

Statistical analysis of experimental data

Least-squares method (2)

Aleksander Filip Żarnecki



Lecture 09
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Least-squares method (2)

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

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:

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

assuming σ_i are known

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

χ^2 distribution

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

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

Properties of the χ^2 distribution

(Gamma pdf: see lecture 03)

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

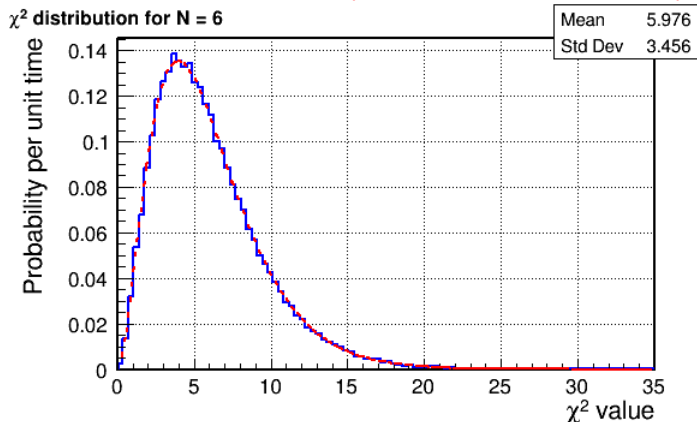
$$\mathbb{V}(\chi^2) = \frac{k}{\lambda^2} = 2N$$

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

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

χ^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 χ^2

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

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

Distribution of χ_{red}^2 is again described by Gamma pdf with

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

Properties of the distribution:

$$\langle \chi_{red}^2 \rangle = 1 \quad \mathbb{V}(\chi_{red}^2) = \sigma_{\chi_{red}^2}^2 = \frac{2}{N}$$

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

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 \mathbf{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.

One of the examples is the polynomial series:

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

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_l :

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

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:

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

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

Parameter fit

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

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

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 , $l = 0 \dots M$ (for polynomial fit of order M , $M + 1$ parameters).

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

For uniform uncertainties it is then:

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

quite simple to implement...

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Values of μ_i depend on some **controlled variables** x_i and a set of model parameters \mathbf{a} :

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We look for the best estimate of \mathbf{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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(lecture 08)

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(lecture 08)

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 expand χ^2 in a series:

$$\chi^2(\mathbf{a}) = \chi^2(\mathbf{a}_0) - 2 \mathbf{b} \cdot (\mathbf{a} - \mathbf{a}_0) + \dots$$

where vector \mathbf{b} is the negative gradient of χ^2 :

$$\mathbf{b} = -\frac{1}{2} \nabla \chi^2(\mathbf{a}_0) \quad b_j = -\frac{1}{2} \frac{\partial \chi^2}{\partial a_j} = \sum_{i=1}^N \frac{y_i - \mu_i}{\sigma_i^2} \cdot \frac{\partial \mu_i}{\partial a_j}$$

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Vector \mathbf{b} defines the direction of steepest χ^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...

Iterative procedure

(Brandt)

We can try to be “smarter”. Expanding χ^2 to quadratic term:

$$\chi^2(\mathbf{a}) = \chi^2(\mathbf{a}_0) - 2 \mathbf{b} \cdot (\mathbf{a} - \mathbf{a}_0) + (\mathbf{a} - \mathbf{a}_0)^T \mathbb{A} (\mathbf{a} - \mathbf{a}_0) + \dots$$

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

$$\mathbb{A}_{jk} = \left. \frac{1}{2} \frac{\partial^2 \chi^2}{\partial a_j \partial a_k} \right|_{\mathbf{a}=\mathbf{a}_0}$$

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In this approximation, we can calculate the expected position of the χ^2 minimum:

$$\nabla \chi^2(\mathbf{a}) = -2 \mathbf{b} + 2 \mathbb{A} (\mathbf{a} - \mathbf{a}_0)$$

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In this approximation, we can calculate the expected position of the χ^2 minimum:

$$\nabla \chi^2(\mathbf{a}) = -2 \mathbf{b} + 2 \mathbb{A} (\mathbf{a} - \mathbf{a}_0) = 0$$

$$\Rightarrow \mathbf{a}_m = \mathbf{a}_0 + \mathbb{A}^{-1} \mathbf{b}$$

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 .

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If our “initial guess” is close to the true (global) minimum, procedure based on the Hessian matrix inversion is very efficient and converges fast.

However, it can be unstable, if we start too far from the actual minimum...

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Iterative procedure based on the gradient calculation is much slower, but it much more robust. **It finds the minimum even when starting from a parameter space point far away from it.**

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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:

$$\mathbf{a}_{i+1} = \mathbf{a}_i + \lambda^{-1} \mathbf{b} \quad (\lambda \equiv 1/\varepsilon) \quad \mathbf{a}_{i+1} = \mathbf{a}_i + \mathbb{A}^{-1} \mathbf{b}$$

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 the value of λ determines 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 $\lambda \rightarrow 0$

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The key element proposed by D.W.Marquardt (1963) was to use variable λ 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 χ^2 value of χ_0^2 .
Assume $\lambda_0 = 0.01$.

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- 2 Calculate matrix \mathbf{A} and vector \mathbf{b} for current \mathbf{a}_i .

Marquardt Minimization

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Assume $\lambda_0 = 0.01$.

- 2 Calculate matrix \mathbb{A} and vector \mathbf{b} for current \mathbf{a}_i .

- 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 χ_{i+1}^2

Marquardt Minimization

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and calculate the corresponding value of χ_{i+1}^2

- 4 Compare with the previous iteration:

- If $\chi_{i+1}^2 < \chi_i^2$:
 \Rightarrow accept the new parameter set and decrease λ by factor 10
- If $\chi_{i+1}^2 \geq \chi_i^2$:
 \Rightarrow keep old parameter values ($\mathbf{a}_{i+1} = \mathbf{a}_i$) and increase λ by factor 10

Marquardt Minimization

(Brandt)

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- 5 Iterate points 2–4 until required precision reached

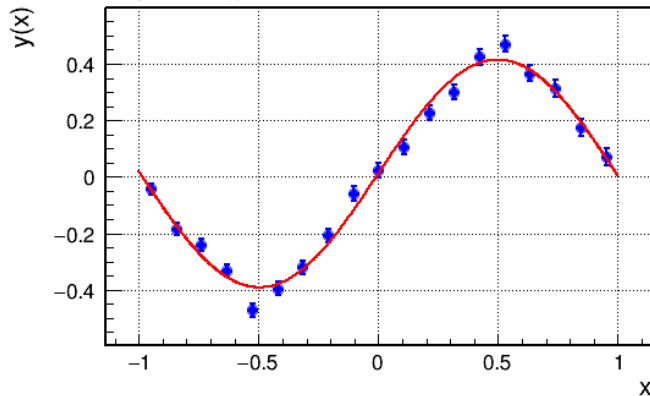
Marquardt Minimization example

09_fit1.ipynb

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Fitting Fourier series to
example data set

General fit Npar = 4 $\chi^2 = 40.84 / 15$



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

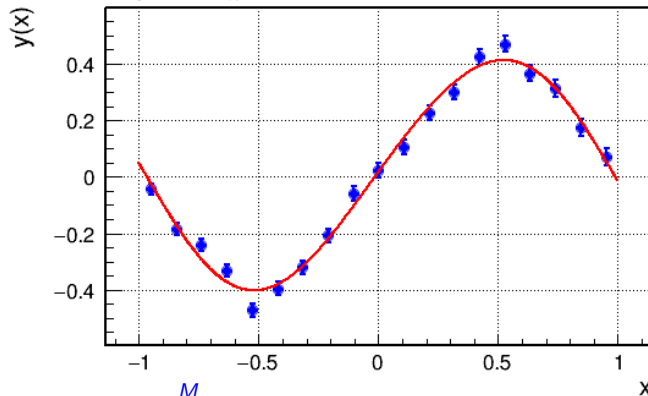
Marquardt Minimization example

09_fit1.ipynb

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Fitting Fourier series to
example data set

