Unfolding in HEP Experiments

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- The Unfolding Problem
- The Origin of Difficulties
- Regularisation Methods
- Conclusions

(1) The unfolding problem

- Measurements in HEP experiments
  - Requirements
  - Example
- Integral equation
  - Notation
  - Conditions in HEP
- Matrix equation
  - Standard solution
- Simplifying solutions
  - Bin-by-bin correction
  - Another method
  - Conclusion about simpl. methods
- Statistical considerations
  - Correlated errors
  - Example from a publication

Requirements ...

on data points in a physics publication:

- accuracy
- no dependence on physics assumptions in MC simulation
- no or small correlations between data points

Comparison of data points with theoretical models or other data difficult or impossible in case of large correlations between data points. Error bars can not represent size of correlations!

If correlations are big:

- publish full covariance matrix of data points,
- use full covariance matrix (i.e. inverse as a weight matrix) in fits, detailed comparsions etc.

Measurements in High Energy Physics

- finite detector resolution: *smearing* of measured quantities
- detector effects like non-linear response
- limited acceptance (trigger, cuts): loss of events

... and physical effects:

- radiation of photons (ISR, FSR)
- Fermi motion within the nucleus
- fragmentation (partons $\rightarrow$ hadrons)

Integral equation

Notation:

$$
\begin{aligned}
x &= \text{true variable} \\
f(x) &= \text{true distribution of } x \\
y &= \text{measured variable} \\
g(y) &= \text{measured distribution of } y \\
b(y) &= \text{background distribution, included in } g(y) \\
A(y,x) &= \text{resolution function (response function),} \\
&\ \text{defined by set of Monte Carlo events,} \\
&\ \text{using } f_0(x)
\end{aligned}
$$

Integral equation for *unknown* $f(x)$:

$$
\begin{aligned}
g(y) &= \int A(y,x) f(x)\,\mathrm{d}x + b(y) \\
&\Rightarrow \int A(y,x) f_0(x) f_{\mathrm{mult}}(x)\,\mathrm{d}x + b(y) \\
&\Rightarrow \int A'(y,x) f_{\mathrm{mult}}(x)\,\mathrm{d}x + b(y)
\end{aligned}
$$

Monte Carlo $f_0(x)$ absorbed in $A'(y,x)$

final result: $\quad f(x) \equiv f_0(x) \cdot f_{\mathrm{mult}}(x)$

Example: Measurement of $\mathrm{d}\sigma/\mathrm{d}y$
in neutral current neutrino (narrow band beam) nucleon interactions.
Measurement of the distribution of inelasticity y, with

$$
\begin{aligned}
y &= \frac{E_{\mathrm{had}}}{E_\nu} \qquad 0 \le y \le 1 \\
f(y) &= Q + \bar{Q} \cdot (1-y)^2
\end{aligned}
$$

Measured variables:
hadronic energy E_{had} and radius r of vertex.
Narrow band beam energy flux $\Phi(E_\nu, r)$ has two-peak structure, with peak position r-dependent (from decay of π and K mesons).

Matrix equation

Integral equation simplified as matrix equation:

$$\begin{aligned} g(y) &= \int A(y,x)f(x)\,\mathrm{d}x \\ \mathbf{g} &= A\,\mathbf{f}\,. \end{aligned}$$

Representation of:

- true $f(x)$ by histogram $\mathbf{f}$ with n bins
- measured $g(y)$ by histogram $\mathbf{g}$ with m bins
- $A(y,x)$ by m-by-n matrix A

A single element if vector $\mathbf{g}$:

$$g_i = \sum_{j=1}^{n} A_{ij} f_j$$

Interpretation:

- A_{ij} = probability, to measure an event from true bin f_j in bin g_i,
- column $A_{\bullet j}$ is detector response to true element f_j,
- all elements $A_{ij} \geq 0$ by definition.

Conditions in HEP experiments

- data are *events* = set (n-tuple) of $[y]$ values
- limited statistics of measured events
- resolution finite, systematic shifts, etc.
- resolution (response) function only known implicitly, as a set of $[y|x]$ pairs from the simulation
- limited statistics of simulated events

Case $m = n$: standard solution by inversion

$$\begin{aligned} \mathbf{f} &= A^{-1}\,\mathbf{g} \\ V_f &= \left(A^{-1}\right)\ V_g \left(A^{-1}\right)^T \end{aligned}$$

error propagation

Inverse matrix A^{-1} has mainly negative off-diagonal elements (negative correlations between bins).

The standard solution is statistically correct, but is usually wildly fluctuating, due to a lack of stability.

Standard solution

Case $m > n$: Least squares method

weight matrix $W = V_g^{-1}$ $\qquad V_g =$ Cov. Matrix

Minimum of

$$\begin{aligned} S(\mathbf{f}) &= \left(\mathbf{g}^{\text{meas}} - A\mathbf{f}\right)^T W \left(\mathbf{g}^{\text{meas}} - A\mathbf{f}\right) \\ &= \text{const} + 2\mathbf{f}^T A^T W \mathbf{g}^{\text{meas}} + \mathbf{f}\left(A^T W A\right)\mathbf{f} \end{aligned}$$

Solution: derivative = 0:

$$A^T W \mathbf{g}^{\text{meas}} + \left(A^T W A\right)\mathbf{f} = 0$$

$$\begin{aligned} f &= \left(A^T W A\right)^{-1} A^T W \ \cdot \mathbf{g}^{\text{meas}} = B \cdot \mathbf{g}^{\text{meas}} \\ V_f &= B V_g B^T \\ &= \left(A^T W A\right)^{-1} A^T W \ V_g \ W A \left(A^T W A\right)^{-1} \\ &= \left(A^T W A\right)^{-1} \end{aligned}$$

