 + a_2 \sin(a_0\ x) + a_3 \cos(a_0\ x)$$

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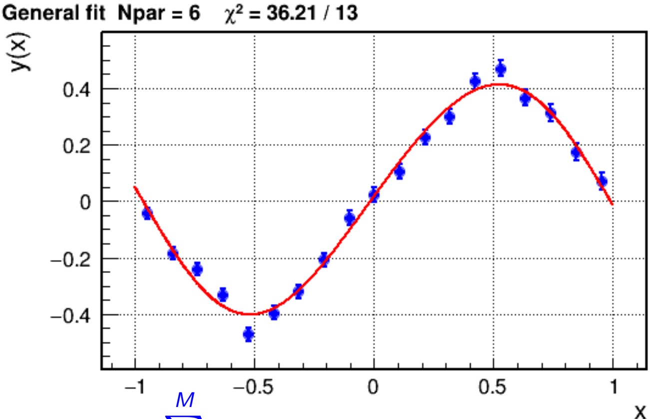


$$y(x) \quad = \quad a_1 + \sum_{n=1}^{M} a_{2n} \sin(n a_0 x) + a_{2n+1} \cos(n a_0 x) \qquad M = 2$$

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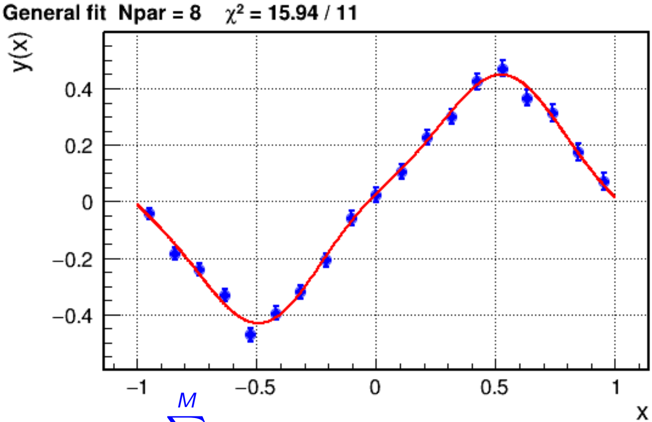
Fitting Fourier series to example data set




$$y(x) \quad = \quad a_1 + \sum_{n=1}^{M} a_{2n} \sin(n a_0 x) + a_{2n+1} \cos(n a_0 x) \qquad M = 3$$

## Marquardt Minimization example

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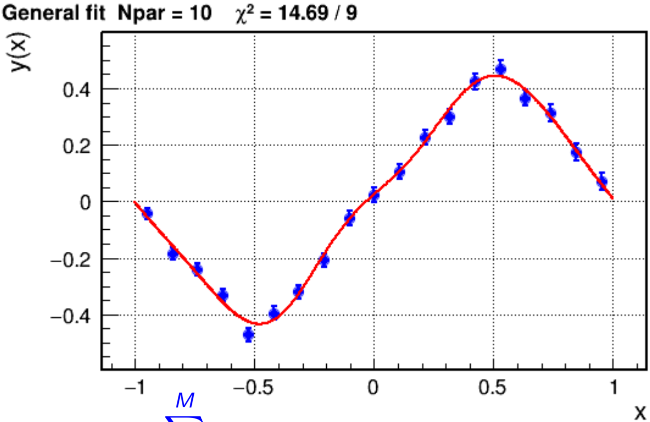


$$y(x) = a_1 + \sum_{n=1}^{M} a_{2n} \sin(n a_0 x) + a_{2n+1} \cos(n a_0 x) \qquad M = 4$$

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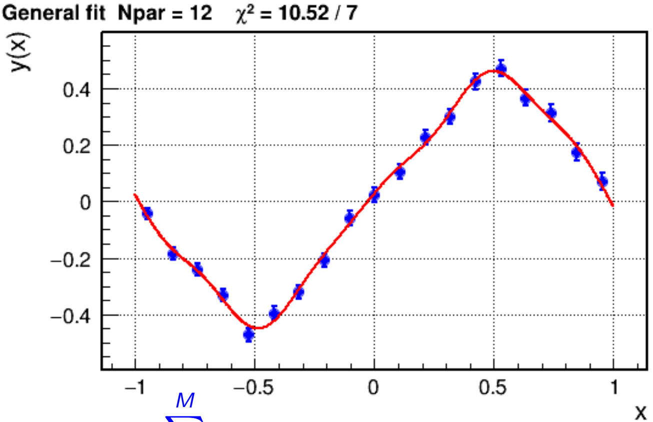
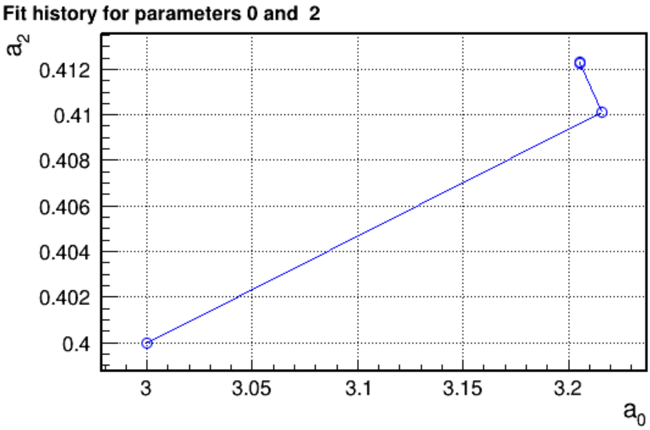



$$y(x) = a_1 + \sum_{n=1}^{M} a_{2n} \sin(n a_0 x) + a_{2n+1} \cos(n a_0 x) \qquad M = 5$$

## Marquardt Minimization example

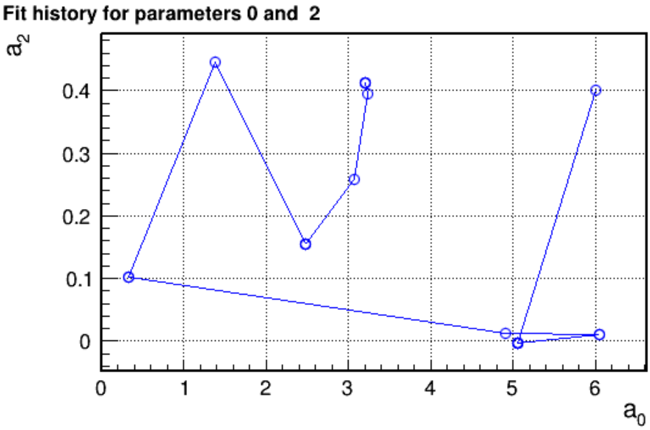
Fit converges fast when the initial values are "correct" $(a_0 = 3)$




$$y(x) = a_1 + a_2 \sin(a_0\ x) + a_3 \cos(a_0\ x)$$

## Marquardt Minimization example

Much slower convergence when the initial values are "wrong" $(a_0 = 6)$

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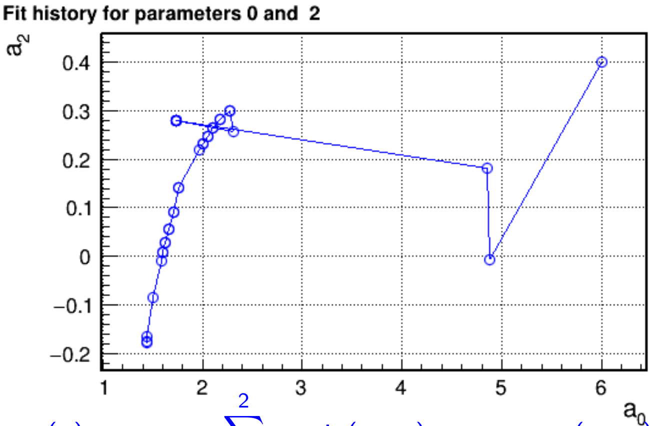
## Marquardt Minimization example

