

Statistical analysis of experimental data

Systematic uncertainties

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Lecture 10

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Systematic uncertainties

- 1 Systematic effects
- 2 Estimating systematic uncertainties
- 3 Including systematic effects
- 4 Reducing variables
- 5 Homework

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

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

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:

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

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

$$\mathbb{A}_{jk} = \left. \frac{1}{2} \frac{\partial^2 \chi^2}{\partial a_j \partial a_k} \right|_{\mathbf{a}=\mathbf{a}_0} \approx \sum_{i=1}^N \frac{1}{\sigma_i^2} \cdot \frac{\partial \mu_i}{\partial a_j} \cdot \frac{\partial \mu_i}{\partial a_k} \quad \left(\text{neglecting } \frac{\partial^2 \mu_i}{\partial a_j \partial a_k} \right)$$

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

$$\begin{aligned} \nabla \chi^2(\mathbf{a}) &= -2 \mathbf{b} + 2 \mathbb{A} (\mathbf{a} - \mathbf{a}_0) = 0 \\ \Rightarrow \mathbf{a}_m &= \mathbf{a}_0 + \mathbb{A}^{-1} \mathbf{b} \end{aligned}$$

and we can try to “jump” directly to the minimum...

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 λ 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 $\lambda \rightarrow 0$

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...

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 (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 also consider it as a way to compare two different estimates of the variance of the measurement, and check if they are compatible.

We define the random variable F as:

introduced by R.A.Fisher in 1924

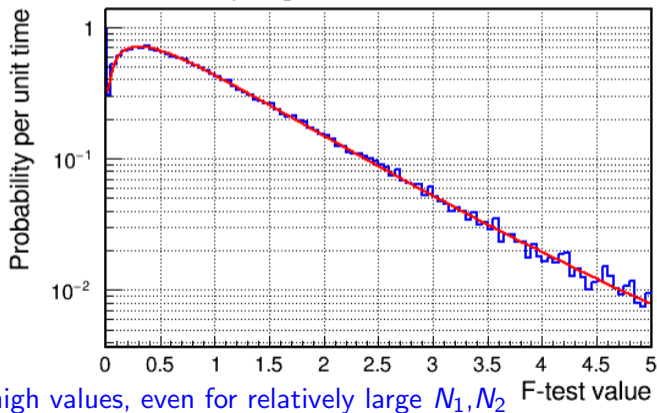
$$F = \frac{\chi_1^2/N_1}{\chi_2^2/N_2}$$

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

Example distributions of the Fisher's F variable

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

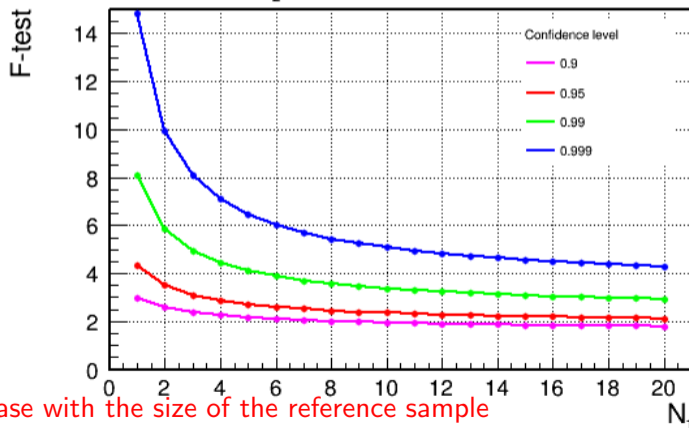


Significant tail of high values, even for relatively large N_1, N_2

F-test

Plot 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?**

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

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

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:

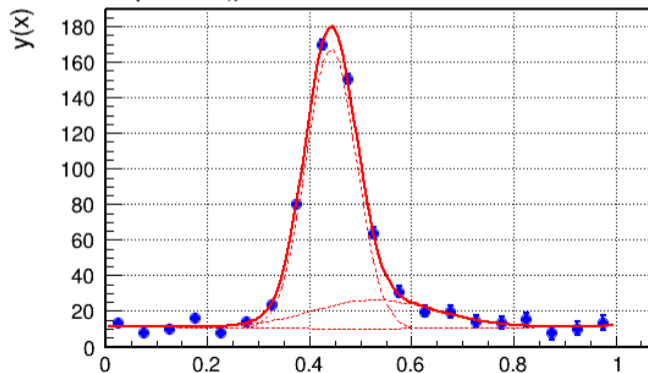
$$F = \frac{\Delta\chi^2/\Delta m}{\chi_{(m)}^2/(N-m)}$$

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

F-test for fit model

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

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



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 $\chi^2(\mathbf{a})$.

However, we now need to look for this minimum taking additional constraints into account:

$$w_k(\mathbf{a}) = 0 \quad k = 1 \dots K$$

where number of constraints K should be lower than number of parameters M .

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

Example

We would like to fit polynomial model to a series of measurements where the azimuthal 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 $\theta \rightarrow \pm\pi$:

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

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

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

We can write these equations the matrix form:

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

$\tilde{\mathbb{A}}$

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 $\tilde{\mathbb{A}}$** .

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

(seems to work for linear problems)

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

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Statistical uncertainties

We have considered numerical results of experiments as random variables.

Probability to obtain given numerical result was described by PDF.

Results of a repeated experiment were considered as independent variables.

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Uncertainties of the results were related to the fluctuations in the measurement due to:

- actual nature of the physics process studied (lecture 01)
eg. exponential distribution for decay time measurement
- finite precision of our instruments
eg. precision with which decay time is measured in the detector
- inhomogeneity of the population studied
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Uncertainties related to fluctuations of the individual measurement results are usually referred to as **statistical uncertainties**.