... or Maximum Likelihood Method (Poisson statistics in bin):
Minimum of

$$-2\ln\mathcal{L}\left(\mathbf{f}\right)$$

Numerical example: (in case of absence of statistical errors)

$$\mathbf{f} = \begin{pmatrix} 100 \\ 121 \\ 81 \\ 64 \end{pmatrix} \qquad \text{yields measurement} \qquad \mathbf{g} = \begin{pmatrix} 104.2 \\ 108.8 \\ 85.6 \\ 67.4 \end{pmatrix}$$

$$\text{Unfolding} \quad A^{-1} \begin{pmatrix} 104.2 \\ 108.8 \\ 85.6 \\ 67.4 \end{pmatrix} \Rightarrow \begin{pmatrix} 100 \\ 121 \\ 81 \\ 64 \end{pmatrix}$$

Solution is correct for all input vectors $\mathbf{g}$.

Numerical example:

$$\varepsilon = \text{migration probability} = 0.4$$

$$A = \begin{pmatrix} 1-\varepsilon/2 & \varepsilon/2 & 0 & 0 \\ \varepsilon/2 & 1-\varepsilon & \varepsilon/2 & 0 \\ 0 & \varepsilon/2 & 1-\varepsilon & \varepsilon/2 \\ 0 & 0 & \varepsilon/2 & 1-\varepsilon/2 \end{pmatrix}$$

$$= \begin{pmatrix} 0.8 & 0.2 & 0.0 & 0.0 \\ 0.2 & 0.6 & 0.2 & 0.0 \\ 0.0 & 0.2 & 0.6 & 0.2 \\ 0.0 & 0.0 & 0.2 & 0.8 \end{pmatrix}$$

Inverse matrix:

$$A^{-1} = \begin{pmatrix} 1.38 & -0.52 & 0.19 & -0.05 \\ -0.52 & 2.10 & -0.76 & 0.19 \\ 0.19 & -0.76 & 2.10 & -0.52 \\ -0.05 & 0.19 & -0.52 & 1.38 \end{pmatrix}$$

has negative (and positive) off-diagonal elements.

Another simplifying unfolding method (popular for multiplicity distributions):

$\mathbf{g} = A\,\mathbf{f}$ with A from Monte Carlo.

Assume certain true vector $\mathbf{f}^{\mathrm{MC}}$, calculate *measured* vector $\mathbf{g}^{\mathrm{MC}} = A\,\mathbf{f}^{\mathrm{MC}}$, and define new matrix B by

$$B_{ij} = A_{ij}\,\left(\frac{f_j^{\mathrm{MC}}}{g_i^{\mathrm{MC}}}\right)$$

for use in the *unfolding* equatiuon

$$\mathbf{f} = B\,\mathbf{g} \qquad\qquad B \neq A^{-1}$$

Note: this so called *equation* is valid *only* for the vector $\mathbf{g} = \mathbf{g}^{\mathrm{MC}}$.

Based on interpretation:

- the row $B_{i\bullet}$ contains the distribution of events in the true bins, which are measured in bin i.

Simplifying methods

Bin-by-bin correction (Unsmearing)

The contents of each data bin are multiplied by the **ratio**

- of the number of entries generated
- to the number reconstructed in the same bin.

Simulation: $\mathbf{g}^{\mathrm{MC}} = A\,\mathbf{f}^{MC}$

Note: matrix A not explicitly needed.

Correction: applied iteratively

$$f_i = g_i^{\mathrm{meas}} \times \left(\frac{f_i^{\mathrm{MC}}}{g_i^{\mathrm{MC}}}\right) = g_i^{\mathrm{meas}} \times \textbf{ratio}$$

Very popular in HEP (... quickly converging), but

- valid only in the case of pure *acceptance* correction (no migration between bins),
- **not** quickly converging,
- converges to the same solution as matrix inversion, if converging at all.

Different numerical values(1. and 2. element interchanged):

$$\mathbf{f} = \begin{pmatrix} 121 \\ 100 \\ 81 \\ 64 \end{pmatrix} \qquad \text{yields measurement} \quad \mathbf{g} = \begin{pmatrix} 116.8 \\ 100.4 \\ 81.4 \\ 67.4 \end{pmatrix}$$

$$\textit{Unfolding } B \begin{pmatrix} 116.8 \\ 100.4 \\ 81.4 \\ 67.4 \end{pmatrix} \Rightarrow \begin{pmatrix} 108.1 \\ 117.1 \\ 77.4 \\ 63.4 \end{pmatrix} \neq \begin{pmatrix} 121 \\ 100 \\ 81 \\ 64 \end{pmatrix}$$

Result is wrong!

Conclusion: result of this method correct only if correct result already used as input; otherwise the result is biased.

Example: A as before. Assume solution:

$$\mathbf{f} = \begin{pmatrix} 100 \\ 121 \\ 81 \\ 64 \end{pmatrix} \qquad \text{yields measurement} \qquad \mathbf{g} = \begin{pmatrix} 104.2 \\ 108.8 \\ 85.6 \\ 67.4 \end{pmatrix}$$

$$\text{matrix } B = \begin{pmatrix} 0.77 & 0.18 & 0 & 0 \\ 0.23 & 0.67 & 0.28 & 0 \\ 0 & 0.15 & 0.57 & 0.24 \\ 0 & 0 & 0.15 & 0.76 \end{pmatrix}$$

$$\textit{Unfolding} \quad B \cdot \begin{pmatrix} 104.2 \\ 108.8 \\ 85.6 \\ 67.4 \end{pmatrix} \Rightarrow \begin{pmatrix} 100 \pm 7.9 \\ 121 \pm 8.1 \\ 81 \pm 5.7 \\ 64 \pm 6.2 \end{pmatrix}$$

Result correct, but error (calculated by standard error propagation) even smaller than Poisson error.