General fit Npar = 6 $\chi^2 = 36.21 / 13$



$$y(x) = a_1 + \sum_{n=1}^M a_{2n} \sin(na_0x) + a_{2n+1} \cos(na_0x) \quad M = 2$$

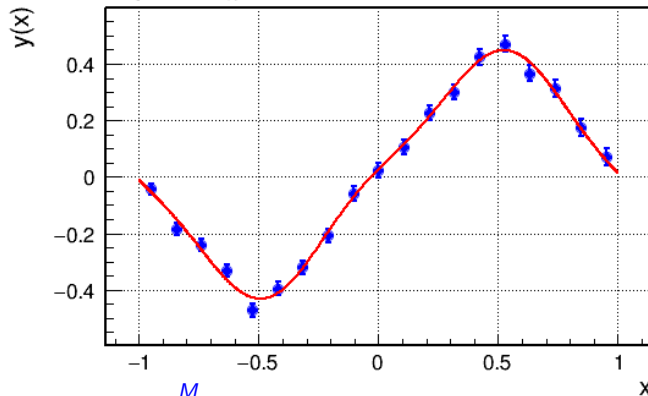
Marquardt Minimization example

09_fit1.ipynb

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Fitting Fourier series to
example data set

General fit Npar = 8 $\chi^2 = 15.94 / 11$



$$y(x) = a_1 + \sum_{n=1}^M a_{2n} \sin(na_0x) + a_{2n+1} \cos(na_0x) \quad M = 3$$

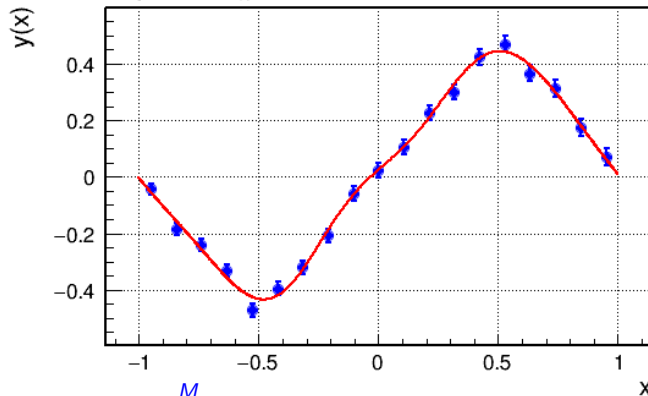
Marquardt Minimization example

09_fit1.ipynb

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Fitting Fourier series to
example data set

General fit Npar = 10 $\chi^2 = 14.69 / 9$



$$y(x) = a_1 + \sum_{n=1}^M a_{2n} \sin(na_0x) + a_{2n+1} \cos(na_0x) \quad M = 4$$

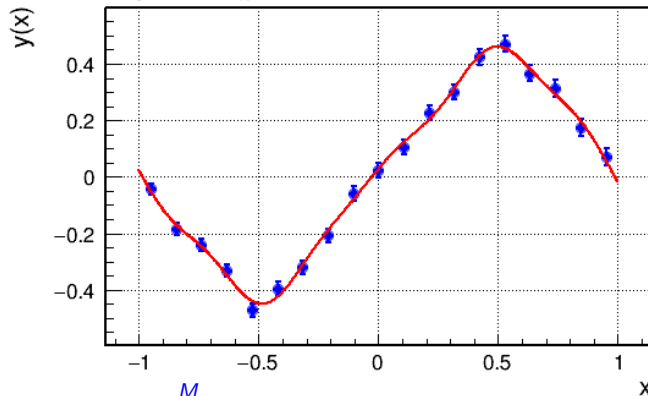
Marquardt Minimization example

09_fit1.ipynb

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Fitting Fourier series to
example data set

General fit Npar = 12 $\chi^2 = 10.52 / 7$



$$y(x) = a_1 + \sum_{n=1}^M a_{2n} \sin(na_0x) + a_{2n+1} \cos(na_0x) \quad M = 5$$

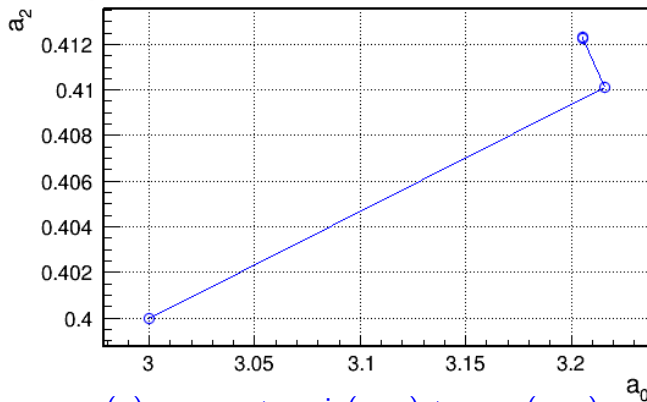
Marquardt Minimization example

09_fit2.ipynb

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

Fit history for parameters 0 and 2



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

Marquardt Minimization example

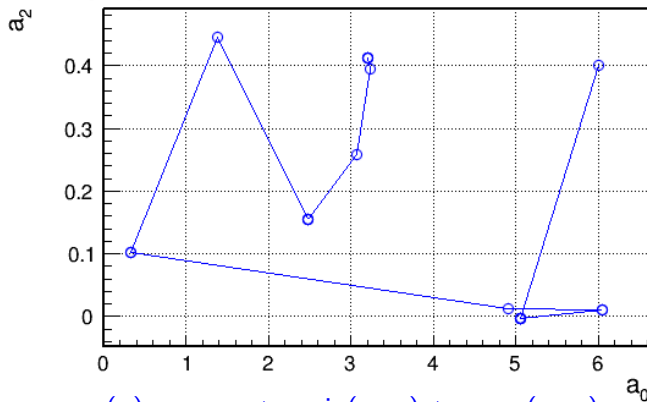
Much slower convergence when the initial values are “wrong”

09_fit2.ipynb

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($a_0 = 6$)

