

# UNFOLDING / DECONVOLUTION

- Direct and inverse processes

Suppose we want to measure some variable  $x$  using a detector that has a response function that "deforms" or "transforms" in some way. The variable  $x$  into  $y$ .

~~Y = f(x)~~

If  $f(x)$  is the PDF of  $x$ , and  $r(x, y)$  is the response function (also called kernel function), the PDF of  $y$  will be:

$$g(y) = \int r(x, y) f(x) dx [+ b(y)] \rightarrow \text{Fredholm integral}$$

↓                      ↓  
Convolution of  $f$  and  $r$

~~possible noise~~ ~~background~~ or ~~bkg~~

Typically,  $r$  induces a "smearing" which broadens the nests structures present in the original distributions.

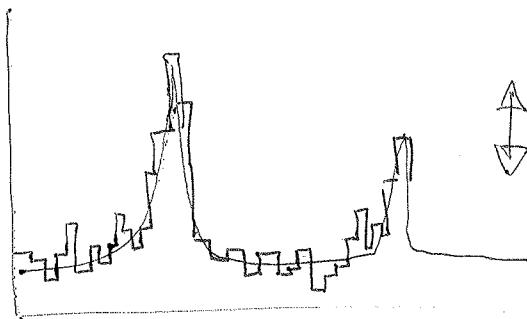
- Example:
- Energy resolution for an X-ray detector
  - Space resolution induced by lens aberrations on telescope image

Possible ~~eff~~ "distortions" are:

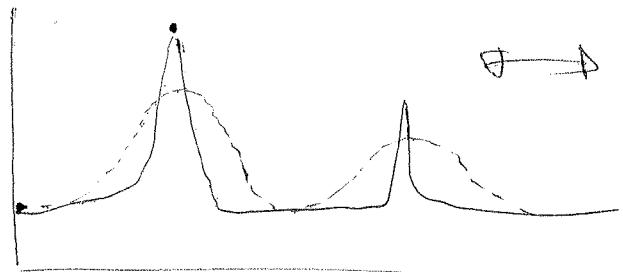
- Statistical fluctuations (e.g. due to Poisson statistics) if the data are binned
- Smearing due to limited resolution = migration of counts between bins
- Reduced efficiency
- Non-linear detector response

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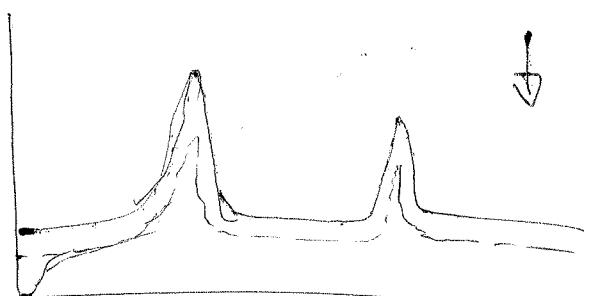
→ Statistical fluctuations due to  
e.g. Poisson statistics in bins:



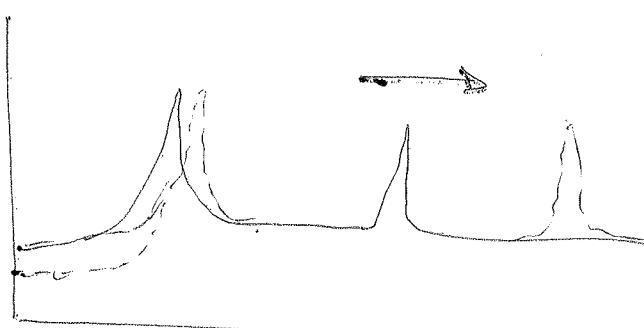
→ Smearing, i.e. migration of counts between bins due to resolution of detector:



→ Reduction of counts due to  
non-uniform efficiency

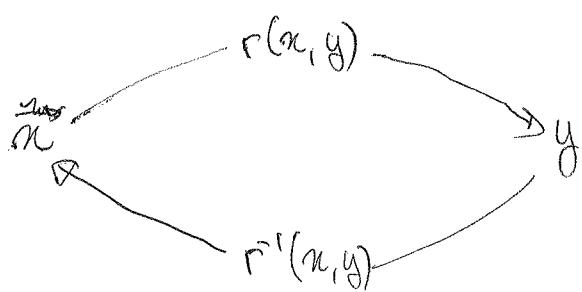


→ Deformation of distribution due  
to non-linear detector response



Usually, we see a combination of all these effects!