The standard solution (inversion) usually produces a wildly fluctuating result.

Conclusions about simplifying methods:

- the fast solution of a system of linear equations by *inversion* is replaced by a very slow *iterative* method, which is stopped rather early;
- if the slow method converges, it will converge to the same *fluctuating* result;
- fluctuating intermediate unfolding results are smoothed (or even fitted to parametrizations);
- simplifying methods have no statistical basis (but people say: *they work*);
- results are usually biased towards the expectation.

. . . the basic underlying assumption of the method is that the relative frequencies occurring in the response matrix derived from the Monte Carlo generator are the same as in the real data. Otherwise, the unfolded multiplicity distribution will be biased towards the generator distribution . . . .

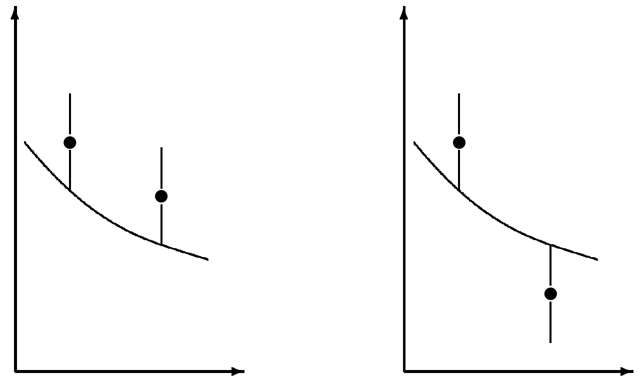
. . . one should note that this kind of unfolding procedure is model dependent and provides a reliable correction of the data only if the multiplicity distributions observed at the detector level for real events are well reproduced by the fully simulated events. This is the case for our analysis . . .

from publications

Numerical example: $\sigma_1 = \sigma_2 = \sigma$

two deviations $\Delta = \pm 1\,\sigma$

$$\chi^2 = \begin{cases} 2/(1+\rho) & \text{same sign} \\ 2/(1-\rho) & \text{opposite sign} \end{cases}$$



Probability from χ^2

	same sign	opposite sign
$\rho = 0$	37 %	37 %
$\rho = +0.9$	59 %	0.0005 %
$\rho = -0.9$	0.0005 %	59 %

Difficult interpretation of *common* deviations of > 1 data point in case of *correlated* ($\rho \neq 0$) data points.

Correlations

Case of two *correlated* variables:

$$\text{Covariance matrix} \quad V = \begin{pmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 \end{pmatrix}$$

$$\begin{aligned} \sigma_{1,2} &= \text{standard deviations of the variables} \\ \rho &= \text{correlation coefficient} \qquad -1 < \rho < +1 \end{aligned}$$

The χ^2 value Wert for a deviation Δ from a theroretical prediction is given by:

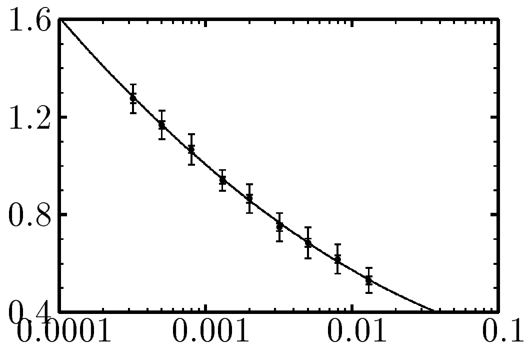
$$\chi^2 = \Delta^T \left(V^{-1}\right) \Delta$$

with the inverse of the covariance matrix

$$V^{-1} = \frac{1}{(1-\rho^2)} \begin{pmatrix} 1/\sigma_1^2 & -\rho/\sigma_1\sigma_2 \\ -\rho/\sigma_1\sigma_2 & 1/\sigma_2^2 \end{pmatrix}$$

Example from a publication

Result of bin-by-bin *unsmearing* correction:



Fit of parabola to the data shows: **either**

- errors to big (by factor > 5), **or**
- fluctuations too small.

data points are strongly correlated (positive correlation).

- effective rank of set of data points is only 2 ... 3.

Origin of correlations?

Given a measurement:

$$\begin{aligned} \mathbf{g} &= \text{vector of } m \text{ data points} \\ V_g &= \text{covariance matrix, rank } m \\ & \quad \text{(often diagonal for direct data)} \end{aligned}$$

Transformation:

$$\mathbf{f} = \text{vector of } n \text{ parameters}$$

by linear transformation of vector $\mathbf{g}$ by matrix B.

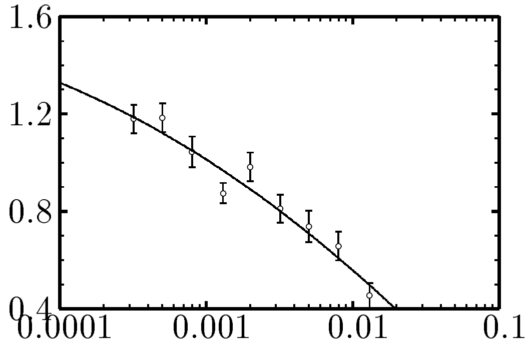
$$\begin{aligned} \mathbf{f} &= B\,\mathbf{g} \\ V_f &= B\,V_g\,B^T \qquad \text{(error propagation)} \end{aligned}$$

Rank of matrix V_f is $(\leq) m$.
If $n > m$ oder even $n \gg m$: matrix singular,
Diagonal elements small for large positive correlation between parameters.