Fit history for parameters 0 and 2



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

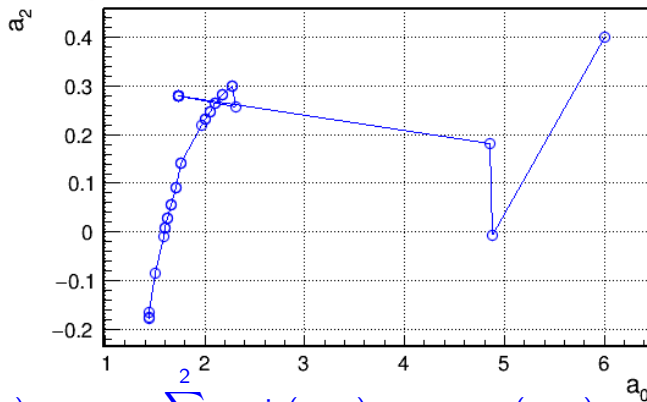
Marquardt Minimization example

09_fit2.ipynb

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

Fit history for parameters 0 and 2



$$y(x) = a_1 + \sum_{n=1}^2 a_{2n} \sin(na_0x) + a_{2n+1} \cos(na_0x)$$

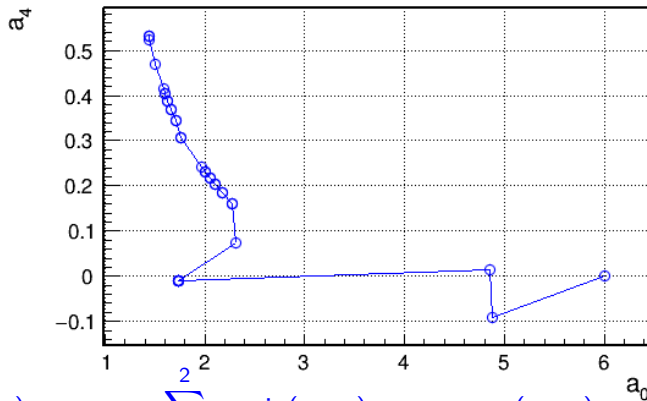
Marquardt Minimization example

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

Fit history for parameters 0 and 4



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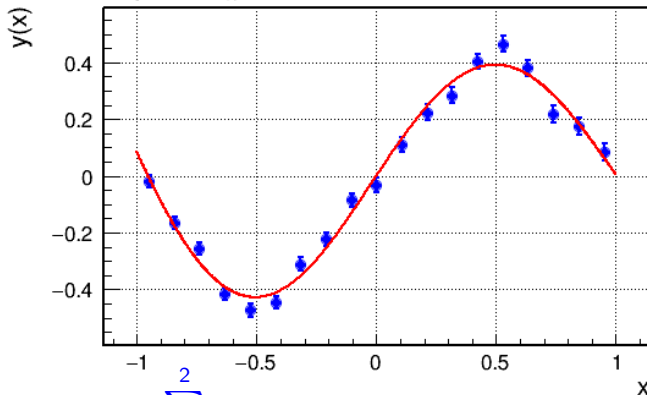
Marquardt Minimization example

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

General fit Npar = 6 $\chi^2 = 43.78 / 13$

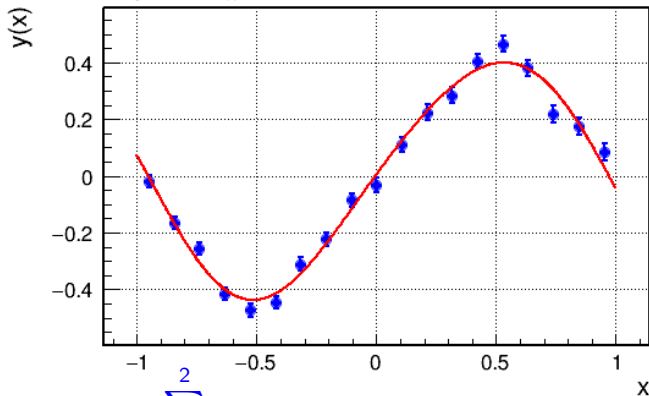


$$y(x) = a_1 + \sum_{n=1}^2 a_{2n} \sin(na_0x) + a_{2n+1} \cos(na_0x)$$

Marquardt Minimization example

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

General fit Npar = 6 $\chi^2 = 38.37 / 13$



$$y(x) = a_1 + \sum_{n=1}^2 a_{2n} \sin(na_0x) + a_{2n+1} \cos(na_0x)$$

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)

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

Comparison of variances

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

However, we can also 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.

One can consider it as a procedure to compare two different estimates of the variance of the measurement, and check if they are compatible.

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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 χ_1^2 and χ_2^2 are χ^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:

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

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

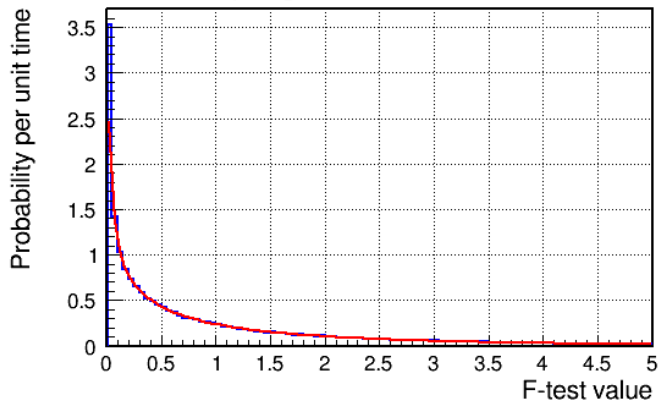
(for $N_2 \gg N_1$; ratio variance is dominated by the variance of the reduced χ^2 with N_1 d.o.f.)

F variable distribution

[09_F-test.ipynb](#)[Open in Colab](#)

Example distributions of the Fisher's F variable

F-test distribution for $N_1=1$, $N_2=20$



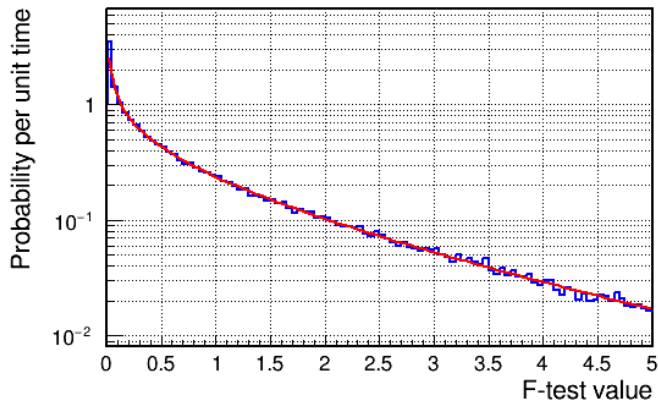
F variable distribution

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Example distributions of the Fisher's F variable

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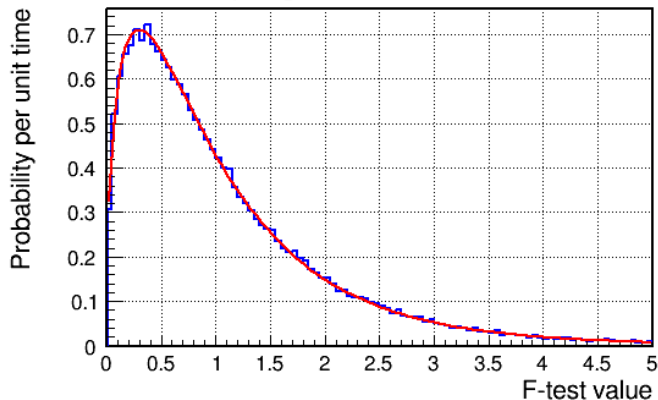
F variable distribution

09_F-test.ipynb

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Example distributions of the Fisher's F variable

F-test distribution for $N_1=3$, $N_2=20$



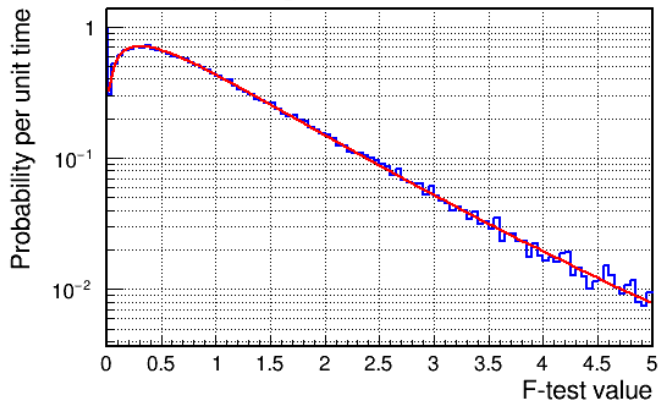
F variable distribution

09_F-test.ipynb

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Example distributions of the Fisher's F variable

