Unfolding algorithms and RooUnfold

- **Unfolding algorithms:**
  - **Extracted from slides by T. Adye at PHYSTAT 2016 and K. Reygers lectures at Heilderbeg Univ.**
  - **S. Smitt and D. Britzger, DESY Stat School 2014**
  - **S. Schmitt , QCDHS conference in 2016**

Unfolding

- Unfolding: estimate truth distribution from measurement, distorted by
  - detector effects
  - statistical fluctuations
- truth distribution: cross sections or similar quantities
- Unfolding is also referred to as "correction for detector effects"

- Integral equation of 1st kind

  $$\int k(x,y) f(y)\,dy + \delta(x) = g(x)$$

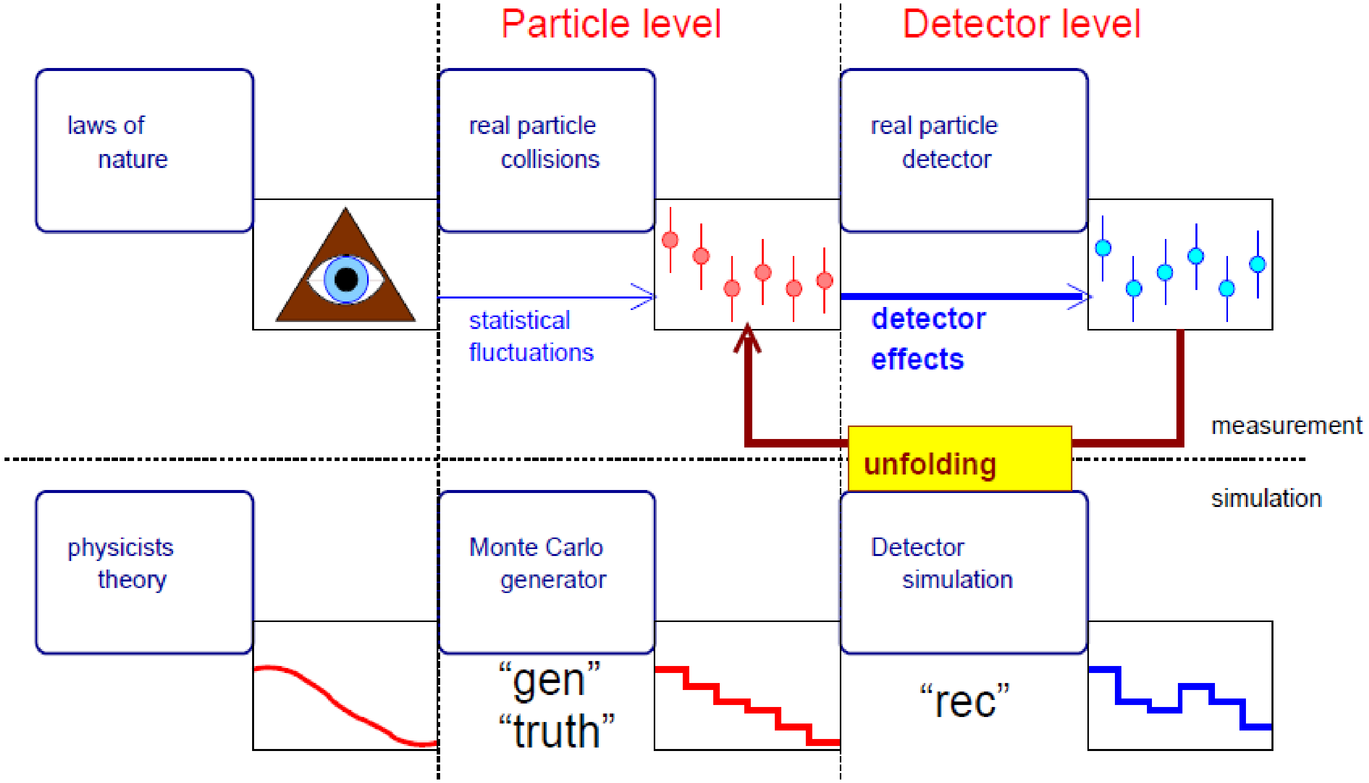
  given observations $g(x)$

  the kernel $k(x,y)$

  and fluctuations $\delta(x)$

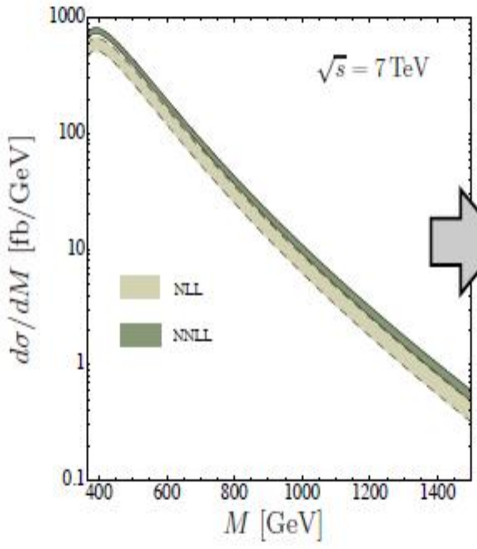
  estimate the truth $f(y)$
- k(x,y): detector effects, background, etc
- g(x) has uncertainties
- k(x,y) has syst. uncertainties
  $\rightarrow$ not covered in this talk

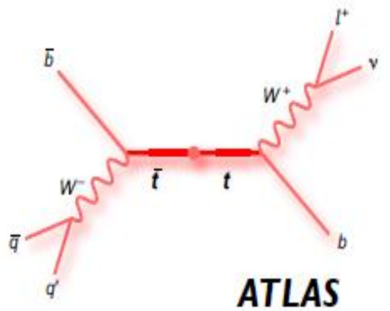
What is unfolding

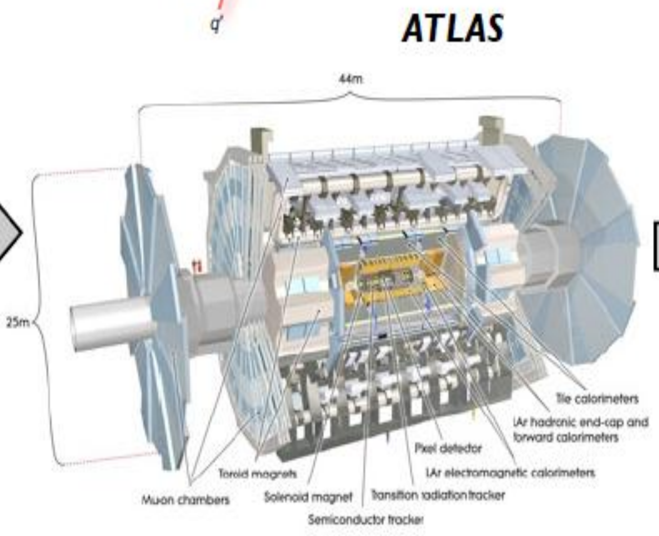


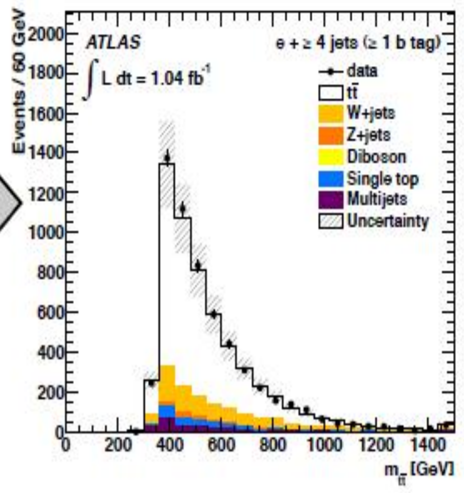
- Obtain measurements independent of detector effects, using the simulation
- Propagate statistical uncertainties back to particle level
- Require results to be independent of theory assumptions

ATLAS analysis example





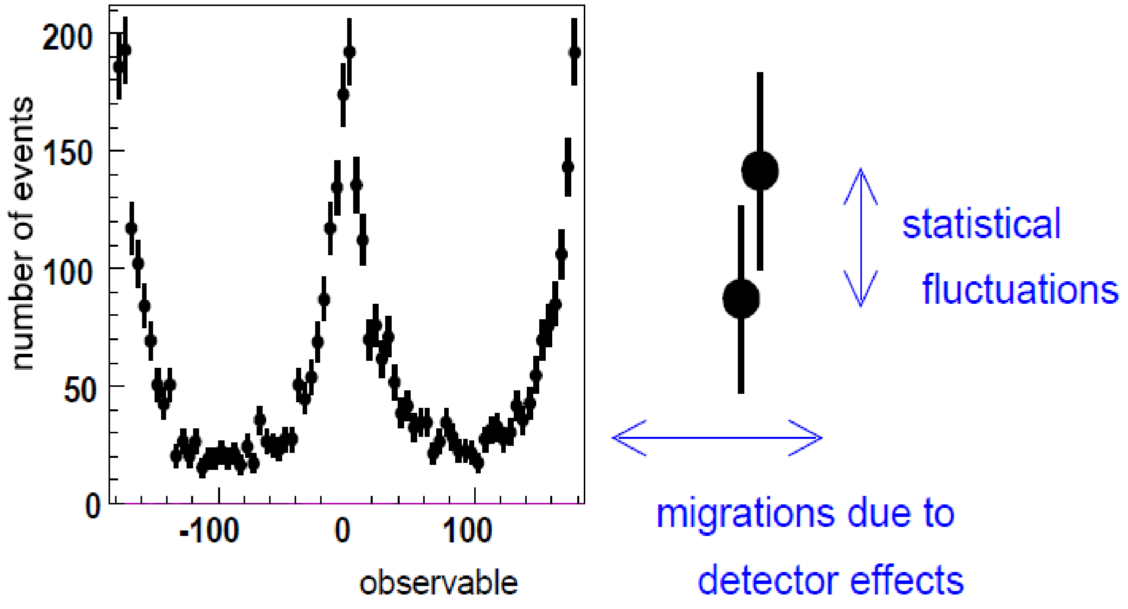

ATLAS
44m
25m
Tile calorimeters
LAr hadronic end-cap and forward calorimeters
Pixel detector
LAr electromagnetic calorimeters
Toroid magnets
Muon chambers
Solenoid magnet
Transition radiation tracker
Semiconductor tracker



G. Aad *et al.* [ATLAS Collaboration], Eur. Phys. J. C **72** (2012) 2039, arXiv:1203.4211 [hep-ex].

Migrations and stat. fluctuations

Histogram of observed event counts is affected by statistical fluctuations (vertical axis) and detector effects (horizontal axis)



Unfolding: correct for migration effects in the presence of statistical fluctuations

Result: estimator of the "truth" and its covariance matrix (statistical uncertainties)

Formal definitions

- measurements are given by event (jet, track, ...) counts, grouped in bins x_i^{rec}
- Bins are defined by regions in phase-space (observables)
- Not covered: unbinned methods
- Detector effects: detector response matrix A

  A_{ij}: probability that event from truth bin j is found in rec bin i

  Expected number of events in bin i: $\mu_i = \sum A_{ij} x_j^{\text{truth}}$

- Statistical fluctuations: Poisson distribution or Gaussian approximation

$$P(Y_i = y_i^{\text{rec}}) = \frac{\exp[-\mu_i](\mu_i)^{y_i}}{y_i!}$$

Testing unfolding results

The A is response matrix, x true vector and μ is observed one at the detector level

$$Ax + b = \mu , \qquad A_{ij} = \frac{N_{ij}^{\mathrm{MC,rec} \wedge \mathrm{gen}}}{N_j^{\mathrm{MC,gen}}} .$$

obtained from simulation

As experiment is performed, y_i are observed instead of μ_i
and the difference is amplified with unfolding procedure.
For low statistics counting experiment:

- Poisson distribution: $P(y_i;\mu_i) = \exp(-\mu_i)(\mu_i)^{y_i}/y_i!$

For larger statistics:

- Gaussian distribution with fixed μ_i and covariance matrix V_{yy}

The result of the unfolding is estimator of the truth distribution, $\hat{x}$
and corresponding uncertainties and correlations

$$\delta_j = \sqrt{(V_{xx})_{jj}}, \qquad \text{and} \qquad \rho_{jk} = \frac{(V_{xx})_{jk}}{\delta_j \delta_k}$$

The global correlation coefficient of bin j : $\rho_j = \sqrt{1 - \left((V_{xx})_{jj} \left(V_{xx}{}^{-1}\right)_{jj}\right)^{-1}}$

Testing unfolding results

- **Data tests:**
  - **verify normalisation:** $Y_{\text{fold}} = Y_{\text{data}}$

$$Y_{\text{unf}} := \sum_{i=1}^{M} (A\hat{x} + b)_i \qquad \text{and} \qquad Y_{\text{data}} := \sum_{i=1}^{M} y_i$$

fold

  - **calculate** $\chi_A^2 = (A\hat{x} + b - y)^{\text{T}}(V_{yy})^{-1}(A\hat{x} + b - y)$

    which one expects to find distributed with

    degress of freedom $M_y - M_x$

$$\rho_{\text{avg}} = \frac{1}{M_x}\sum_{j=1}^{M_x}\rho_j$$

  - **calculate average global correlation coefficient**

    one expexts to find non-zero global correlation coefficient in presence non-negligible migrations.

Testing unfolding results

- Closure tests:
  - unfold MC generated sample with A matrix obtained with same MC, tests technical correctnest of the procedure
  - unfold MC generated sample using A matrix obtained with different MC (different model)
  - Apply Poissonian statistical fluctuations to folded MC (detector level), unfold. Repeat several times, take average

$$\boldsymbol{x}^{\text{avg}} = \langle \hat{\boldsymbol{x}} \rangle, \qquad \text{and} \qquad (V_{xx}^{\text{avg}})_{jk} = \langle (\hat{x}_j - x_j^{\text{avg}})(\hat{x}_k - x_k^{\text{avg}}) \rangle$$

  - Modify truth distribution, use same unfolding matrix A, repeat several times, confirm that results unbiased

$$\chi^2_{\text{truth}} = (\hat{\boldsymbol{x}} - \boldsymbol{x}^{\text{truth}})^{\text{T}} V_{xx}{}^{-1} (\hat{\boldsymbol{x}} - \boldsymbol{x}^{\text{truth}})$$

Unfolding methods

- Bin-by-bin "correction"
- Matrix methods:
  - Matrix inversion
  - "Bayesian" [D'Agostini 1995]
  - "Iterative" [D'Agostini 1995 iterated]
  - Fraction fit: TUnfold
  - Regularised unfolding: TUnfold

(truth+background) × detector × stat.fluctuations $\longrightarrow$ measurement

Result: estimator of truth $\longleftarrow$unfolding algorithm $\longleftarrow$ measurement

Toy example from arXiv:1611.01927

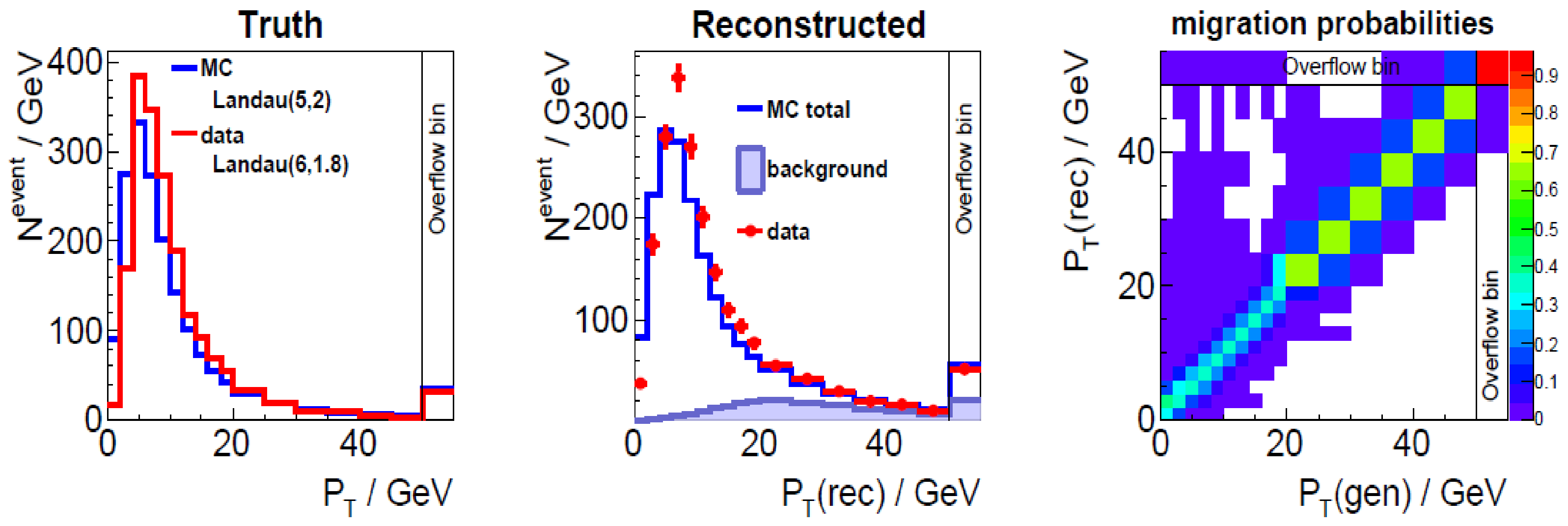


Figure 1. Toy example, distribution on truth level (left), on reconstructed level (middle), response matrix (right).