(2) Origin of difficulties in unfolding

- The case $n = m = 2$
  - A numerical example
- Unfolding of periodic functions
  - A numerical example
- Lower limit of the bin width
- Conclusions

Figure shows size of *expected* fluctuations for same error size: (simulated random data points with same error size around fitted positions)



Note: the fit of a parabola to the simulated data points has the opposite sign of curvature: due to the large errors the sign of the curvature is unkown!

Inverse matrix:

$$A^{-1} = \frac{1}{1-2\varepsilon}\begin{pmatrix} 1-\varepsilon & -\varepsilon \\ -\varepsilon & 1-\varepsilon \end{pmatrix}$$

General expression for the resultant covariance matrix:

$$V_f = \frac{1}{(1-2\varepsilon)^2}\begin{pmatrix} (1-\varepsilon)^2 g_1 + \varepsilon^2 g_2 & -\varepsilon(1-\varepsilon)(g_1+g_2) \\ -\varepsilon(1-\varepsilon)(g_1+g_2) & (1-\varepsilon)^2 g_2 + \varepsilon^2 g_1 \end{pmatrix}$$

The case $n = m = 2$

Only $n = 2$ possible true values and only $m = 2$ possible measured values.
ε is the probability for migration out of original bin.

$\varepsilon = 0.5$ means: **no** measurement.

$$\begin{pmatrix} g_1 \\ g_2 \end{pmatrix} = \begin{pmatrix} 1-\varepsilon & \varepsilon \\ \varepsilon & 1-\varepsilon \end{pmatrix} \cdot \begin{pmatrix} f_1 \\ f_2 \end{pmatrix}$$

or short:

$$\mathbf{g} = A\mathbf{f}$$

Unfolding by inversion:

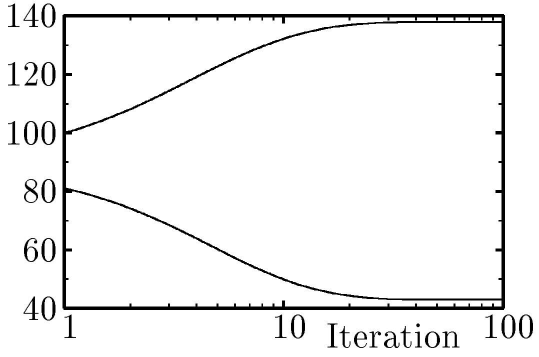
$$\boxed{\begin{aligned} \mathbf{f} &= A^{-1}\mathbf{g} \\ V_f &= A^{-1}\, V_g\, A^{-1} \end{aligned}}$$

Example:

- Classification of events as NC and CC,
- ε is the probability for wrong classification.

What about the bin-by-bin acceptance correction method in this case?

Parameter f_1 and f_2 versus iteration number:



The method converges (of course) to the *same* values as the inversion method, but extremely slow (linear convergence).

$$f_1 = 138 \pm 13.8 \qquad\qquad f_2 = 43 \pm 4.8$$

The errors are too small (correlation by finite resolution is ignored).

A numerical example:

Measurement and covariance matrix are:

$$\begin{aligned} g_1 &= 100 \pm 10 \\ g_2 &= 81 \pm 9 \end{aligned} \qquad V_g = \begin{pmatrix} 100 & 0 \\ 0 & 81 \end{pmatrix}$$

Result of unfolding by inversion:

ε	$\hat{f}_1$	$\hat{f}_2$	ρ
0	100 ± 10	81 ± 9	0
0.1	102.4 ± 11.3	78.6 ± 10.2	-0.22
0.4	138 ± 35	43 ± 33	-0.92
0.5	$\pm\infty$	$\pm\infty$	singular

- Statistical errors magnified because of finite resolution (migration probability ε)!

Effect in detail for $\varepsilon = 0.4$:

$$A^{-1} = \frac{1}{1-2\varepsilon} \begin{pmatrix} 1-\varepsilon & -\varepsilon \\ -\varepsilon & 1-\varepsilon \end{pmatrix} = \begin{pmatrix} 3 & -2 \\ -2 & 3 \end{pmatrix}$$

$$\begin{aligned} \hat{f}_1 &= 3 \cdot g_1 - 2 \cdot g_2 = 300 - 162 = 138 \\ \sigma &= \sqrt{3^2 \cdot 100 + 2^2 \cdot 81} = 35 \qquad (\gg 10) \end{aligned}$$

Unfolding of periodic functions

Discussion of a special case with *analytical* formula for the unfolding.

Assumption:

- $f(x)$ periodic (period $= 2\pi$)
- Gaussian x resolution (standard deviation $= \sigma$)

Representation of $f(x)$ as Fourier sum:

$$f(x) = \frac{a_0}{2} + \sum_{\nu=1}^{\infty} \left(a_\nu \cos \nu x + b_\nu \sin \nu x \right)$$

The sin and cos functions form an orthogonal system of functions.

$$a_\nu = \frac{1}{\pi} \int_0^{2\pi} f(x) \cos \nu x \, \mathrm{d}x$$

Properties :

- Asymptotic behavior of the Fourier coefficients

$$c_\nu = \sqrt{a_\nu^2 + b_\nu^2} = \mathcal{O}\left(\frac{1}{|\nu|^{r+1}} \right) ,$$

  if r-th derivative of $f(x)$ continuous.

