

# **Statistical Methods in Particle Physics**

## **9. Unfolding**

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WS 2017/18**

# Deconvolution

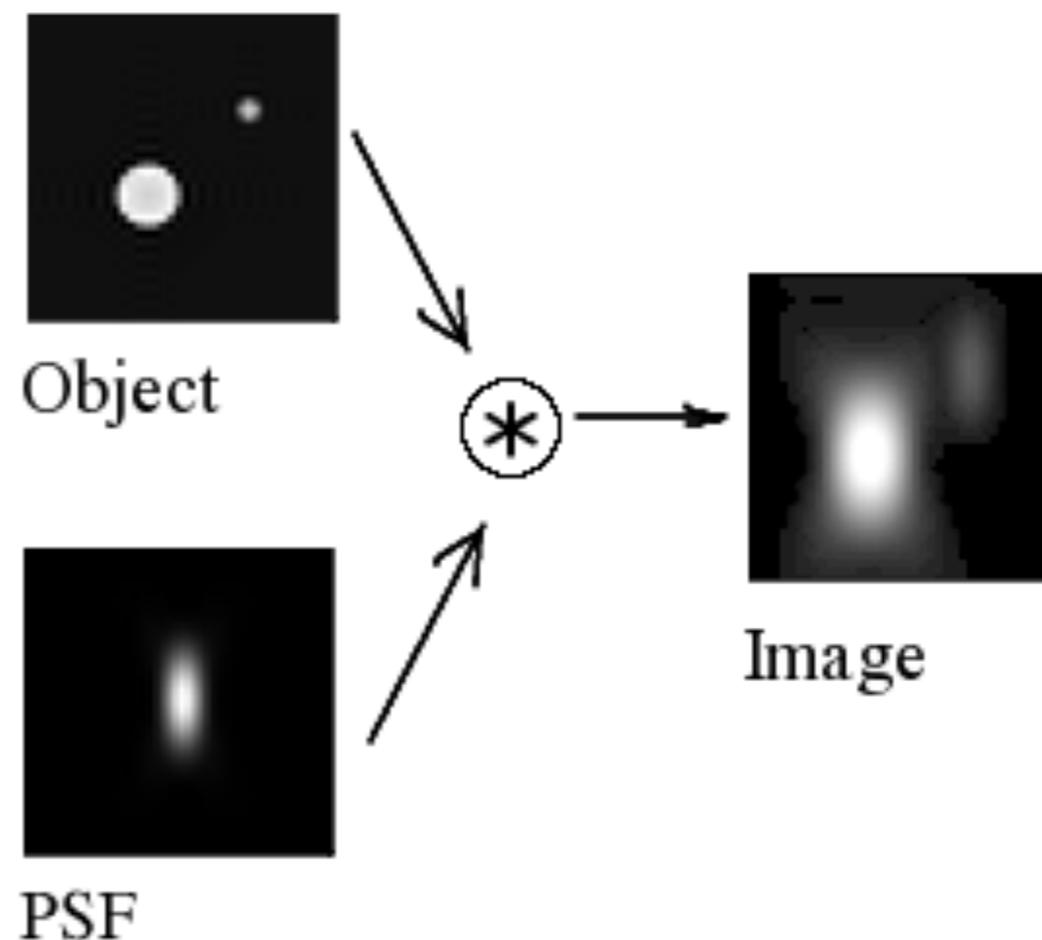
Finite resolution of the detector smears the quantities we're interested in.

Goal:  
smeared information  
→ original information

This is called *deconvolution* or *unfolding*

"Inverse problem"

Problem can be ill-posed in the sense that unfolded result can be very sensitive to small perturbations in the data



Example:

Smearing of a telescope image

[https://en.wikipedia.org/wiki/Point\\_spread\\_function](https://en.wikipedia.org/wiki/Point_spread_function)

# To Unfold or Not to Unfold?

[C. Pruneau,  
Data Analysis Techniques for Physical Scientists]

From S. Oser's lecture:

The most important advice I can give about deconvolution is “Don't”.

It's a lot of work, and often produces biased or otherwise unsatisfactory results. Moreover it's often unnecessary.

“Forward fitting” is much easier

- ▶ Take theory prediction
- ▶ Convolve it with the response of the detector
- ▶ Compare smeared theory directly with the data

# When Unfolding Makes Sense

1. Results from experiment A and B with different response function are to be compared
2. It is too complicated to publish the response function of the detector along with the data
  - ▶ Detector response might be very complex, e.g., time dependent
  - ▶ Sometimes computer code reflecting the response would have to be published
  - ▶ Danger that future users don't use the filter correctly

# Examples

- Multiplicity distributions  $P(N_{\text{ch}})$

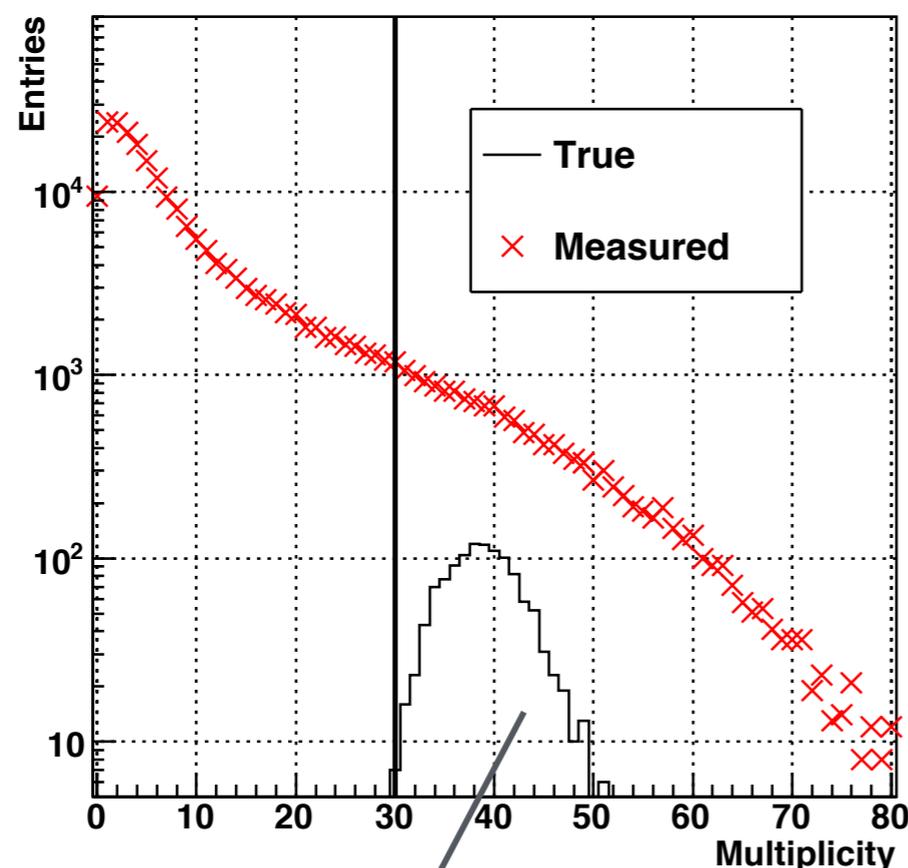
- ▶ Measured multiplicity differs from true charged particle multiplicity due to detector effects (efficiency, fake hits, ...)