"Wrong" initial values can result in incorrect result $(a_0 = 6)$

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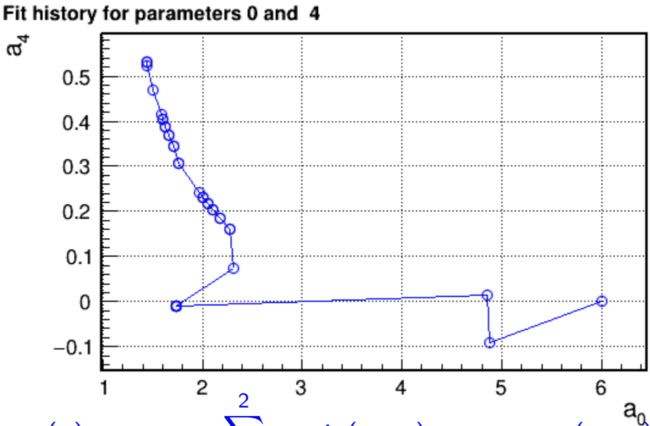


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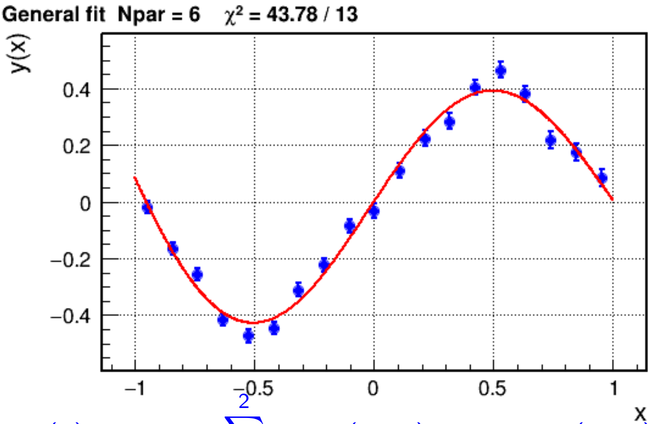


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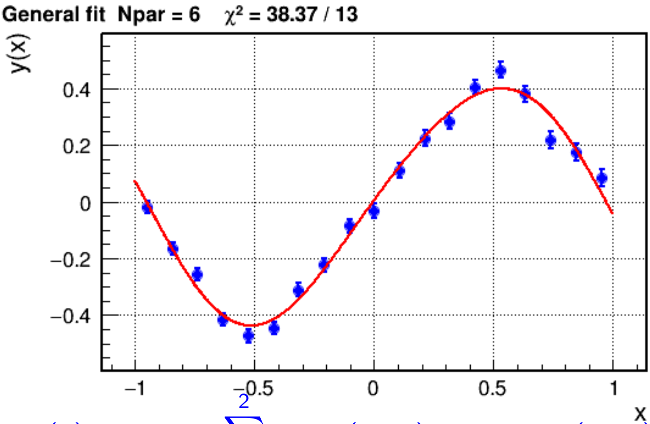
## Marquardt Minimization example

Result of the same fit with "correct" initial values $(a_0 = 3)$




$$y(x) = a_1 + \sum_{n=1}^{2} a_{2n} \sin(n a_0 x) + a_{2n+1} \cos(n a_0 x)$$

## Using derivatives

There are many different algorithms with multiple implementations (libraries and programs) for least-square fits of model parameters.

However, general algorithms need to be based on numerical calculation of model function derivatives.

Using dedicated code, with analytical derivative calculation (as in the presented examples) has advantages:

- number of calls to model function significantly reduced (speed)
- better precision of derivatives/numerical stability
- possibility to tune fit performance to particular needs
  to further improve fit efficiency

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- possibility to tune fit performance to particular needs to further improve fit efficiency

When large number of fits is to be performed to similar sets of data, one should consider implementing his/hers own fit procedure...

## Least-squares method (2)

## Comparison of variances

If the precision of the measurement is known, we can calculate the $\chi^2$ value resulting from the fit (or arithmetic averaging in the simplest case) to verify the consistency of the procedure (uncertainty estimate in particular).

However, we can also try to compare two independent series of measurements to check, if they are consistent. We can do it even, if our estimate of experimental uncertainties is not very reliable.

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We define the random variable $F$ as: introduced by R.A.Fisher in 1924

$$F = \frac{\chi_1^2/N_1}{\chi_2^2/N_2}$$

where $\chi_1^2$ and $\chi_2^2$ are $\chi^2$ values (or sample variances if we set $\sigma \equiv 1$) of the two independent measurements with $N_1$ and $N_2$ degrees of freedom.

## $F$ variable distribution

Distribution of the Fisher's $F$ variable is given by:

$$f(F; N_1, N_2) \;=\; A(N_1, N_2)\; F^{\,\frac{N_1}{2}-1} \left(1 + \frac{N_1}{N_2}\, F\right)^{-\frac{N_1+N_2}{2}}$$

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Expected (mean) value of $F$ is slightly above one:

$$\langle F \rangle \;=\; \frac{N_2}{N_2 - 2} \qquad\qquad N_2 > 2$$

and the variance is:

$$\mathbb{V}(F) \;=\; \frac{2}{N_1} \cdot \frac{N_2^2 (N_1 + N_2 - 2)}{(N_2 - 2)^2 (N_2 - 4)}$$

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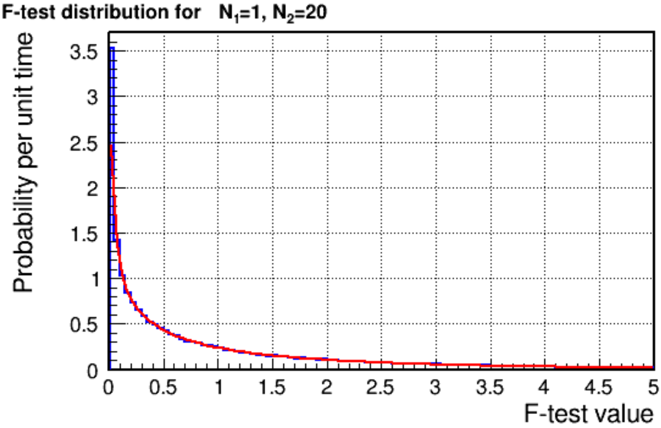
$$\mathbb{V}(F) \;\approx\; \frac{2}{N_1}$$

(for $N_2 \gg N_1$ given by the variance of the reduced $\chi^2$ with $N_1$ d.o.f.)