F-test distribution for $N_1=3$, $N_2=20$

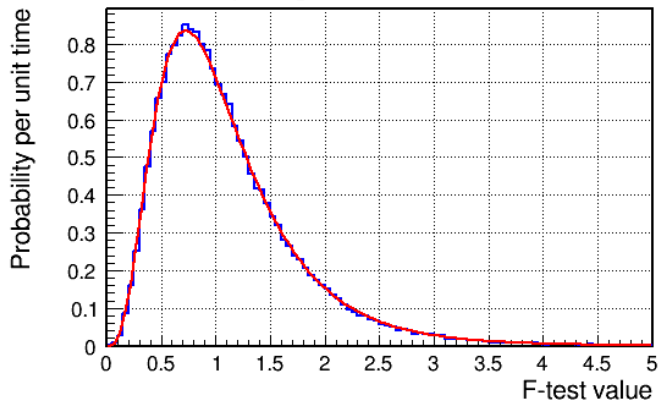


F variable distribution

[09_F-test.ipynb](#)[Open in Colab](#)

Example distributions of the Fisher's F variable

F-test distribution for $N_1=10$, $N_2=20$



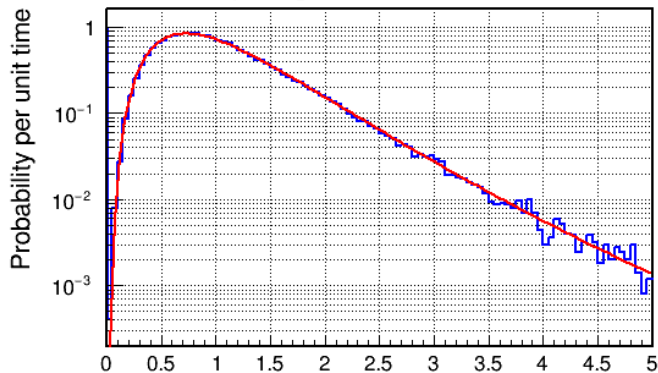
F variable distribution

09_F-test.ipynb

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Example distributions of the Fisher's F variable

F-test distribution for $N_1=10, N_2=20$



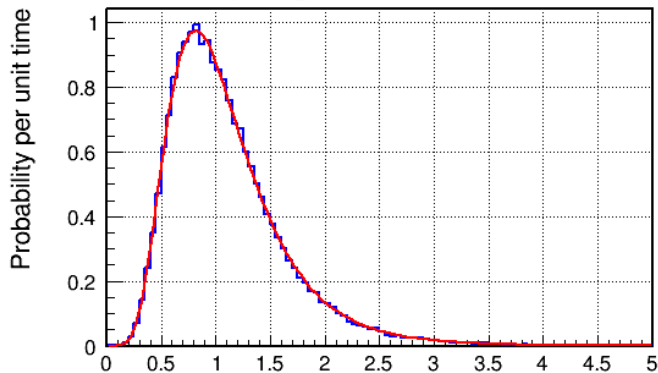
Significant tail of high values, even for relatively large $N_1, N_2 \dots$ F-test value

F variable distribution

[09_F-test.ipynb](#)[Open in Colab](#)

Example distributions of the Fisher's F variable

F-test distribution for $N_1=20, N_2=20$



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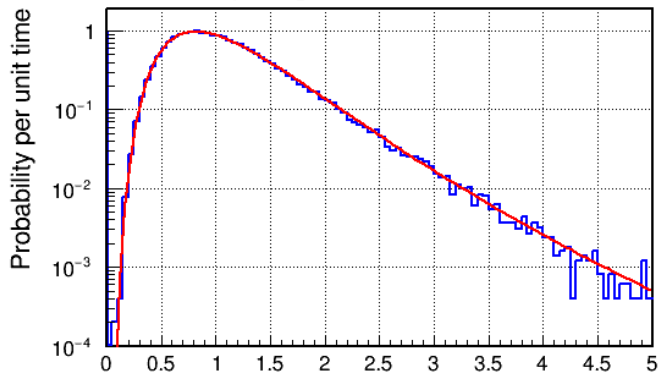
F variable distribution

09_F-test.ipynb

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Example distributions of the Fisher's F variable

F-test distribution for $N_1=20, N_2=20$



Significant tail of high values, even for relatively large $N_1, N_2 \dots$ F-test value

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:

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

F-test

(Brandt)

“Critical values” of F for small numbers of degrees of freedom N_1 and N_2

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

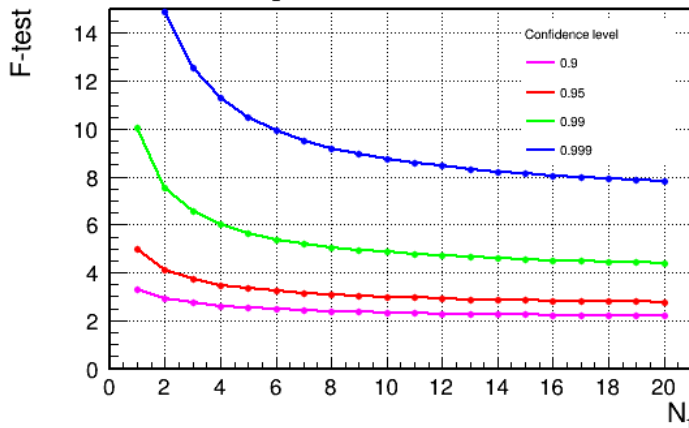
F-test

09_F-limit.ipynb

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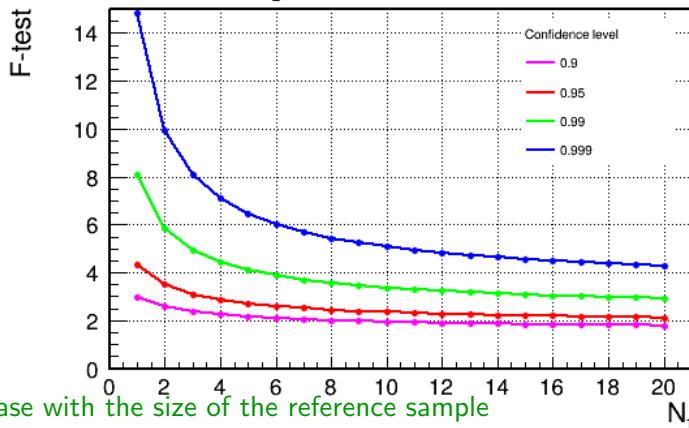
Plot of “critical values” of F for $N_2 = 10$

Critical F-test curves for $N_2 = 10$



F-test

09_F-limit.ipynb

 Open in ColabPlot of “critical values” of F for $N_2 = 20$ Critical F-test curves for $N_2 = 20$ 

Variations decrease 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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$$\chi^2_{(m-\Delta m)} = \chi^2_{(m)} + \Delta\chi^2$$

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$$\chi_{(m-\Delta m)}^2 = \chi_{(m)}^2 + \Delta\chi^2$$