- Curvature

$$\int_0^{2\pi} \left| f''(x) \right|^2 \, \mathrm{d}x = \pi \sum_{\nu=1}^{\infty} c_\nu^2 \nu^4$$

In general a *few* Fourier terms sufficient for an accurate description of function $f(x)$ (higher order terms become soon very small).

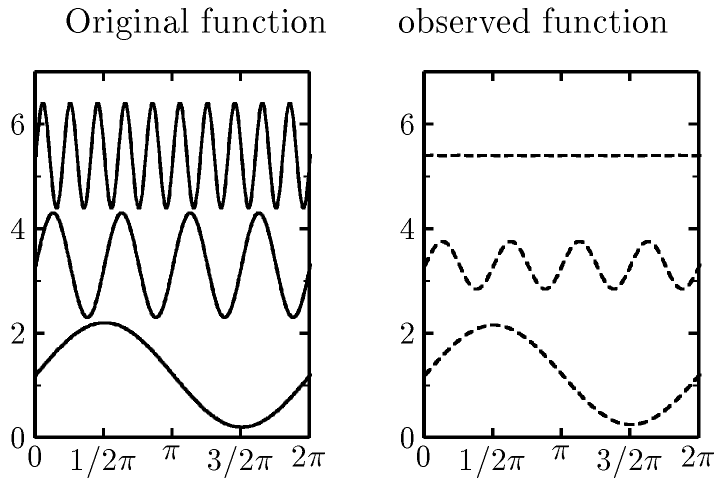
The result of **folding** of $f(x)$ with a Gaussian resolution function (standard deviation σ) is the *observed* function $g(y)$:

$$g(y) = \int_{-\infty}^{+\infty} \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(y-x)^2}{2\sigma^2}\right) f(x)\,\mathrm{d}x \ ,$$

which is again periodic, with Fourier coefficients

$$\begin{aligned} \alpha_\nu &= a_\nu \ \exp\left(-\tfrac{\nu^2\sigma^2}{2}\right) \\ \beta_\nu &= b_\nu \ \exp\left(-\tfrac{\nu^2\sigma^2}{2}\right) \end{aligned}$$

Note: each single coefficient is modified (damped), independent of all other coefficients!



Unfolding is very simple: correct the *measured* coefficients α_ν und β_ν by multiplication with factors

$$\exp\left(+\frac{\nu^2\sigma^2}{2}\right)$$

in order to get the coefficients a_ν und b_ν back.

A numerical example

Test function = sum of three Breit-Wigner functions:

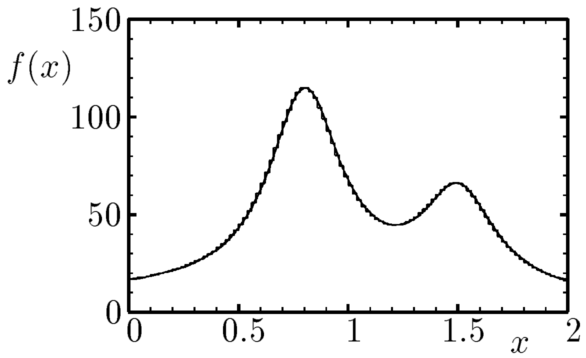
$$f(x) = \sum_{k=1}^{3} b_k \frac{g_k^2}{(x - x_k)^2 + g_k^2}$$

... interpreted as a periodic function function within interval $0 \ldots 2\pi$

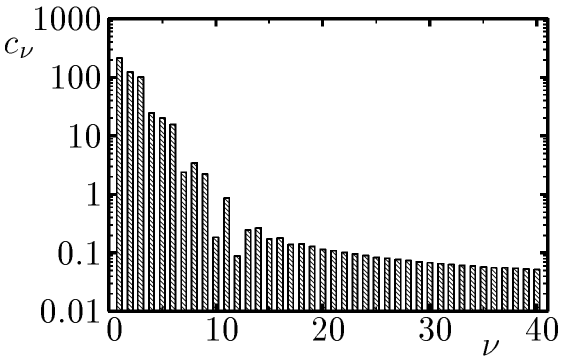
- Fourier analysis
- effect of finite resolution
- effect from statistical errors
- combination of the two effects

Fourier analysis of test function

Test function as a histogram (100 bins):



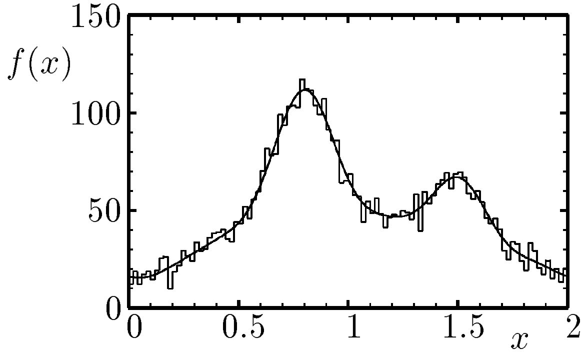
Fourier coeff. $c_\nu = \sqrt{a_\nu^2 + b_\nu^2}$ on a log. scale:

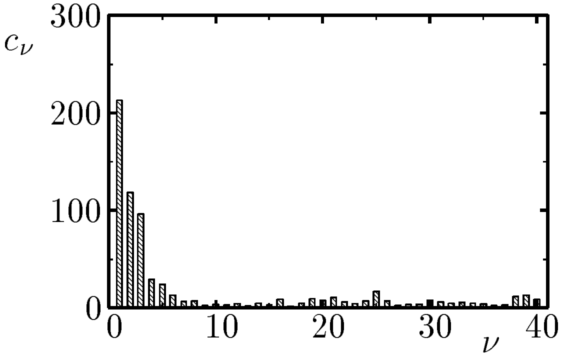


Coefficients $c_\nu \to 0$ for large ν as $1/\nu^2$.
Coefficients up to $\nu = 9$ are sufficient for the accurate parametrization of the test function (see curve in top figure = representation of terms up to $\nu = 9$.