## *F* variable distribution

Example distributions of the Fisher's *F* variable



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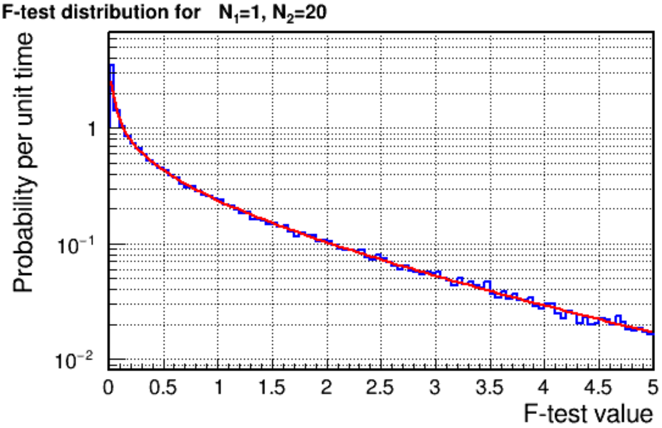

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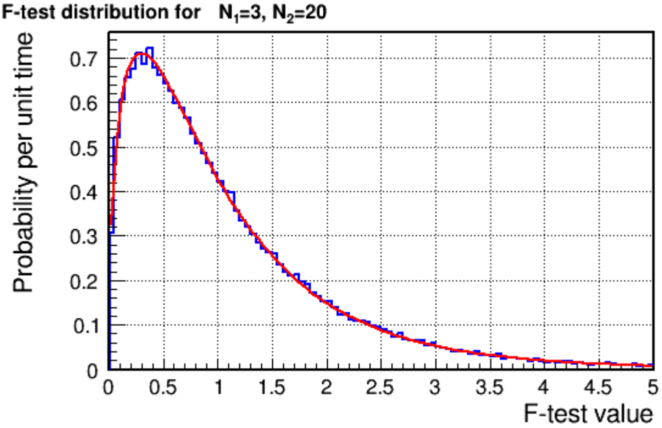

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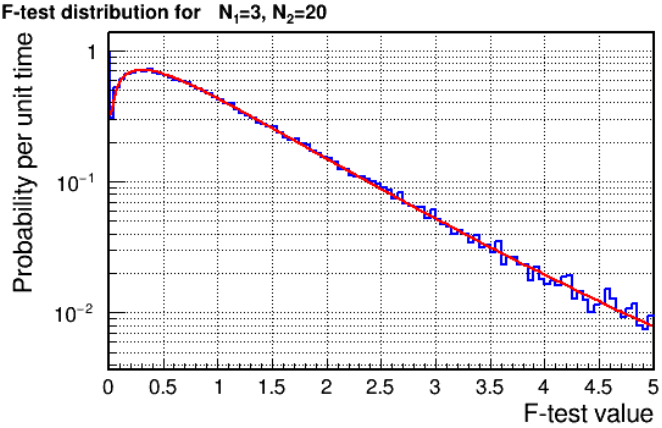

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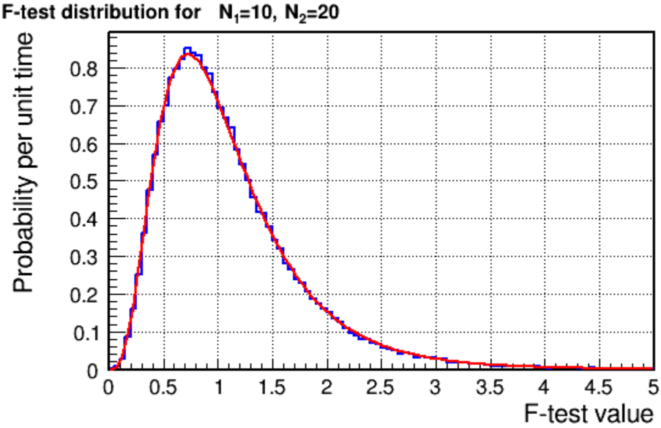

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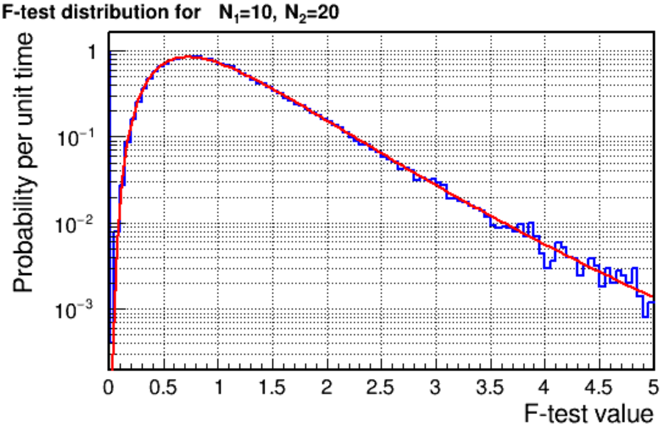


Significant tail towards high values, even for relatively large $N_1, N_2$

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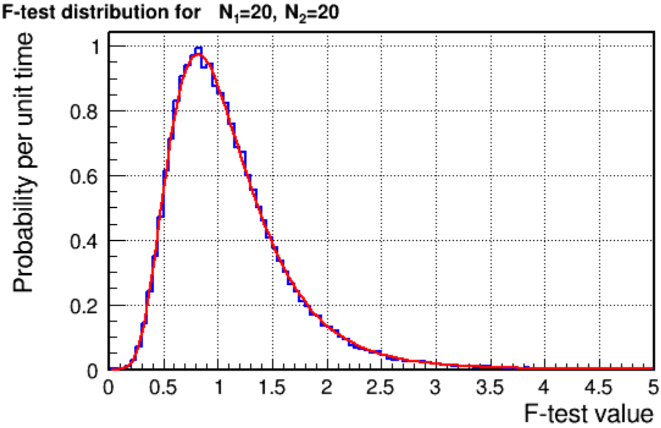


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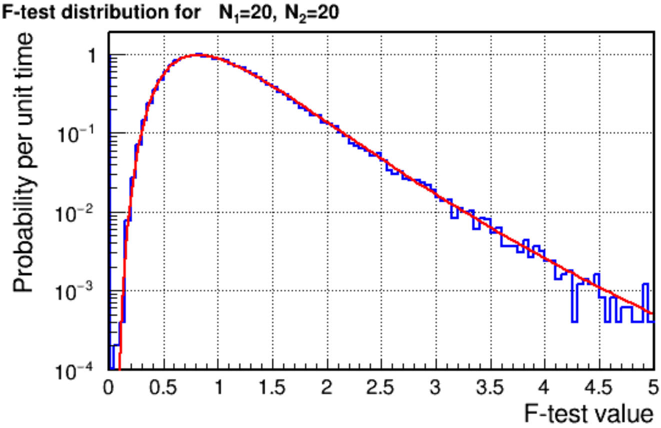


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## $F$-test

When the calculated value of $F$ is large, $F \gg 1$, we can conclude that the two considered data sets are not consistent...

However, we need to be careful, as large fluctuations possible!

Conclusion can depend on the assumed confidence level for $F$, i.e. the maximum probability we allow for given (or higher) value to result from the statistical fluctuations in the (consistent) data sets.

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We can define critical value of $F$, $F_{crit}$, corresponding the the frequentist upper limit for given confidence level CL:

$$\int_0^{F_{crit}} dF\, f(F) \;=\; \mathrm{CL} \qquad\qquad \int_{F_{crit}}^{+\infty} dF\, f(F) \;=\; 1 - \mathrm{CL} \;=\; p$$