- $p_T$  spectra, e.g.,  $\pi^0$  spectrum measured with a calorimeter

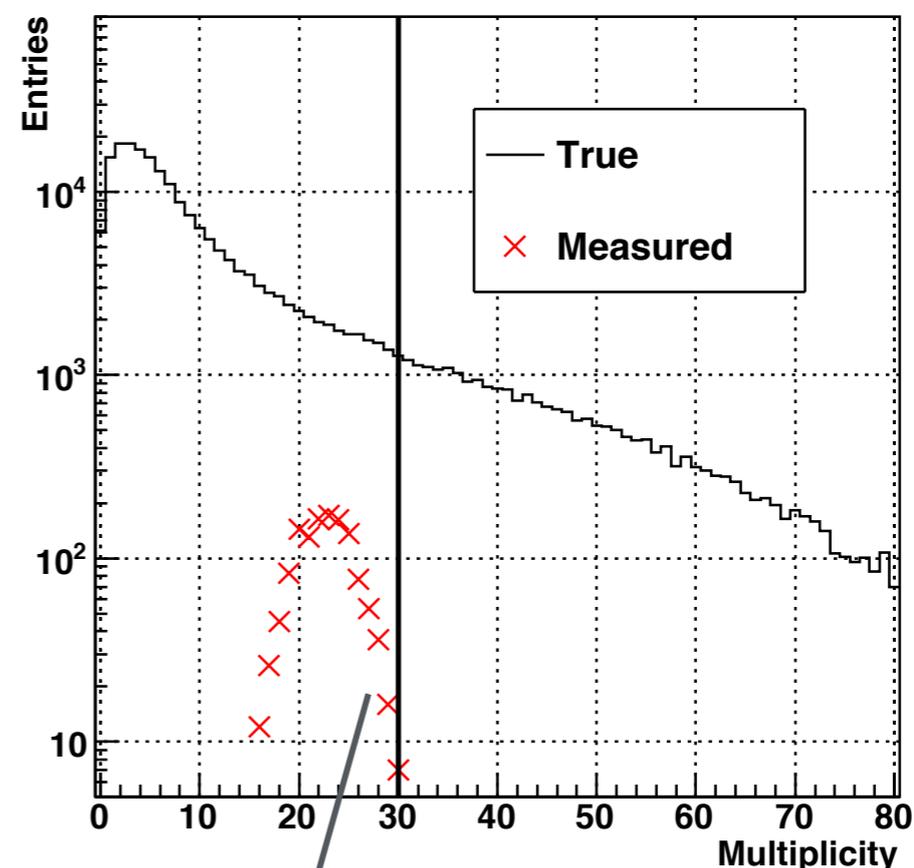
- ▶ finite energy resolution and shower overlaps in a calorimeter affect the  $p_T$  of the reconstructed shower

Example: multiplicity distributions in pp collisions

arXiv:0912.0023



true  $N$ 's contributing to measured  $N = 30$



measured  $N$ 's for a true  $N = 30$

# Response Matrix (I)

Suppose that we deal with continuous variables (e.g., transverse momentum)

$f_t(x_t)$  : distribution of true values (normalized to unity)

$f_m(x_m)$  : distribution of measured values (normalized to unity)

$f_b(x_m)$  : distribution of background (normalized to unity)

Response function  $R$ :

$$R(x_m|x_t) = \underbrace{r(x_m|x_t)}_{\text{"smearing"}} \times \underbrace{\varepsilon(x_t)}_{\text{"efficiency"}} \quad \text{probability (density) to observe } x_m \text{ given } x_t$$

By construction, one has

$$\int_{\Omega_m} r(x_m|x_t) dx_m = 1$$

# Response Matrix (II)

Further definitions:

$m_{\text{tot}}$  : number of true events

$n_{\text{tot}}$  : number of measured events

$b_{\text{tot}}$  : number of background events

$$\mu_{\text{tot}} = E[m_{\text{tot}}], \quad \nu_{\text{tot}} = E[n_{\text{tot}}], \quad \beta_{\text{tot}} = E[b_{\text{tot}}]$$

It is practical to work with discrete bins. E.g., probability to find true in bin  $j$ :

$$p_j = \int_{\text{bin } j} dx_t f_t(x_t), \quad \mu_j = \mu_{\text{tot}} \times p_j$$

Ignoring backgrounds, the measured number of entries in bin  $i$  is:

$$\begin{aligned} \nu_i &= \mu_{\text{tot}} \int_{\Omega_t} dx_t \text{Prob}(x_m \text{ in } i | \text{true } x_t, \text{ detected}) \\ &\quad \times \text{Prob}(\text{detect } x_t) \times \text{Prob}(\text{produce } x_t) \\ &= \mu_{\text{tot}} \int_{\text{bin } i} dx_m \int_{\Omega_t} dx_t r(x_m | x_t) \varepsilon(x_t) f_t(x_t) \end{aligned}$$

# Response Matrix (III)

Further definitions:

$$\begin{aligned} \nu_i &= \mu_{\text{tot}} \int_{\text{bin } i} dx_m \sum_{j=1}^M \int_{\text{bin } j} dx_t r(x_m|x_t) \varepsilon(x_t) f_t(x_t) \\ &= \sum_{j=1}^M \int_{\text{bin } i} dx_m \int_{\text{bin } j} dx_t \frac{r(x_m|x_t) \varepsilon(x_t) f_t(x_t)}{\mu_j / \mu_{\text{tot}}} \mu_j \end{aligned}$$

This may be written as

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

with the components of the response matrix

$$R_{ij} = \frac{\int_{\text{bin } i} dx_m \int_{\text{bin } j} dx_t r(x_m|x_t) \varepsilon(x_t) f_t(x_t)}{\int_{\text{bin } j} dx_t f(x_t)}$$

# Response Matrix (IV)

In other words:

$$R_{ij} = \text{Prob}(\text{observed in bin } i | \text{true in bin } j)$$

Obviously, summing the response matrix over  $i$  gives the efficiency:

$$\sum_{i=1}^N R_{ij} = \varepsilon_j$$

In compact matrix form (including background):

$$\nu_i = \sum_{j=1}^M R_{ij} \mu_j + \beta_i \qquad \vec{\nu} = R \vec{\mu} + \vec{\beta}$$

Response matrix depends on  $f_t(x_t)$  which we want to know. However, if we make the bins small enough  $f_t(x_t) \approx \text{const.}$  within a bin and drops from the ratio:

$$R_{ij} = \frac{\int_{\text{bin } i} dx_m \int_{\text{bin } j} dx_t r(x_m | x_t) \varepsilon(x_t) f_t(x_t)}{\int_{\text{bin } j} dx_t f(x_t)} \approx \frac{1}{\Delta x_{t,j}} \int_{\text{bin } i} dx_m \int_{\text{bin } j} dx_t r(x_m | x_t) \varepsilon(x_t)$$

# Unfolding by Inverting the Response Matrix (I)

We have

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

Replace  $\vec{v}$  by  $\vec{n}$  to obtain an obvious estimator for the true distribution:

$$\hat{\vec{\mu}} = R^{-1}(\vec{n} - \vec{\beta})$$

This solution minimizes

$$\chi^2(\vec{\mu}) = (\vec{v}(\vec{\mu}) - \vec{n})^T V^{-1}(\vec{v}(\vec{\mu}) - \vec{n}) \quad \text{where} \quad V_{i,j} = \text{cov}[n_i, n_j]$$