At this point, we have 2 possibilities:



a) Include the response function  
in the fit, and fit  $r(y)$   
(That's what we have done  
so far)

b) Invert the response function  
and fit  $x$   
↳ Unfolding

## • Convolution and Fourier Transform

In most cases,  $r$  depends only on the difference of  $x-y$ , so it depends just on one variable:  $r(x-y) = r(x-y)$ .

In general, we will denote the convolution as  $\otimes$ .

Let's take the Fourier Transform of  $g$ :

$$\hat{g}(k) = \int_{-\infty}^{+\infty} g(y) e^{-iky} dy$$

$$\text{Conversely: } g(y) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \hat{g}(k) e^{iky} dk$$

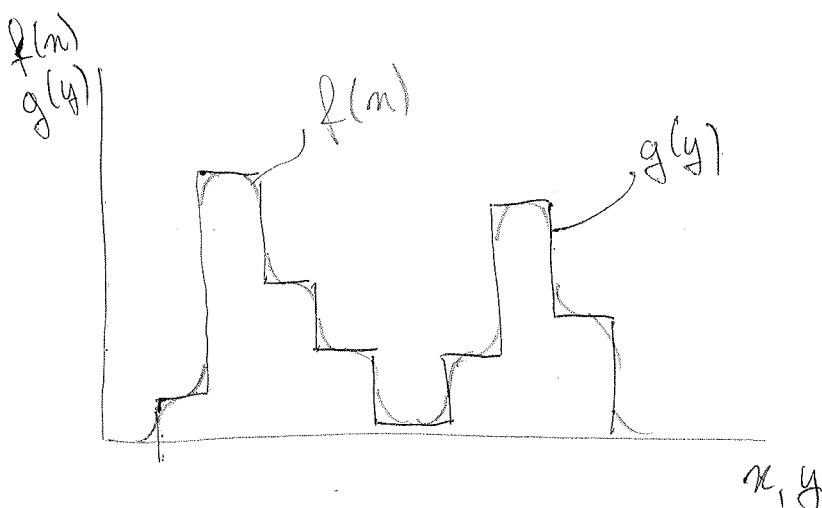
One can demonstrate that:  $\widehat{g \otimes r} = \hat{g} \cdot \hat{r}$

Conversely:  $\widehat{g \cdot r} = \hat{g} \otimes \hat{r}$

→ Example: Gaussian smearing

$$\text{Take } r(x-y) = \frac{1}{2\pi\sigma} \exp\left(-\frac{(x-y)^2}{2\sigma^2}\right)$$

$$\hat{r}(k) = e^{-ik\mu} \exp\left(-\frac{\sigma^2 k^2}{2}\right)$$



## • Discrete data

In many cases, the data are available in form of histograms, where every bin contains some number of counts ~~with an expect  $n_i$~~  with an expect  $n_i$ :

$$\text{with an expectation value } v_i : \quad v_i = \langle n_i \rangle = \int_{\delta n_i} f(n) dn \quad i=1, \dots, N,$$

In principle, also  $y$  the original variable can be distributed among multiple bins, which can be of a different size:

$$\mu_j = \int_{\delta y_j} g(y) dy \quad j=1, \dots, M \quad M \text{ can be different from } N$$

The relation between  $\mu_j$  and  $v_i$  will be:

$$v_i = \sum_{j=1}^M R_{ij} \mu_j$$

$R = N \times M$  matrix = response matrix

If we also have some background  $b$  affecting  $n$ , we'll have:

$$v_i = \sum R_{ij} \mu_j + b_i$$

$$\vec{v} = R \vec{\mu} + \vec{b}$$

## • Unfolding by inversion of the response matrix

Suppose we measure an experimental binned distribution  $\vec{n} = (n_1, \dots, n_N)$  and we want to find an estimate for the original distribution  $\vec{\mu}$ .