## *F*-test (Brandt)

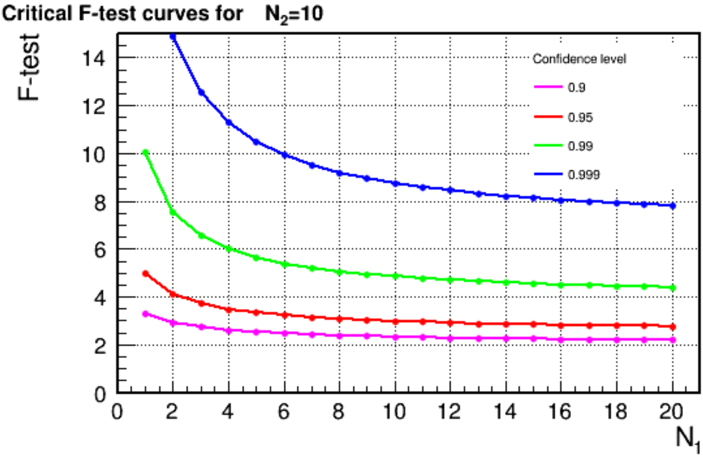
"Critical values" of $F$ for small numbers of degrees of freedom $N_1$ and $N_2$

$$\text{CL} = 0.950 = P = \int_0^{F_P} f(F; f_1, f_2)\,\mathrm{d}F$$

| $N_2$ $f_2$ \ $N_1$ $f_1$ | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 161.4 | 199.5 | 215.7 | 224.6 | 230.2 | 234.0 | 236.8 | 238.9 | 240.5 | 241.9 |
| 2 | 18.51 | 19.00 | 19.16 | 19.25 | 19.30 | 19.33 | 19.35 | 19.37 | 19.38 | 19.40 |
| 3 | 10.13 | 9.552 | 9.277 | 9.117 | 9.013 | 8.941 | 8.887 | 8.845 | 8.812 | 8.786 |
| 4 | 7.709 | 6.944 | 6.591 | 6.388 | 6.256 | 6.163 | 6.094 | 6.041 | 5.999 | 5.964 |
| 5 | 6.608 | 5.786 | 5.409 | 5.192 | 5.050 | 4.950 | 4.876 | 4.818 | 4.772 | 4.735 |
| 6 | 5.987 | 5.143 | 4.757 | 4.534 | 4.387 | 4.284 | 4.207 | 4.147 | 4.099 | 4.060 |
| 7 | 5.591 | 4.737 | 4.347 | 4.120 | 3.972 | 3.866 | 3.787 | 3.726 | 3.677 | 3.637 |
| 8 | 5.318 | 4.459 | 4.066 | 3.838 | 3.687 | 3.581 | 3.500 | 3.438 | 3.388 | 3.347 |
| 9 | 5.117 | 4.256 | 3.863 | 3.633 | 3.482 | 3.374 | 3.293 | 3.230 | 3.179 | 3.137 |
| 10 | 4.965 | 4.103 | 3.708 | 3.478 | 3.326 | 3.217 | 3.135 | 3.072 | 3.020 | 2.978 |

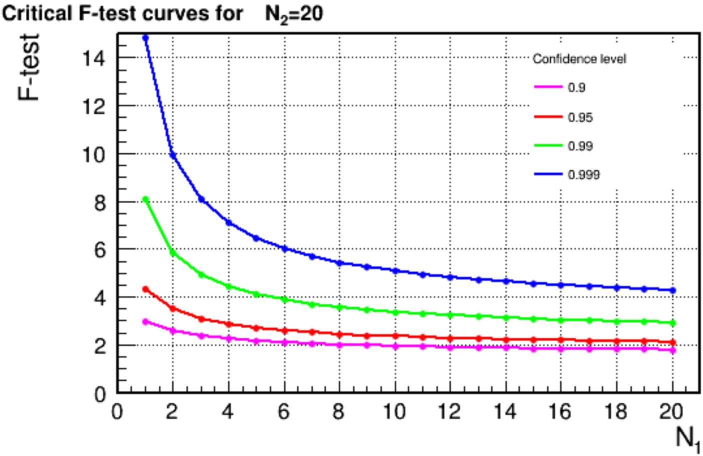
## $F$-test

Plot of "critical values" of $F$ for $N_2 = 10$



## $F$-test

Plot of “critical values” of $F$ for $N_2$ =20




Variations decresase with the size of the reference sample

## $F$-test for fit model (Bonamente)

It turns out that the $F$ variable can also be used to test our fit model.

Let us assume we have a model with $m$ adjustable (free) parameters, which we apply to the set of $N$ data points. Are all model parameters relevant?

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We can consider "reduced" version of model with $m - \Delta m$ parameters. It is clear that the resulting $\chi^2$ value will be larger:

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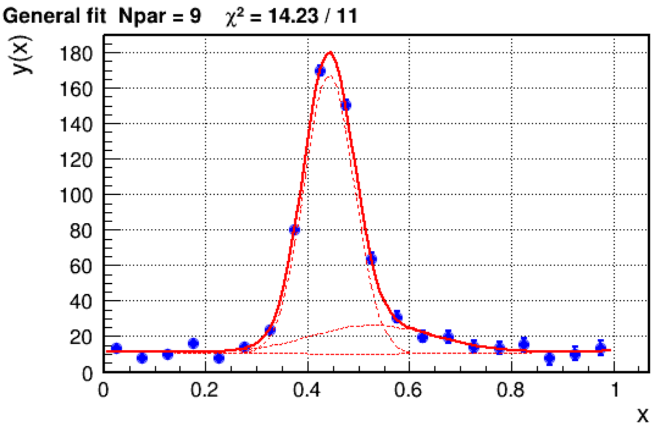
If reduced model is equivalent to the "full" one, distribution of $\Delta\chi^2$ is given by the $\chi^2$ distribution with $\Delta m$ degrees of freedom. We can test this hypothesis by considering:

$$F = \frac{\Delta\chi^2/\Delta m}{\chi^2_{(m)}/(N-m)}$$

where we need to note that $\chi^2_{(m)}$ and $\Delta\chi^2$ are independent.

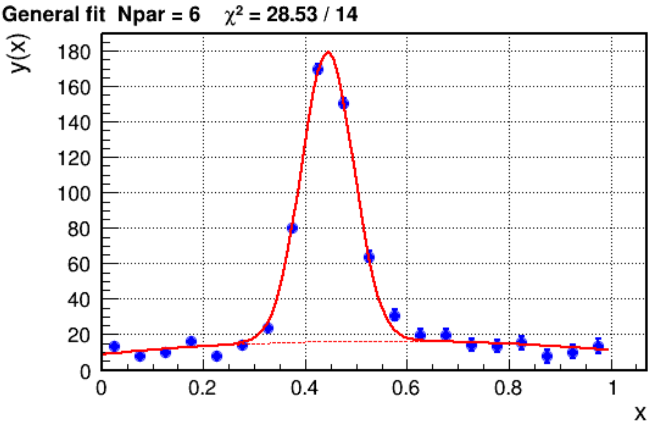
## $F$-test for fit model

Example of $F$-test application. We try to fit the data with polynomial background (3 parameters) and two Gaussian peaks (3+3 parameters).



## *F*-test for fit model

Example of *F*-test application. Is the second signal component really needed?! Fit with one peak gives a reasonable description of the data.



## $F$-test for fit model

Example of $F$-test application.

$$N = 20 \qquad m = 9$$

$$\chi^2_{(m)} \approx 14.23 \qquad \chi^2_{(m)}/(N-m) \approx 1.294$$

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There is about 5% chance that the improvement in the fit result, when adding the second signal component, was only due to the statistical fluctuations in the data...

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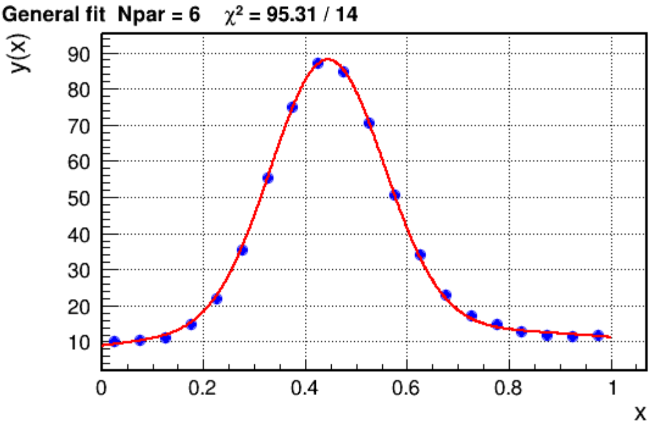
Second component fit result misleading: $A_2 = 4.950 \pm 1.523$ $(3.25\sigma)$

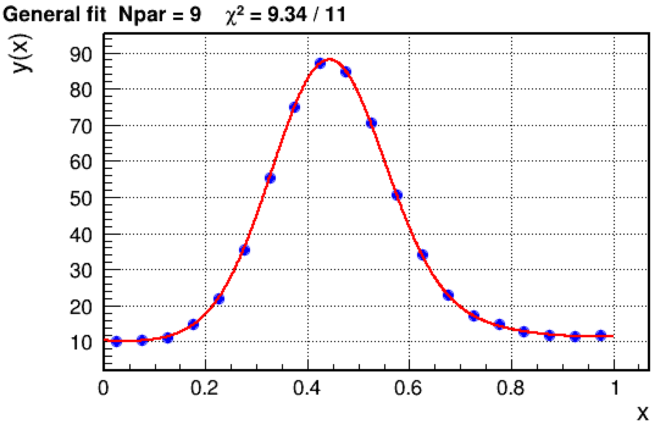
## *F*-test for fit model

Example (2). Significantly reduced measurement errors.
Fit with one signal component.