It can be shown that the covariance matrix of the solution is given by

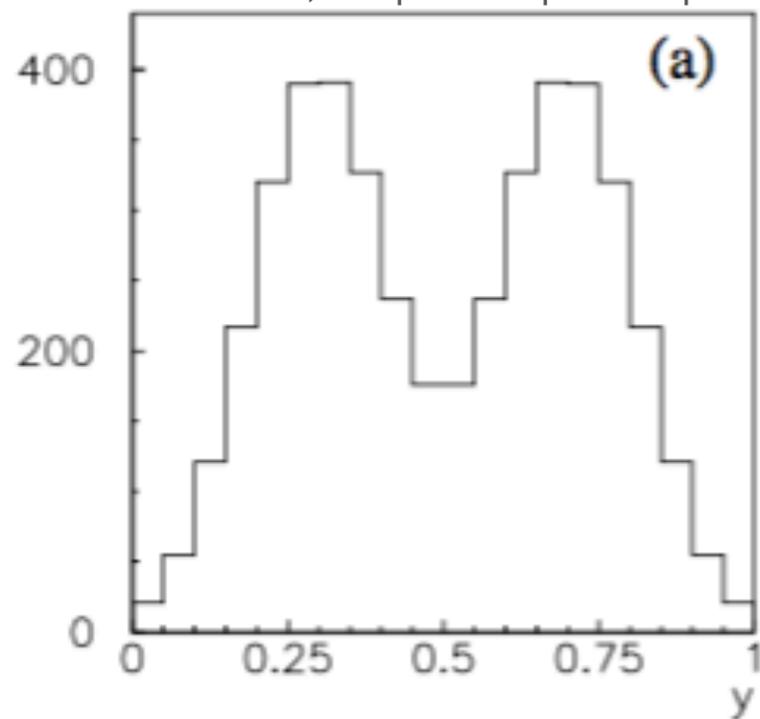
$$U = R^{-1} V (R^{-1})^T$$

# Unfolding by Inverting the Response Matrix (II)

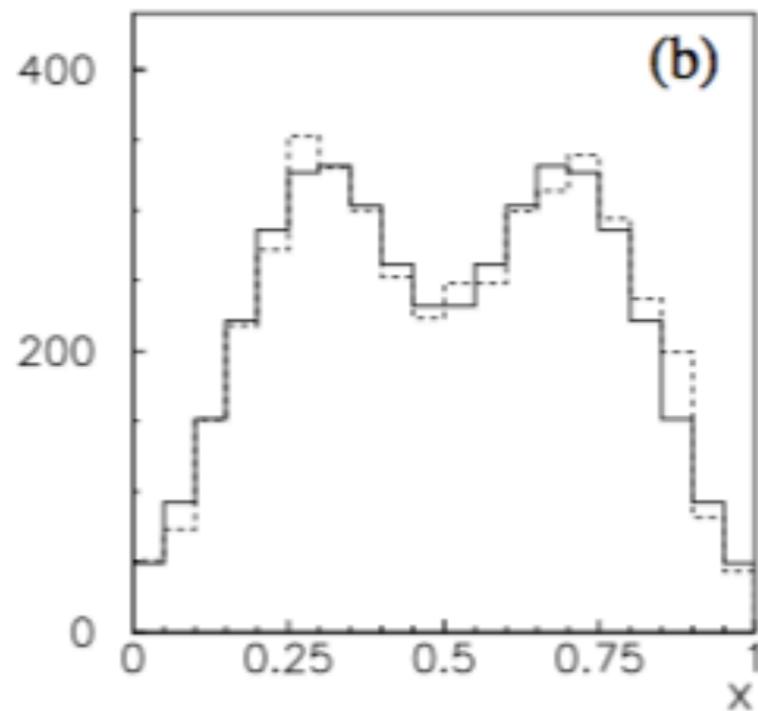
It can also be shown that matrix inversion is unbiased and has minimal variance.

This sounds good ... let's try it.

