

UNFOLDING / DECONVOLUTION

• Direct and inverse processes

Suppose we want to measure some variable ~~z~~ using a detector that has a response function that "deforms" or "transforms" in some way the variable ~~z~~ into ~~z~~ x

~~z~~

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:

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

\downarrow
Convolution of f and r

\rightarrow possible noise ~~or big~~

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

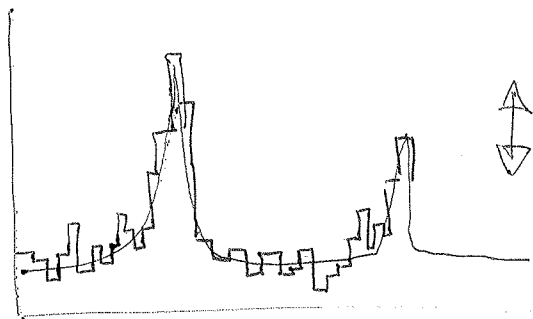
Examples: - Energy resolution for an X-ray detector
- Space resolution induced by lens ~~at~~ aberrations on Telescope image

Possible ~~effect~~ "distortions" are:

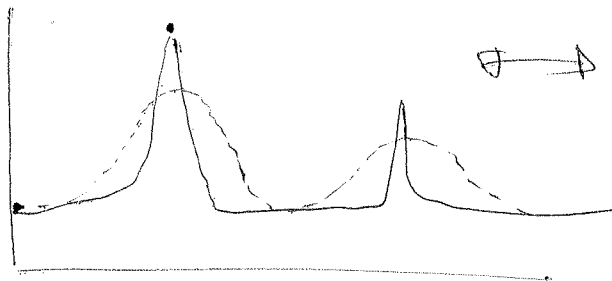
- \rightarrow Statistical fluctuations (e.g. due to Poisson statistics) if the data are binned
- \rightarrow Smearing due to limited resolution = migration of counts between bins
- \rightarrow Reduced efficiency
- \rightarrow Non-linear detector response

See next page

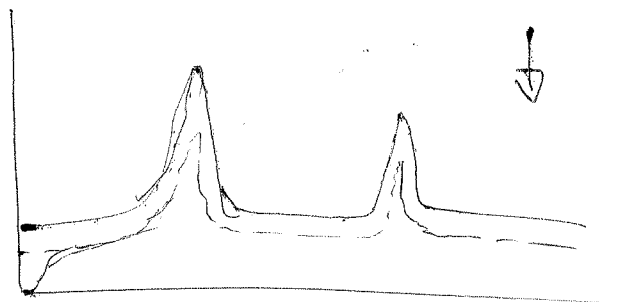
→ Statistical fluctuations due to
e.g. Poisson statistics in bins:



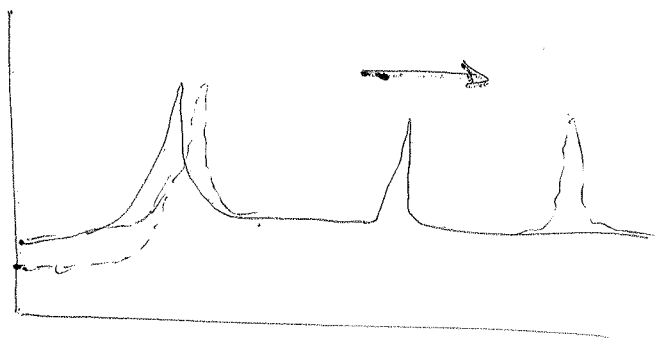
→ Smearing, i.e. migration of counts between bins due to resolution of detector:



→ Reduction of counts due to
non-unitary efficiency

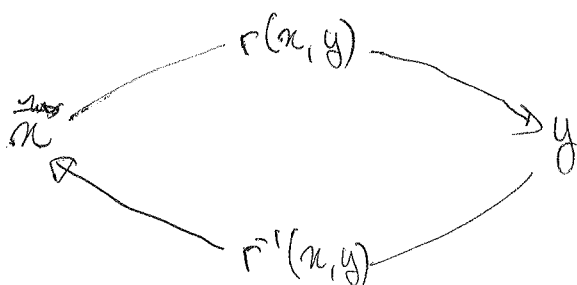


→ Deformation of distribution due
to non-linear detector response



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 y
(that's what we have done
so far)

b) Invert the response function
and fit x
↳ Unfolding

Unf. 2

• 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 :

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

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

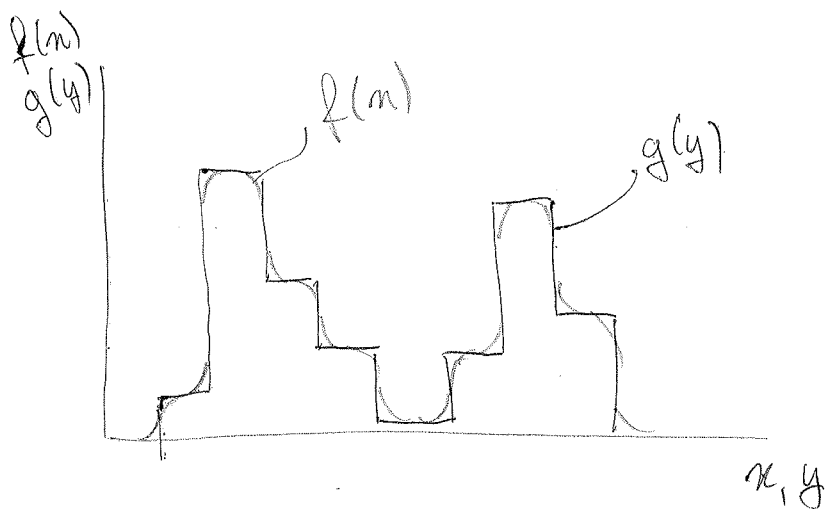
One can demonstrate that: $\widehat{g \otimes r} = \hat{g} \cdot \hat{r}$