We can use the max-L method:

$$L(\vec{n} | \vec{\mu}) = \prod_{i=1}^N \text{Poisson}(n_i | v_i(\vec{\mu})) = \prod_{i=1}^N \text{Poisson}\left(n_i | \sum_{j=1}^M R_{ij} \mu_j + b_i\right)$$

The solution is found by inverting the matrix.

$$\text{Assuming } N=M \text{ for simplicity: } \hat{\vec{\mu}} = R^{-1}(\vec{n} - \vec{b})$$

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The covariance matrix of the expected bin entries  $\hat{\mu}_i$  is:

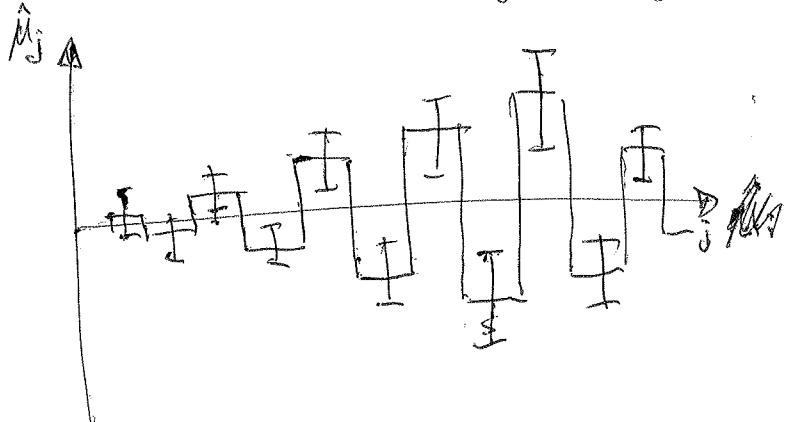
$$U = R^{-1} V (R^{-1})^T \text{ where } V \text{ = covariance matrix of data } n_i$$

$$V_{ij} = S_{ij} v_j \text{ because of Poisson precn.}$$

The issue is that then each bin  $\hat{\mu}_j$  is strongly anti-correlated with its neighbour  $\hat{\mu}_{j\pm 1}$  because of the off-diagonal entries of  $U$ .

This is cured by statistical fluctuations in the data reflecting into strong anti-correlations rather than into the uncertainty on  $\hat{\mu}_j$ , as one would expect.

One gets something like:



- Bin-by-bin correction

One possible solution is to correct  $n_i$  using the ratio of expected values before and after unfolding:

$$\hat{\mu}_i = \frac{\mu_i^{\text{est}}}{v_i^{\text{est}}} (n_i - b_i) \quad \text{where: } \mu_i^{\text{est}}, v_i^{\text{est}} \text{ are obtained from simulation.}$$

$v_i^{\text{est}}$  has no background

Problem: This approach introduces a bias that drives  $\hat{\mu}_i$  towards  $\mu_i^{\text{exp}}$ :

$$\langle \hat{\mu}_i \rangle - \mu_i = \left( \frac{\mu_i^{\text{est}}}{v_i^{\text{est}}} - \frac{\mu_i}{v_i - b_i} \right) (v_i - b_i)$$

In this way, we risk to hide real discrepancies!

## • Regularized unfolding

We have this situation:

- The max-L based matrix inversion is unbiased by construction, but is affected by a large variance.
- Any other method can reduce the variance, but will be biased.

What we can do is to impose some condition ~~on~~ on the "smoothness" of the values to be estimated  $\hat{\mu}$ , quantified by some function  $S(\hat{\mu})$ . These methods are called "regularized unfolding".

In practice, instead of minimizing  $\Lambda = -2 \ln L$ , we minimize:

$$\phi(\hat{\mu}) = \Lambda(\hat{\mu}) + \gamma^2 S(\hat{\mu}), \text{ where } \gamma = \text{"regularization strength"}$$

If  $\gamma = 0 \Rightarrow$  max-L estimate

If  $\gamma \gg 0 \Rightarrow \hat{\mu}$  is extremely smooth, but insensitive to measured data  $\vec{n}$

→ Normalization issue:

The total measured yield  $n = \sum n_i$  might differ from the expected yield  $v = \sum v_i$ .