Cowan, <http://inspirehep.net/record/599644>

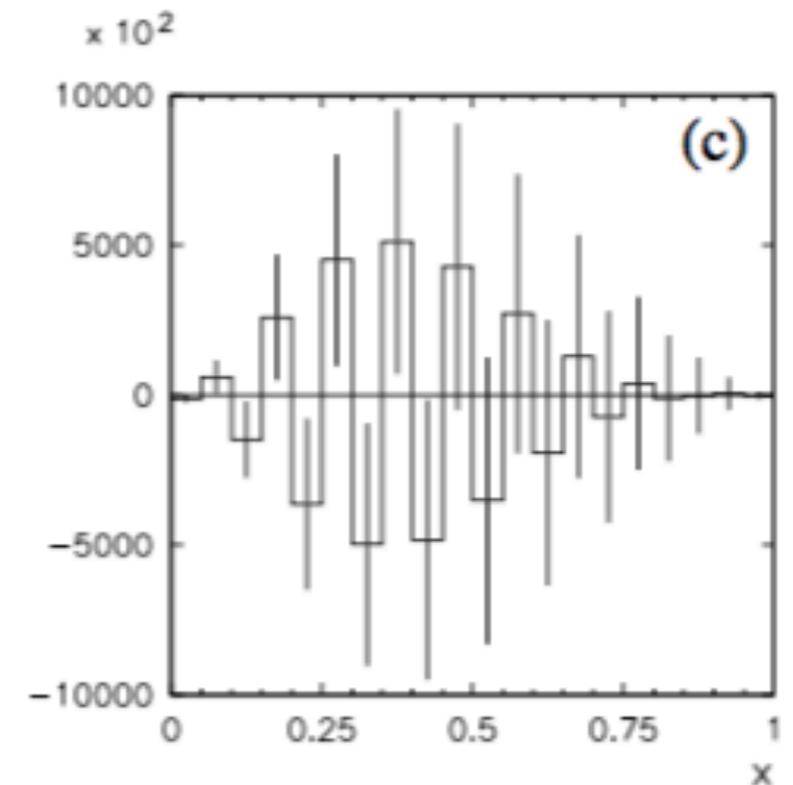


true distribution  $\vec{\mu}$



solid line:  $\vec{v} = R\vec{\mu}$

dashed line:  
sampled data  $\vec{n}$  from  $\text{Poisson}(n_i, \nu_i)$



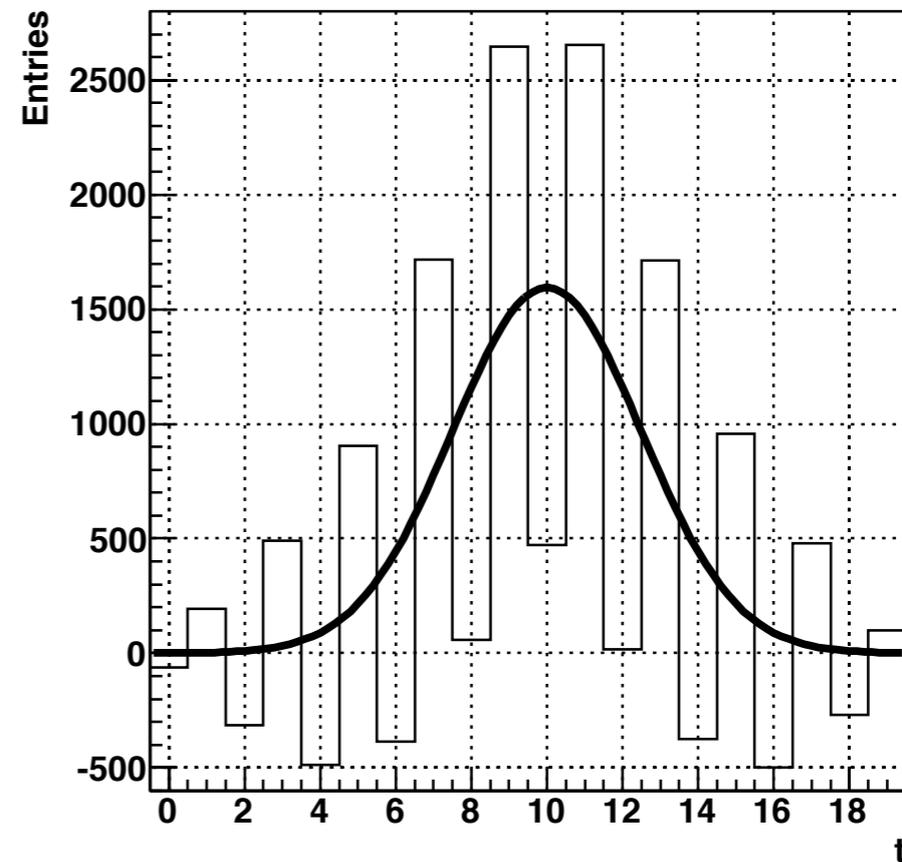
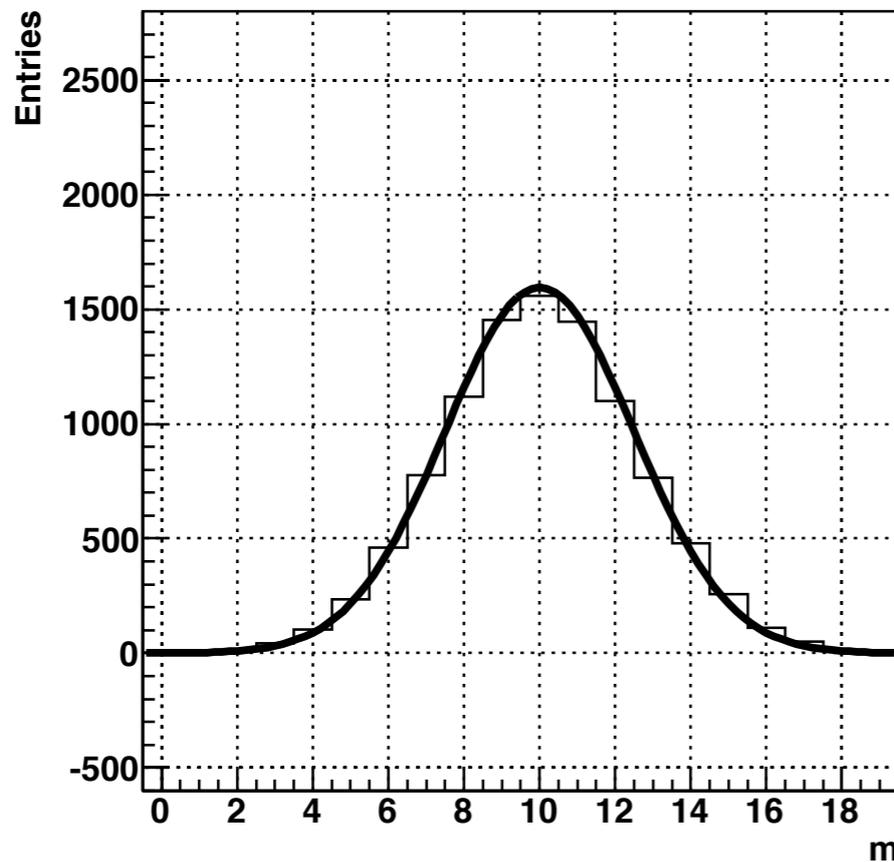
estimate  $\hat{\vec{\mu}} = R^{-1}\vec{n}$

This looks like a disaster ... unfolded distribution very different from the true one

# Unfolding by Inverting the Response Matrix (III)

Another example:

$$R = \begin{pmatrix} 0.75 & 0.25 & 0 & \dots \\ 0.25 & 0.50 & 0.25 & 0 \\ 0 & 0.25 & 0.50 & 0.25 \\ & & 0 & 0.25 & 0.50 \\ \vdots & & & & \ddots \end{pmatrix}.$$



Same conclusion: we don't get the desired (smooth) answer

# What's Wrong with the Matrix Inversion Method?

Unbiased, minimum variance, actually also a ML estimator ... all very nice!

The result is not wrong, it is just not desirable

- ▶ Does not really look like the original distribution
- ▶ Large correlation between bins

"Applying the response matrix  $R$  smears out fine structure  
→ applying  $R^{-1}$  creates (usually unwanted) structure"

More desirable solution by adding (smoothness) constraints.  
However, this will produce a bias.

The art of unfolding is to find an acceptable balance between bias and smoothness.

# Bin-by-Bin Method (I)

Used very often, but has issues ...

Assume shape of true spectrum and determine correction factor for each bin (usually determined from Monte Carlo simulation):

$$\mu_i = C_i(n_i - \beta_i) \qquad C_i = \frac{\mu_i^{\text{MC}}}{\nu_i^{\text{MC}}}$$

Works if smearing (bin-to-bin sharing) is negligible, only loss due to finite efficiency:

$$R_{ij} \approx \delta_{ij}\varepsilon_j$$

Obviously works, too, if MC = nature.

Expectation value for corrected data:

$$E[\hat{\mu}_i] = C_i E[n_i - \beta_i] = C_i(\nu_i - \beta_i) \equiv C_i \nu_i^{\text{sig}}$$

# Bin-by-Bin Method (II)

Inserting the  $C_i$ 's one can determine the bias:

$$E[\hat{\mu}_i] = \frac{\mu_i^{\text{MC}}}{\nu_i^{\text{MC}}} \nu_i^{\text{sig}} = \underbrace{\left( \frac{\mu_i^{\text{MC}}}{\nu_i^{\text{MC}}} - \frac{\mu_i}{\nu_i^{\text{sig}}} \right)}_{\text{bias}} \nu_i^{\text{sig}} + \mu_i$$

no bias only if  
MC = nature

Covariance matrix of the corrected data (smearing fluctuations independent between bins)

$$U_{ij} = \text{cov}[\hat{\mu}_i, \hat{\mu}_j] = C_i C_j \underbrace{\text{cov}[n_i^{\text{sig}}, n_j^{\text{sig}}]}_{0 \text{ for } i \neq j} = C_i^2 \text{Var}[n_i^{\text{sig}}] \delta_{ij}$$

## Iterative bin-by-by method

- ▶ Start with plausible guess of true spectrum
- ▶ Apply correction to measurement
- ▶ Generate new correction factors from corrected spectrum of previous iteration
- ▶ And so on ... usually a few iterations sufficient

# Regularized Unfolding

Matrix inversion is the maximum likelihood solution:

Independent  
Poisson  
fluctuations:

$$\ln L(\vec{\mu}) = \sum_{i=1}^M (n_i \ln \nu_i - \nu_i)$$

ML estimator:  $\hat{\nu} = \vec{n}$   
 $\rightarrow \hat{\mu} = R^{-1}(\vec{n} - \vec{\beta})$

Idea: accept solutions that are close to maximum likelihood estimate:

$$\ln L(\vec{\mu}) \geq \ln L(\vec{\mu}_{\max}) - \Delta \ln L(\vec{\mu})$$

Define a smoothness function  $S$  that gets bigger when the unfolded solution becomes smoother.