Effects due to statistical errors

Histogram with error ±5 in each bin:

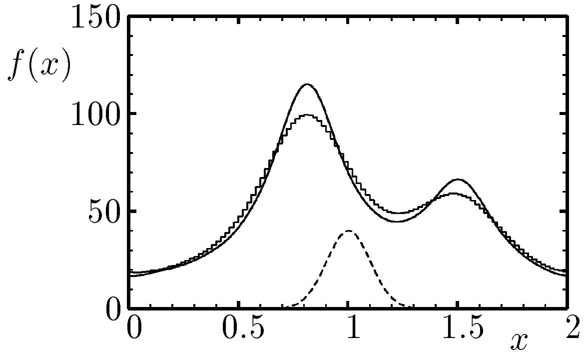


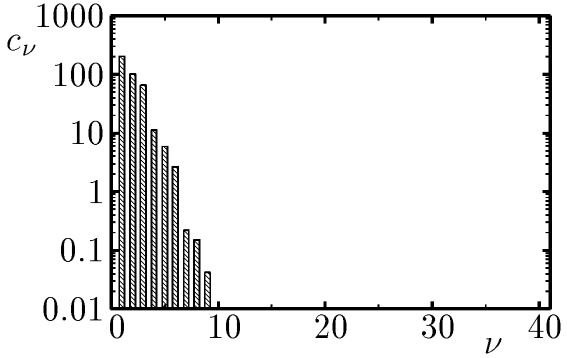


Statistical measurement errors generate a *constant* error (noise) for the coefficients. Only the first coefficients up to $\nu = 6 \ldots 8$ are **significant** (curve in top figure reconstructed from the first 6 coefficients).

Effects of finite resolution

Histogram of the function(curve) after **folding** with a Gaussian resolution function ($\sigma = 0.1$, dashed curve):





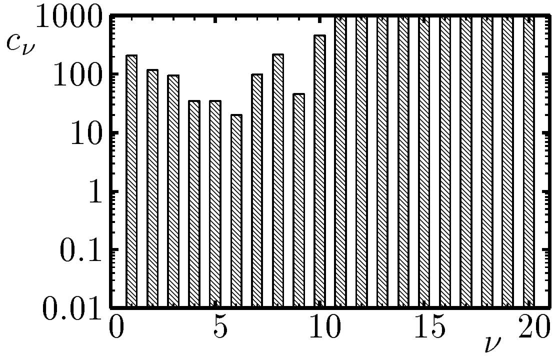
Coefficients $c_\nu \to 0$ much faster because of finite resolution.

Corrections of Fourier coefficients

Coefficients α_ν and β_ν corrected by factor:

$$\exp\left(+\frac{\nu^2\sigma^2}{2}\right)$$

Plot of corrected coefficients c_ν:

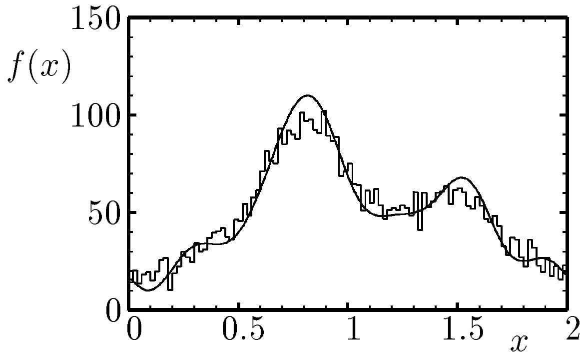


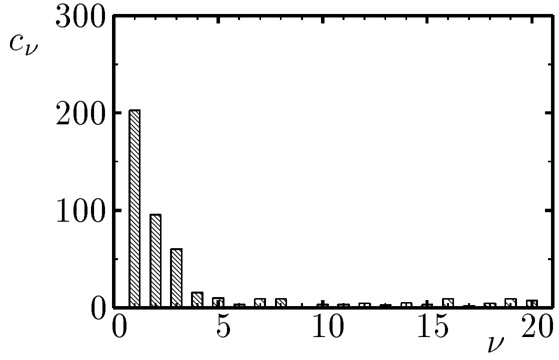
Cut-off necessary at $\nu = 6$ in order to avoid large fluctuations by *noise*.

(*Regularisation*)

Effects ...

by the finite resolution **plus** statistical errors:





Coefficients up to $\nu \approx 6$ significant. Curve (top figure) reconstructed from the coefficients up to $\nu = 6$.

Conclusions

- Limited resolution has the effect of negative correlations between adjacent corrected data points and of large fluctuation of data points
- cut-off essential to suppress enlarged statistical fluctuations (regularisation)
- Cut-off index critical
- bin width ≥ 2 standard deviations

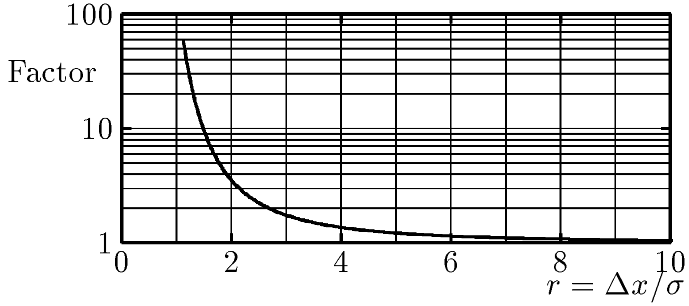
Lower limit of the bin width

Cut-off at $\nu = \nu_0$ means:

$$1 + 2 \times \nu_0 \quad \text{significant coefficients only}$$

Representation of result in bins (with integration of corrected function within bins) with limitation to $1 + 2 \times \nu_0$ bins (number of degrees of freedom).