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

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

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

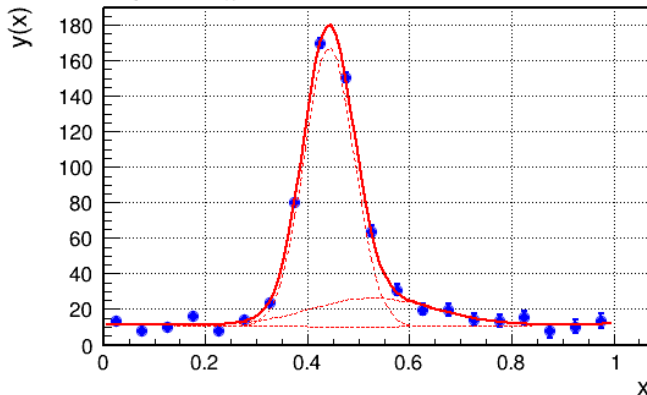
F-test for fit model

09_fit3.ipynb

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

General fit Npar = 9 $\chi^2 = 14.23 / 11$



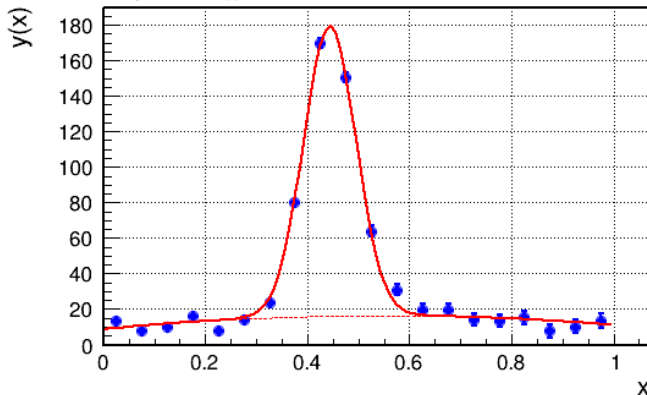
F-test for fit model

[09_fit3.ipynb](#)[Open in Colab](#)

Example of F -test application. Is the second signal component really needed?!

Fit with **one peak** gives a reasonable description of the data as well.

General fit Npar = 6 $\chi^2 = 28.53 / 14$



F-test for fit model

Example of F -test application.

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

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

F-test for fit model

Example of F -test application.

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

$$\Delta\chi^2 \approx 14.33 \quad \Delta\chi^2/\Delta m \approx 4.777$$

F-test for fit model

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$$F \approx 3.69$$

$$p \approx 0.047$$

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...

F-test for fit model

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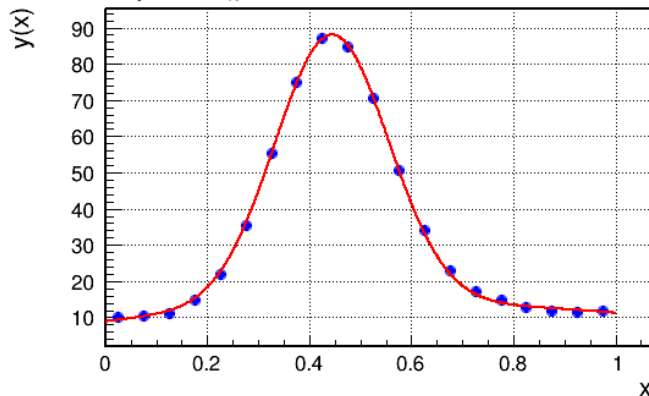
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Second component fit result misleading: $A_2 = 4.950 \pm 1.523$ (3.25σ)

F-test for fit model

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

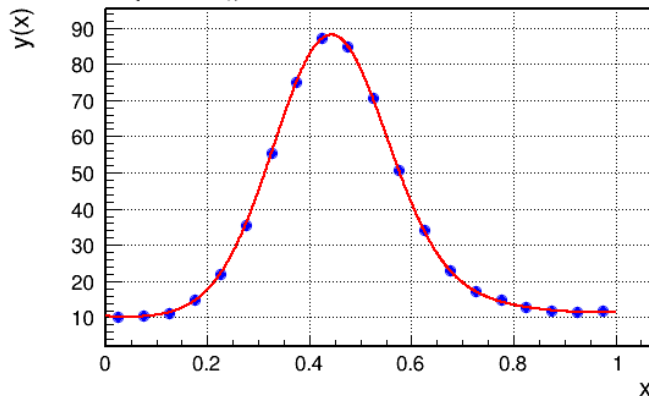
General fit Npar = 6 $\chi^2 = 95.31 / 14$



F-test for fit model

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

General fit Npar = 9 $\chi^2 = 9.34 / 11$



F-test for fit model

Example (2) of F -test application.

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

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

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

$$F \approx 33.75$$

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

corresponding to about 4.3σ deviation...

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

Least-squares method (2)

- 1 Non-linear fit procedure
- 2 F -test
- 3 Constrained fit**
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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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- 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 χ^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 independent model variables. \Rightarrow 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, $w \in [-1, +1]$.

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

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

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:

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

⇒ we have independent constraints on even and odd parameters.

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

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

Model reduction example

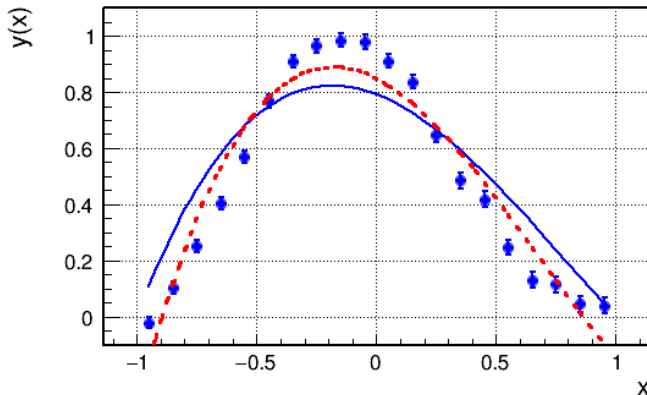
09_reduce.ipynb

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Example polynomial fit **without** and **with** model constraints

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

Linear fit Npar = 4 $\chi^2 = 283.37 / 16$ red.: $\chi^2 = 674.03 / 18$ p = 0.00098



3rd order polynomial not describing data at all

Model reduction example

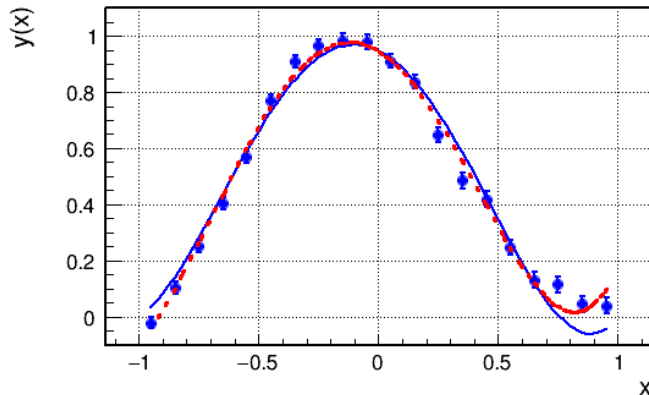
09_reduce.ipynb

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Example polynomial fit **without** and **with** model constraints

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

Linear fit Npar = 5 $\chi^2 = 35.97 / 15$ red.: $\chi^2 = 90.5 / 17$ p = 0.00099



4th order polynomial fit still not satisfactory...

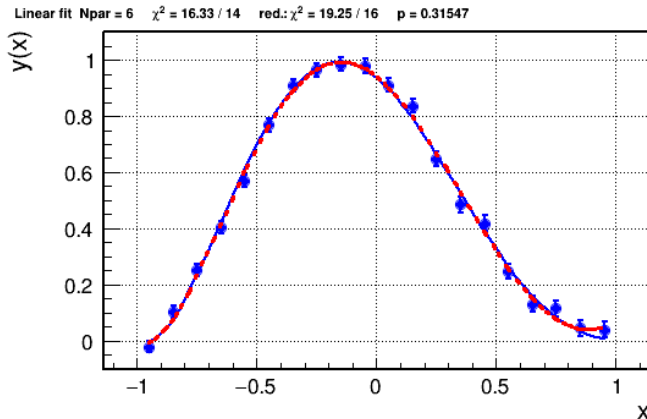
Model reduction example

09_reduce.ipynb

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Example polynomial fit **without** and **with** model constraints

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



Reasonable description of the data.