We can include an extra term:

$$\phi(\hat{\mu}) = \Lambda(\hat{\mu}) + \gamma^2 S(\hat{\mu}) + \lambda(n - v)$$

At this point we "just" have to choose  $S(\hat{\mu})$ .

## • Tikhonov Regularization

Let's choose:  $S(\vec{\mu}) = (\mathbf{L}\vec{\mu})^\top \mathbf{L}\vec{\mu}$

where  $\mathbf{L}$  is a  $n \times k$  matrix.

→ In the simplest case,  $\mathbf{L} = \mathbf{I}$ , therefore:  $S(\vec{\mu}) = \sum_j \mu_j^2$

In this way, the term  $\gamma^2 S(\vec{\mu})$  damps the ones with large deviations of  $\mu_j$  from zero.

→ Another choice is:

$$\mathbf{L} = \begin{pmatrix} -1 & 1 & 0 & \dots & 0 \\ 1 & -2 & 1 & & \vdots \\ 0 & 1 & -2 & \ddots & 1 & 0 \\ \vdots & & & \ddots & 1 & 0 \\ 0 & \dots & 0 & \ddots & -1 \end{pmatrix}$$

In fact, if we have a function approximated by a histogram  $h$  with bin size  $\delta$ , the first two derivatives are:

$$h_i' = \frac{h_i - h_{i-1}}{\delta}$$

$$h_i'' = \frac{h_{i-1} - 2h_i + h_{i+1}}{\delta^2}$$

So  $\mathbf{L}$  is an approximation of the 2<sup>nd</sup> derivative of  $\vec{\mu}$  as approximation of  $g(y)$ .

$S(\vec{\mu})$  would correspond to:

$$S \approx \int \left( \frac{d^2 g(y)}{dy^2} \right)^2 dy$$

In this way, large 2<sup>nd</sup> derivatives that induce high-frequency oscillations are damped.

## • Iterative unfolding

Another approach is to repeat the unfolding:

$$\mu_j^{(k+1)} = \mu_j^{(k)} \sum_{i=1}^N \frac{R_{ij}}{\varepsilon_j} \frac{n_i}{\sum_{p=1}^N R_{ip} \mu_p^{(k)}} + \text{noise}$$

with  $\varepsilon_j = \sum_i R_{ij}$

We start from  $\mu_j^{(0)} = \mu_j^{\text{est}}$  and proceed for  $K$  iterations, with ~~K large~~  
 $K$  of order 100.

This approach can be motivated using Bayes' Theorem.

Take a number of "cover"  $C_j$ ,  $j = 1, \dots, M$

and a number of "effect"  $E_i$ ,  $i = 1, \dots, N$

Then:  $P(C_j | E_i) = \frac{P(E_i | C_j) \pi_0(C_j)}{\sum_{k=1}^M P(E_i | C_k) \pi_0(C_k)}$

$C_j$  = event generated in bin  $j$  of original histogram

$E_i$  = event observed, after detector effects, in bin  $i$  of  $n$  histogram

$P(E_i | C_j)$  = response matrix  $R_{ij}$

$$\pi_0(C_j) = \frac{\mu_j^{(0)}}{n^{\text{obs}}} \quad n^{\text{obs}} = \sum_{i=1}^N n_i$$

Therefore:  $P(C_j | E_i) = \frac{R_{ij} \mu_j^{(0)}}{\sum_{k=1}^M R_{ik} \mu_k^{(0)}}$

The experimental distribution  $\vec{n} = (n_1, \dots, n_N)$  is the number of occurrences of each effect  $E_i$ :  $n_i = n(E_i)$

The expected number of events  $\mu_j^{(1)}$  assigned to each cause  $C_j$  is:

$$\mu_j^{(1)} = \hat{n}(C_j) = \sum_{i=1}^N n(E_i) \frac{P(C_j | E_i)}{\varepsilon_j} = \mu_j^{(0)} \sum_{i=1}^N \frac{E_{ij}}{\varepsilon_j} \frac{n_i}{\sum_{k=1}^N P_{ik} \mu_k^{(0)}}$$

- Other methods

This was just a brief introduction.

Other possible values are:

- Singular Value Decomposition (SVD)
- Slope constrained unfolding
- Fully Bayesian unfolding