Magnification factor for statistical errors due to limited resolution (migration):



Smallest bin width is $\Delta x \approx 2 \times \sigma \qquad (r \approx 2)$

Overview

Regularisation: start from standard solution, but add term $\tau \cdot R(\mathbf{f})$ to the Likelihood function or χ^2-expression:

$$-2 \ln \mathcal{L}(\mathbf{f}) + \tau \cdot R(\mathbf{f})$$

- τ = regularisation parameter

Different expressions for $R(\mathbf{f})$:

- curvature $R = \int |f''(x)|^2 \, \mathrm{d}x$
- magnitude $R = \int |f(x)|^2 \, \mathrm{d}x$
- maximum entropy $R = \sum_j f_j \ln f_j / \varepsilon_j$

In case of curvature:

- τ small: no effect of regularisation
- τ large: resulting function will be **linear**

Regularisation has been introduced by Thikhonov.

(3) Regularisation methods

- Overview
- Practical experimental problems
- Splines and B splines
- Determining the regularisation parameter
- Data points
- A numerical example

Practical problems

Knowledge of resolution function $A(y, x)$ essential, but:

- problems in the event generation,
- problems in the detector simulation,
- problems in the measurement (data taking, reconstruction),
- MC statistics too small.

The most important practical problem in unfolding is **control** of the resolution function!

Unfolding procedure has to include back-projection of result (by reweighting of MC events) for comparison of distributions of many measured variables.

- $f(x)$ has to be smooth (use of spline function instead of histogram).

Different technical realisations:

- SVD Approach to Data Unfolding (A. Höcker, V. Kartvelishvili)
  Singular Value Decomposition, curvature, MC-TH-95-15
- Entropy Method (M. Schmelling)
  NIM A 340 (1994) 209
- RUN Algorithmus (V. B.)
  Curvature, B-Splines, DESY 84-118, OPAL TN 361 (1996)

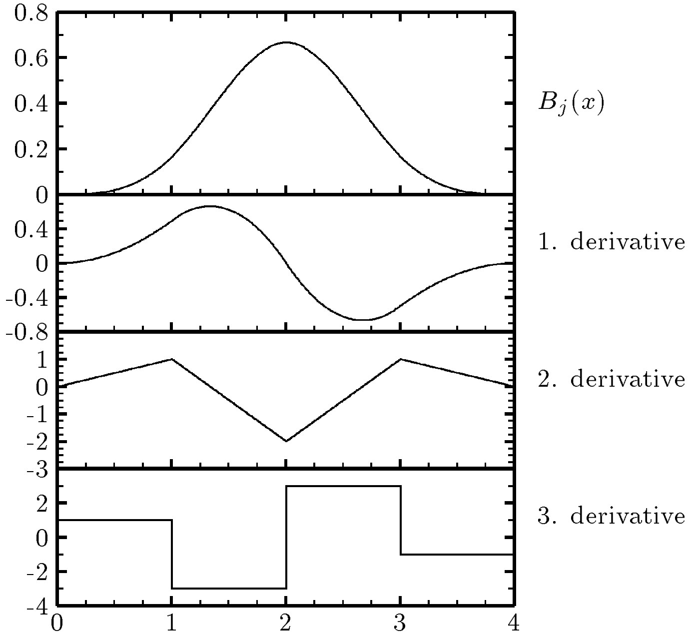
These methods contain explicitly regularisation in a controlled way.

Note: The simplifying methods (bin-by-bin correction and others) contain, implicitly, a much stronger regularisation of the result.

B splines

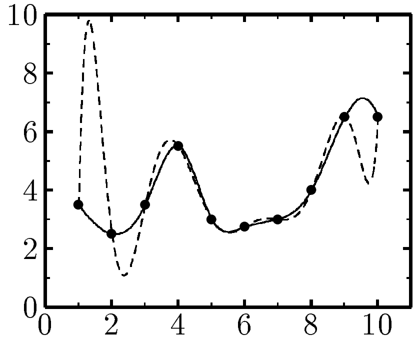
Cubic B splines:

- not equal to zero in limited x interval,
- made out of four polynomials of third degree
- jump in the third derivative



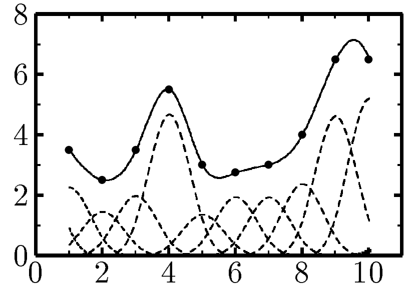
Interpolation by spline functions

Example: Interpolation of 10 data points by cubic spline functions (full curve) und polynomial of 9.th degree (dashed):



Representation by B splines (with local support):

$$f(x) = \sum_j a_j \, B_j(x) \qquad B_j(x) = \text{ cubic B spline}$$



with diagonal matrix S, with solution

$$a_j'^{\,\mathrm{reg}} = \left(\frac{1}{1 + \tau S_{jj}} \right) a_j'^{\,\mathrm{unreg}}$$

(curvature S_{jj} is increasing rapidly, resulting in a damping of coeffients with high value of index j).