A heavy particle is produced with pT and decay into two massless particles.
Ebegy and angles of the decay products are smeared with resolution functions.
The observed pT is calculted as vector sum of two reconstructed particles.
Background is also generated and contribute mostly at high pT.
For pT distribution at „truth” Level landau distribution is used, with different parameters for MC and data. The difference between both parametrisations is clearly visible. The MC sample is used to derive response matrix.

„Bin-by-bin”

- Assumption: migration effects are “small” so they can be “corrected” using a multiplicative factor
- The factor is determined from MC
- Two variants:
  - Simple bin-by-bin
  - Bin-by-bin with background subtraction

Bin-by-bin correction factors

- Very simple method:

$$x_i = (y_i - b_i)\boxed{\frac{N_i^{\text{gen}}}{N_i^{\text{rec}}}} \leftarrow \text{Correction factor}$$

y_i : observed in bin i

b_i : expected backround in bin i

N_i^{gen} : MC truth in bin i

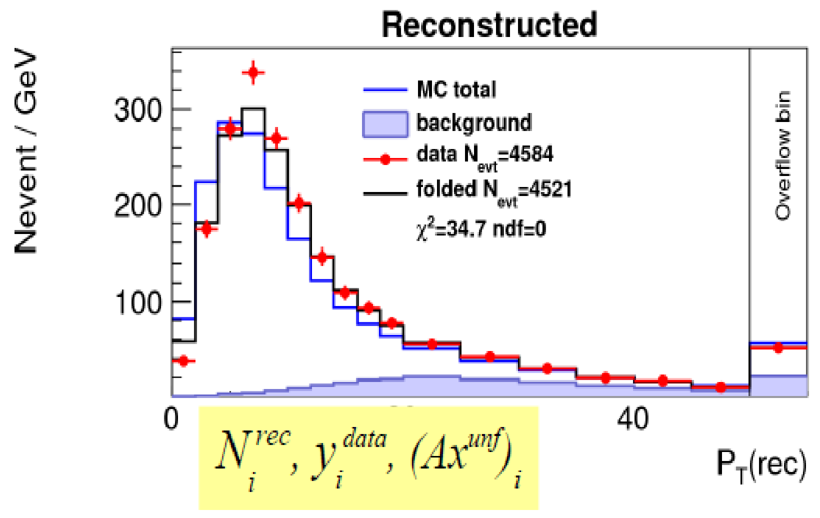
$N_i^{\text{rec}} = \sum_j A_{ij} N_i^{\text{gen}}$: MC reconstructed in bin i

Results "looks nice"

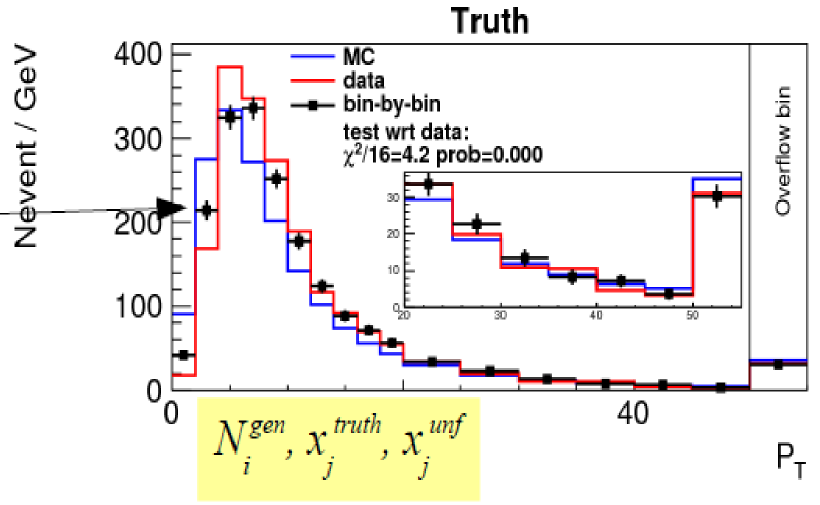
No statistical bin-to-bin correlations

but

Method is wrong, fails very basic tests



$N_i^{rec},\ y_i^{data},\ (Ax^{unf})_i$



$N_i^{gen},\ x_j^{truth},\ x_j^{unf}$

Simple „Bin-by-bin": why is it wrong?

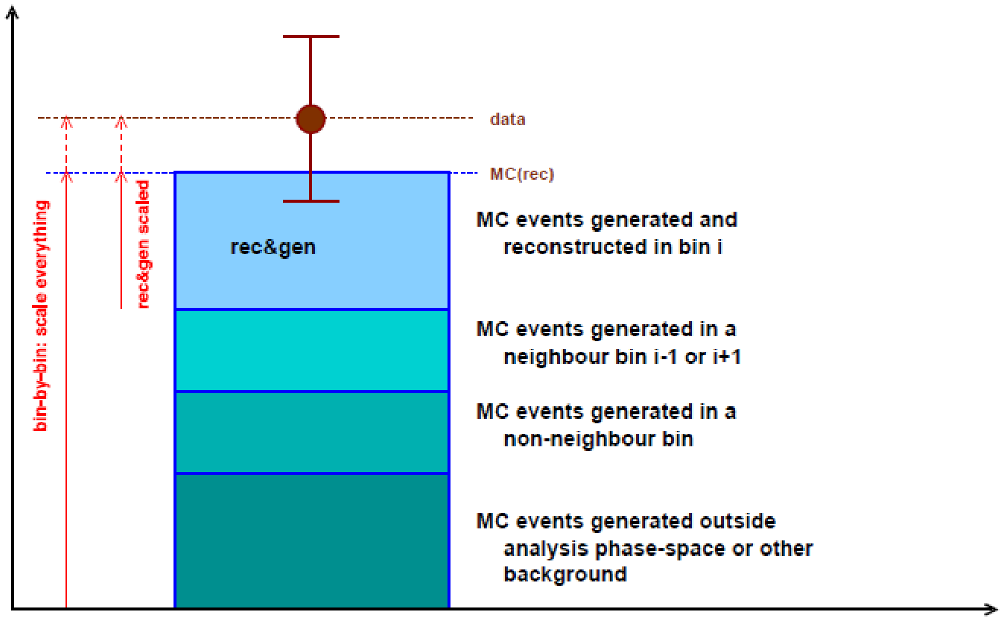
- Migrations are additive, while BBB correction is multiplicative → wrong type of correction

$$x_i^{\text{BBB}} = x_i^{\text{gen}} \frac{y_i^{\text{data}}}{y_i^{\text{rec}}}$$

- It should be:

$$x_i^{\text{BBBSUB}} = x_i^{\text{gen}} \frac{y_i^{\text{data}} - \left(y_i^{\text{rec}} - y_i^{\text{rec\&gen}}\right)}{y_i^{\text{rec\&gen}}}$$

$$= x_i^{\text{gen}} \frac{y_i^{\text{data}} - y_i^{\text{rec}}\left(1 - P_i\right)}{y_i^{\text{rec}} P_i}$$


data
MC(rec)
bin-by-bin: scale everything
rec&gen scaled
rec&gen
MC events generated and reconstructed in bin i
MC events generated in a neighbour bin i-1 or i+1
MC events generated in a non-neighbour bin
MC events generated outside analysis phase-space or other background

- Relevant quantity: purity

$$P_i = \frac{y_i^{\text{rec\&gen}}}{y_i^{\text{rec}}}$$

Matrix methods

- All matrix methods are based on the matrix of probabilities:

$$\text{Expected number of events in bin } i: \ \mu_i = \sum A_{ij} x_j^{\text{truth}}$$

- The A_{ij} are calculated from Monte Carlo

$$A_{ij} = \frac{y_{ij}^{\text{rec,gen}}}{y_j^{\text{gen}}} \text{ and the reconstruction efficiencies are } \varepsilon_j = \sum_i A_{ij}$$

- A_{ij} is normalized to the generated number of events in bin j, so it is (largely) model independent, only depends on the detector response.

Matrix inversion

- If the number of bins is equal on gen and rec level: A is a square matrix

  → invert it

folding equation: $y = Ax + b$

invert matrix: $x = A^{-1}(y - b)$

Covariance: $V_{xx} = A^{-1} V_{yy} (A^{-1})^T$

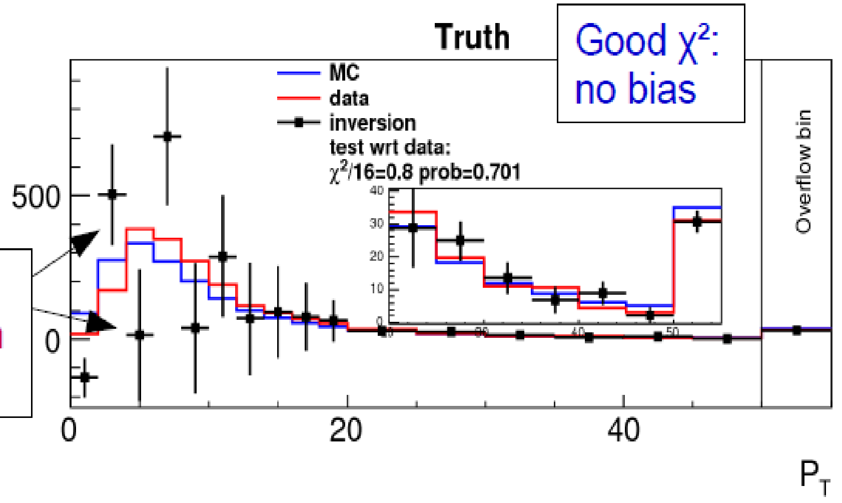
correlation coefficients: $\rho_{ij} = \dfrac{(V_{xx})_{ij}}{\sqrt{(V_{xx})_{ii}(V_{xx})_{jj}}}$

y : measurements

V_{yy} : covariance matrix of measurements

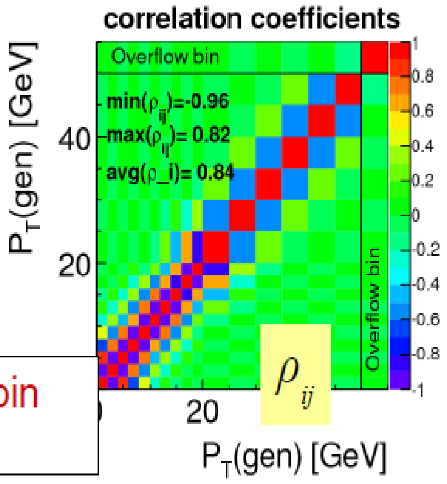
b : background

A : matrix of migrations

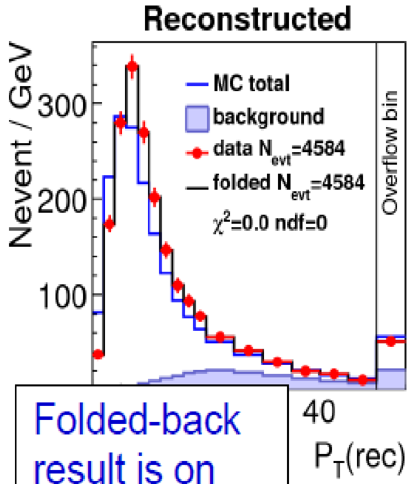


Good χ^2: no bias

Unfolded result exhibits bin-to-bin oscillations



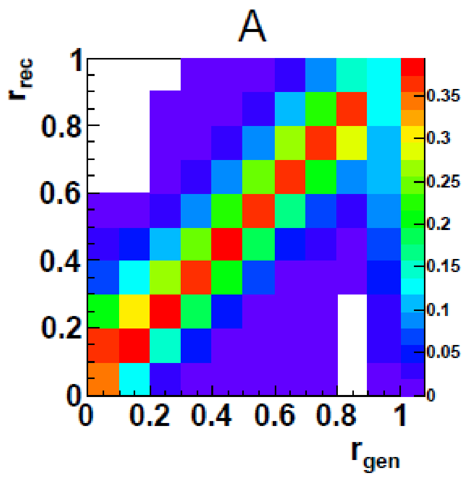
Large bin-to-bin correlations

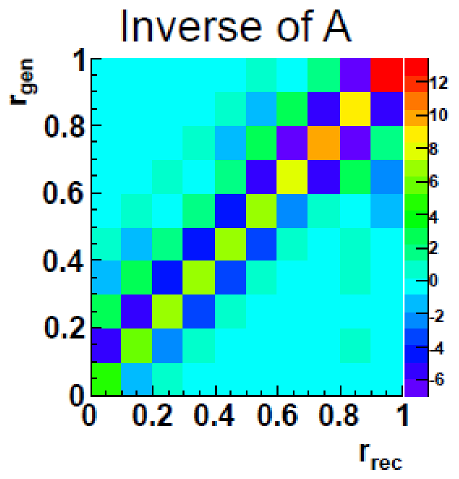


Folded-back result is on the data

Cause of large fluctuations

- Matrix inversion: creates large negative off-diagonals
  $\rightarrow$ statistical fluctuations of the data are amplified
- Possible improvements
  - Avoid matrix inversion "Bayesian" or "Iterative"
  - Use more reconstructed bins $\rightarrow$ TFractionFitter, TUnfold
  - Regularisation:
    TSVDUnfold, TUnfold





Template fit

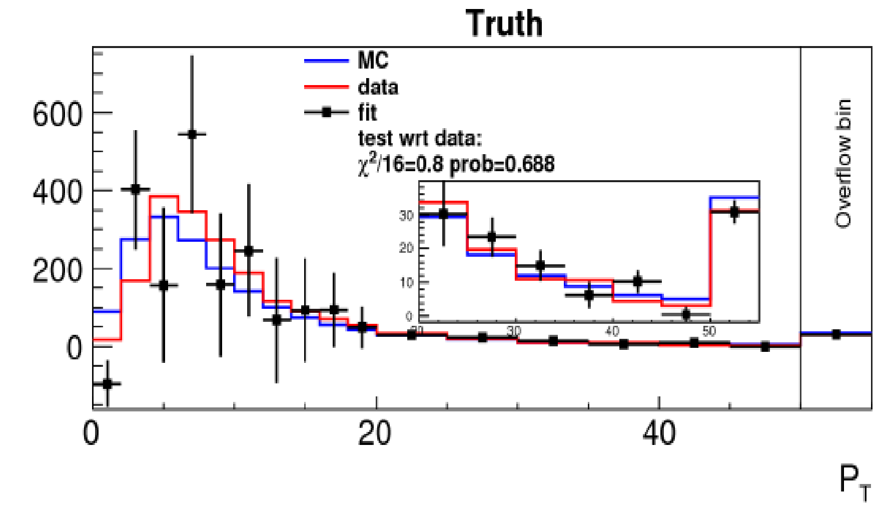
- Choose larger number of reconstructed bins than truth bins → least-square fit
- Idea: use more information → obtain better result?