The task then is to maximize

$$\Phi(\vec{\mu}) = \alpha \ln L(\vec{\mu}) + S(\mu)$$

$\alpha$  depends on  $\Delta \ln \vec{\mu}$ ,  
 $\alpha \rightarrow \infty$  give ML solution

smoothness function

# Tikhonov Regularization

Measure of smoothness = mean square of  $k$ -th derivative of deconvoluted function  $f$ :

$$S[f] = - \int dx \left( \frac{d^k f}{d^k x} \right)^2 \quad k = 1, 2, 3, \dots$$

Minus sign makes  $S$  big when derivative is small

Tikhonov for  $k = 2$  with  $\log L = -\chi^2/2$ :

$$S(\vec{\mu}) = - \sum_{i=1}^{M-2} (-\mu_i + 2\mu_{i+1} - \mu_{i+2})^2$$

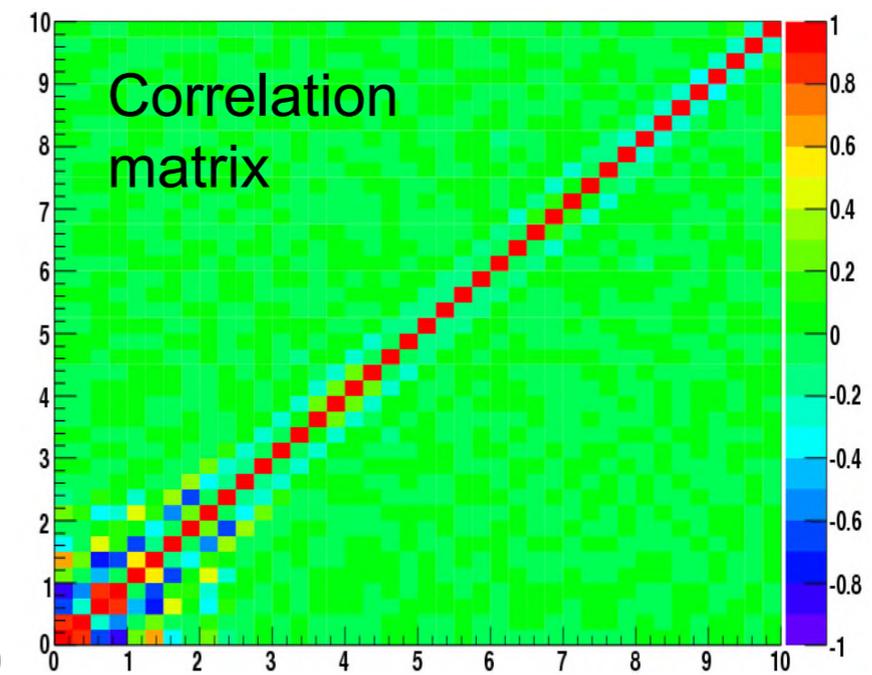
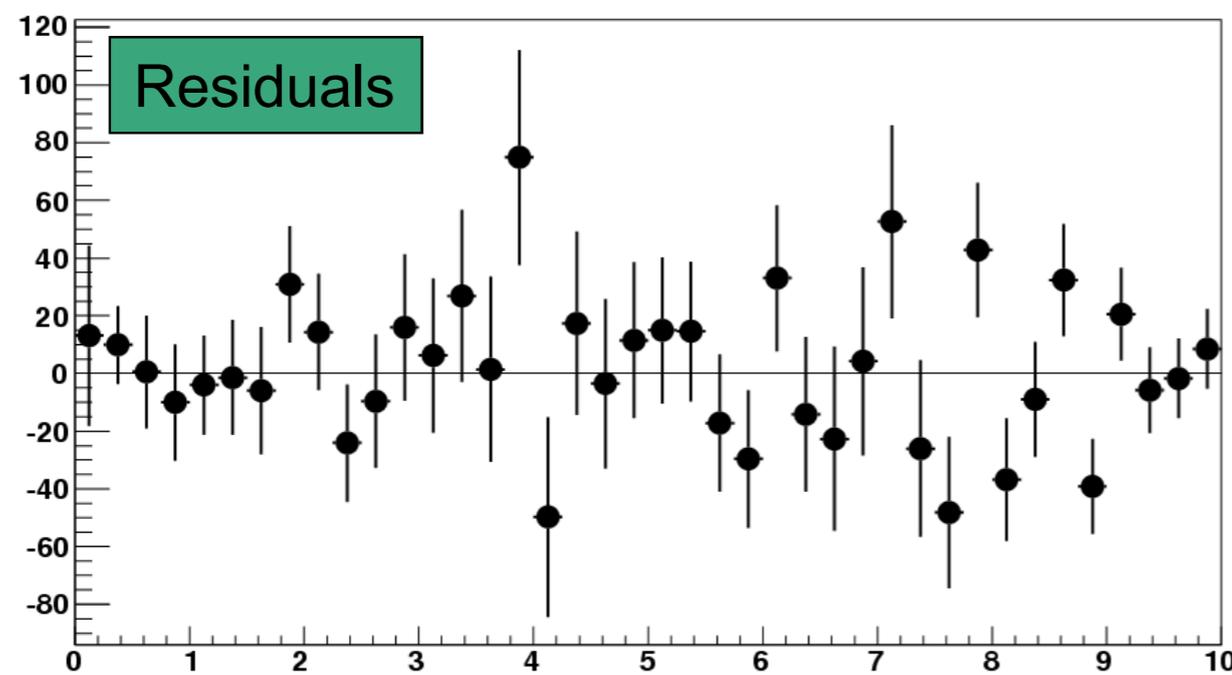
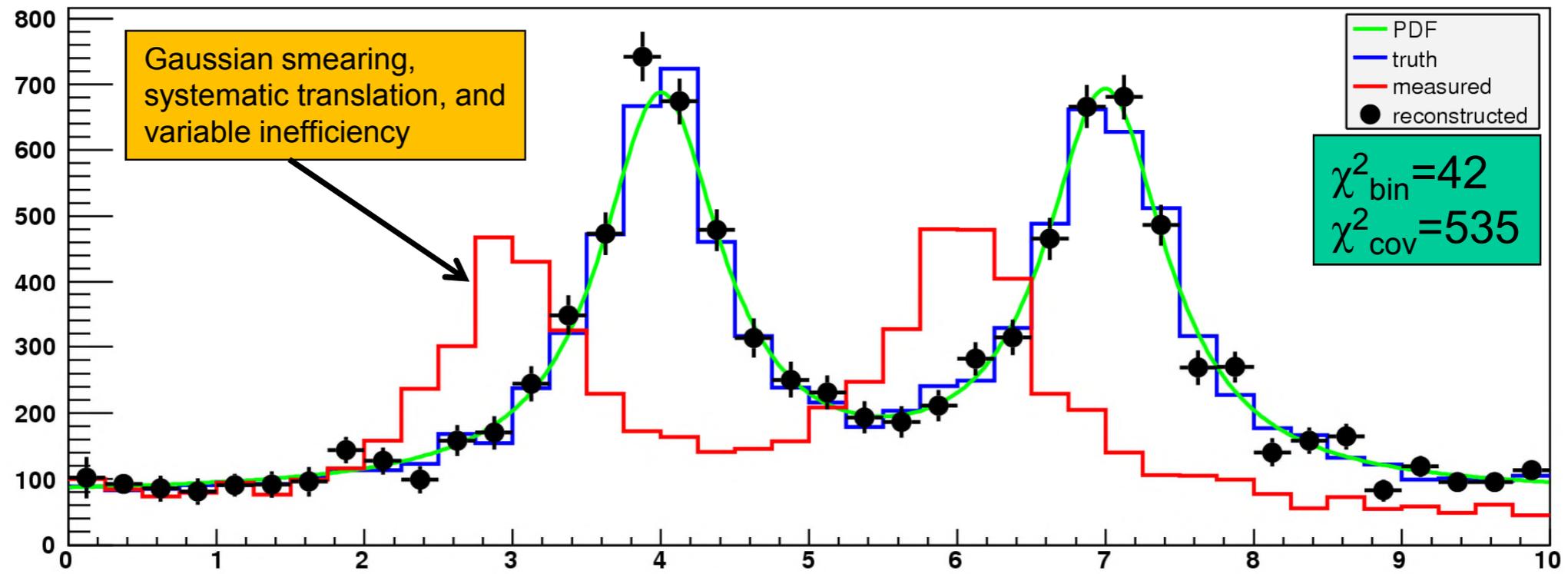
Implementation by A. Höcker, V. Kartvelishvili: *Singular Value Decomposition*  
(NIM A372 (1996) 469, hep-ph/9509307, TSVDUnfold in ROOT)