## *F*-test for fit model

Example (2). Significantly reduced measurement errors.
Fit with two signal components.



## $F$-test for fit model

Example (2) of $F$-test application.

$$N = 20 \quad m = 9 \quad \Delta m = 3$$

$$\chi^2_{(m)} \approx 9.34 \qquad \chi^2_{(m)}/(N-m) \approx 0.849$$

$$\Delta\chi^2 \approx 85.97 \qquad \Delta\chi^2/\Delta m \approx 28.66$$

$$F \approx 33.75$$
$$p \approx 8 \cdot 10^{-6}$$

corresponding to about 4.3 $\sigma$ deviation...

Can not yet be claimed as discovery, but significant enough to be shown...

## Least-squares method (2)

## Model constraints

Different quantities measured in our experiment can be related.

Relations, which are usually given in form of equations, can be due to theoretical predictions, model assumptions or experimental constraints.
For example:

- measurements of energy and momentum of the particle, are related by the invariant mass formula $E^2 = p^2 + m^2$
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- contribution of different components to the measured distribution can be constrained by the total normalization of the sample
- distributions can be constrained by the acceptance of the detector
- we can make additional assumptions regarding eg. symmetry of the distribution or asymptotic behavior

## Model constraints

We consider set of $N$ measurement points $(x_i, y_i)$, which can be compared to model predictions depending on parameters $\mathbf{a}$ in terms of the $\chi^2$ value:

$$\chi^2(\mathbf{a}) = \sum_{i=1}^{N} \frac{(y_i - \mu(x_i, \mathbf{a}))^2}{\sigma_i^2}$$

Best estimate of $\mathbf{a}$ should correspond to the minimum of $\chi^2(\mathbf{a})$.

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How can we find the best parameter values in this case?

## Model reduction

The first approach is to reduce number of model parameters, using constraints to eliminate some of the model variables.

We thus reduce the problem with $M$ model parameters to problem with $M' = M - K$ independent parameters. (method of elements)

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## Example

We would like to fit polynomial model to a series of measurements where the polar angle $\theta \in [-\pi, +\pi]$ is the controlled variable:

$$\mu(x; \mathbf{a}) = \sum_{k=0}^{M-1} a_k \left(\frac{\theta}{\pi}\right)^k = \sum_k a_k \, x^k$$

where we introduced $x = \frac{\theta}{\pi}$ for simplicity.

And we expect that the distribution should vanish for $\theta \to \pm\pi$:

$$\mu(-1; \mathbf{a}) = \mu(+1; \mathbf{a}) = 0 \qquad K = 2$$

## Model reduction example

Our constraints give us direct relations between model parameters:

$$\mu(+1; \mathbf{a}) = \sum_k a_k \, (+1)^k = 0$$

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We can add and subtract these two equations to obtain:

$$\sum_{k=0,2,4...} a_k = 0 \quad \text{and} \quad \sum_{k=1,3,5...} a_k = 0$$

$\Rightarrow$ we have independent constrains on even and odd parameters.

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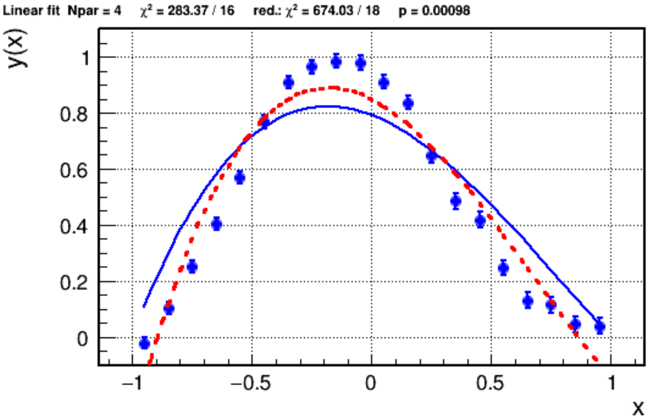
We can reduce number of parameters to $M' = M - 2$ by writing parameters for two highest terms (for even $M$) as:

$$a_{M-2} = -\sum_{k=0,2,4\ldots}^{M-4} a_k \qquad \text{and} \qquad a_{M-1} = -\sum_{k=1,3,5\ldots}^{M-3} a_k$$

## Model reduction example

Example polynomial fit without and with model constraints

$$\mu(-1) = \mu(+1) = 0$$




3rd order polynomial not describing data at all

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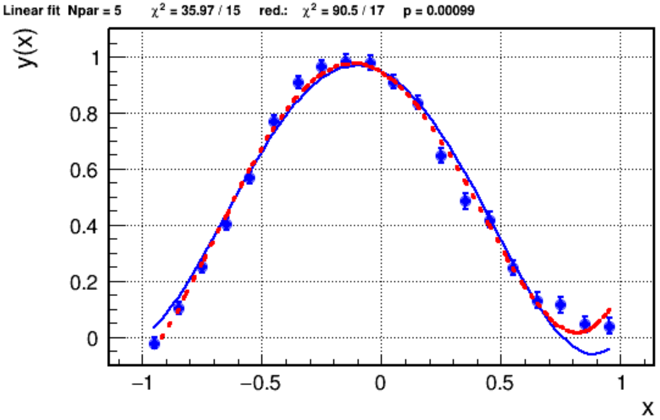


$4^{th}$ order polynomial fit still not satisfactory...

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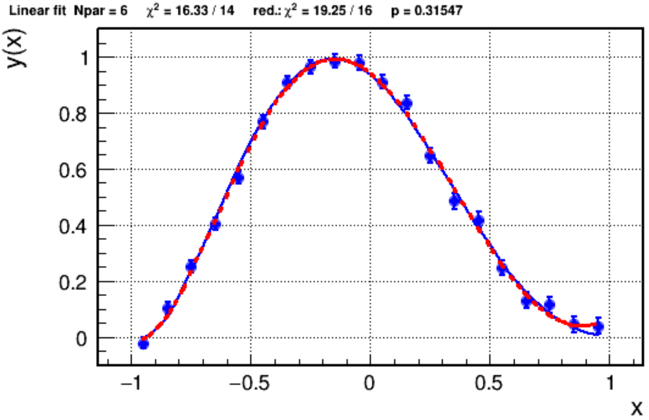


Reasonable description of the data.