Systematic uncertainties

Particle physics experiments are quite complex, and so is the data analysis.

We frequently use Monte Carlo methods to correct for different effects.

Simplest example is the (differential) cross section measurement:

$$\sigma_i = \frac{N_i}{\varepsilon_i A_i \mathcal{L}}$$

where: N_i is the measured number of events (in given bin i), ε - event selection efficiency, A - detector acceptance and \mathcal{L} - integrated luminosity.

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Statistical uncertainty of the extracted cross section value is due to the Poisson fluctuations in the number of reconstructed events.

But we also need to take into account that other factors (ε_i , A_i , \mathcal{L}) are also known with finite precision \Rightarrow **systematic uncertainties**

Sources of systematic uncertainties

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(Bonamente) The term **systematic error** designates sources of error that systematically **shift the signal** of interest either too high or too low. Sources of systematic errors need to be identified to correct the **erroneous offset**. A typical example is an instrument that is miscalibrated and systematically reports measurements that have an erroneous offset.

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(Barlow; quotes after J. Orear, *Notes on Statistics for Physicists*)

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"**Systematic effects**" is a general category which includes effects such as background, selection bias, scanning efficiency, energy resolution, angle resolution, variation of counter efficiency with beam position and energy, dead time, etc.

Systematic effects are not a problem, if we understand them and know how to model them precisely (**correct the final result for systematic error**).

Sources of systematic uncertainties

Systematic uncertainty is the uncertainty in the estimation of systematics.

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Systematic effects and their uncertainties are often estimated based on separate, independent experiments. This is the case for both the experimental uncertainties (eg. detector calibration, alignment) as well as those related to the theoretical model (eg. value of the coupling parameter, particle masses, assumed cross sections).

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The maximum-likelihood approach can be used to estimate the impact of systematic effect and the resulting uncertainty of the measurement.

Likelihood function of the procedure used to constrain the systematic effect should be folded into the likelihood function of the main experiment.

Systematic uncertainties

In our simple example of cross section measurement:

$$\sigma_i = \frac{N_i}{\varepsilon_i A_i \mathcal{L}}$$

the statistical uncertainty on σ_i is due to Poisson fluctuations in N_i :

$$\sigma_{stat} = \frac{\sigma_{N_i}}{\varepsilon_i A_i \mathcal{L}} = \frac{\sqrt{N_i}}{\varepsilon_i A_i \mathcal{L}} = \frac{\sigma_i}{\sqrt{N_i}}$$

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Uncertainty on $\varepsilon_i A_i$ can result from many different sources (including eg. energy calibration), but one should also take into account contribution from the finite statistics of the Monte Carlo events:

$$\sigma_{r_i} = \sqrt{\frac{r_i(1-r_i)}{N^{MC}}} \quad (\text{binomial distribution})$$

$$r_i = \varepsilon_i A_i$$

where N^{MC} is the total number of (unweighted) Monte Carlo events (before selection)

Systematic uncertainties

The resulting systematic uncertainty on the cross section measurement:

$$\sigma_{\text{sys}(MC)} = \sigma_i \cdot \frac{\sigma_{r_i}}{r_i} = \sigma_i \cdot \sqrt{\frac{1 - r_i}{r_i N_i^{MC}}} = \sigma_i \cdot \sqrt{\frac{1 - r_i}{N_i^{MC}}}$$

where N_i^{MC} is the number of MC events accepted in cross section bin i .

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In general, arbitrary level of correlation (when more than one effect is taken into account) is possible for systematic uncertainties...

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Extended model

We considered outcome of our experiment y_i as a random variable with given probability density function (usually assumed to be Gaussian)

$$f(y_i) = G(y_i; \mu_i, \sigma_i)$$

where, in the general case, the uncertainty of the measurement was given by (the square root of) the variance of the distribution:

$$\sigma_{(stat) i}^2 = \mathbb{V}(y_i) = \langle (y_i - \mu_i)^2 \rangle$$

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This is how we can define the statistical uncertainty: uncertainty of the measurement when the expected value (and other parameters of pdf) are precisely known:

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

with controlled variable x_i and all model parameters \mathbf{a} fixed.

Extended model

To describe systematic effects, we need to introduce additional parameters in the model:

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We usually assume some nominal, expected values of these parameters, \mathbf{s}_0 .

Uncertainties of these parameters, σ_s , are then what contributes to the systematic uncertainty of our measurements:

$$\mu_i = \mu(x_i; \mathbf{a}, \mathbf{s}) = \mu(x_i; \mathbf{a}, \mathbf{s}_0) + \sum_j \frac{\partial \mu_i}{\partial s_j} \cdot (s_j - s_{0,j})$$

$$\mu_i = \mu_0(x_i; \mathbf{a}) + \sum_j \frac{\partial \mu_i}{\partial s_j} \sigma_{s_j} \cdot \delta_j \quad \delta_j = \frac{s_j - s_{0,j}}{\sigma_{s_j}}$$

where we introduce variations δ_j scaled to unit normal distribution ($\mu = 0, \sigma = 1$)

Extended model

Assuming there is no systematic bias in the measurement (or we already corrected for it), averaging over \mathbf{s} we should get:

$$\mathbb{E}(\mu_j) = \mu_0(x_j; \mathbf{a})$$

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$$= \sigma_{(stat) i}^2 + \sum_j \left(\frac{\partial \mu_i}{\partial s_j} \right)^2 \sigma_{s_j}^2$$

where we assume independent sources of systematic variations.