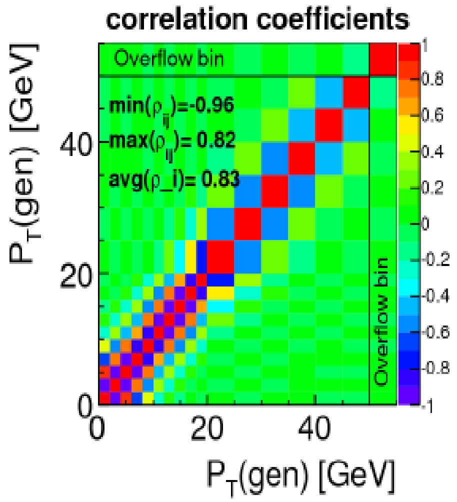
$$\chi^2 = (y - b - Ax)^T V_{yy}^{-1} (y - b - Ax)$$

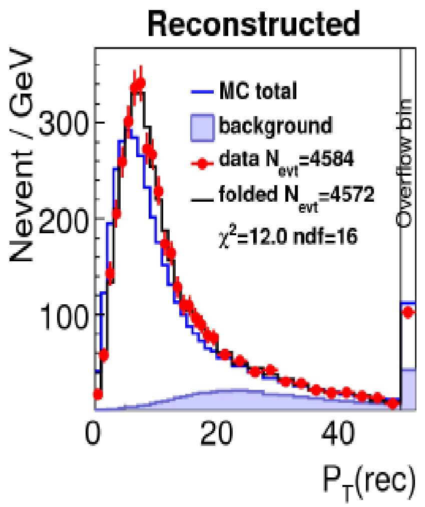
y : measurements
V_{yy} : covariance matrix of measurements
b : background
A : matrix of migrations
A_{ij} : MC template for truth bin j

$$x = (A^T V_{yy}^{-1} A)^{-1} A^T V_{yy}^{-1} (y - b)$$

covariance of x : $V_{xx} = (A^T V_{yy}^{-1} A)^{-1}$







Template fit with area constraint

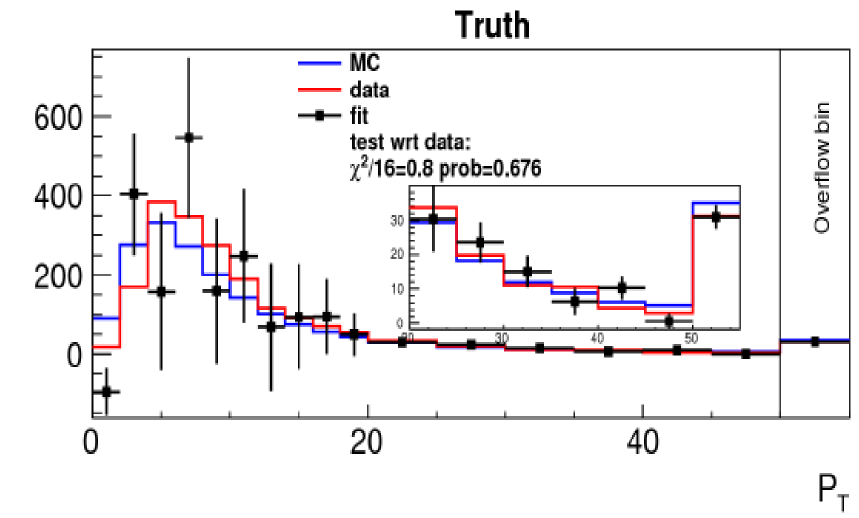
- Template with with constraint on the total number of events
- Basic idea: preserve normalisation for the folded-back result by adding the constraint

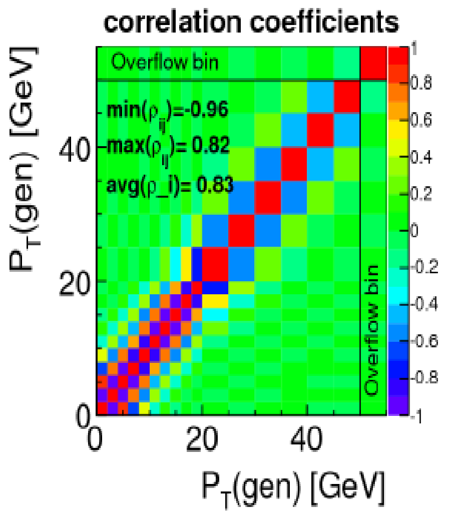
$$\sum (y_i - b_i) = \sum_{i,j} A_{ij} x_j$$

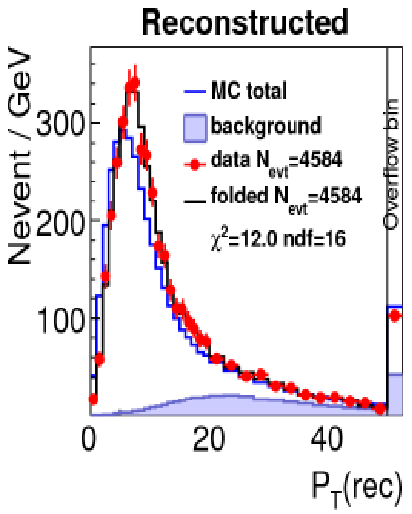
- Technical implementation: see TUnfold documentation

→ Result does not change much over unconstrained template fit, but normalisation is recovered

$[N_{data} = N_{fold} = 4584]$







Tikhonov regularisation

- Basic idea: add terms to the likelihood which damp oscillations in the result.

$$\chi^2 = (y - b - Ax)^T V_{yy}^{-1} (y - b - Ax) + \tau^2 (L(x - x_B))^T L(x - x_B)$$

y : measurements
V_{yy} : covariance matrix of measurements
b : background
A : matrix of migrations
x_B : regularisation bias
L : regularisation conditions
τ : regularisation strength

In addition, apply area constraint to preserve normalisation

- Regularisation bias x_B: set to zero or to MC truth
- Regularisation conditions L: set to unity matrix [or mimic second derivatives, “curvature”]
- Regularisation strength τ: “small” number

$$\tau \ll 1/\sigma$$

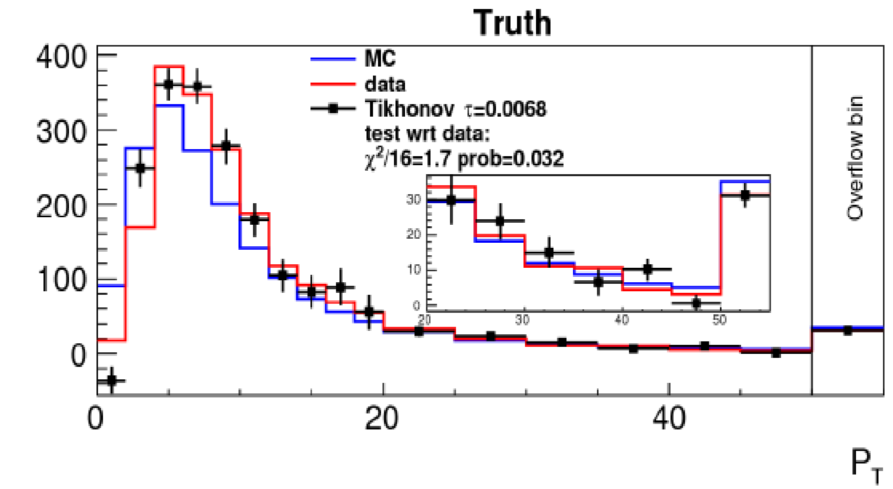
where σ~uncertainty after unfolding

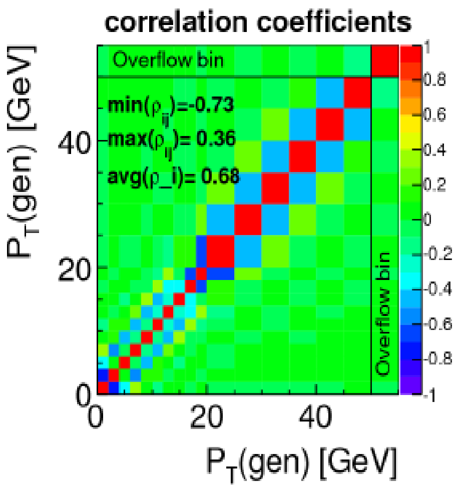
Tikhonov regularisation (eg. TUnfold)

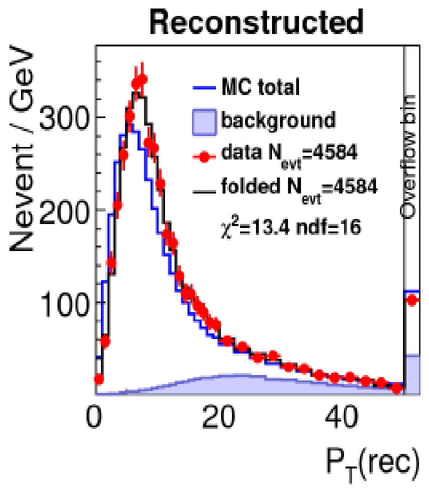
- Basic idea: add terms to the likelihood which damp oscillations in the result.
- This is working well: no oscillations, moderate correlations and uncertainties

  Basic tests look reasonable

- Question: objective to choose τ







Iterative method

Ratio data to folded
→ iterate until ~1

$$x_j^{(N+1)} = x_j^{(N)} \sum_i \frac{A_{ij}}{\epsilon_j} \frac{y_i}{\sum_k A_{ik} x_k^{(N)}}$$

efficiency: $\epsilon_j = \sum_i A_{ij}$

start values: $x_j^{(-1)}$ [e.g. MC truth]

iterate until N is sufficiently large

- Original works by Shepp/Vardi 1982, Kondor 1983, Mülthei/Schorr 1987
- Re-invented by D'Agostini 1995 as "Iterative Bayesian unfolding"

Note: efficiency is absorbed in a redefinition of A, x in the original works: x'=εx and A'=A/ε

- Mathematical properties (Shepp/Vardi 1982 and Mülthei/Schorr 1987)
  - Ultimately converges to a maximum of the (Poisson) Likelihood

    → like matrix inversion but with all x≥0
  - Convergence is very slow
- Use in HEP:
  - Stop after N iterations → result will be "smooth" [regularized] but is biased to the start value

Regularisation strength:

Tikhonov: τ ↔ Iterative: N_{iter}

Iterative method with background

$$x_j^{(N+1)} = x_j^{(N)} \sum_i \frac{A_{ij}}{\epsilon_j} \frac{y_i - b_i}{\sum_k A_{ik} x_k^{(N)}}$$

efficiency: $\epsilon_j = \sum_i A_{ij}$

start values: $x_j^{(-1)}$ [e.g. MC truth]

OR

$$x_j^{(N+1)} = x_j^{(N)} \sum_i \frac{A_{ij}}{\epsilon_j} \frac{y_i}{\sum_k A_{ik} x_k^{(N)} + b_i}$$

efficiency: $\epsilon_j = \sum_i A_{ij}$

start values: $x_j^{(-1)}$ [e.g. MC truth]

- Background could be subtracted from the data
- Or: background could be added to the folded MC in the denominator. This guarantees the desired property $x \geq 0$
- D'Agostini suggests to include the background normalisation as extra bin x_{n+1}. This also guarantees $x \geq 0$ but results in an extra parameter → make sure to then include a background control bin in the set of measurement bins

Evaluation of the covariance matrix

- Matrix inversion methods (with or without Tikhonov regularisation): covariance matrix is calculated analytically

- Iterative methods: non-linear, covariance matrix calculation in general has to be done by other means

- Replica method
  - Apply statistical fluctuations on the data histogram

    $\rightarrow$ N replicas of the data
  - Repeat the unfolding for each replica
  - Covariance is estimated from RMS of the results
- Bootstrap method:

  similar idea, but based on events

  $\rightarrow$ test complete analysis chain

Iterative method: 0th iteration

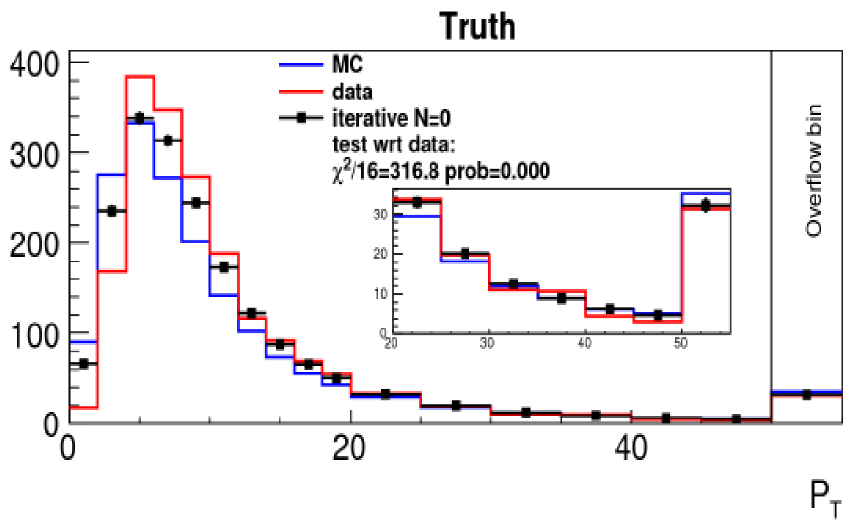
$$x_j^{(N+1)} = x_j^{(N)} \sum_i \frac{A_{ij}}{\epsilon_j} \frac{y_i}{\sum_k A_{ik} x_k^{(N)} + b_i}$$

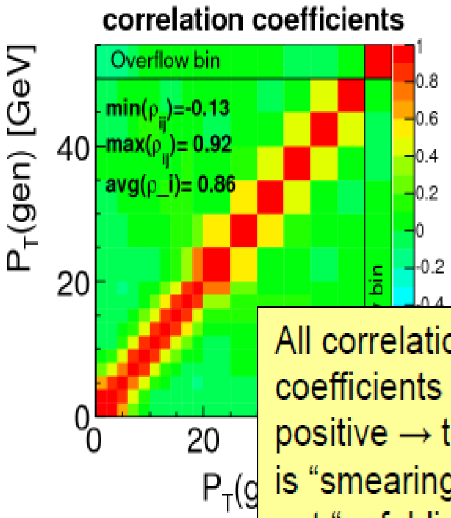
efficiency: $\epsilon_j = \sum_i A_{ij}$

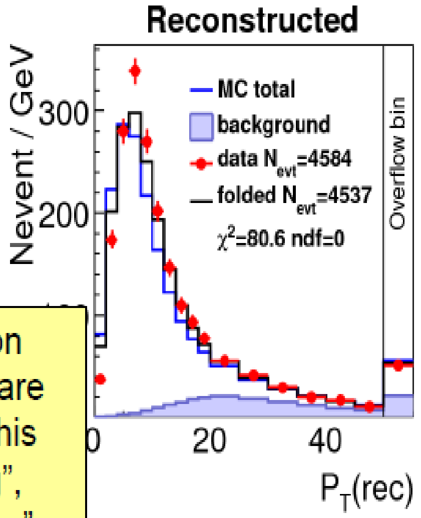
start values $x_j^{(-1)}$ set to MC truth