## Model reduction example

Example polynomial fit without and with model constraints

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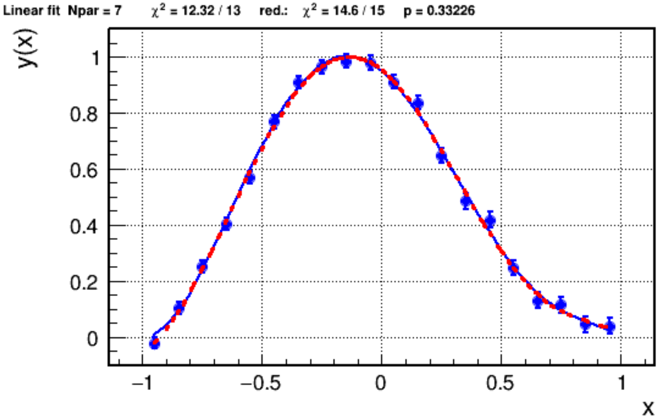


Even better description of the data. Constraints hardly affect the fit...

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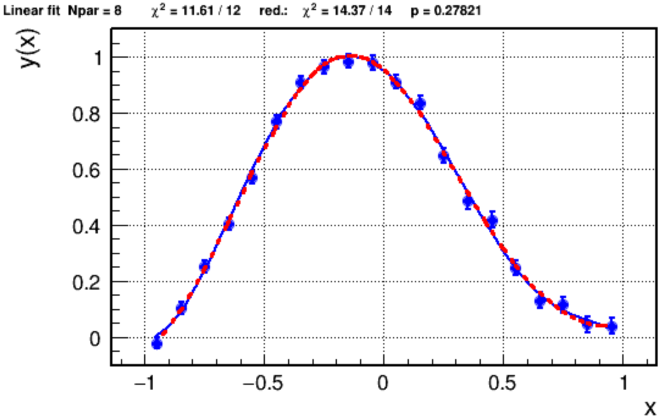



Even better description of the data. Constraints hardly affect the fit...

## Model reduction test

for linear constraints !

We can use $F$-test to verify, if data are consistent with constraints.

We follow the procedure described previously: we have a model with $m$ free parameters and $\Delta m$ constraints, which we test on the set of $N$ data points

Constrained ("reduced") model has $m - \Delta m$ parameters and results in higher $\chi^2$:

$$\Delta\chi^2 = \chi^2_{\text{reduced}} - \chi^2_{\text{full}} \geq 0$$

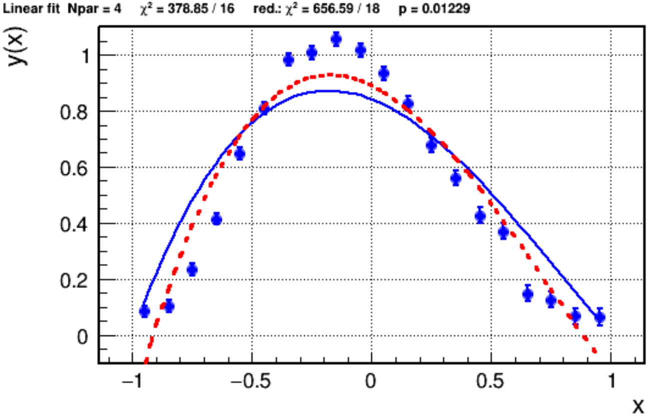
To test if the reduced model is equivalent to the "full" one, we consider:

$$F = \frac{\Delta\chi^2/\Delta m}{\chi^2_{\text{full}}/(N-m)} \qquad \text{and} \qquad p = \int_F^{+\infty} dF' \, f(F')$$

$p$ value (indicated in the plots) describe the probability of given $\chi^2$ change (when imposing constraints) due to statistical fluctuations only.

## Model reduction example (2)

Example polynomial fit without and with model constraints, to inconsistent data set




$3^{rd}$ order polynomial not describing data at all

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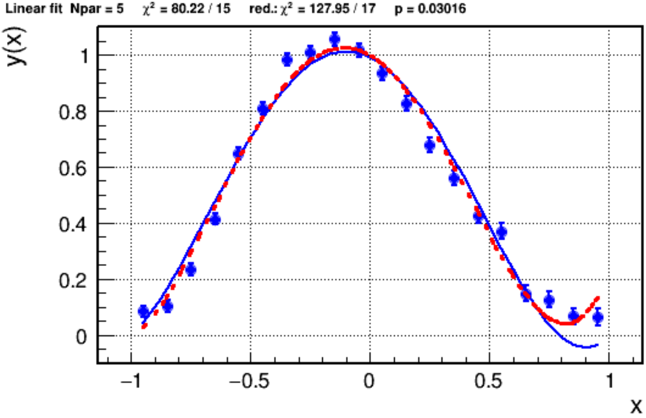


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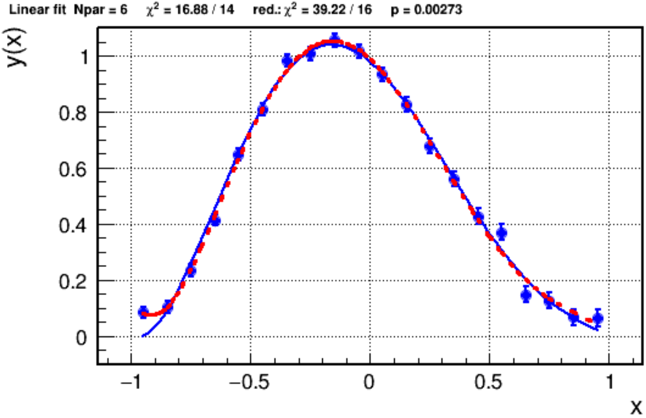
## Model reduction example (2)

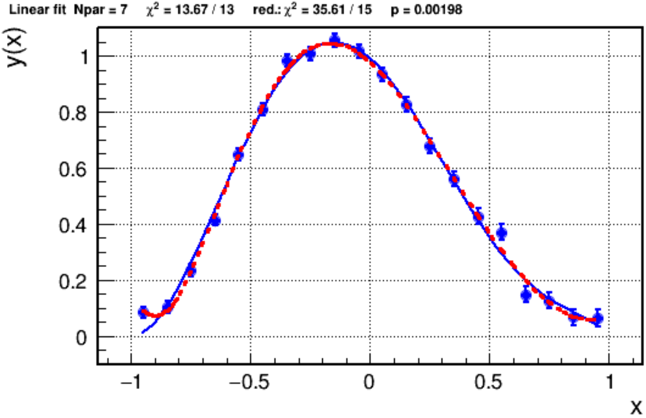
Example polynomial fit without and with model constraints, to inconsistent data set




Reasonable description of the data only without constraints...

## Model reduction example (2)

Example polynomial fit without and with model constraints, to inconsistent data set (generated with $\mu(-1) = \mu(+1) = 0.05$)




*p* value indicates that data is not consistent with constraints...

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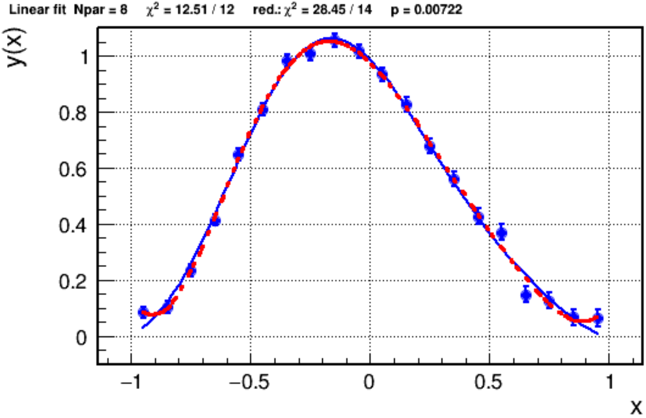


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## Model reduction

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However, elimination of variables is not always possible or can result in problems with minimization / numerical instabilities.

Also, when iterative fit procedure is to be used, initial parameter values should be "guessed", but imposing constraints "by hand" can be difficult.

$\Rightarrow$ while model reduction is a preferred solution, resulting in higher fit efficiency in most cases, we need an alternative...