Model reduction example

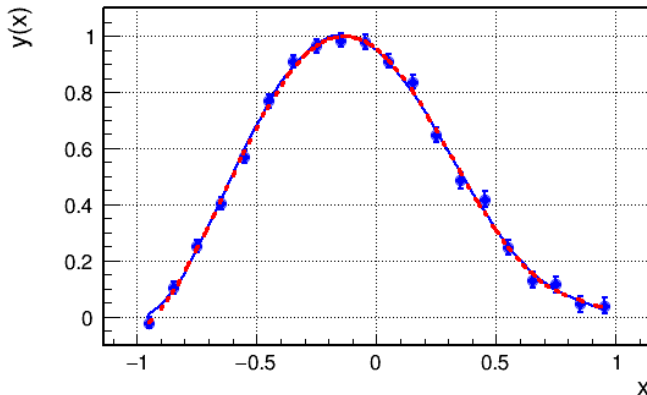
09_reduce.ipynb

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Example polynomial fit **without** and **with** model constraints

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

Linear fit Npar = 7 $\chi^2 = 12.32 / 13$ red.: $\chi^2 = 14.6 / 15$ p = 0.33226



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

Model reduction example

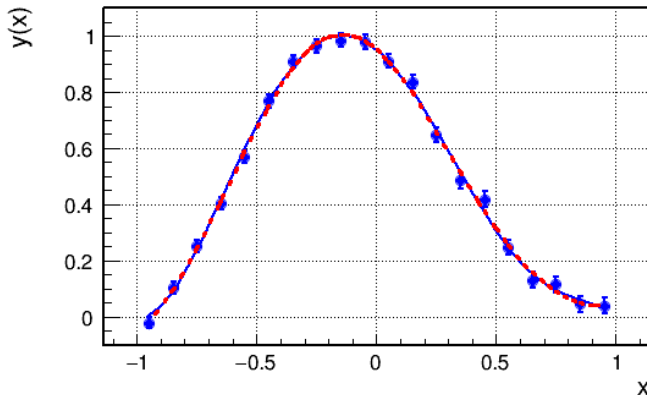
09_reduce.ipynb

 Open in Colab

Example polynomial fit **without** and **with** model constraints

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

Linear fit Npar = 8 $\chi^2 = 11.61 / 12$ red.: $\chi^2 = 14.37 / 14$ p = 0.27821



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 Δm constraints, which we test on the set of N data points

Constrained (“reduced”) model has $m - \Delta m$ parameters and results in higher χ^2 :

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

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

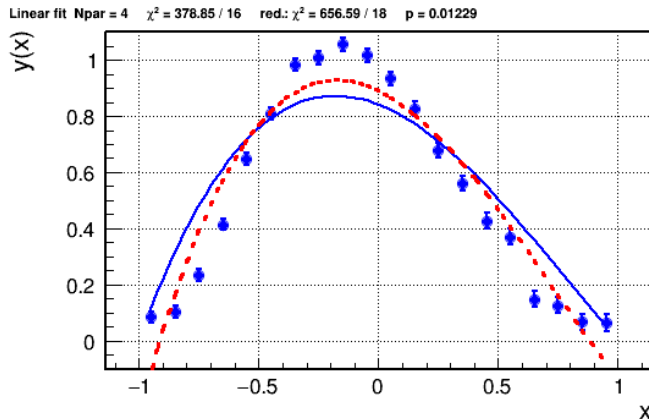
$$F = \frac{\Delta\chi^2 / \Delta m}{\chi_{\text{full}}^2 / (N - m)} \quad \text{and} \quad p = \int_F^{+\infty} dF' f(F')$$

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

Model reduction example (2)

(generated with $\mu(-1) = \mu(+1) = 0.05$)

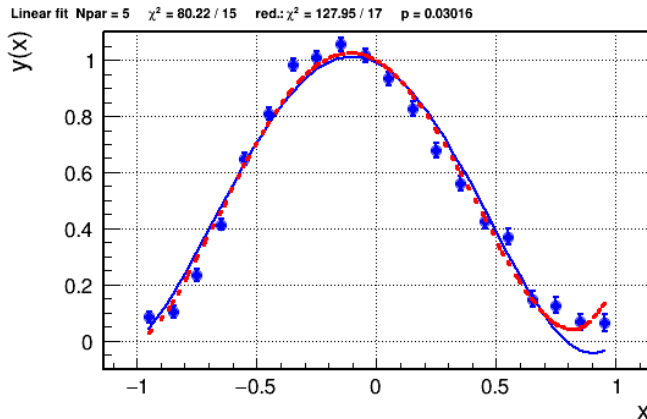
Example polynomial fit **without** and **with model constraints**, to inconsistent data set



3rd order polynomial not describing data at all

Model reduction example (2)

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



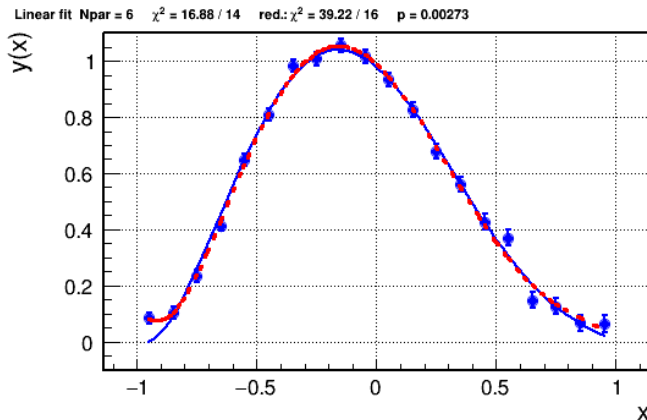
4th order polynomial fit still not satisfactory...

Model reduction example (2)

09_reduce2.ipynb

 Open in Colab

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



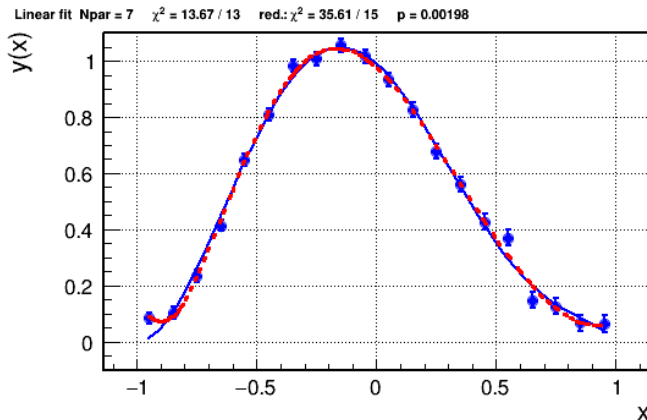
Reasonable description of the data only without constraints...

Model reduction example (2)

09_reduce2.ipynb

 Open in Colab

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

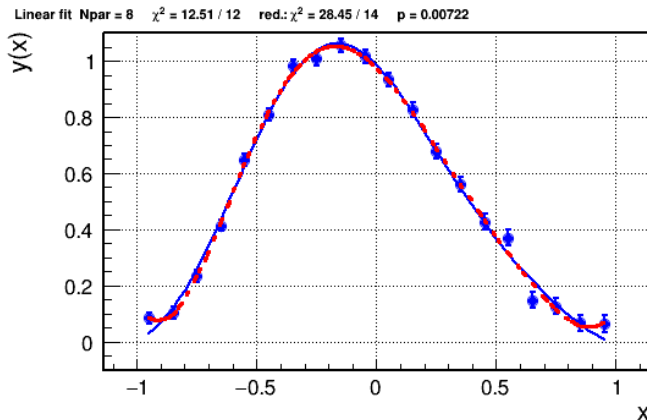


p value indicates that data is not consistent with constraints...