- 0th iteration: "Bayesian unfolding" from 1995 D'Agostini paper
- Result "looks nice", very small uncertianties, but fails all tests

$\rightarrow$ the method has to be iterated





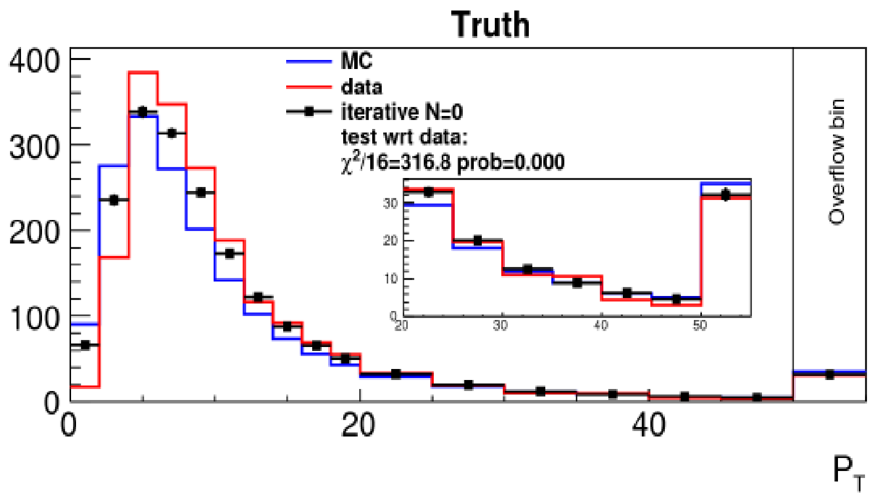


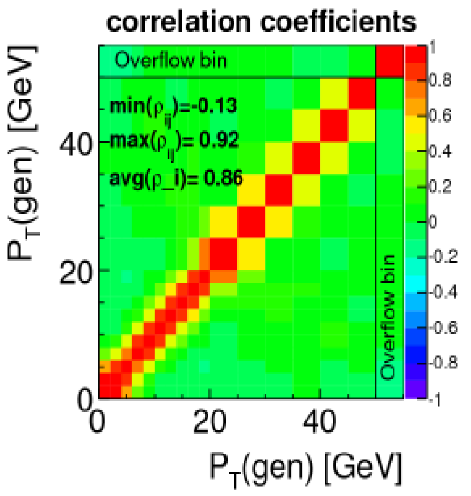
All correlation coefficients are positive → this is "smearing", not "unfolding"

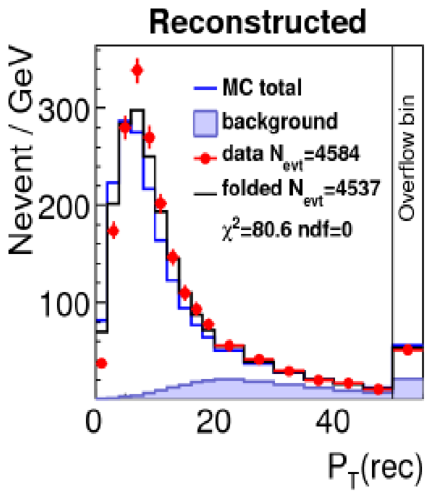
Iterative method: 1st iteration

$$x_j^{(N+1)} = x_j^{(N)} \sum_i \frac{A_{ij}}{\epsilon_j} \frac{y_i}{\sum_k A_{ik} x_k^{(N)} + b_i}$$

- Convergence rate is expected to grow quadratically with the number of bins [Mülthei/Schorr 1987]
- Look at 1st iteration
  - Neighboring bins have positive correlation (expect: negative)
  - Shape not described
  - Folded-back different from data
  - → have to iterate further



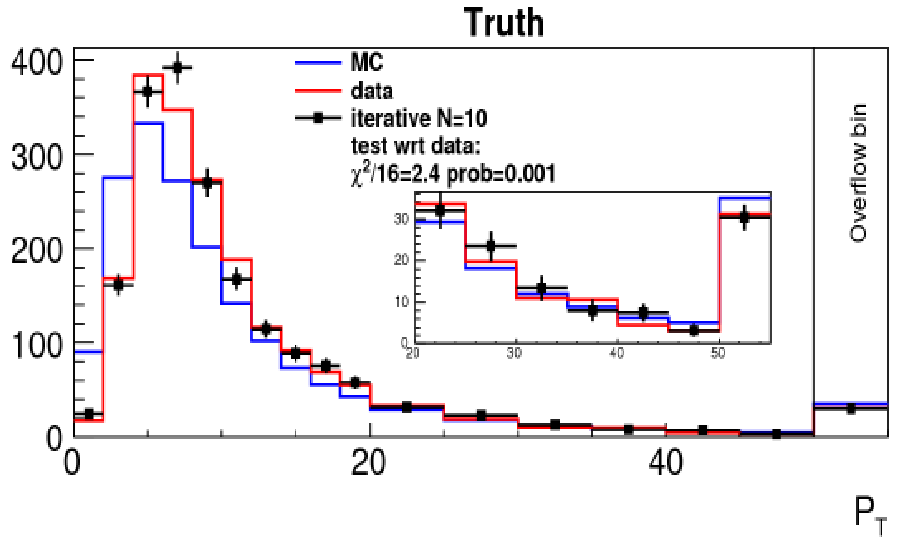


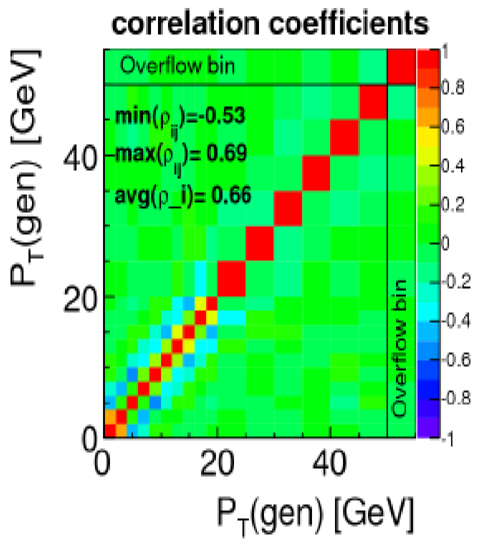


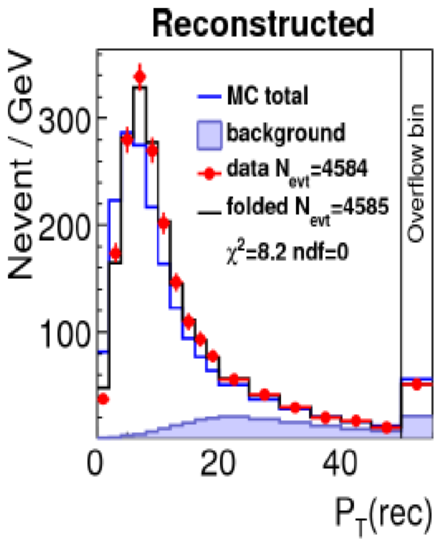
Iterative method: 10th iteration

$$x_j^{(N+1)} = x_j^{(N)} \sum_i \frac{A_{ij}}{\epsilon_j} \frac{y_i}{\sum_k A_{ik} x_k^{(N)} + b_i}$$

- Convergence rate is expected to grow quadratically with the number of bins [Mülthei/Schorr 1987]
- Look at 10th iteration
  - Similar to Tikhonov with strong regularisation



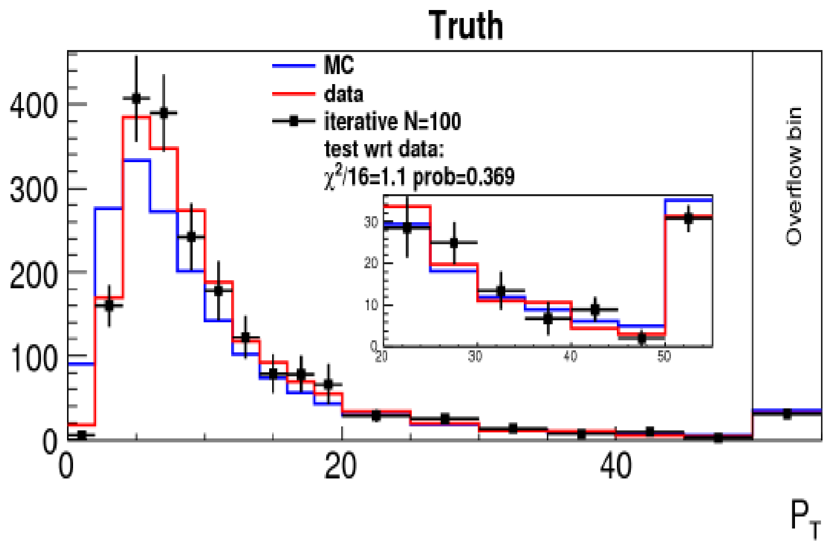


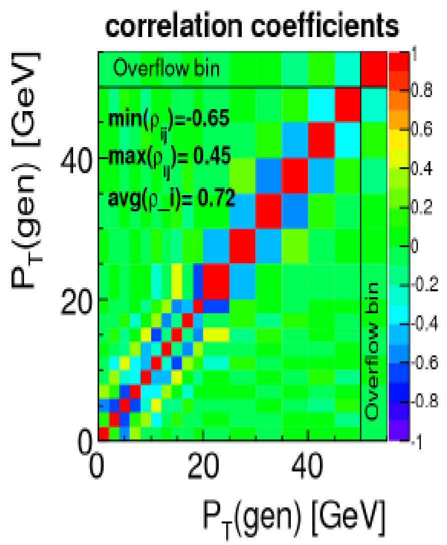


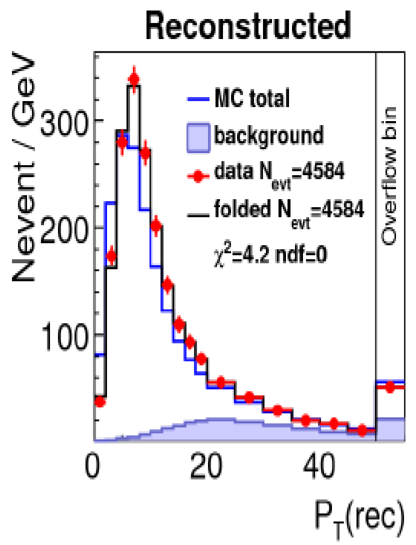
Iterative method: 100th iteration

$$x_j^{(N+1)} = x_j^{(N)} \sum_i \frac{A_{ij}}{\epsilon_j} \frac{y_i}{\sum_k A_{ik} x_k^{(N)} + b_i}$$

- Convergence rate is expected to grow quadratically with the number of bins [Mülthei/Schorr 1987]
- Look at 100th iteration
  - Similar to Tikhonov with weak regularisation



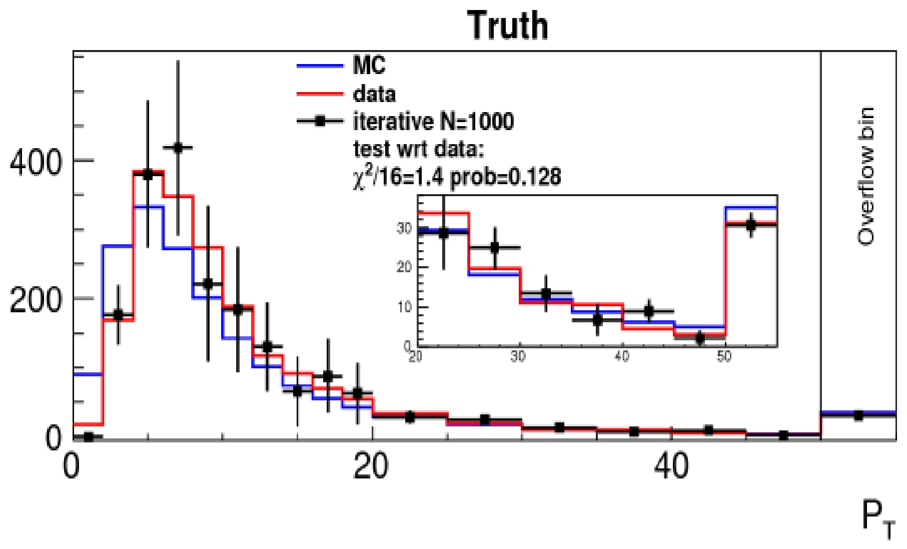


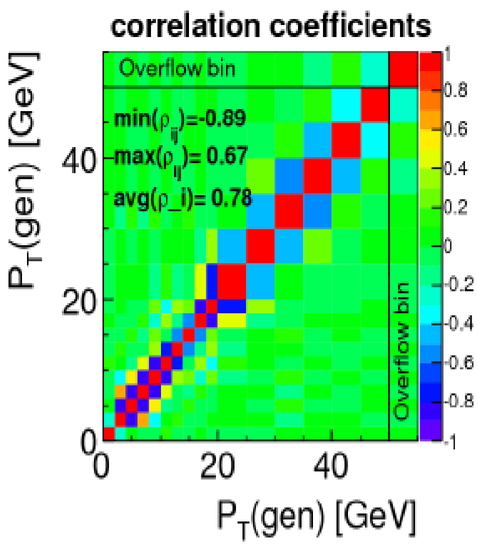


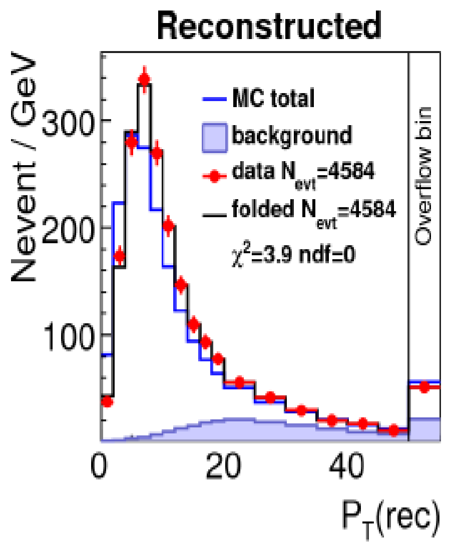
Iterative method: 1000th iteration

$$x_j^{(N+1)} = x_j^{(N)} \sum_i \frac{A_{ij}}{\epsilon_j} \frac{y_i}{\sum_k A_{ik} x_k^{(N)} + b_i}$$

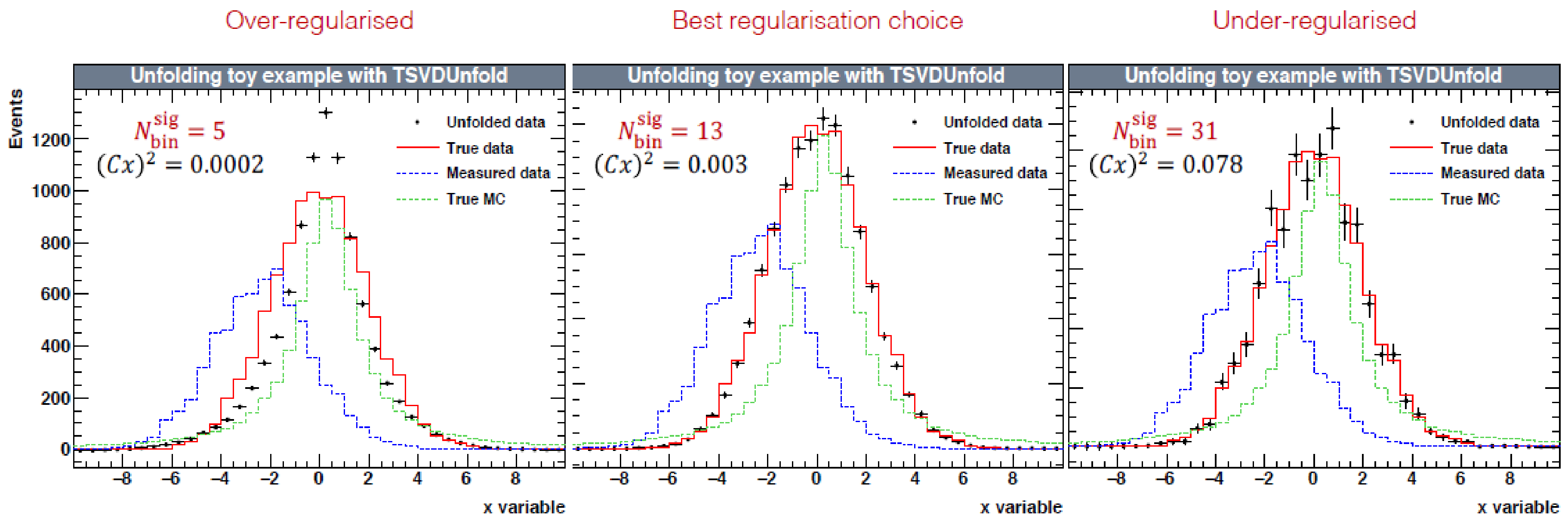
- Convergence rate is expected to grow quadratically with the number of bins [Mülthei/Schorr 1987]
- Look at 1000th iteration
  - Similar to matrix inversion, but all guaranteed to be x≥0
  - Objective to choose number of iterations? Scan of correlation?