## Method of Lagrange Multipliers (Behnke)

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

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Our problem is now reduced to finding parameters $\mathbf{a}$ and $\boldsymbol{\lambda}$ fulfilling

$$\frac{\partial \mathcal{L}}{\partial a_j} = 0 \qquad \text{and} \qquad \frac{\partial \mathcal{L}}{\partial \lambda_k} = 0$$

(without any additional constraints)

## Method of Lagrange Multipliers

Writing the full formula for $\mathcal{L}$: $\mu_i = \mu(x_i; \mathbf{a})$

$$\mathcal{L}(\mathbf{a}, \boldsymbol{\lambda}) = \sum_{i=1}^{N} \frac{(y_i - \mu_i)^2}{\sigma_i^2} + \sum_{k=1}^{K} 2\, \lambda_k\, w_k(\mathbf{a})$$

We obtain a set of $M + K$ equations for the same number of parameters:

$$\frac{\partial \mathcal{L}}{\partial a_j} = -2 \sum_{i=1}^{N} \frac{(y_i - \mu_i)}{\sigma_i^2} \frac{\partial \mu_i}{\partial a_j} + 2 \sum_{k=1}^{K} \lambda_k \frac{\partial w_k}{\partial a_j} \qquad j = 1 \ldots M$$

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$$\frac{\partial \mathcal{L}}{\partial \lambda_k} = 2\, w_k(\mathbf{a}) = 0 \qquad k = 1 \dots K$$

Adding constraints modifies the resulting system of equation for **a**...

## Method of Lagrange Multipliers

Let us consider the linear problem (linear in **a**):

$$\mu(x;\mathbf{a}) = \sum_{j=1}^{M} a_j \; f_j(x) \qquad \text{and} \qquad w_k(\mathbf{a}) = \sum_{j=1}^{M} d_{k,\,j} \; a_j \; - \; c_k$$

Our set of equations can be now presented as:

$$\sum_{j=1}^{M} \left( \sum_{i=1}^{N} \frac{f_l(x_i) \; f_k(x_i)}{\sigma_i^2} \right) a_j + \sum_{k=1}^{K} d_{k,\,l} \; \lambda_k = \sum_{i=1}^{N} \frac{f_l(x_i) \; y_i}{\sigma_i^2} \qquad l = 1 \ldots M$$

$$\sum_{j=1}^{M} d_{k,\,j} \; a_j = c_k \qquad k = 1 \ldots K$$

## Method of Lagrange Multipliers

We can write these equations the matrix form:

$$\underbrace{\left(\begin{array}{c|c} \mathbb{A} & \mathbb{D} \\ \hline \mathbb{D}^{\mathsf{T}} & 0 \end{array}\right)}_{\tilde{\mathbb{A}}} \cdot \left(\begin{array}{c} \mathbf{a} \\ \hline \boldsymbol{\lambda} \end{array}\right) = \left(\begin{array}{c} \mathbf{b} \\ \hline \mathbf{c} \end{array}\right)$$

where: $\mathbb{A}_{jk} = \sum_{i=1}^{N} \frac{f_j(x_i)\, f_k(x_i)}{\sigma_i^2}$ , $\mathbb{D}_{jk} = d_{k,\,j}$ and $b_j = \sum_{i=1}^{N} \frac{f_j(x_i)\, y_i}{\sigma_i^2}$

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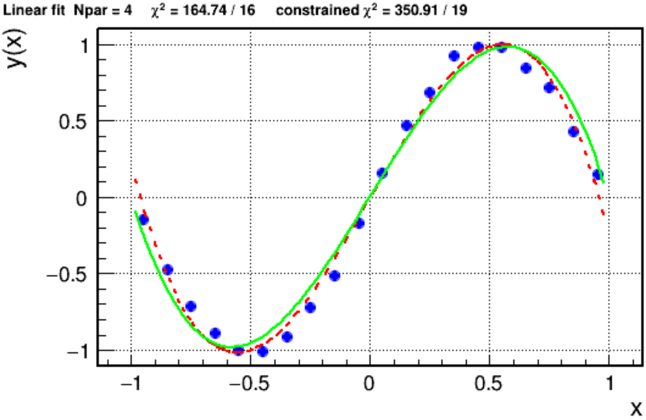
Covariance matrix for **a** can be extracted as:

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

(seems to work for linear problems).

## Lagrange Multipliers example

Fitting $\sin(\pi x)$ with polynomial. Constraints: $\mu(-1) = \mu(0) = \mu(+1) = 0$.




$3^{rd}$ order polynomial

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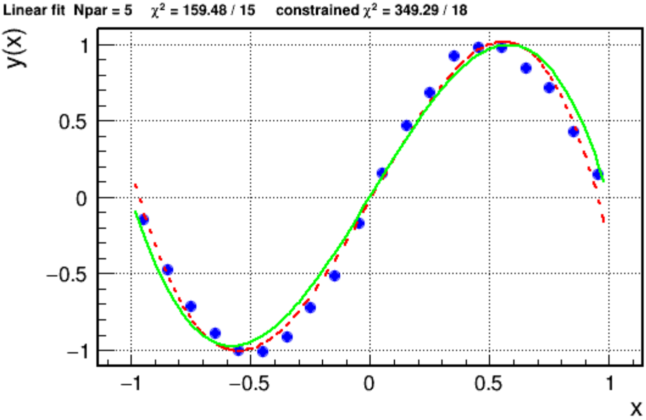


No improvement adding $x^4$ term...

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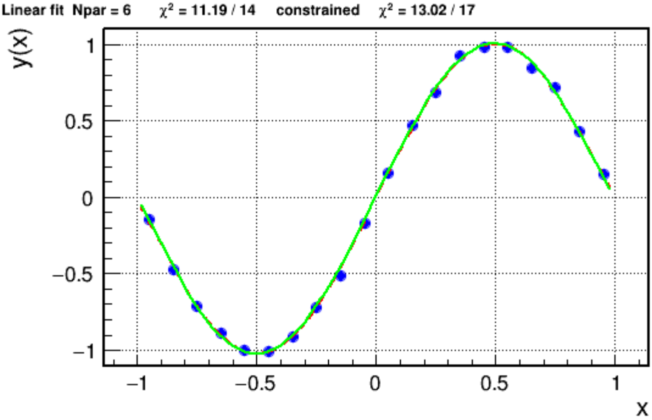
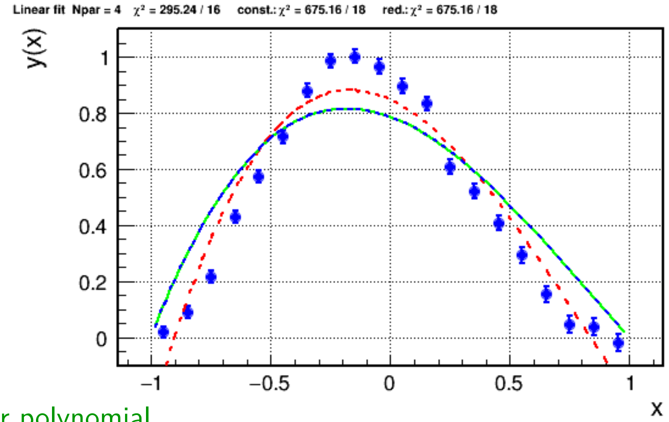



Good description when $x^5$ term included...

## Lagrange Multipliers example (2)

Comparing two approaches to polynomial fit with constraints.