Minimizes  $\chi^2(\vec{\mu}) + \tau \sum_i [(\mu_{i+1} - \mu_i) - (\mu_i - \mu_{i-1})]^2$

Advice on how to choose  $\tau$  in the paper

# RooUnfold with SVD Algorithm

$k = 30$



<http://hepunix.rl.ac.uk/~adye/software/unfold/RooUnfold.html>

Tim Adye, Unfolding in HEP, <https://indico.cern.ch/event/671301/contributions/2745801>

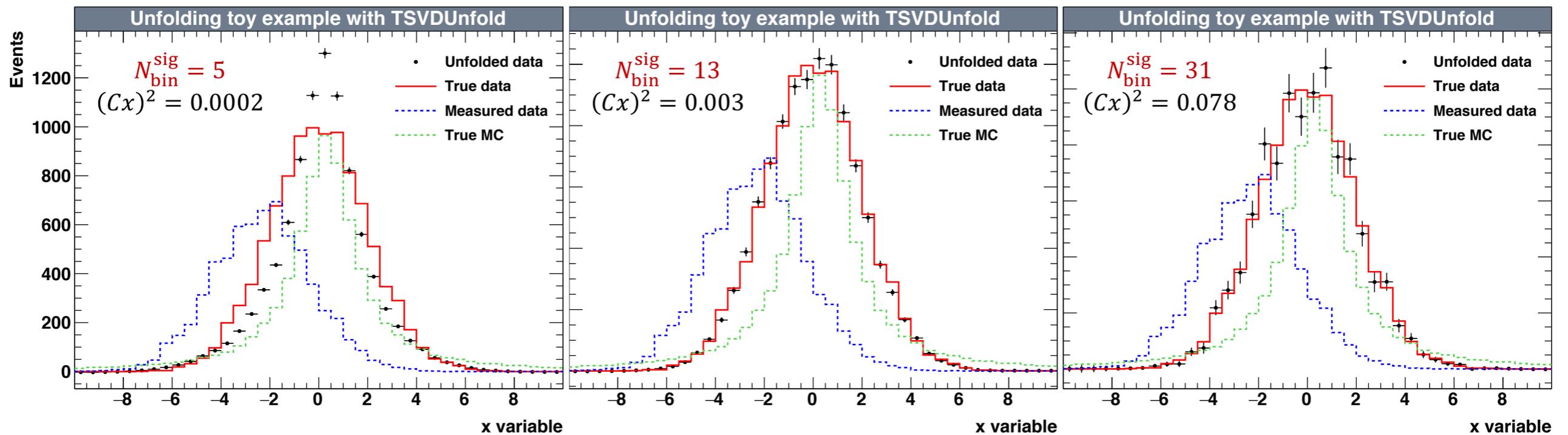
# Over- and Under-Regularized Unfolding

Andreas Höcker, <https://indico.cern.ch/event/634037/>

Over-regularised

Best regularisation choice

Under-regularised



The parameter determines the strength of the regularization

- ▶  $\tau$  too small  $\rightarrow$  oscillations
- ▶  $\tau$  too large  $\rightarrow$  unfolded spectrum biased towards MC

# Regularization Based on Entropy (I)

Shannon entropy of a discrete probability distribution:

$$H = - \sum_{i=1}^M p_i \ln p_i$$

all  $p_i$  equal  $\rightarrow$  maximum entropy (max. smoothness)

$p_i = 1$ , all others 0  $\rightarrow$  minimum entropy

Use entropy as regulation function:

$$S(\vec{\mu}) = H(\vec{\mu}) = - \sum_{i=1}^M \frac{\mu_i}{\mu_{\text{tot}}} \ln \frac{\mu_i}{\mu_{\text{tot}}}$$

This gives the distribution with the maximum entropy consistent within the selected tolerance with the ML solution

Entropy related to number of different ways  $\mu_{\text{tot}}$  objects can be distributed to obtain histogram  $\vec{\mu} = (\mu_1, \dots, \mu_M)$

$$\Omega(\vec{\mu}) = \frac{\mu_{\text{tot}}!}{\mu_1! \cdot \dots \cdot \mu_M!}$$

Stirling's approximation

$\rightsquigarrow$

$$\ln \Omega(\vec{\mu}) \approx \mu_{\text{tot}} H(\vec{\mu})$$

# Relation of Maximum Entropy Regularization and Bayesian Approach

With a certain prior belief we obtain in the Bayesian approach:

$$f(\vec{\mu}|\vec{n}) \propto L(\vec{n}|\vec{\mu}) \cdot \pi(\vec{\mu})$$

Maximum entropy prior:

$$\pi(\vec{\mu}) \propto \Omega(\vec{\mu}) = \exp(\mu_{\text{tot}} H(\vec{\mu}))$$

Logarithm of Bayesian posterior distribution:

$$\begin{aligned} \ln f(\vec{\mu}|\vec{n}) &\propto \ln L(\vec{n}|\vec{\mu}) + \ln \pi(\vec{\mu}) \\ &= \ln L(\vec{n}|\vec{\mu}) + \mu_{\text{tot}} H(\vec{\mu}) \end{aligned}$$

We see: Bayesian approach = maximum likelihood with entropy regularization  
(with  $\alpha = 1/\mu_{\text{tot}}$ )

# Cross Entropy Regularization

Maximum entropy regularizations penalizes deviation from flat distribution.