Over- and Under-Regularised Unfolding



The parameter determines the strength of the regularization

- τ too small → oscillations
- τ too large → unfolded spectrum biased towards MC

Selection of other unfolding methods

- SVD [Hoecker et al, 1995]
  - Equivalent to matrix inversion with Tikhonov regularisation, parameter τ from Eigenvalue analysis
- Shape-constrained unfolding [Kuusela, Panaretos 2015]
- Improved D'Agostini [2010]
- Fully Bayesian [Choudalakis 2012]

RooUnfold package

- Provide a framework for different algorithms
  - Can compare performance directly, with common user code
    - RooUnfold takes care of different binning, normalisation, efficiency conventions
  - Can use common RooUnfold utilities
    - Write once, use for all algorithms
  - Currently implement or interface to iterative Bayes, SVD, TUnfold, unregularised matrix inversion, and bin-by-bin correction factors algorithms
- Simple OO design
  - "response matrix" object can be filled separately from training sample
    - in a different routine, or a different program (ROOT I/O support)
- Simple interface for the user
  - From program, ROOT/CINT script, or interactive ROOT prompt
  - Fill with histograms, vectors/matrices,… or direct methods:
    - `response->Fill(`x_{measured}, x_{true}`)` and `Miss(`x_{true}`)` methods takes care of normalisation
  - Results as a histogram with errors, or vector and covariance matrix

RooUnfold features

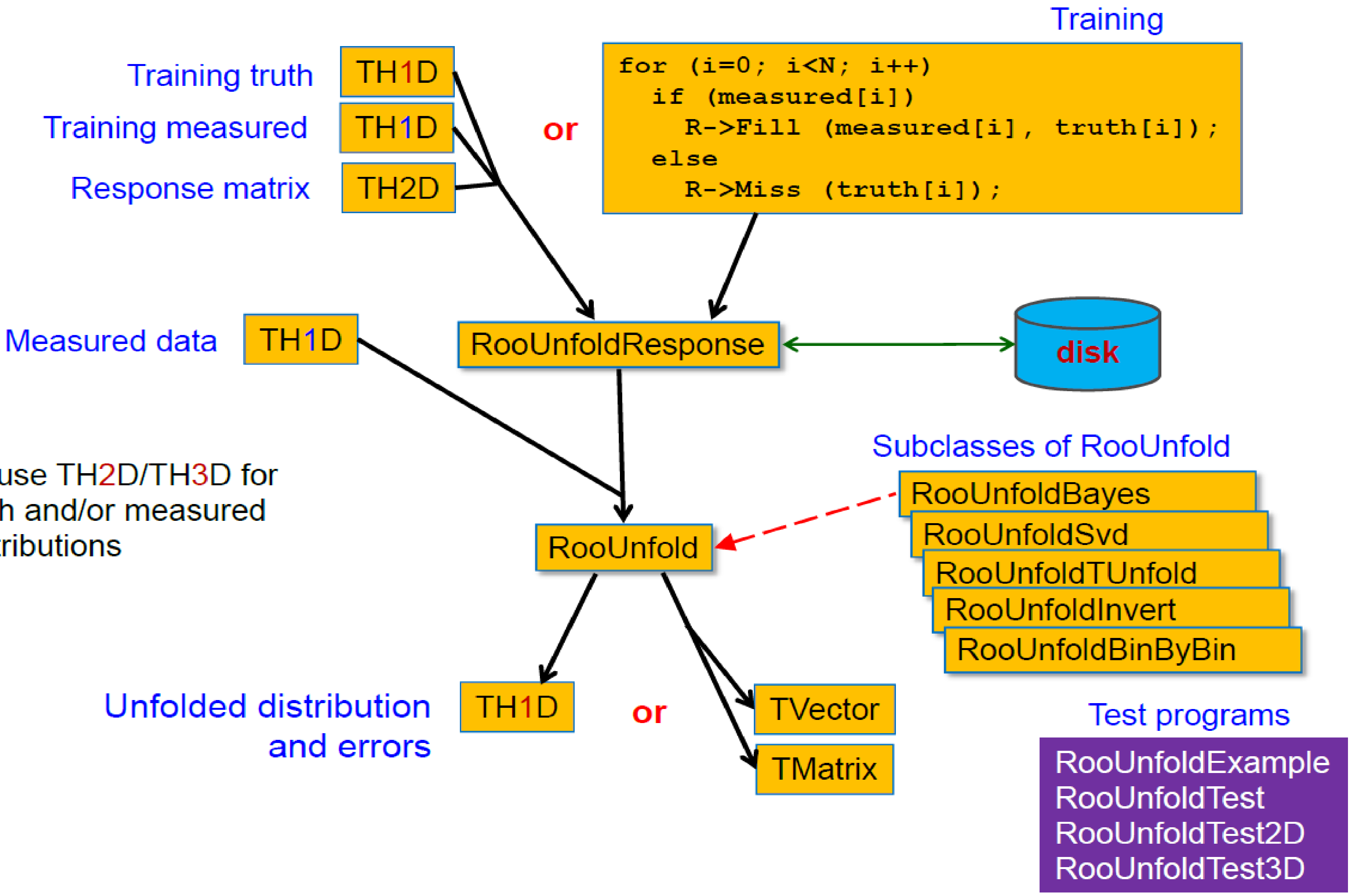
- Supports different binning scenarios
  - multi-dimensional distributions (1D, 2D, and 3D)
  - Different binning (or even dimensionality) for measured and truth
  - Option to include or exclude histogram under/overflow bins in the unfolding
- Supports different methods for error computation (simple switch). In order of increasing CPU time:
  - No error calculation (uses √N)
  - bin-by-bin errors (no correlations)
  - full covariance matrix from the propagation of measurement errors in the unfolding, or
  - covariance matrix from MC toys
    - useful to test error propagation and when it is inaccurate
- These details are handled by the framework, so don’t need to be implemented for each algorithm

RooUnfold testing

- Calculates resolutions, pulls, and χ^2
- Includes a toy MC test framework, allowing selection of different
  - PDFs and PDF parameters
  - binning
  - 1D, 2D, 3D tests
  - unfolding methods and parameters
  - Test procedures for the regularisation parameter and errors

  and plotting results from a single command

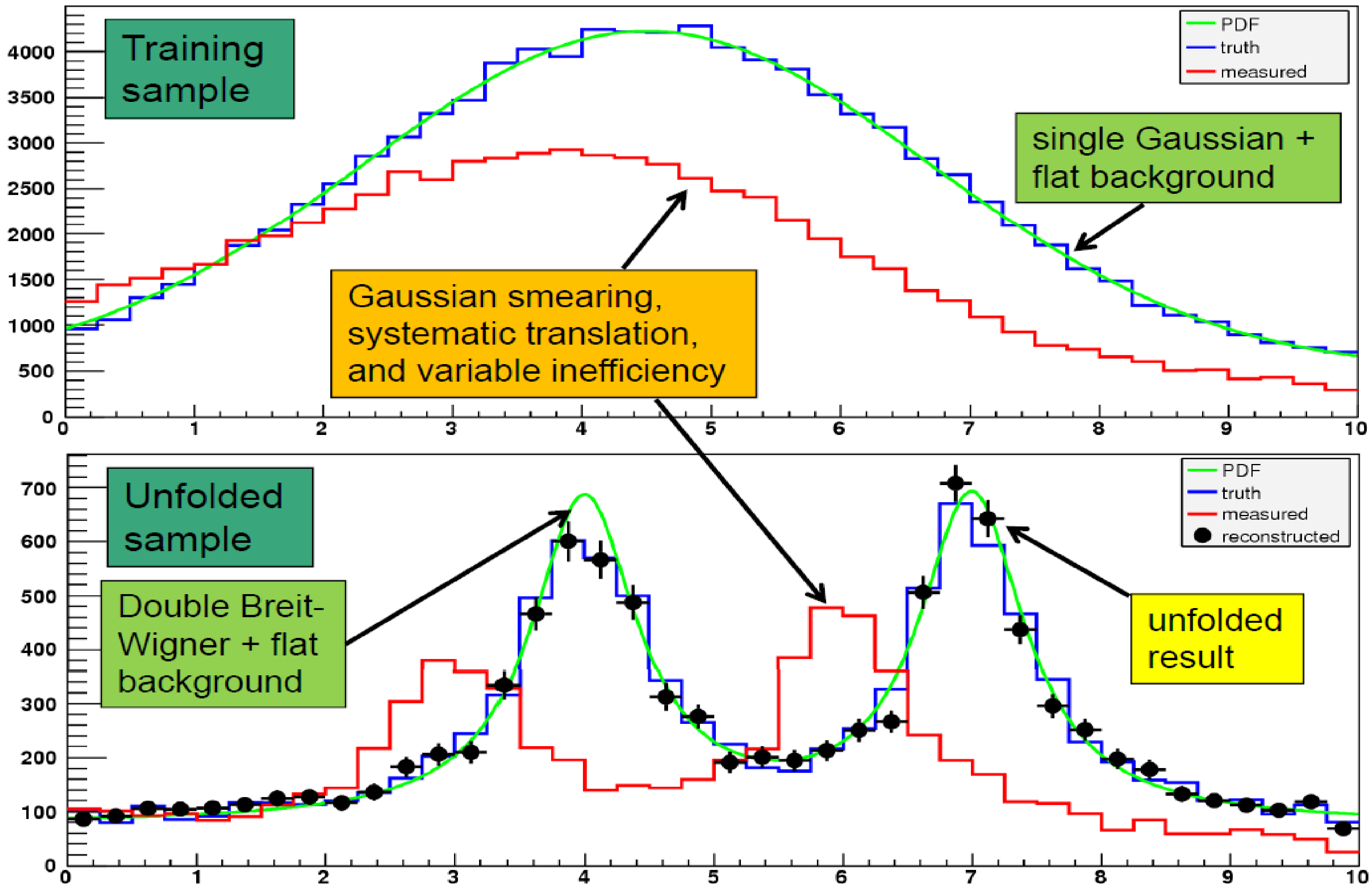
RooUnfold classes



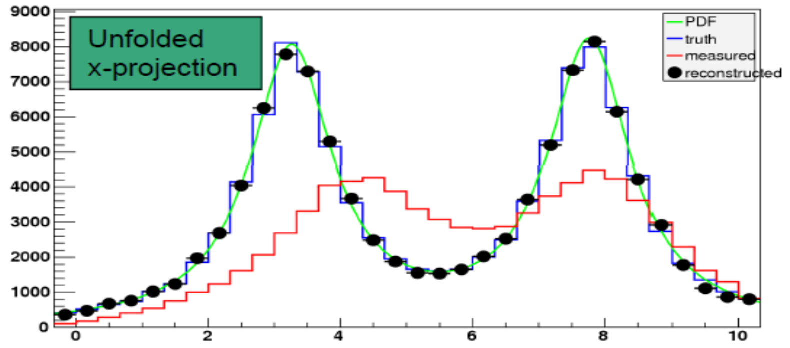
```
for (i=0; i<N; i++)
  if (measured[i])
    R->Fill (measured[i], truth[i]);
  else
    R->Miss (truth[i]);
```

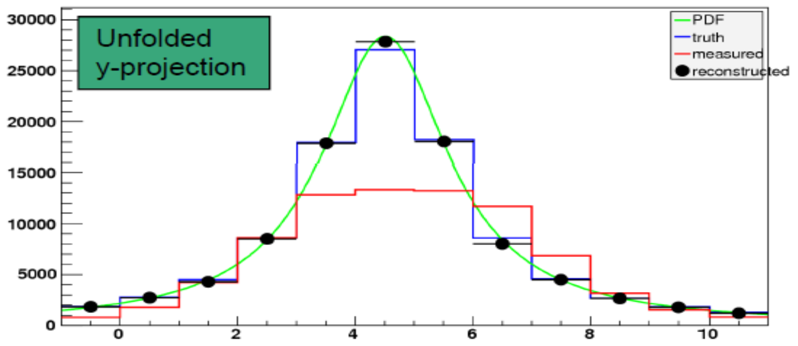
RooUnfoldExample
RooUnfoldTest
RooUnfoldTest2D
RooUnfoldTest3D

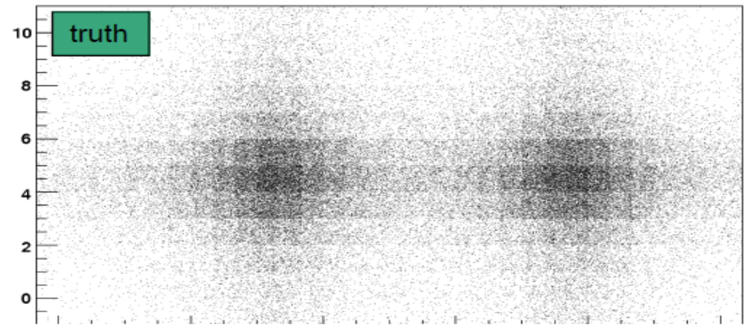
RooUnfold example (Bayes)

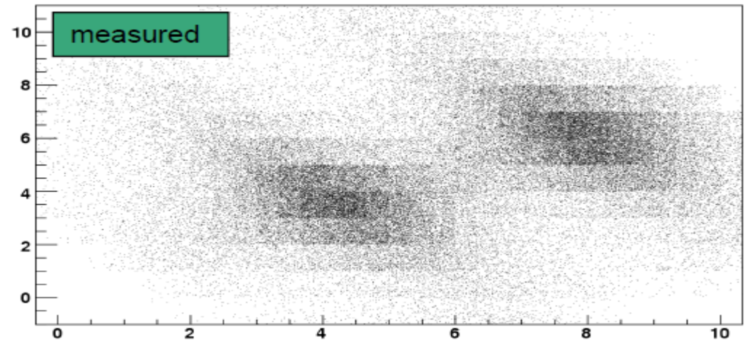


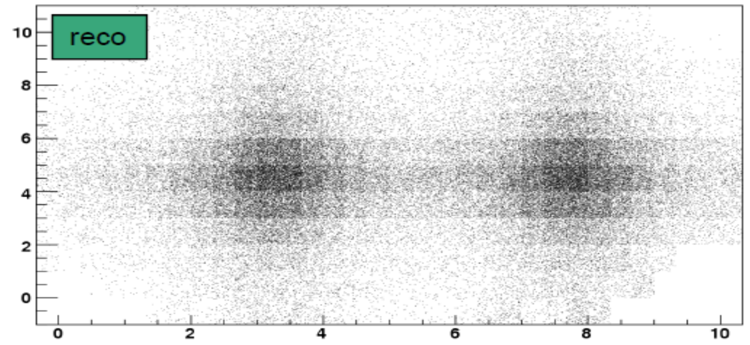
RooUnfold example (Bayes)