Extended model

Covariance matrix for the series of measurements y_i :

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where mixed terms vanish, as systematic variations and statistical fluctuations are independent

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where covariance matrix for statistical uncertainties is diagonal:

$$\mathbb{C}_{ij}^{(stat)} = \begin{cases} \sigma_{(stat)}^2 & \text{for } i = j \\ 0 & i \neq j \end{cases}$$

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statistical fluctuations are independent

systematic uncertainties result in correlations of expectations:

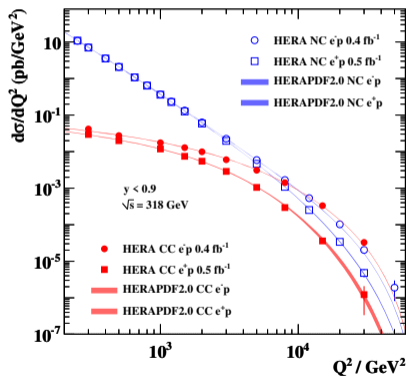
$$\mathbb{C}_{ij}^{(sys)} = \sum_k \left(\frac{\partial \mu_i}{\partial s_k} \right) \left(\frac{\partial \mu_j}{\partial s_k} \right) \sigma_{s_k}^2$$

We can no longer treat measurements as independent...

Example SM predictions from HERA

measurement already discussed in lecture 06

H1 and ZEUS



NC and CC DIS cross sections comparable for the highest Q^2 values

$$Q^2 \sim M_Z^2, M_W^2$$

Combined QCD+EW analysis shows good agreement with SM predictions

Phys. Rev. D 93 (2016) 092002, [arXiv:1603.09628](https://arxiv.org/abs/1603.09628)

How were systematic uncertainties on the SM predictions calculated?

Example

Let us focus on the “PDF uncertainties”, i.e. uncertainties related to our knowledge of the Parton Distribution Functions (PDF) of the proton.

Cross section for NC and CC DIS $e^\pm p$ scattering are given in terms of the quark density functions. In the leading order:

$$\frac{d^2\sigma_{CC}^{e^\pm p}}{dx dQ^2} = \frac{G_F^2}{4\pi} \left(\frac{M_W^2}{M_W^2 + Q^2} \right)^2 \begin{cases} u + c + (1-y)^2(\bar{d} + \bar{s} + \bar{b}) & \text{for } e^- p \\ (1-y)^2(d + s + b) + \bar{u} + \bar{c} & \text{for } e^+ p \end{cases}$$

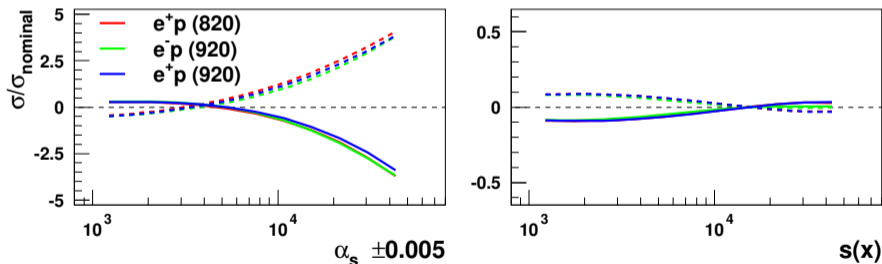
where u, d, s, c, b are quark densities ($\bar{u}, \bar{d} \dots$ - antiquark) in the proton, extracted by fitting QCD evolution equations to the large set of data from many experiments (not only DIS).

However, one has to take into account uncertainties of the input data, as well as uncertainties related to different assumptions in the fit...

Example

Analysis of HERA data was based on the QCD fit results implemented in EPDFLIB library

It provided not only the **nominal parton density values**, but also density values corresponding to **variations of different “systematic parameters”**.

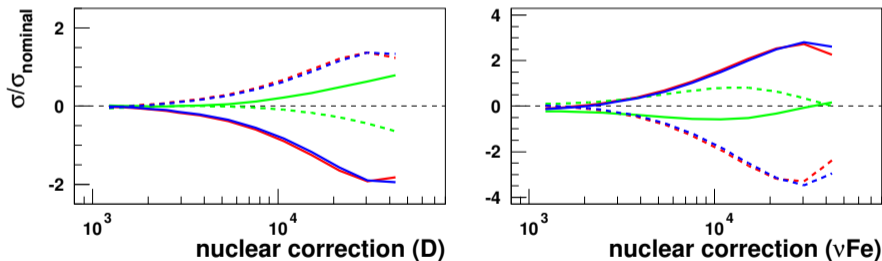


Variations of the three considered NC DIS data sets as a function of Q^2 for up (solid) and down (dashed) variation of systematic parameters (as indicated in labels)

Example

Analysis of HERA data was based on the QCD fit results implemented in EPDFLIB library

It provided not only the **nominal parton density values**, but also density values corresponding to **variations of different “systematic parameters”**.

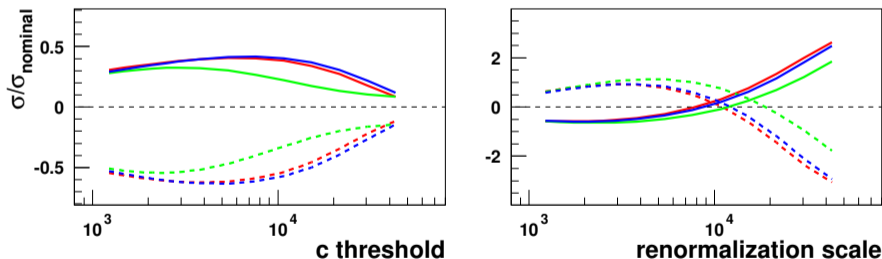


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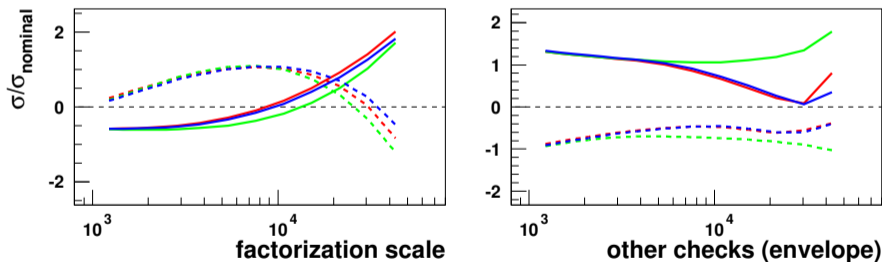