Model reduction example (2)

[09_reduce2.ipynb](#)[Open in Colab](#)

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



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Model reduction

After fitting the reduced model, constraints can be used to extract **values of eliminated parameters** and their uncertainties can be calculated from **standard error propagation**...

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When trying to reduce the number of parameters, one should consider redefining the parameter basis in such a way that constraints depend only on selected parameters.

Can be essential for numerical stability...

Model reduction

After fitting the reduced model, constraints can be used to extract **values of eliminated parameters** and their uncertainties can be calculated from **standard error propagation...**

When trying to reduce the number of parameters, one should consider redefining the parameter basis in such a way that constraints depend only on selected parameters.

Can be essential for numerical stability...

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.

⇒ 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 λ_k - Lagrange multipliers

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

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

(without any additional constraints)

Method of Lagrange Multipliers

Writing the full formula for \mathcal{L} :

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

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

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

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

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

Adding **constraints** modifies the resulting system of equation for \mathbf{a} ...

Method of Lagrange Multipliers

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

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

Our set of equations can be now presented as:

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

Method of Lagrange Multipliers

We can write these equations the matrix form:

$$\left(\begin{array}{c|c} \mathbb{A} & \mathbb{D} \\ \hline \mathbb{D}^\top & 0 \end{array} \right) \cdot \begin{pmatrix} \mathbf{a} \\ \boldsymbol{\lambda} \end{pmatrix} = \begin{pmatrix} \mathbf{b} \\ \mathbf{c} \end{pmatrix}$$

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 $b_j = \sum_{i=1}^N \frac{f_j(x_i) y_i}{\sigma_i^2}$

and the problem can be solved by inverting matrix $\tilde{\mathbb{A}}$.

Method of Lagrange Multipliers

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and the problem can be solved by inverting matrix $\tilde{\mathbb{A}}$.

Covariance matrix for \mathbf{a} can be extracted as:

(seems to work for linear problems)

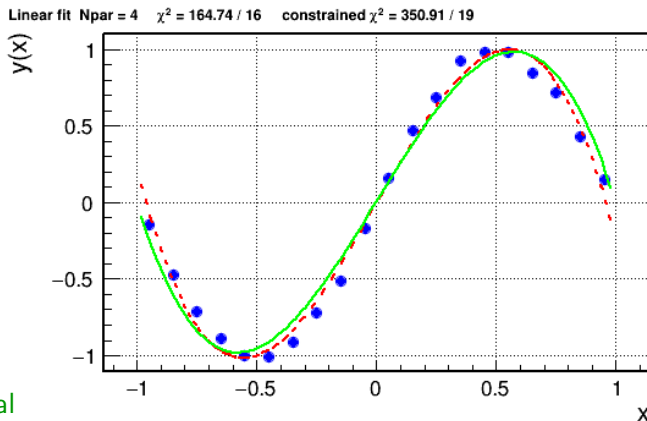
$$(\mathbb{C}_{\mathbf{a}})_{ij} = (\tilde{\mathbb{A}}^{-1})_{ij} \quad i, j = 1 \dots M$$

Lagrange Multipliers example

09_const.ipynb

 Open in Colab

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

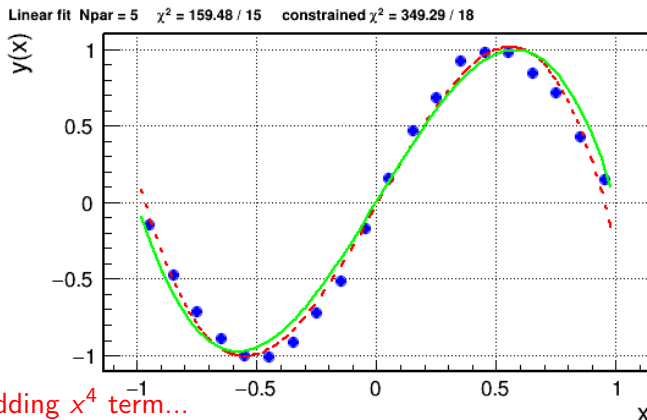


Lagrange Multipliers example

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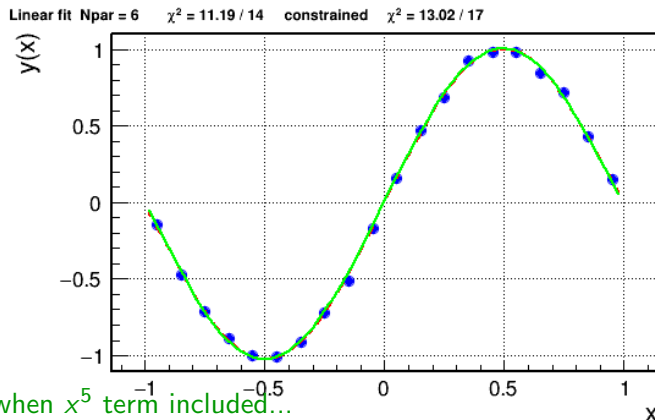
No improvement adding x^4 term...

Lagrange Multipliers example

09_const.ipynb

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



Good description when x^5 term included...

Lagrange Multipliers example (2)

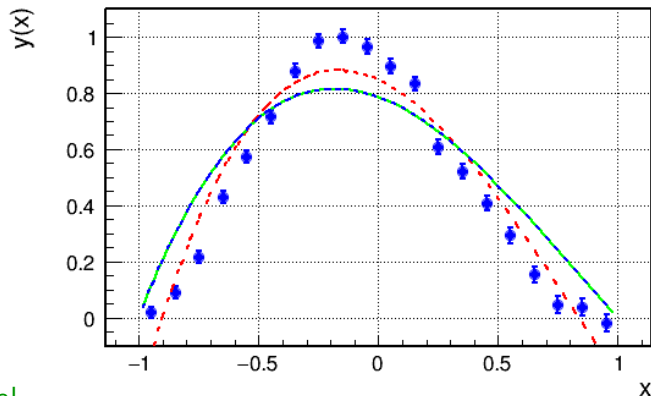
09_const2.ipynb

 Open in Colab

Comparing two approaches to polynomial fit with constraints.

Fit approach: **unconstrained** Lagrange multipliers model reduction

Linear fit Npar = 4 $\chi^2 = 295.24 / 16$ const.: $\chi^2 = 675.16 / 18$ red.: $\chi^2 = 675.16 / 18$



3rd order polynomial

Lagrange Multipliers example (2)

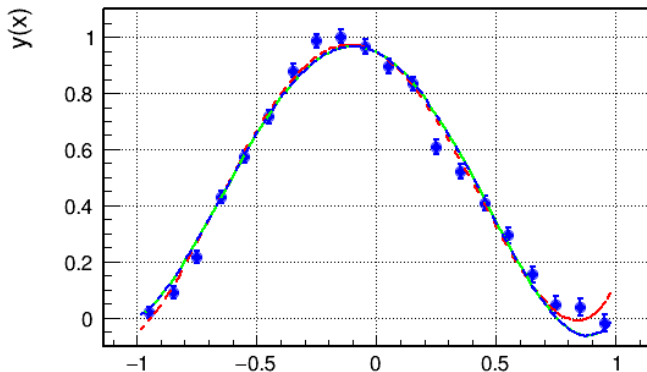
09_const2.ipynb

 Open in Colab

Comparing two approaches to polynomial fit with constraints.