In some situations that might be the right assumption.

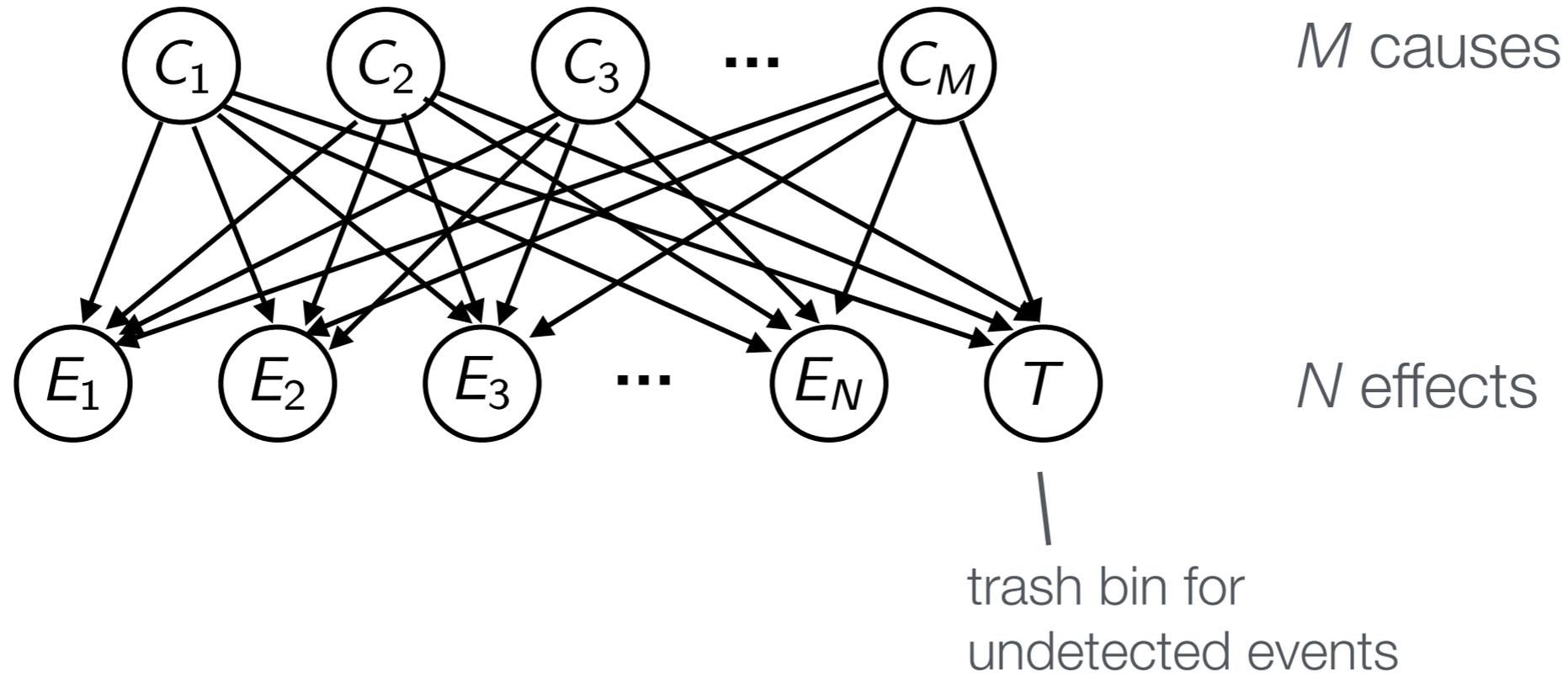
But if we have prior knowledge that the true events approximately follow some distribution  $q$ , then we might want to use cross entropy:

$$K(f; q) = - \sum_{i=1}^M f_i \ln \frac{f_i}{Mq_i}$$

If reference distribution is flat, this reduces to regular entropy.

# Bayesian Unfolding (I)

Causal network:



Response matrix:

$$R_{ji} = P(E_j | C_i, I)$$

$I$ : prior knowledge about probabilities of the causes  $C_i$

$$E[n_j | \mu_i] = P(E_j | C_i, I) \cdot \mu_i = R_{ji} \cdot \mu_i$$

# Bayesian Unfolding (II)

Bayes theorem:

$$P(C_i|E_j, I) = \frac{P(E_j|C_i, I) \cdot P(C_i|I)}{\sum_{k=1}^M P(E_j|C_k, I) \cdot P(C_k|I)}$$

We can write this as

$$\theta_{ij} := P(C_i|E_j, I) = \frac{R_{ji} \cdot P(C_i|I)}{\sum_{k=1}^M R_{jk} \cdot P(C_k|I)}$$

Estimate for number of true events in bin  $i$  given that we measure  $n_j$  events in bin  $j$ :

$$\mu_i|n_j = \frac{P(C_i|E_j, I) \cdot n_j}{\epsilon_i} = \frac{\theta_{ij} \cdot n_j}{\epsilon_i}$$

# Bayesian Unfolding (III)

Summing over all observed bins:

$$\mu_i | \vec{n} = \frac{1}{\varepsilon_i} \sum_{j=1}^N \theta_{ij} \cdot n_j$$

By definition we can write the efficiency as

$$\varepsilon_i = \sum_{j=1}^N P(E_j | C_i, I) = \sum_{j=1}^N R_{ji}$$

Response matrix usually from Monte Carlo simulation.

# Bayesian Unfolding (IV)

This procedure is applied iteratively:

- Choose prior distribution  $P(C_i, I)$
- Often prior = measured distribution
- Update prior according to measured values
- iterate
- Limited number of iterations provides implicit regularization