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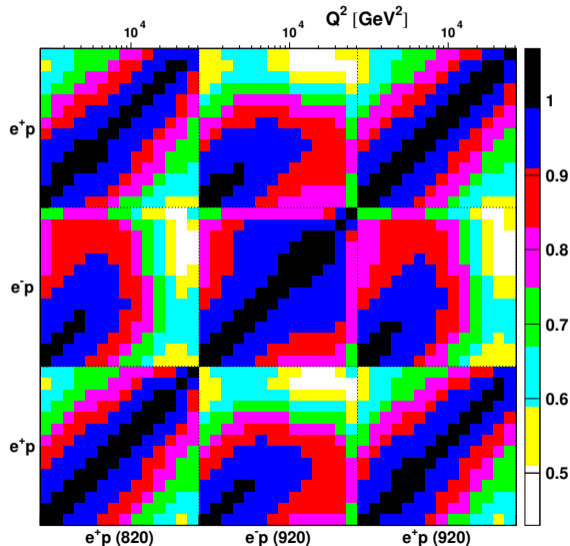


Variations of the three considered NC DIS data sets as a function of Q^2 for up (solid) and down (dashed) variation of systematic parameters (as indicated in labels)

Example

Correlation matrix for the expected high Q^2 NC DIS cross sections:

Must be taken into account when we compare our data to SM predictions



General remarks

One could think that obtaining the proper final result from the analysis (including estimate of the statistical uncertainty) is most important and most difficult. We are almost done...

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But one should also be careful not to overestimate the uncertainties!

Need to distinguish “systematic variations” and “systematic checks” ...

Systematic checks

Usually, there are many parameters in the theoretical model or in the detector descriptions which are known with finite precision. **This is the source of systematic uncertainties.**

And systematic bias, if our estimates of these parameters are wrong.

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Final result of our analysis should not depend on these choice, if our approach is valid, but some variations can occur.

One should be very careful! These variations are often due to the finite MC statistics. One should not include them in the systematic uncertainty estimate.

Otherwise, systematic uncertainties can easily “explode”, if we use large number of “systematic checks” ...

Systematic uncertainties

- 1 Systematic effects
- 2 Estimating systematic uncertainties
- 3 Including systematic effects**
- 4 Reducing variables
- 5 Homework

Example (Toy model)

An experiment is designed to measure an unknown parameter η .

Two measurements are considered (different experiment configurations) corresponding to two random variables x and y related to the physics parameter η :

$$x_{true} = a + \eta$$

$$y_{true} = a + 2 \cdot \eta$$

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We can find the optimum way of extracting η by writing down:

$$\chi^2(\eta) = \left(\frac{x - a - \eta}{\sigma_{stat}} \right)^2 + \left(\frac{y - a - 2\eta}{\sigma_{stat}} \right)^2$$

Example

Looking at the minimum of χ^2 we find:

$$0 = \frac{\partial \chi^2}{\partial \eta} = -\frac{2}{\sigma_{stat}^2} (x - a - \eta + 2(y - a - 2\eta))$$

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This result is not surprising, if we realize that η can be extracted from x and y independently:

$$\eta(x) = x - a \quad \text{and} \quad \eta(y) = \frac{1}{2}(y - a)$$

$$\sigma_{\eta(x)} = \sigma_{stat} \quad \sigma_{\eta(y)} = \frac{1}{2} \sigma_{stat}$$

and minimum of χ^2 corresponds to the **weighted average** of the two measurements, with uncertainty: $\sigma_y = \frac{1}{\sqrt{5}} \sigma_{stat}$

Example

Let us now include **systematic variation** Δ_{sys} of the background estimate a , so that the expected results of the measurement are

$$\langle x \rangle = x_{true} + \Delta_{sys}$$

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$$\eta = \frac{1}{5} x + \frac{2}{5} y - \frac{3}{5} a \Rightarrow \sigma_y^2 = \frac{1}{25} \sigma_{stat}^2 + \frac{4}{25} \sigma_{stat}^2 + \frac{9}{25} \sigma_{sys}^2$$

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but is it the optimal procedure?

Example

We should include systematic variation in **global likelihood**. For Gaussian uncertainties we get:

$$\chi^2(\eta, \delta) = \left(\frac{x - a - \eta - \delta\sigma_{sys}}{\sigma_{stat}} \right)^2 + \left(\frac{y - a - 2\eta - \delta\sigma_{sys}}{\sigma_{stat}} \right)^2 + \delta^2$$

where δ^2 term corresponds to the likelihood of the systematic variation

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We can calculate partial derivatives to get system of equations:

$$\frac{\partial \chi^2}{\partial \eta} : 5\eta + 3\sigma_{sys}\delta = x + 2y - 3a$$

$$\frac{\partial \chi^2}{\partial \delta} : 3\sigma_{sys}\eta + (2\sigma_{sys}^2 + \sigma_{stat}^2)\delta = (x + y - 2a)\sigma_{sys}$$