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

→ Example: Gaussian measuring

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

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



• Discrete data

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

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

In principle, also g the original variable y can be distributed among multiple bins, which can be of a differ :

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

The relation between μ_j and V_i will be :

$$V_i = \sum_{j=1}^{\Pi} R_{ij} \mu_j$$

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

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

$$V_i = \sum_j R_{ij} \mu_j + b_i$$

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

• 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 $\hat{\vec{\mu}}$.

~~We~~ We can use the max-L method :

$$\mathcal{L}(\vec{n} | \vec{\mu}) = \prod_{i=1}^N \text{Poisson}(n_i | V_i(\vec{\mu})) = \prod_{i=1}^N \text{Poisson}(n_i | \sum_{j=1}^{\Pi} R_{ij} \mu_j + b_i)$$

The solution is found by inverting the matrix.

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

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

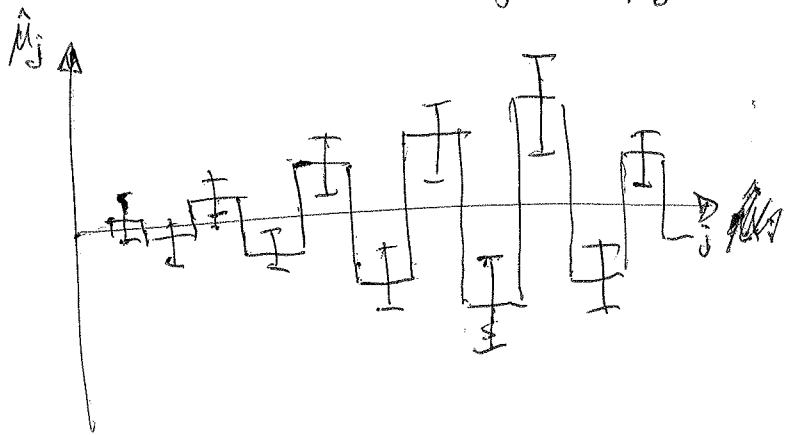
$$U = R^{-1} V (R^{-1})^T \quad \text{where } V = \text{covariance matrix of data } n_i$$

$$V_{ij} = \delta_{ij} v_j \quad \text{because of Poisson process.}$$

The issue is that ~~the~~ each bin $\hat{\mu}_i$ is strongly anti-correlated with its neighbors $\hat{\mu}_{i \pm 1}$ because of the off-diagonal entries of U .

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

One gets something like:



• Bin-by-bin correction

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

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

v_i^{est} has no background

Problem: This approach introduces a bias that drives $\hat{\mu}_i$ towards μ_i^{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- \mathcal{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 ~~off~~ on the "smoothness" of the values to be estimated $\vec{\mu}$, quantified by some function $S(\vec{\mu})$. These methods are called "regularized unfolding".

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

$$\phi(\vec{\mu}) = \Lambda(\vec{\mu}) + \nu^2 S(\vec{\mu}) \quad \text{where } \nu = \text{"regularization strength"}$$

If $\nu = 0 \Rightarrow$ max- \mathcal{L} estimate

If $\nu \gg 0 \Rightarrow \hat{\vec{\mu}}$ 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 $\nu = \sum \nu_i$

We can include an extra-term:

$$\phi(\vec{\mu}) = \Lambda(\vec{\mu}) + \nu^2 S(\vec{\mu}) + \lambda(n - \nu)$$

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

• Tikhonov Regularization

Let's choose: $S(\vec{\mu}) = (L\vec{\mu})^T L\vec{\mu}$

where L is a $n \times k$ matrix.

→ In the simplest case, $L = \mathbb{1}$, therefore: $S(\vec{\mu}) = \sum_j \mu_j^2$

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

→ Another choice is:
$$L = \begin{pmatrix} -1 & 1 & 0 & \dots & 0 \\ 1 & -2 & 1 & & \\ 0 & 1 & -2 & \ddots & 1 & 0 \\ \vdots & & & 1 & -2 & 1 \\ 0 & \dots & 0 & 1 & -1 \end{pmatrix}$$

In fact, if we have a function approximated by a histogram h with bin size δ , 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 L is an approximation of the 2nd derivative of μ 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 2nd derivatives that induce high-frequency oscillations are damped.

- Iterative unfolding

Another approach is to repeat the unfolding:

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

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

We start from $\mu_j^{(0)} = \mu_j^{\text{est}}$ and proceed for K iterations, with 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 of histogram

E_i = event observed, after detector effects, in bin i of a 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:

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

• Other methods

This was just a brief introduction.

Other possible values are:

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