Fit approach: unconstrained    Lagrange multipliers    model reduction

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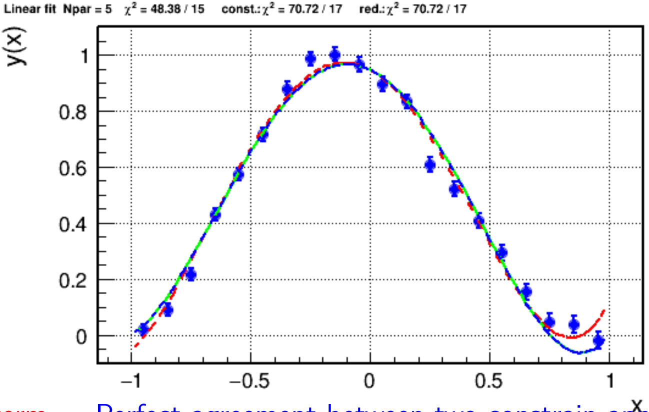


With $x^4$ term Perfect agreement between two constrain approaches

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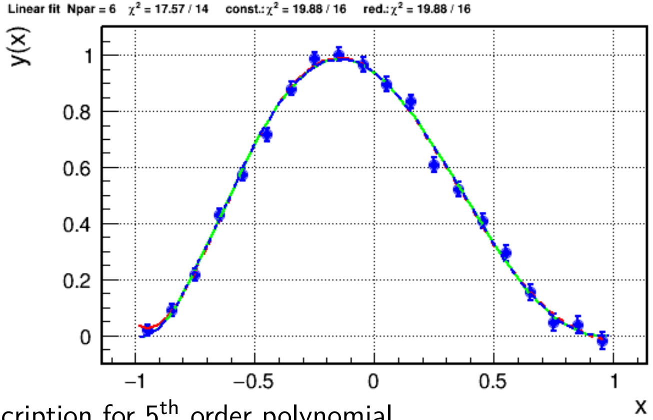


Good description for $5^{th}$ order polynomial...

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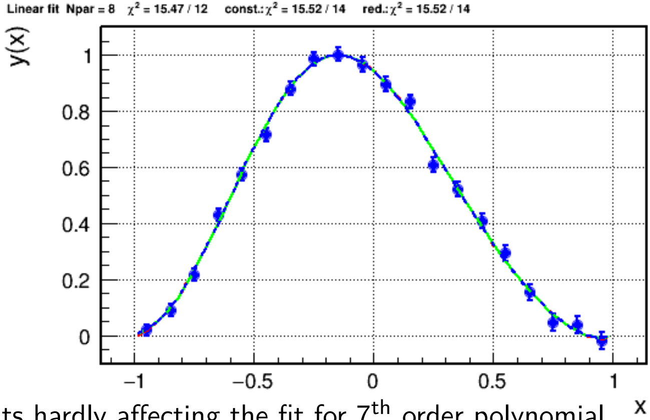


Constraints hardly affecting the fit for $7^{th}$ order polynomial...

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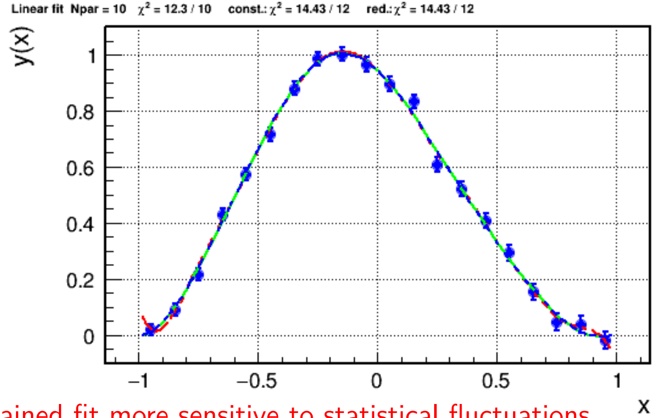



Unconstrained fit more sensitive to statistical fluctuations...

## Least-squares method (2)

## Homework

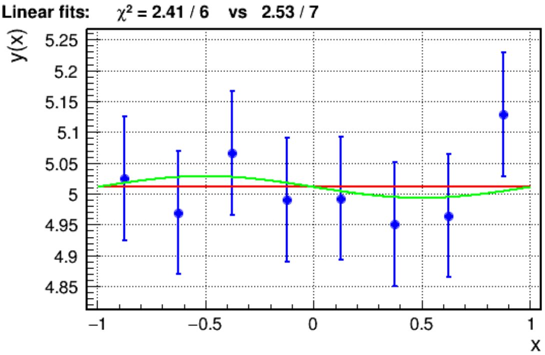
Solutions to be uploaded by December 22.

Consider outcome of the experiment, as illustrated in the figure.

$N = 8$ measurements generated from uniform background model ($\mu = 5$, $\sigma = 0.1$)

Results can be compared to background only model and to background+signal:

$$\mu_b = A$$
$$\mu_{b+s} = B + C \cdot \sin(\pi x)$$



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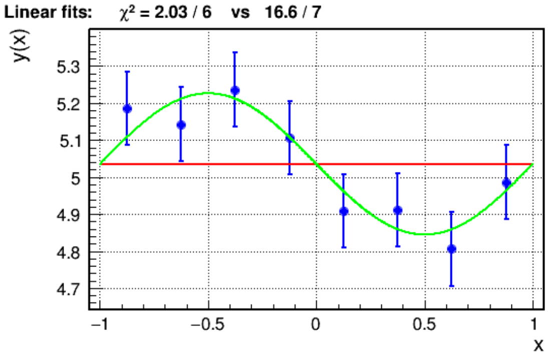

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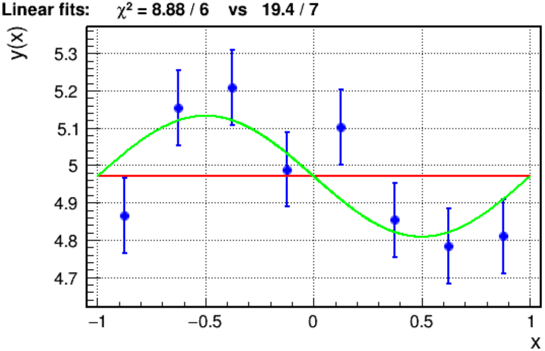


- Estimate probability of fitted $C$ value deviating from zero by more than $3\sigma$

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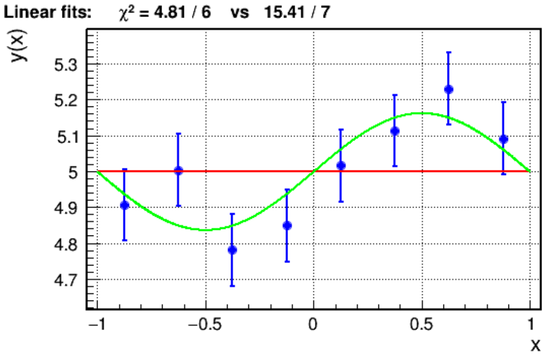


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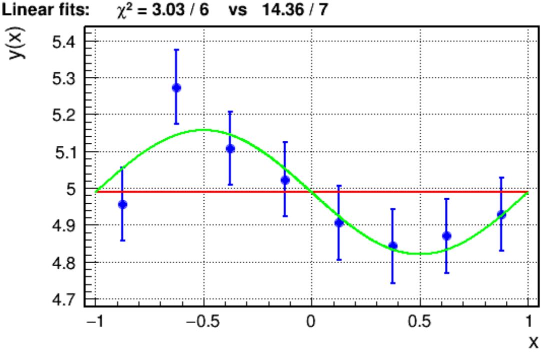


- Estimate probability of fitted $C$ value deviating from zero by more than $3\sigma$
- Verify estimate with simulation

Hint: $\mathbb{A}$ and $\mathbb{C}_{\mathbf{a}}$ do not depend on $y_i$