2D unfolding

2D Smearing, bias, variable efficiency, and variable rotation

RooUnfold algorithms: Iterative Bayes

- Uses the method of Giulio D'Agostini (1995), implemented by Fergus Wilson and Tim Adye
  - Uses repeated application of Bayes' theorem to invert the response matrix
  - Regularisation by stopping iterations before reaching "true" (but wildly fluctuating) inverse
    - Regularisation parameters is the number of iterations, which in principle has to be tuned according to the statistics, number of bins, etc.
      In practice, the results are fairly insensitive to the precise setting.
- Implementation details:
  - Initial prior is taken from training truth, rather than a flat distribution
    - Does not bias result once we have iterated, but perhaps reach optimum faster
  - Takes account of multinomial errors on the data sample but not, by default, uncertainties in the response matrix (finite MC statistics), which is very slow
  - Does not normally do smoothing (can be enabled with an option)

RooUnfold algorithms: SVD

- Uses the method of Andreas Höcker and Vato Kartvelishvili
- Obtains inverse of response matrix using singular value decomposition
  - Use number-of-events matrix to keep track of MC uncertainties
- Regularisation with a smooth cut-off on small singular value contributions (these correspond to high-frequency fluctuations)
  - Replace $s_i^2 \rightarrow s_i^2 / (s_i^2 + s_k^2)$
  - k determines the relative contributions of MC truth and data
    - k too small $\rightarrow$ result dominated by MC truth
    - k too large $\rightarrow$ result dominated by statistical fluctuations
  - k needs to be tuned for the particular type of distribution, number of bins, and approximate sample size
- Unfolded error matrix includes effect of finite MC training statistics (usually small)

RooUnfold algorithms: TUnfold

- Uses the TUnfold method implemented by Stefan Schmitt and included in ROOT
  - RooUnfold includes an interface to this class

- Performs a matrix inversion with 0-, 1-, or 2-order polynomial regularisation of neighbouring bins
  - RooUnfold automatically takes care of packing 2D and 3D distributions and creating the appropriate regularisation matrix required by TUnfold
- TUnfold can determine an optimal regularisation parameter (τ) by scanning the "L-curve" of $\log_{10}(\chi^2)$ vs $\log_{10}(\tau)$.

RooUnfold algorithms: Unregularised

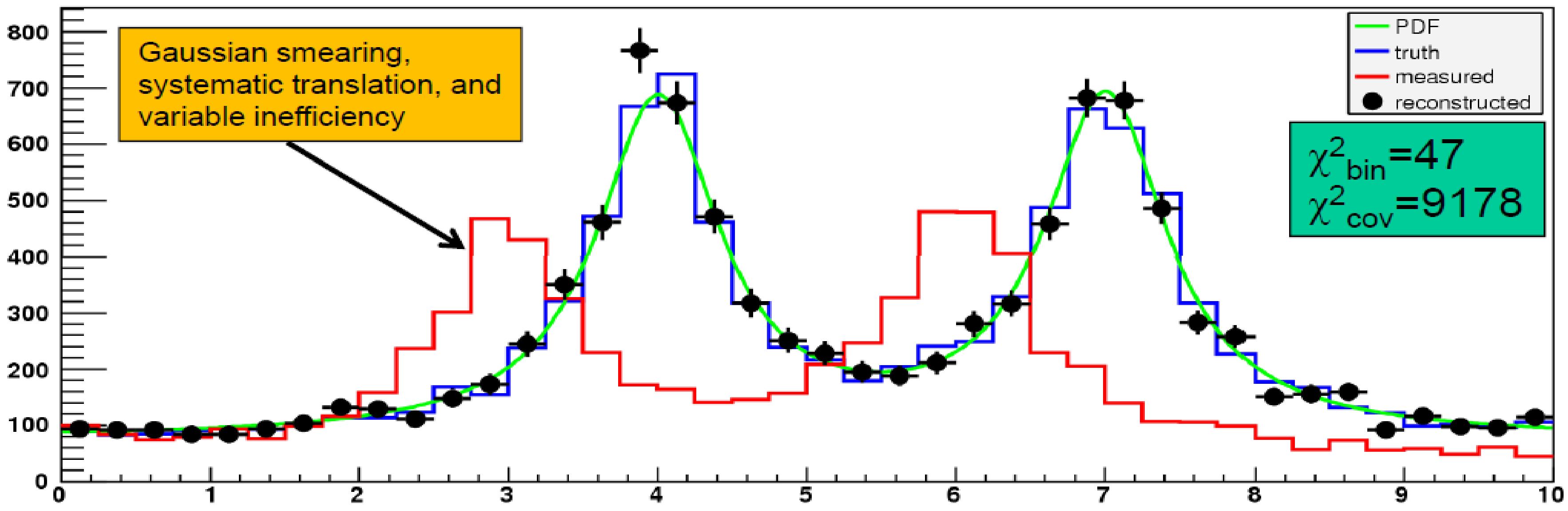
- Very simple algorithms
  - using bin-by-bin correction factors, with no inter-bin migration
  - using unregularised matrix inversion with singular value removal (TDecompSVD)

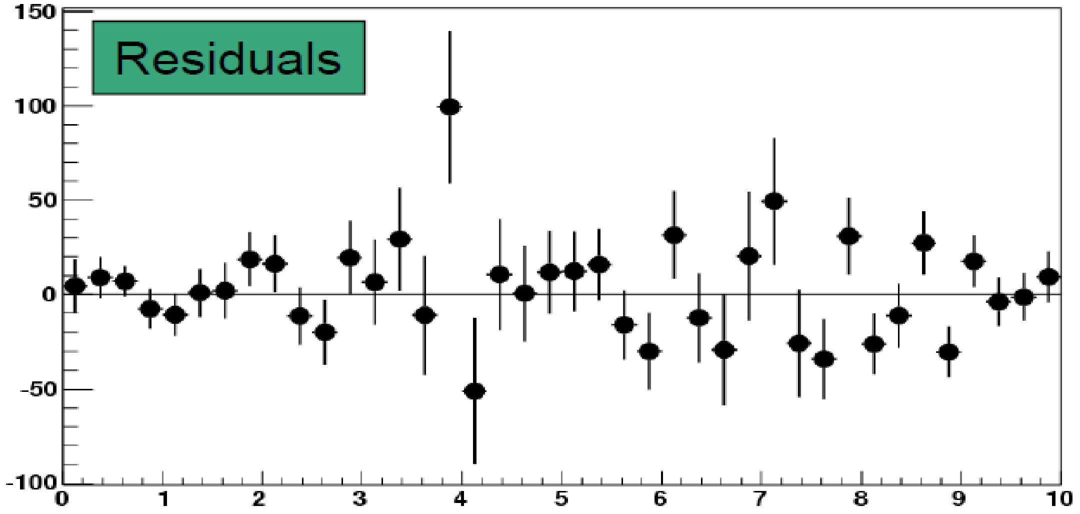
  are included for comparison – and to demonstrate why they should not be used in most cases!

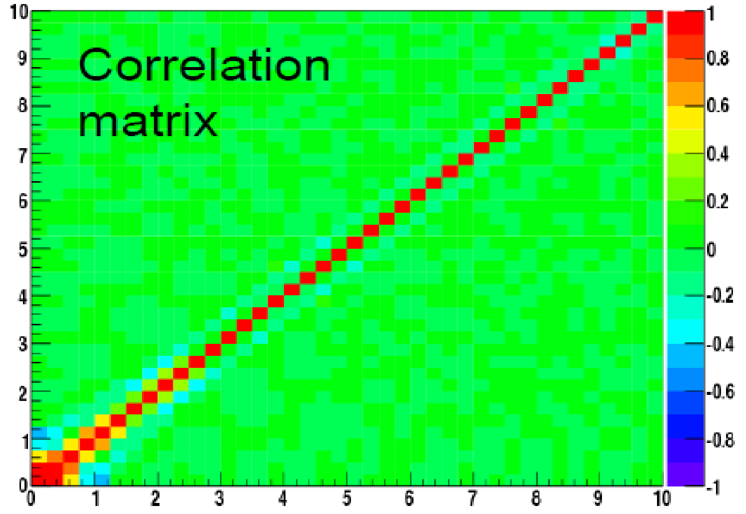
RooUnfold algorithms: comparison

- TUnfold and unregularised matrix inversion require the number of bins, $N_{\text{measured}} \geq N_{\text{true}}$
  - TUnfold claims best results if $N_{\text{measured}} > N_{\text{true}}$, eg. $N_{\text{measured}} = 2N_{\text{true}}$
    - This is a common general recommendation from unfolding experts, but perhaps is most relevant to these types of algorithms with explicit regularisation
    - This is an implicit additional regularisation, since we are “smoothing” two bins into one
- SVD implementation and bin-by-bin methods only support $N_{\text{measured}} = N_{\text{true}}$
  - SVD implementation also only works well for 1D distributions
- The choice of the SVD regularisation parameter has to be done by the user
  - TUnfold can often do this automatically
    - Can we do something similar for the SVD method?
  - The performance of the Bayes method is relatively insensitive to the regularisation parameter (number of iterations)

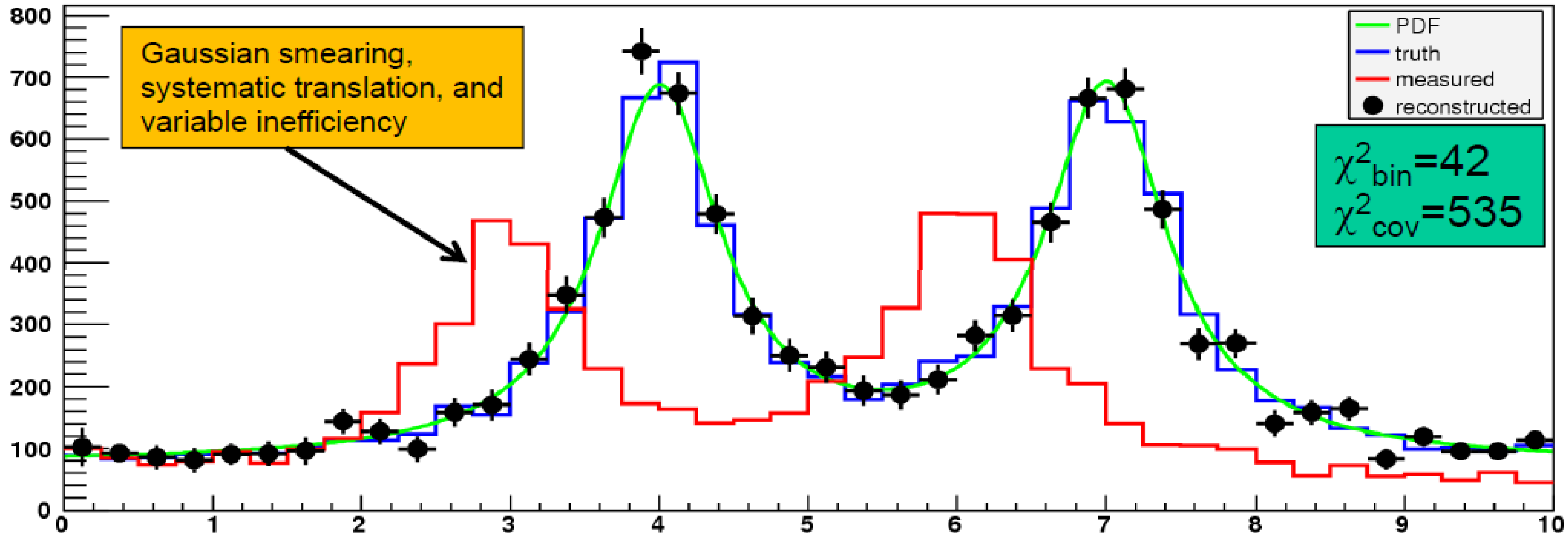
RooUnfold with Bayes algorithm (3 iterations)

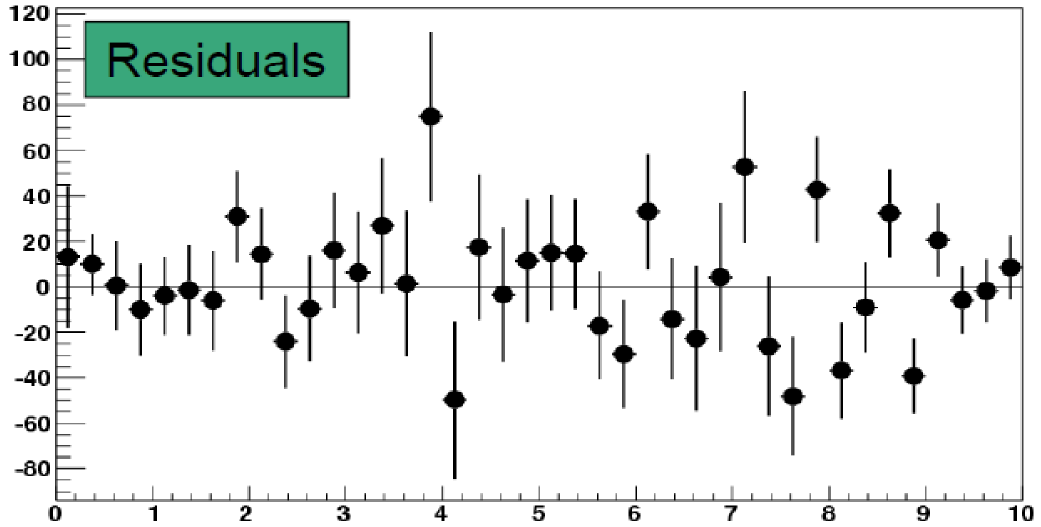


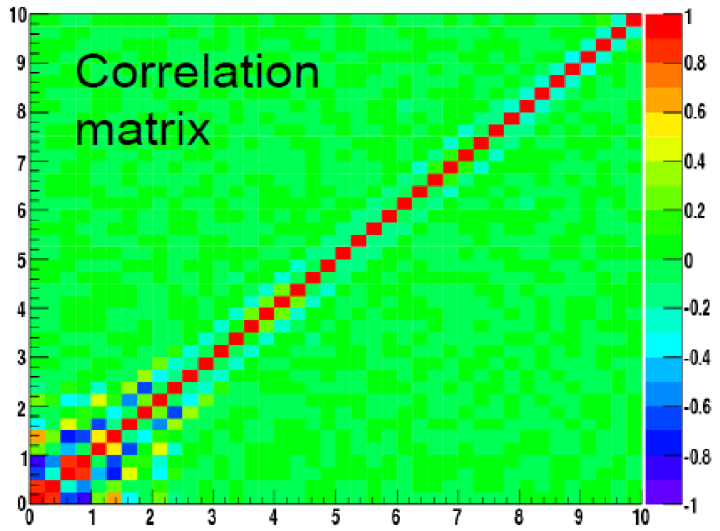




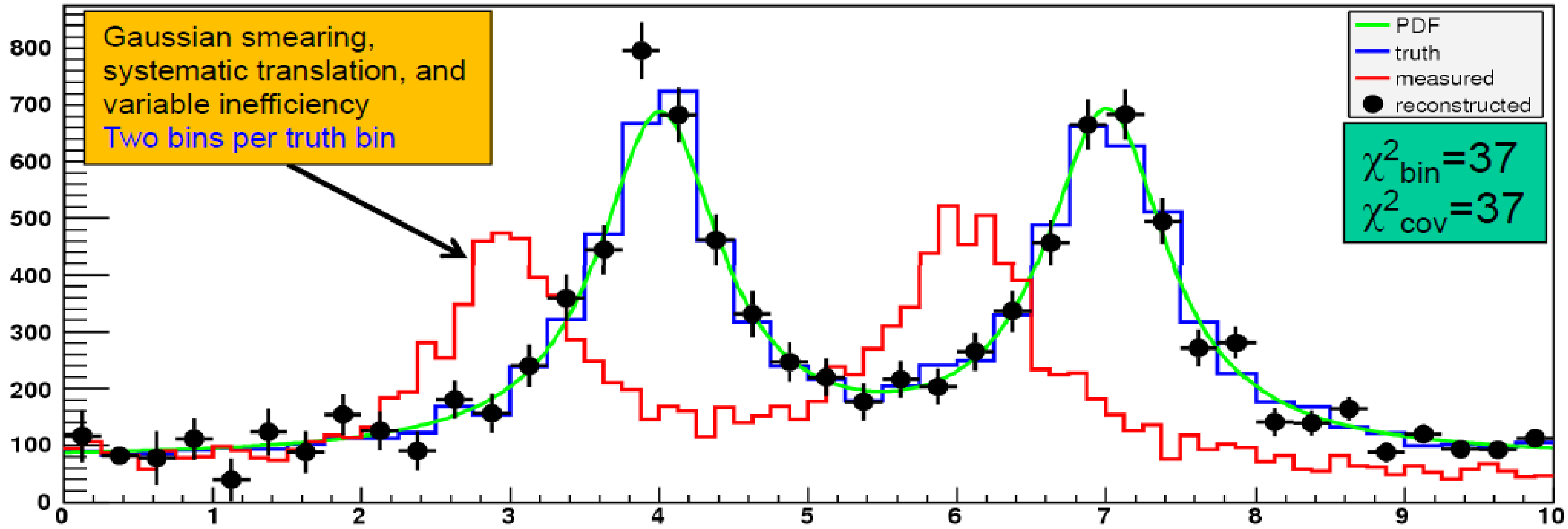
RooUnfold with SVD algorithm (k=30)