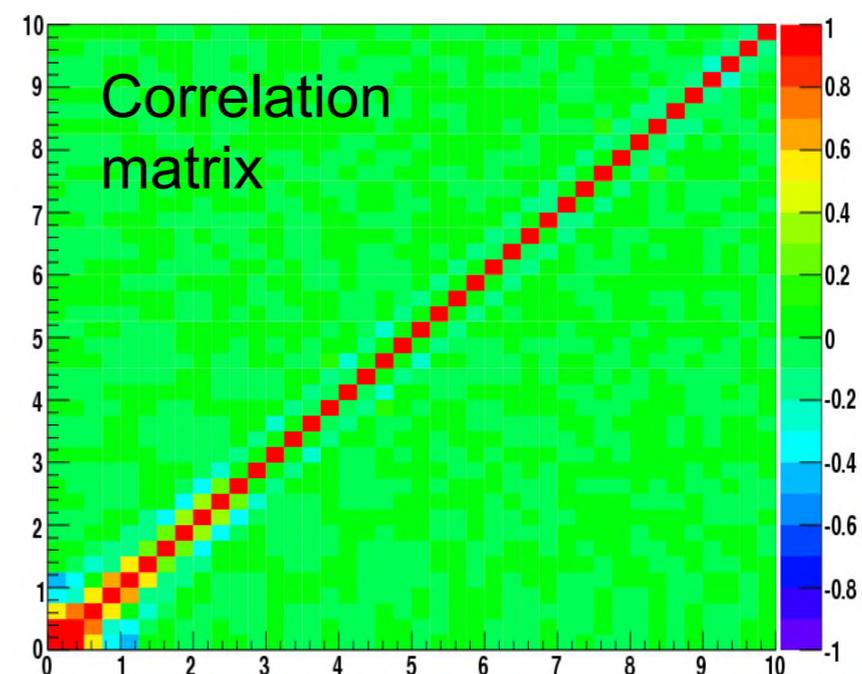
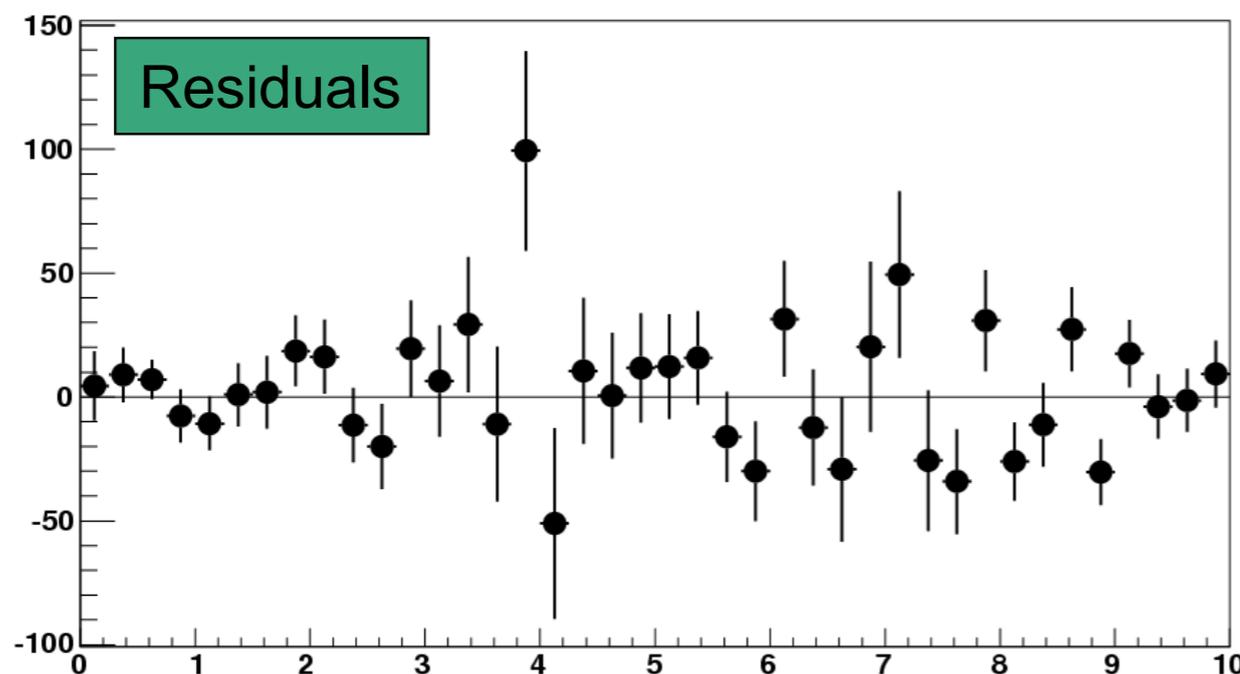
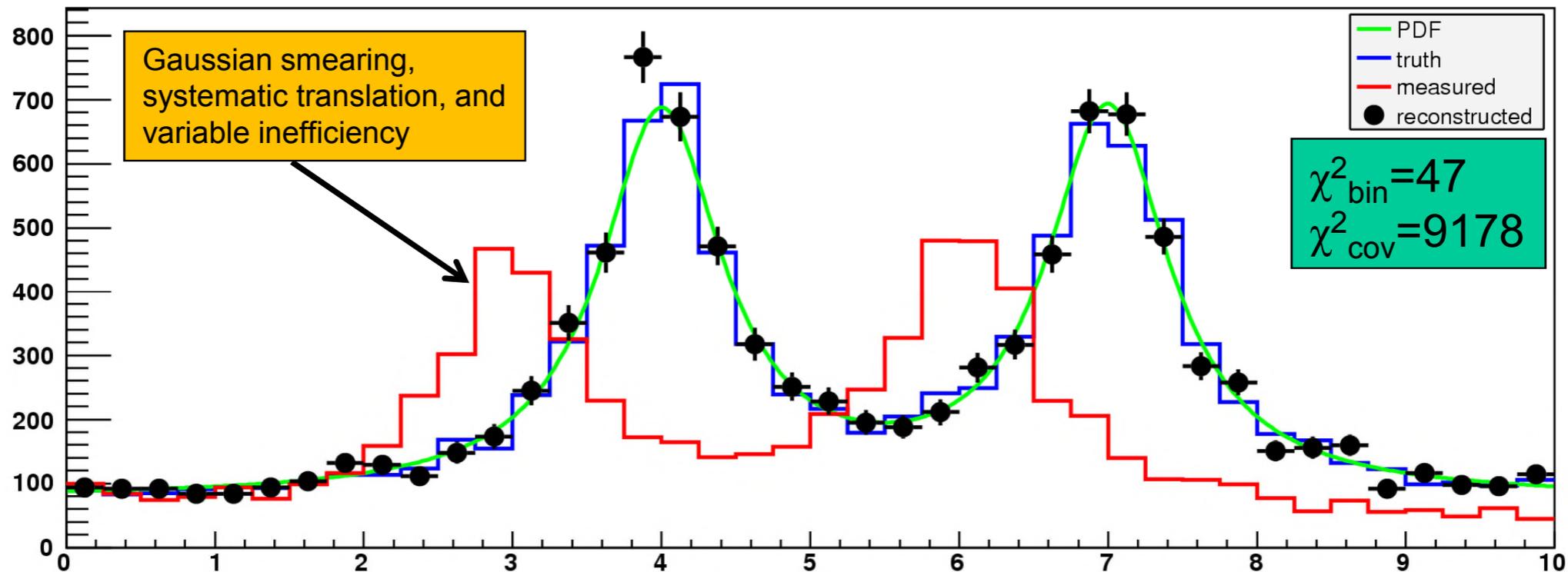
Shepp/Vardi 1982, Mülthei/Schorr 1986

G. D'Agostini, A Multidimensional unfolding method based on Bayes' theorem'', Nucl. Instrum. Meth. A 362 (1995) 487 (see also arXiv:1010.0632)

V. Blobel, Unfolding methods in high-energy physics experiments, <https://cds.cern.ch/record/157405>

# RooUnfold with Iterative Bayesian Algorithm

3 iterations



<http://hepunix.rl.ac.uk/~adye/software/unfold/RooUnfold.html>

Tim Adye, Unfolding in HEP, <https://indico.cern.ch/event/671301/contributions/2745801>

# Which Method to Choose?

There is no "best" method. Depends on the analysis.

Main questions:

How to choose regularization parameters?

After how many iterations to stop in the iterative Bayesian unfolding?

Danger: Regularization and early stopping in iterative unfolding introduce a bias

Don't forget:

in some cases it is most useful to publish folding matrix with the result

Stefan Schmitt, DESY

<http://www.desy.de/~sschmitt/talks/UnfoldStatSchool2014.pdf>