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which we can solve to obtain:

$$\eta = \frac{(2 + f^2)y + (1 - f^2)x - 3a}{5 + f^2} \quad \text{where} \quad f = \frac{\sigma_{sys}}{\sigma_{stat}}$$

Example

For small systematic uncertainties ($\sigma_{sys} \ll \sigma_{stat}$, $f \ll 1$)

$$\eta = \frac{(2 + f^2)y + (1 - f^2)x - 3a}{5 + f^2} \rightarrow \frac{2y + x - 3a}{5}$$

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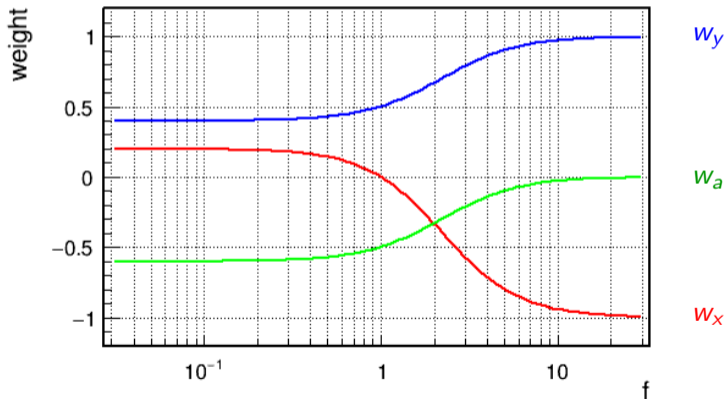
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It is also interesting to note that for ($\sigma_{sys} = \sigma_{stat}$, $f = 1$), measurement of x is not used:

$$\eta = \frac{(2 + f^2)y + (1 - f^2)x - 3a}{5 + f^2} = \frac{y - a}{2}$$

Example

Weights of the two measurements and background estimate



$$\eta = w_x x + w_y y + w_a a$$

Example

How about uncertainty of the extracted η value?

We can obtain it from the covariance matrix:

$$\mathbb{C}_{(\eta,\delta)} = \left(\frac{1}{2} \frac{\partial^2 \chi^2}{\partial a_l \partial a_k} \right)^{-1} = \begin{pmatrix} \frac{5}{\sigma_{stat}^2} & \frac{3\sigma_{sys}}{\sigma_{stat}^2} \\ \frac{3\sigma_{sys}}{\sigma_{stat}^2} & \frac{2\sigma_{sys}^2}{\sigma_{stat}^2} + 1 \end{pmatrix}^{-1}$$

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for $f \rightarrow \infty$

$\rightarrow \sqrt{2} \sigma_{stat}$

$\rightarrow \infty$

General procedure

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

$$\begin{aligned}\mu_i &= \mu(x_i; \mathbf{a}, \mathbf{s}) \\ \chi^2(\mathbf{a}, \mathbf{s}) &= \sum_{i=1}^N \frac{(y_i - \mu(x_i, \mathbf{a}, \mathbf{s}))^2}{\sigma_i^2} + \sum_{k=1}^K \frac{(s_k - s_{0,k})^2}{\sigma_{s_k}^2}\end{aligned}$$

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If systematic parameters are not independent (are correlated)

$$\chi^2(\mathbf{a}') = \sum_{i=1}^N \frac{(y_i - \mu(x_i, \mathbf{a}'))^2}{\sigma_i^2} + \sum_{k,j} (s_k - s_{0,k})(s_j - s_{0,j}) (\mathbb{C}_s)_{j,k}^{-1}$$

General procedure

χ^2 minimization procedure is basically unchanged, only the additional terms (systematic constrains) need to be included in calculations (as we did for the parameter constraints).

Negative gradient of χ^2 uncorrelated systematics

$$b_j = -\frac{1}{2} \frac{\partial \chi^2}{\partial a'_j} = \sum_{i=1}^N \frac{y_i - \mu_i}{\sigma_i^2} \cdot \frac{\partial \mu_i}{\partial a'_j} - \frac{s_j - s_{0,j}}{\sigma_{s_j}^2}$$

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Hessian matrix of second derivatives:

$$A_{jk} = \frac{1}{2} \frac{\partial^2 \chi^2}{\partial a'_j \partial a'_k} = \sum_{i=1}^N \frac{1}{\sigma_i^2} \cdot \frac{\partial \mu_i}{\partial a'_j} \cdot \frac{\partial \mu_i}{\partial a'_k} + \frac{\delta_{jk}}{\sigma_{s_k}^2}$$

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

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Negative gradient of χ^2 general case

$$b_j = -\frac{1}{2} \frac{\partial \chi^2}{\partial a'_j} = \sum_{i=1}^N \frac{y_i - \mu_i}{\sigma_i^2} \cdot \frac{\partial \mu_i}{\partial a'_j} - \sum_k (s_k - s_{0,k}) (\mathbb{C}_s)_{j,k}^{-1}$$

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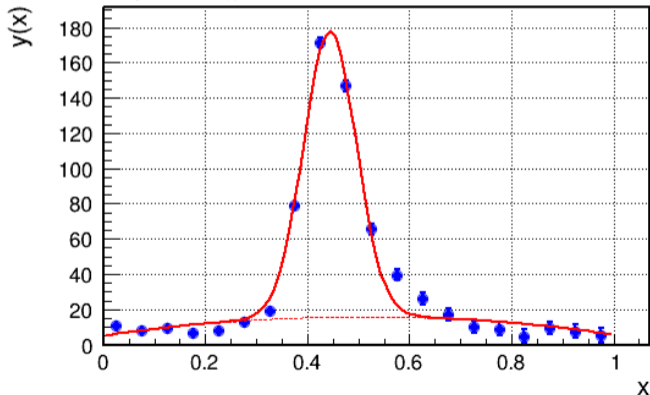
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General procedure example