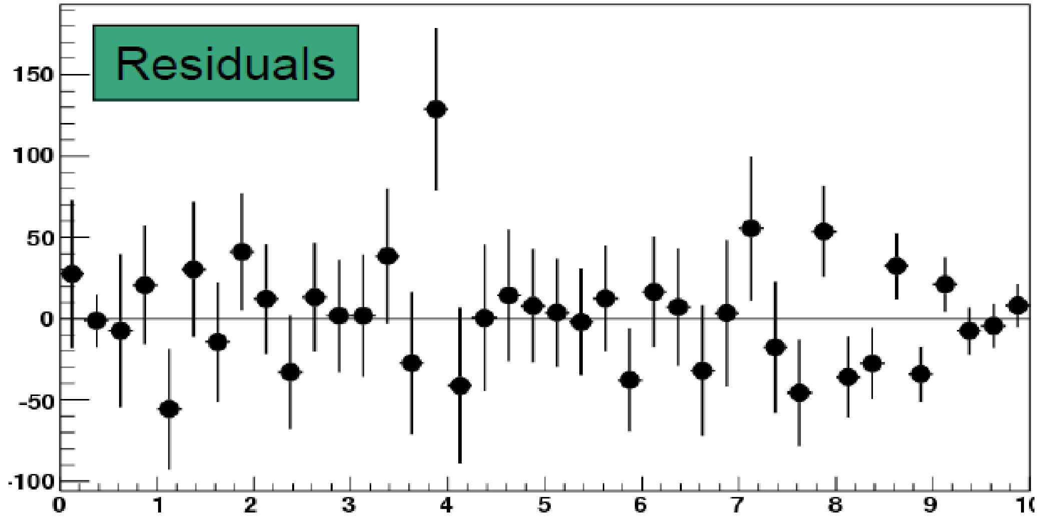


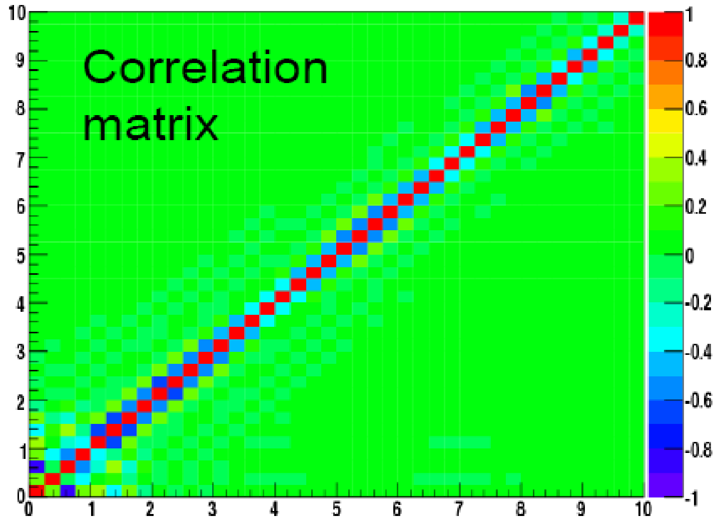




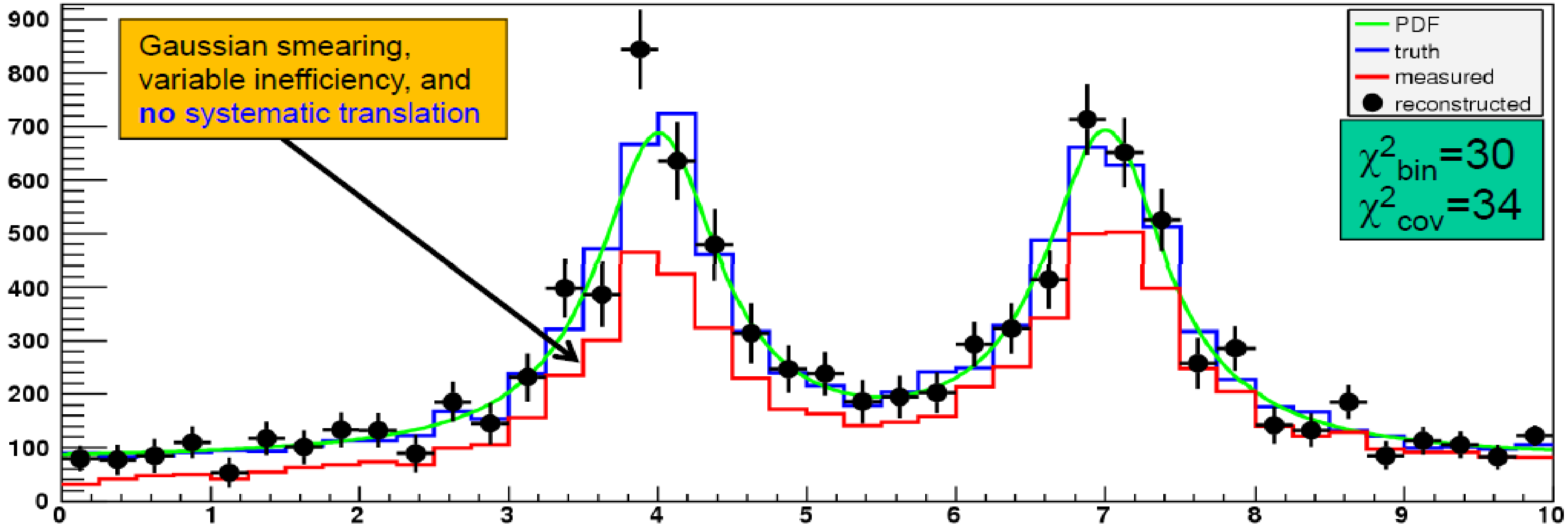
RooUnfold with TUnfold algorithm (τ=0.004)