Fit approach: **unconstrained** Lagrange multipliers model reduction

Linear fit Npar = 5 $\chi^2 = 48.38 / 15$ const.: $\chi^2 = 70.72 / 17$ red.: $\chi^2 = 70.72 / 17$



With x^4 term Perfect agreement between two constrain approaches

Lagrange Multipliers example (2)

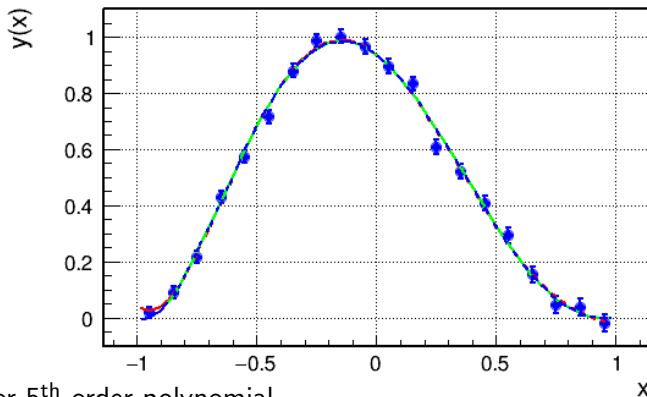
09_const2.ipynb

 Open in Colab

Comparing two approaches to polynomial fit with constraints.

Fit approach: **unconstrained** Lagrange multipliers model reduction

Linear fit Npar = 6 $\chi^2 = 17.57 / 14$ const.: $\chi^2 = 19.88 / 16$ red.: $\chi^2 = 19.88 / 16$



Good description for 5th order polynomial...

Lagrange Multipliers example (2)

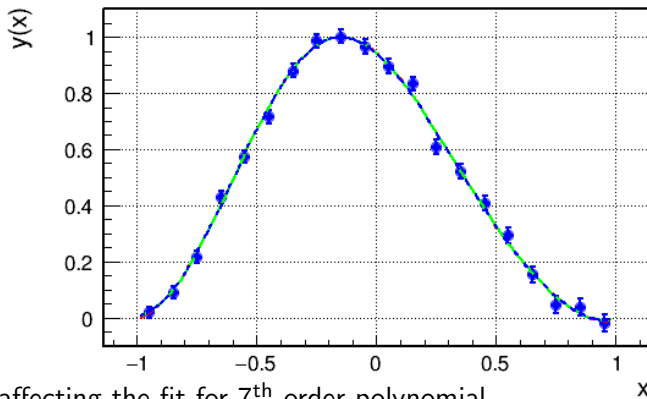
09_const2.ipynb

 Open in Colab

Comparing two approaches to polynomial fit with constraints.

Fit approach: **unconstrained** Lagrange multipliers model reduction

Linear fit Npar = 8 $\chi^2 = 15.47 / 12$ const.: $\chi^2 = 15.52 / 14$ red.: $\chi^2 = 15.52 / 14$



Constraints hardly affecting the fit for 7th order polynomial...

Lagrange Multipliers example (2)

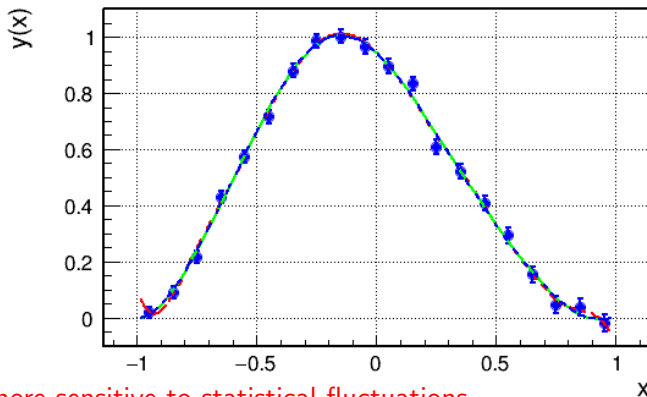
09_const2.ipynb

 Open in Colab

Comparing two approaches to polynomial fit with constraints.

Fit approach: **unconstrained** Lagrange multipliers model reduction

Linear fit Npar = 10 $\chi^2 = 12.3 / 10$ const.: $\chi^2 = 14.43 / 12$ red.: $\chi^2 = 14.43 / 12$



Unconstrained fit more sensitive to statistical fluctuations...

Least-squares method (2)

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

Homework

Solutions to be uploaded by December 21.

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

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

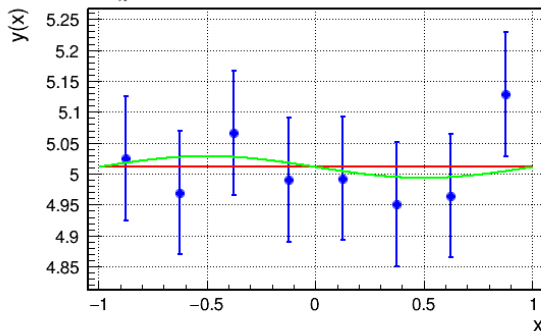
Results can be compared to **background only model** and to **background+signal**:

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

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

Hint: \mathbb{A} and \mathbb{C}_a do not depend on y_i

Linear fits: $\chi^2 = 2.41 / 6$ vs $2.53 / 7$



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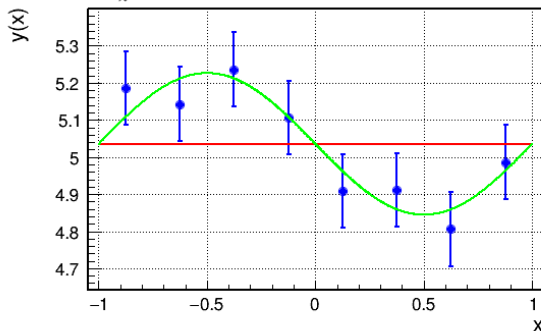
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Linear fits: $\chi^2 = 2.03 / 6$ vs $16.6 / 7$



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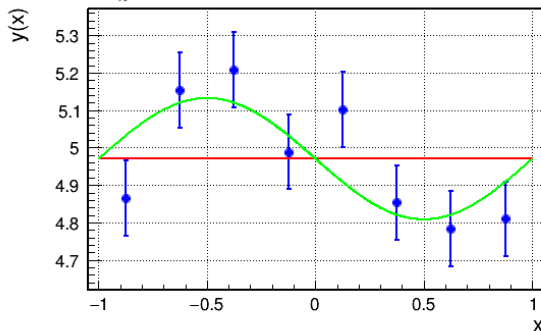
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Linear fits: $\chi^2 = 8.88 / 6$ vs $19.4 / 7$



Homework

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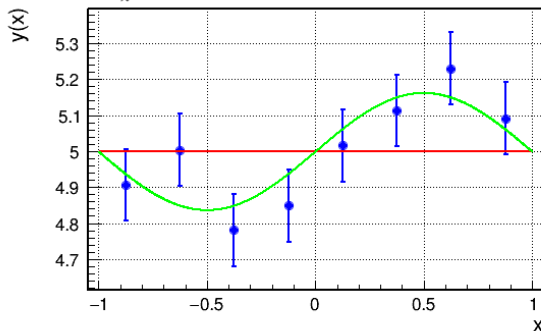
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Linear fits: $\chi^2 = 4.81 / 6$ vs $15.41 / 7$



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

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Hint: \mathbb{A} and \mathbb{C}_a do not depend on y_i

Linear fits: $\chi^2 = 3.03 / 6$ vs $14.36 / 7$