Fitting Gaussian peak on top of background

(lecture 09)

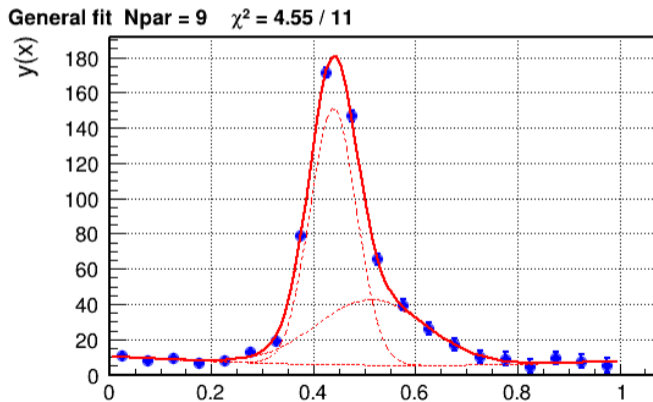
General fit Npar = 6 $\chi^2 = 73.54 / 14$



General procedure example

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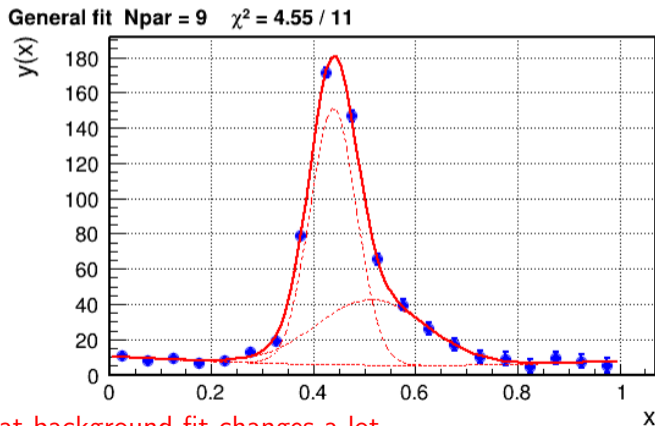


Two peak fit is better, but improvement not very significant, $p = 0.02$ \times

General procedure example

Fitting Gaussian peak on top of background

(lecture 09)



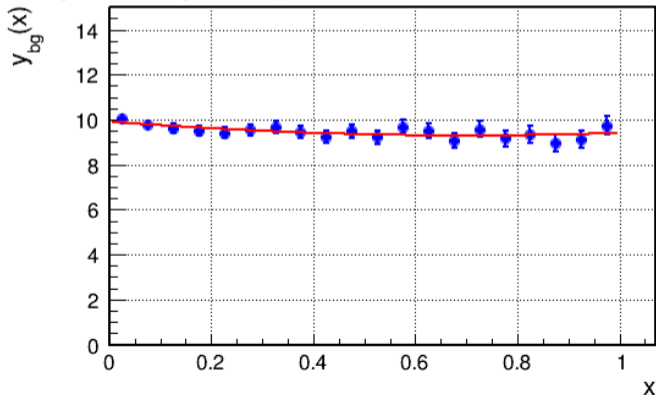
But we also see that background fit changes a lot...

General procedure example

[10_bg_fit.ipynb](#)[Open in Colab](#)

Suppose we can perform an independent background measurement with higher precision and fit parameters of our background model

Background fit Npar = 3 $\chi^2 = 8.14 / 17$



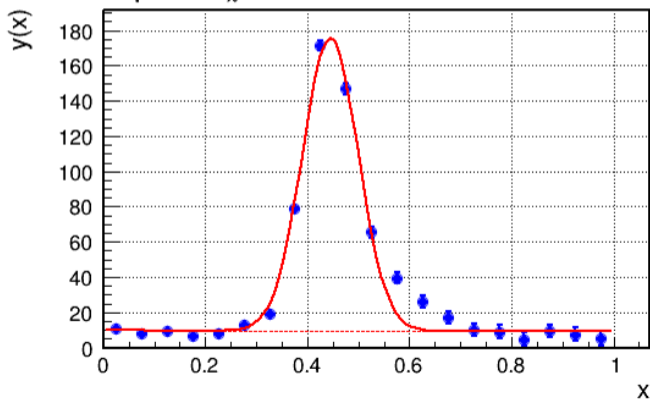
General procedure example

[10_comb_fit_test.ipynb](#)

 [Open in Colab](#)

We can now use parameters from the background fit in signal fit

General fit Npar = 6 $\chi^2 = 93.05 / 14$



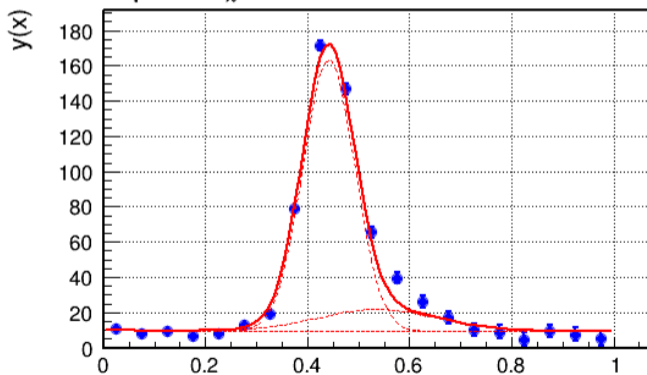
General procedure example

10_comb_fit_test.ipynb

 Open in Colab

We can now use parameters from the background fit in signal fit

General fit Npar = 9 $\chi^2 = 43.78 / 11$



Second peak significance increase from 2.1σ to 4.3σ ($p = 0.9 \cdot 10^{-5}$)

Systematic uncertainties

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- 4 Reducing variables**
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Problem

In the general case, one can consider a huge number of systematic effects, each will contribute to the final systematic uncertainty.