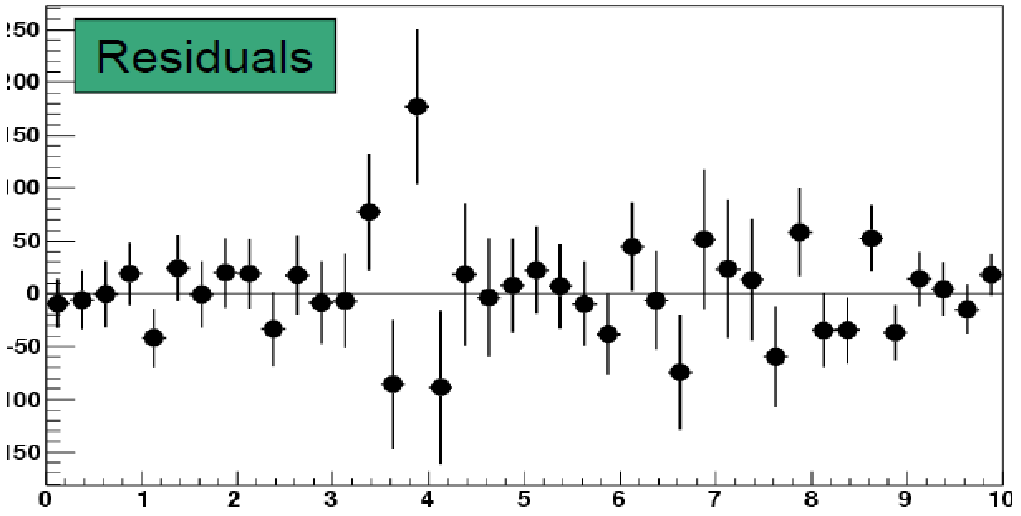


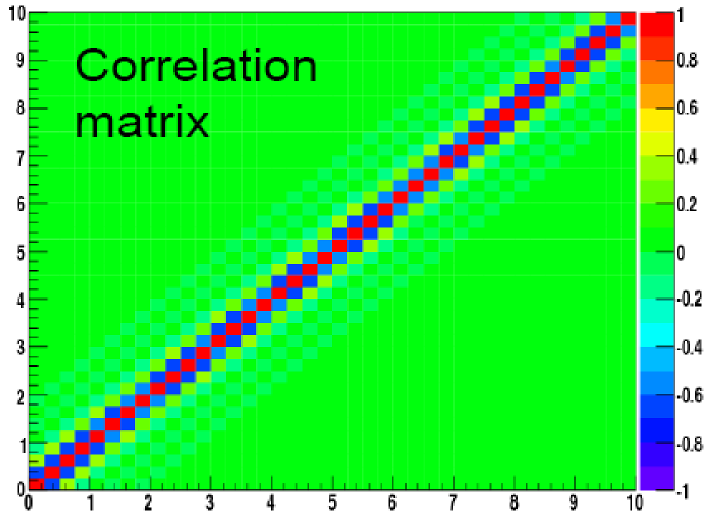




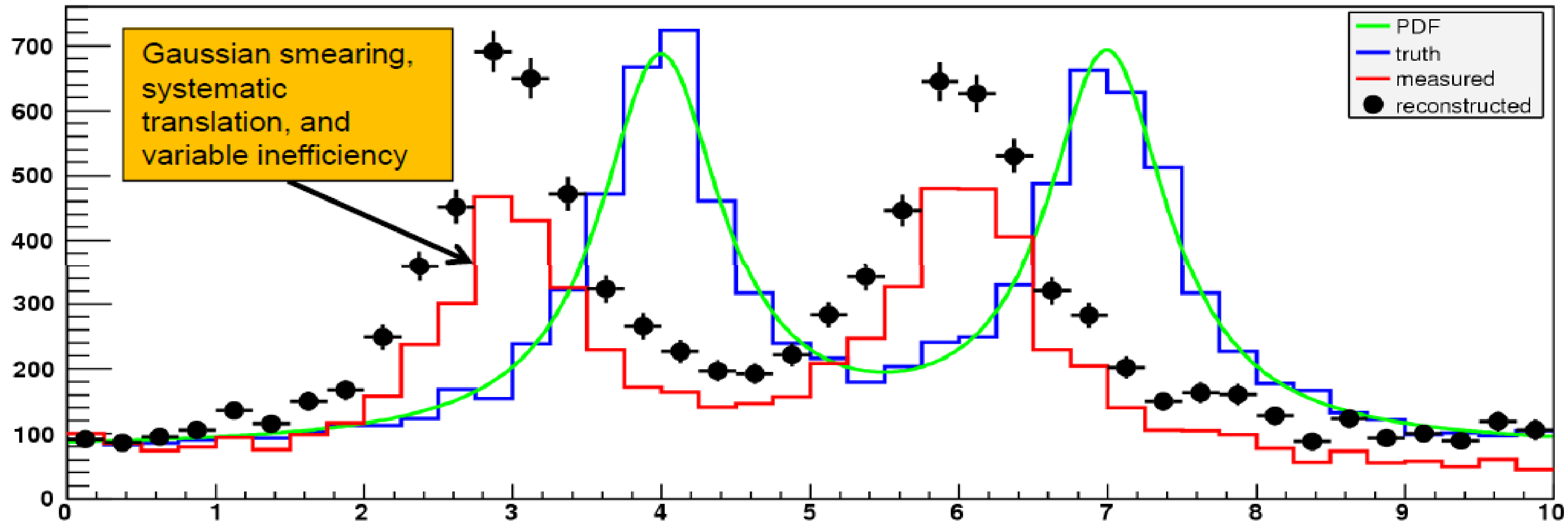
Unregularised matrix inversion

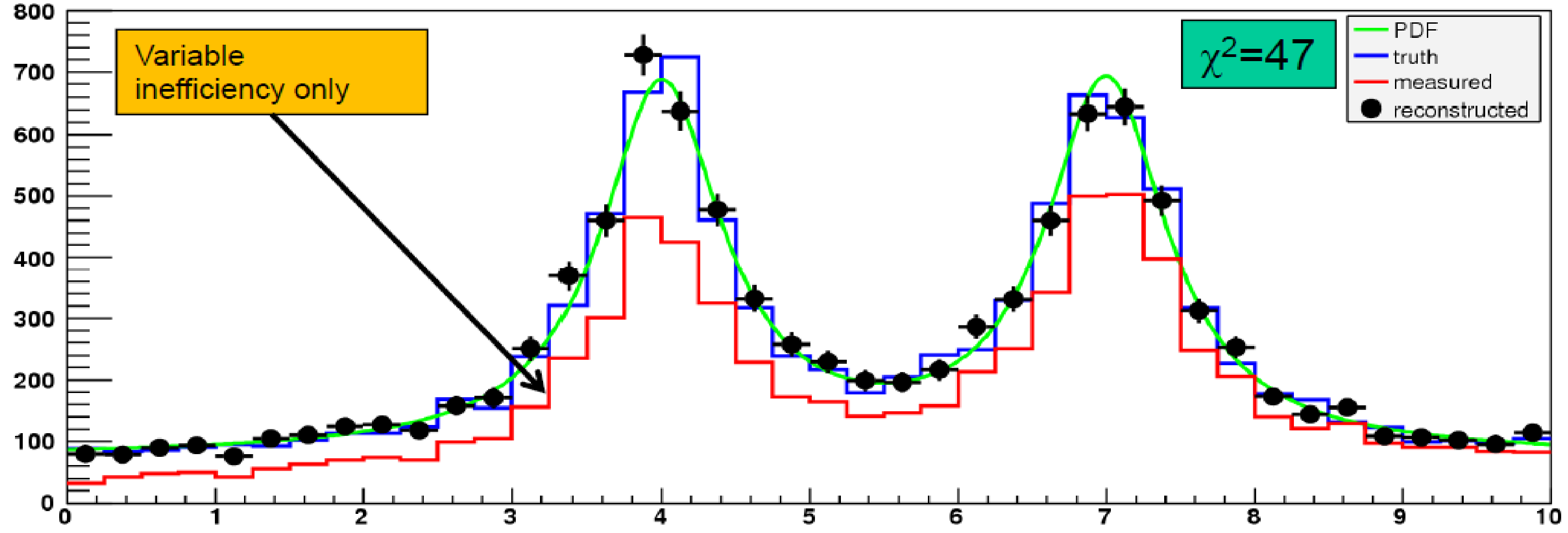






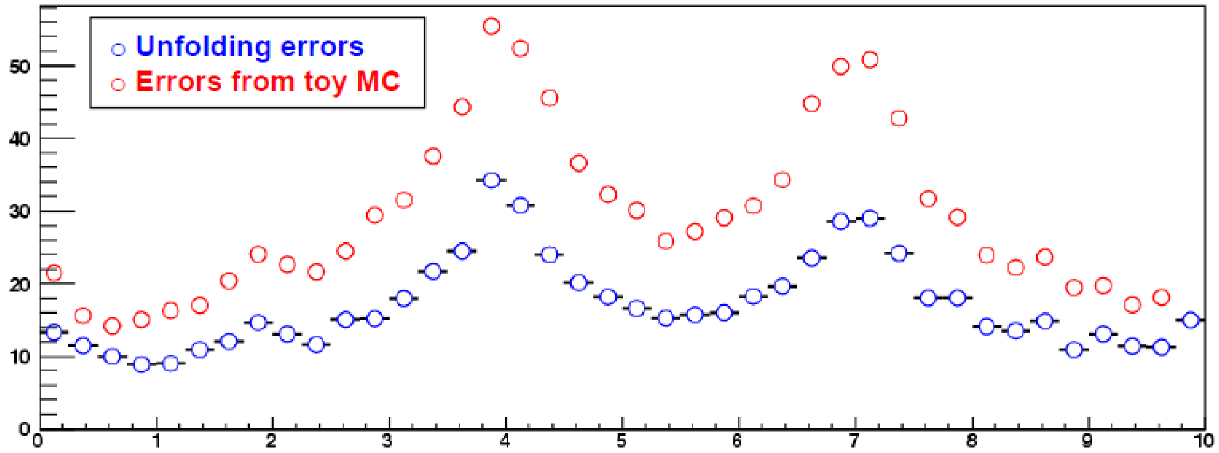
Simple correction factors





Unfolding errors

- All methods return a full covariance matrix of the errors on the unfolded histogram due to uncertainties on the measured distribution.
  - This is often calculated by propagation of errors
    - but not always possible if there are non-linearities or other problems, eg. the iterations in the Bayes method are not handled in D'Agostini's formalism:



- RooUnfold allows the covariance matrix to be calculated from toy MC instead
  - provides a cross-check of the error propagation or replace it if there are problems

Bin-to-bin correlations

- Regularisation introduces inevitable correlations between bins in the unfolded distribution
  - To calculate a correct χ^2, one has to invert the covariance matrix:
    $\chi^2 = (x_m - x_t)^T \mathbf{V}^{-1} (x_m - x_t)$
- However, in many cases, the covariance matrix is poorly conditioned, which makes calculating the inverse problematic
  - Inverting a poorly conditioned matrix involves subtracting large, but very similar numbers, leading to significant effects due to the machine precision

- In any case, χ^2 may not be the best figure of merit
  - could improve χ^2 by relaxing regularisation $\rightarrow$ larger errors, but also larger residuals
  - Is there a better figure of merit?

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

Summary

- Unfolding: get measurements independent of the detector response
- Alternative: publish folding matrix with the result
- Many methods exist, only a few have been compared in this talk
- Big unfolding families investigated in this talk:
  - Matrix inversion +Tikhonov regularisation (parameter τ)
  - Iterative methods + truncation after N_{iter} steps
- Main question: how to choose the regularisation strength.
- Danger to obtain biased results if regularisation is too strong

References

- Bayesian:
  - Nucl.Instrum.Meth. A362 (1995) 487-498
  - arXiv:1010.0632
- TSVDUnfold
  - Nucl.Instrum.Meth.A372 (1996) 469-481
- TUnfold
  - JINST 7 (2012) T10003 [arXiv:1205.6201]

Deconvolution

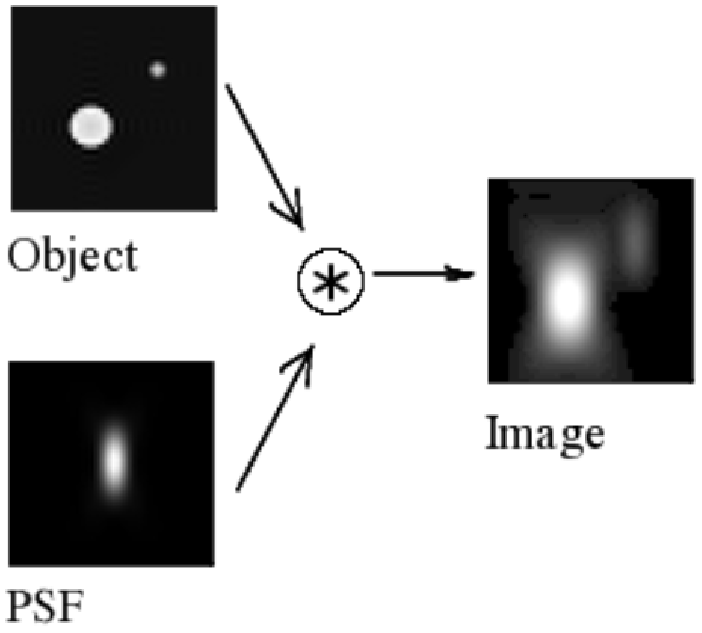
Finite resolution of the detector smears the quantities we're interested in.

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

To Unfold or Not?

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 Make Sense

1. Results from experiment A and B with different response function are to be compared

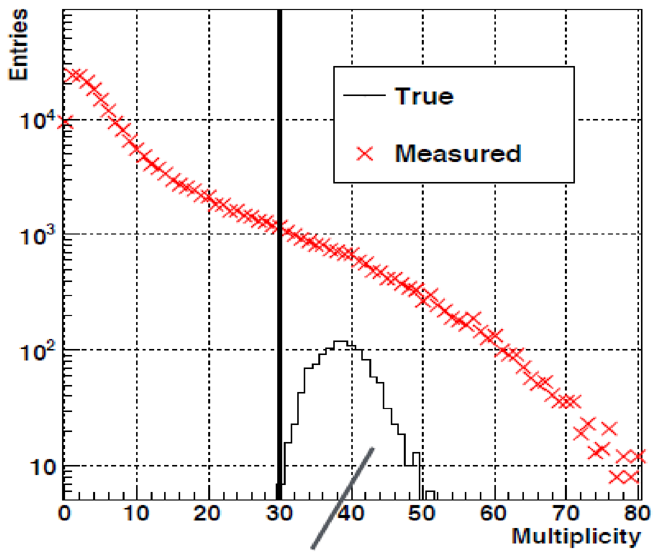
2. It is too complicated to publish the response function of the detector along with the data
   - Detector response might be very complex, e.g., time dependent
   - Sometimes computer code reflecting the response would have to be published
   - Danger that future users don't use the filter correctly

When Unfolding Make Sense

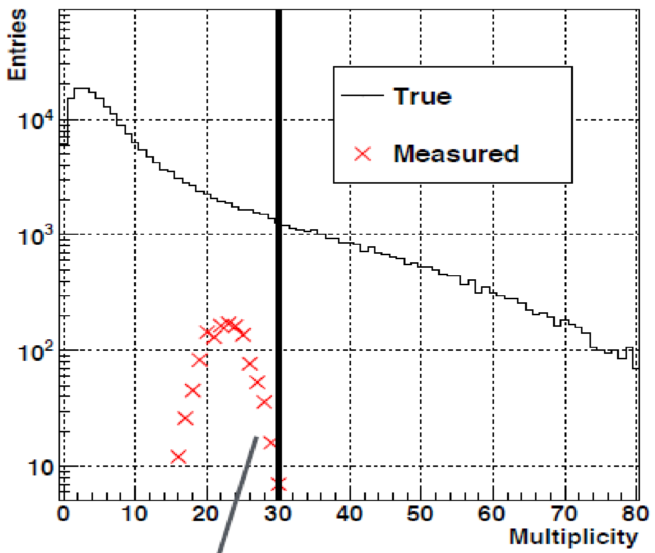
- Multiplicity distributions $P(N_{ch})$
  - Measured multiplicity differs from true charged particle multiplicity due to detector effects (efficiency, fake hits, …)
- p_T spectra, e.g., π^0 spectrum measured with a calorimeter
  - finite energy resolution and shower overlaps in a calorimeter affect 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 continues 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*:

$$R(x_m|x_t) = \underbrace{r(x_m|x_t)}_{\text{"smearing"}} \times \underbrace{\varepsilon(x_t)}_{\text{"efficiency"}}$$

probability (density) to observe x_m given x_t

By construction, one has

$$\int_{\Omega_m} r(x_m|x_t)\,\mathrm{d}x_m = 1$$

Response Matrix (II)

Further definitions:

m_{tot} : number of true events

n_{tot} : number of measured events

b_{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*:

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

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

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

Response Matrix (III)

Further definitions:

$$\nu_i = \mu_{\text{tot}} \int_{\text{bin } i} \mathrm{d}x_m \sum_{j=1}^{M} \int_{\text{bin } j} \mathrm{d}x_t \; r(x_m|x_t)\varepsilon(x_t)f_t(x_t)$$

$$= \sum_{j=1}^{M} \int_{\text{bin } i} dx_m \int_{\text{bin } j} \mathrm{d}x_t \; \frac{r(x_m|x_t)\varepsilon(x_t)f_t(x_t)}{\mu_j/\mu_{\text{tot}}} \mu_j$$

This may be written as

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

with the components of the response matrix

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

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 $f_t(x_t) \approx$ const. within a bin and drops from the ratio:

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

Unfolding by Inverting Responce Matrix (I)

We have

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

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

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

This solution minimizes

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

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

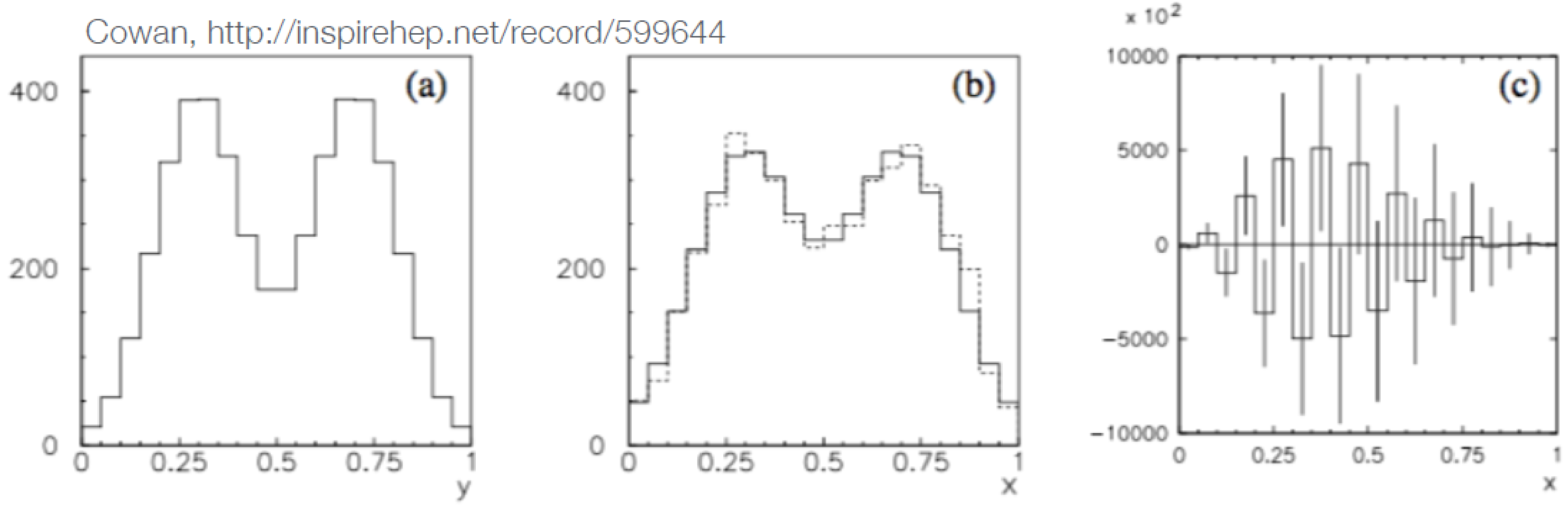
$$U = R^{-1}V(R^{-1})^{\mathsf{T}}$$

Unfolding by Inverting Responce Matrix (II)

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

This sounds good … let's try it.

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



true distribution $\vec{\mu}$

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

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

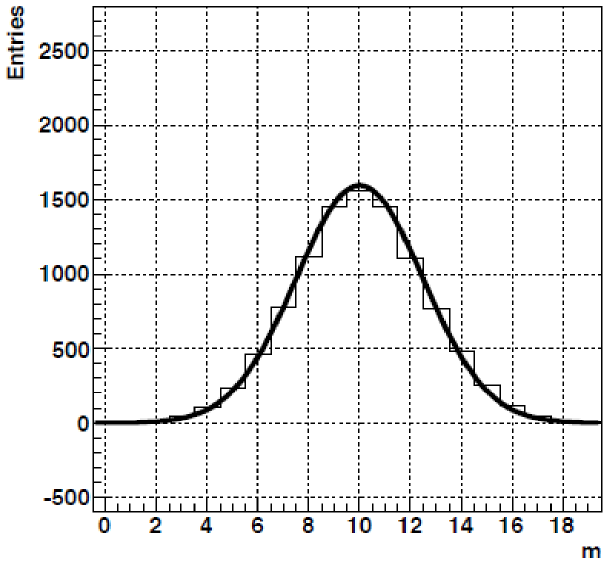
estimate $\hat{\vec{\mu}} = R^{-1}\vec{n}$

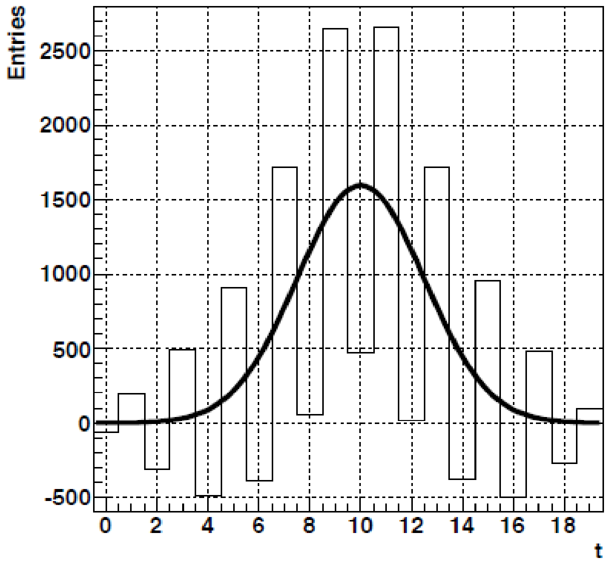
This looks like a disaster … unfolded distribution very different from the true one

Unfolding by Inverting Responce Matrix (III)

Another example:

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





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
$\rightarrow$ 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):

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

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:

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

Bin-by-Bin Method (II)

Inserting the C_i's one can determine the bias:

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

no bias only if MC = nature

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

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

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:

$$\hat{\vec{\nu}} = \vec{n}$$

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

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

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

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

The task then is to maximize

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

α depends on $\Delta \ln \vec{\mu}$,
α → ∞ give ML solution

smoothness function

Tikhonov Regularization

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

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

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 τ in the paper