Effective number of degrees of freedom:

$$m_0 = \sum_{j=1}^{m} \left(\frac{1}{1 + \tau S_{jj}} \right)$$

defines τ ($\tau \approx 1/S_{jj}$ mit $j = m_0$).

- Number of data points equal to effective number of degrees of freedom.

$\boxed{\text{Regularisation by curvature}}$

$$\text{Curvature } = \int \left| f''(x) \right|^2 \, \mathrm{d}x = \mathbf{a}^T C \mathbf{a}$$

with symmetric matrix C:

$$C = \begin{pmatrix} 2 & -3 & 0 & 1 & 0 & 0 & \ldots \\ -3 & 8 & -6 & 0 & 1 & 0 & \\ 0 & -6 & 14 & -9 & 0 & 1 & \\ 1 & 0 & -9 & 16 & -9 & 0 & \\ 0 & 1 & 0 & -9 & 16 & -9 & \\ 0 & 0 & 1 & 0 & -9 & 16 & \\ \vdots & & & & & & \ddots \end{pmatrix}$$

for cubic splines with equidistant knots.

The minimum of

$$-2 \ln \mathcal{L}(a) + \frac{1}{2} \tau \cdot \mathbf{a}^T C \mathbf{a} = \ldots \mathbf{a}^T \mathbf{h} + \frac{1}{2} \mathbf{a}^T H \mathbf{a} + \frac{1}{2} \tau \cdot \mathbf{a}^T C \mathbf{a}$$

has to be determined. Which value of τ?

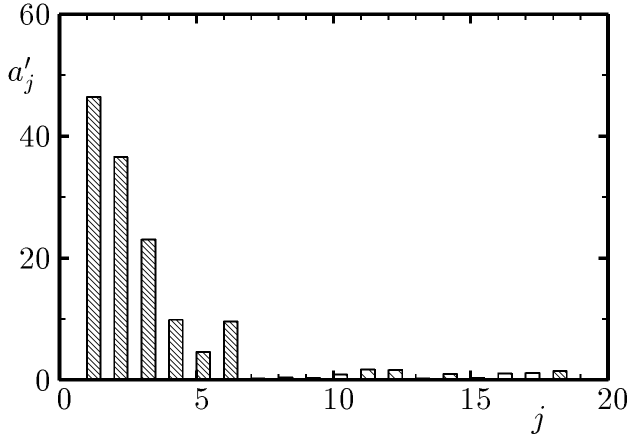
Simultaneous diagonalisation of H and C with parameter transformation ($\mathbf{a} \to \mathbf{a}'$):

$$= \ldots \mathbf{a}'^T \mathbf{a}' + \mathbf{a}'^T S \mathbf{a}'$$

Amplitudes

$$f(x) = \sum_j a_j\, B_j(x) = \sum_j a'_j P_j(x)$$

$$\begin{aligned} B_j(x) &= \text{B-Spline, } \neq 0 \text{ only in small area} \\ P_j(x) &= \text{orthogonal linear combinations} \\ &= \text{(independent)} \end{aligned}$$

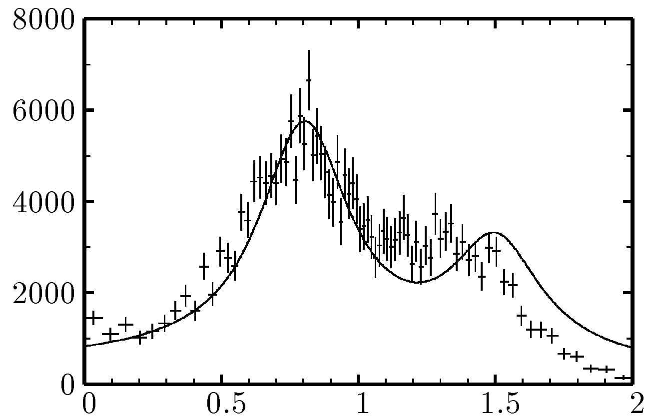


- Coefficients a'_j have variances of 1

Numerical example

Curve = test function (Sum $\sum_i \mathrm{BW}_i$)
Histogram of 10000 generated events:

- Gaussian resolution function with $\sigma = 0.1$
- nichtlinear detector response
- reduced acceptance at both ends



- Width of Histogram bins smaller in the center

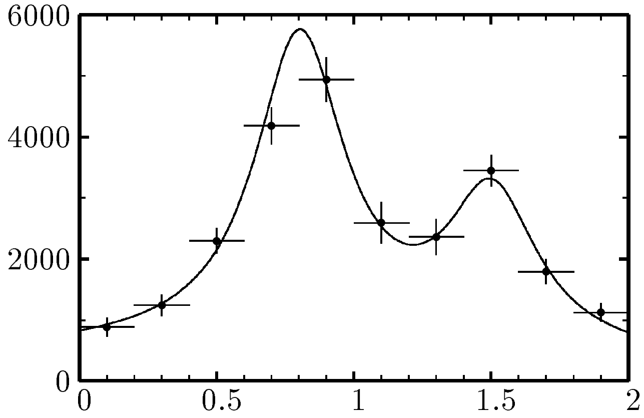
Minimum between the two peaks is filled up!

Conclusions

- Unfolding is necessary for many measurements in HEP experiments
- Unfolding is a difficult statistical and mathematical problem
- It requires a detailed understanding of the detector response
- In use are simplifying methods, which do not have a statistical basis, but they *work* and the results are generally accepted in the HEP community
- Regularisation methods, based on statistical principles, exist, but are not easy to use.

Result of unfolding

- 10 data points by integration over interval
- comparison with input curve



- Minimum between two peaks *visible* again