Number of systematic effects can be larger than the number of relevant model parameters (which we want to extract) or even the number of measurements.

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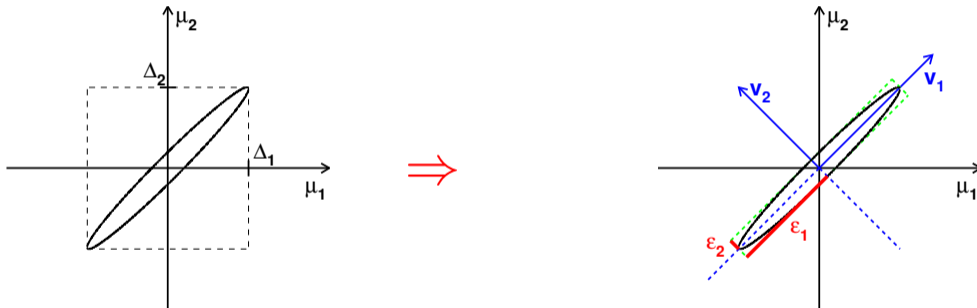
Is there a way to simplify the problem?

Is there a way to reduce the number of systematic variations to consider?

This is also important when we want to model the experiment (eg. with Monte Carlo methods)

Eigenvectors

Correlations between variables can be removed through 'rotation' in the variable space.



This is a problem of finding “eigenvectors” of the covariance matrix. Directions such that:

$$\mathbb{C}_s \cdot \mathbf{v} = \sigma_v^2 \cdot \mathbf{v}$$

Eigenvectors

Eigenvectors of the covariance matrix of systematic parameters define “uncorrelated directions” in the space of systematic parameter variations.

Variations along these directions are independent (uncorrelated).

We can redefine our systematic variables to remove correlations...

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Eigenvalues

Eigenvalues give us the size of variations along given eigenvector ($\sigma_{\mathbf{v}}^2$)

⇒ we can tell what variations are most relevant

By identifying variations which give leading contributions to the covariance matrix, we can limit number of variations considered in our problem.

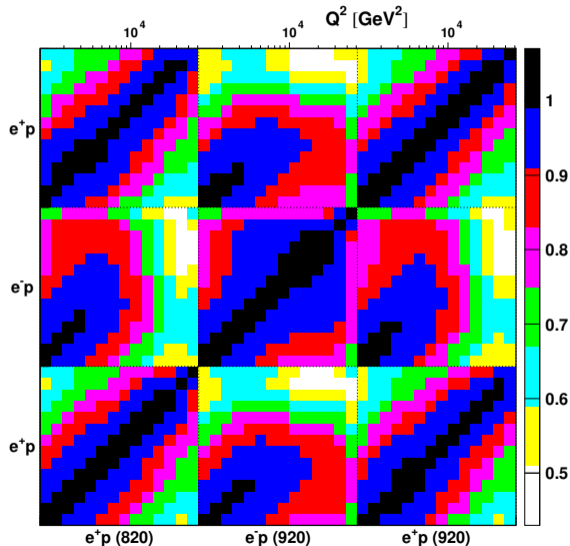
Variations corresponding to eigenvectors with very small eigenvalues can be safely ignored...

In the following, we assume eigenvectors are ordered from highest to lowest eigenvalue.

Eigenvectors

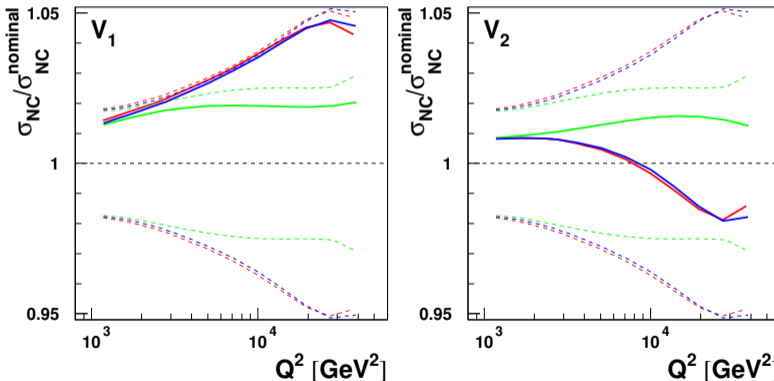
Let us consider uncertainties of the high Q^2 NC DIS cross sections again.

Correlation matrix:



Eigenvectors

Systematic variations corresponding to eigenvectors of correlation matrix:

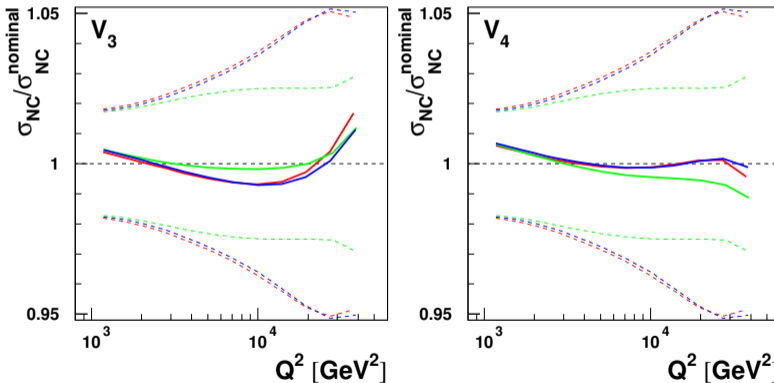


Dominant contribution from the first eigenvector...

(variations relative to the nominal SM

Eigenvectors

Systematic variations corresponding to eigenvectors of correlation matrix:

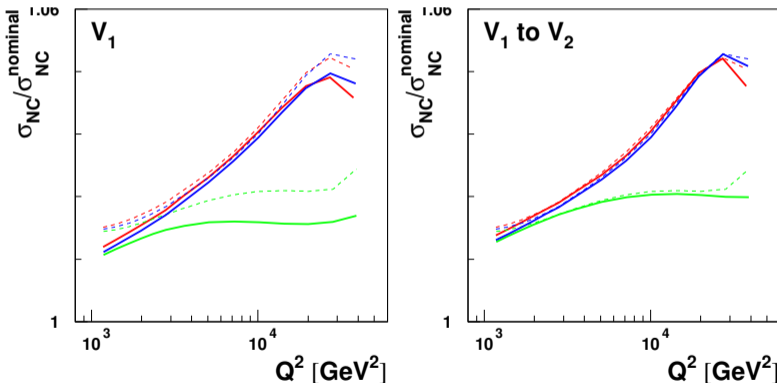


Dominant contribution from the first eigenvector...

(variations relative to the nominal SM

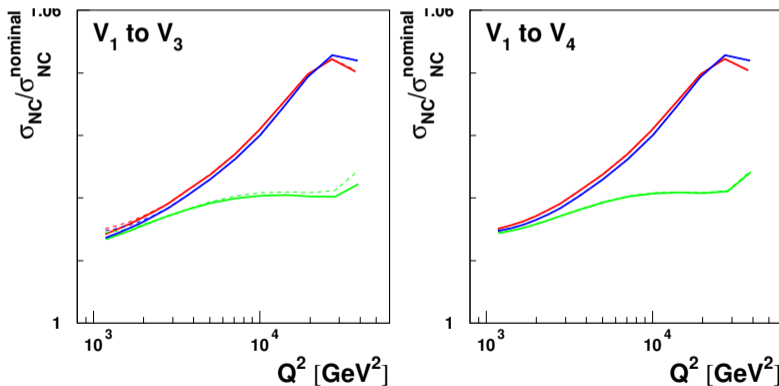
Eigenvectors

Variations corresponding to the sum of eigenvector contributions:



Eigenvectors

Variations corresponding to the sum of eigenvector contributions:



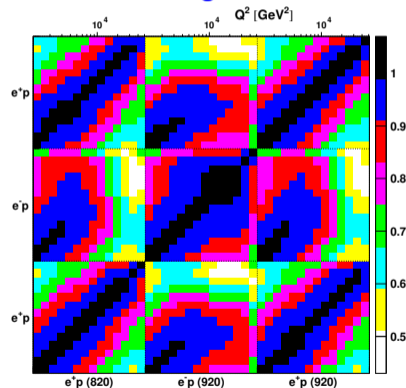
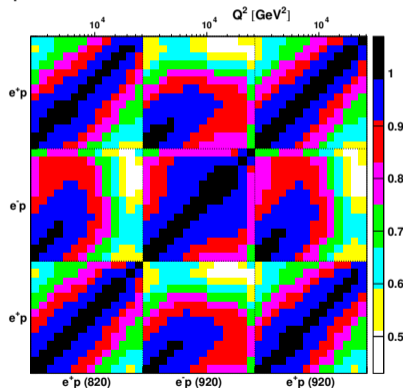
Four first eigenvectors perfectly reproduce total systematic uncertainty

Eigenvectors

Correlation matrix comparison:

Full matrix

Four eigenvectors



Correlations between PDF variations also very well reproduced by the first four eigenvectors

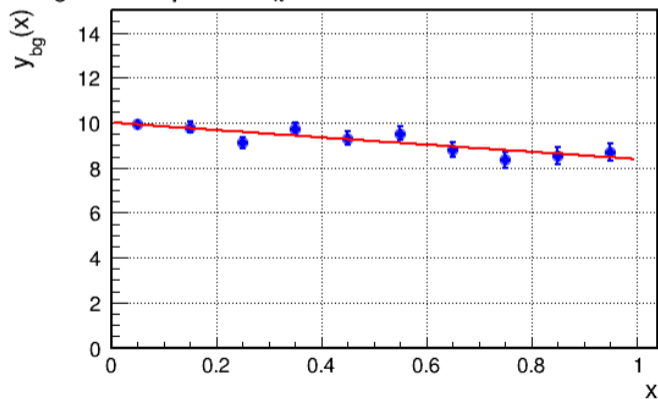
Eigenvectors

10_bg_fit_ev.ipynb

 Open in Colab

Example problem: eigenvectors of background covariance matrix

Background fit Npar = 3 $\chi^2 = 8.89 / 7$



Systematic uncertainties

- 1 Systematic effects
- 2 Estimating systematic uncertainties
- 3 Including systematic effects
- 4 Reducing variables
- 5 Homework

Homework

Solutions to be uploaded by January 11.

Electronic scale is used to weigh two objects, A and B, with masses m_A and m_B . The statistical uncertainty of single measurement is σ_m .

However, we use a support plate, the mass of which, m_0 , is known with uncertainty of σ_0 .

To reduce the impact of this uncertainty we perform three measurements m_j :

- of object A (and plate): $m_1 = m_0 + m_A$
- of object B (and plate): $m_2 = m_0 + m_B$
- of two objects A and B: $m_3 = m_0 + m_A + m_B$

- 1 Try to guess the formula for m_A for $f \rightarrow 0$ and $f \rightarrow \infty$
- 2 Find the optimal (most precise) estimate of m_A as a function of $f = \frac{\sigma_0}{\sigma_m}$.
- 3 Find the uncertainty of the m_A estimate as a function of f .