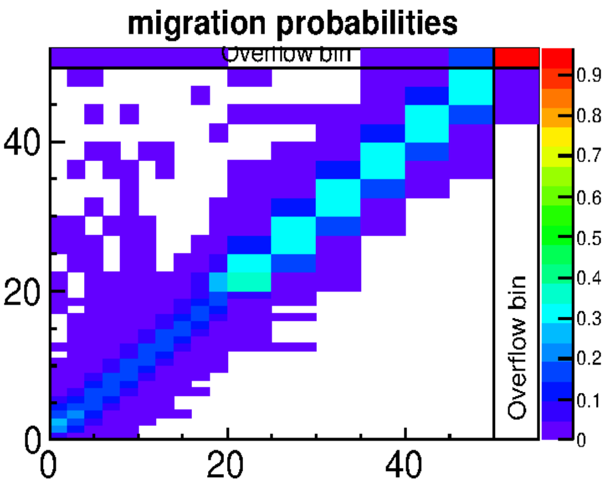
Unfolding methods in HEP

XII Quark Confinement and the Hadron Spectrum

from 29 August 2016 to 3 September 2016

Europe/Athens timezone



CONF12
Thessaloniki, Greece

Stefan Schmitt, DESY

Outline

- Introduction on unfolding
- Example unfolding problem
- Unfolding methods
- Comparison

Introduction

- 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 → not covered in this talk

Unfolding of binned measurements

- This talk: unfolding of binned (discrete) distributions, where bin-to-bin migrations are described by a matrix equation

$$\mu_i = \sum A_{ij} x_j + b_i$$

μ_i : expected measurement in bin i given the truth x

A_{ij} : probability of truth bin j to reconstruct in bin i

x_j : truth in bin j

b_i : background in bin i

$$A_{ij} = \frac{N_{ij}^{\text{MCreco,MCtruth}}}{N_j^{\text{MCtruth}}} \text{ is calculated from MC}$$

- Statistical fluctuations: the observations y_i are drawn from a Poisson distribution

$$P(y_i;\mu_i) = \frac{e^{-\mu_i}\mu_i^{y_i}}{y_i!}$$

- Large sample limit: Gaussian distributions
- Correlated bins: multivariate Gaussians

Unfolding of binned measurements

- This talk: unfolding of binned (discrete) distributions, where bin-to-bin migrations are described by a matrix equation

- Statistical fluctuations: the observations y_i are drawn from a Poisson distribution

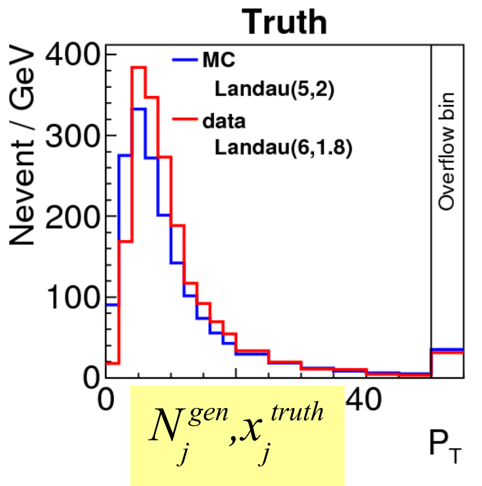
(truth+background) × detector × stat.fluctuations → measurement

Result: estimator of truth ←unfolding algorithm ← measurement

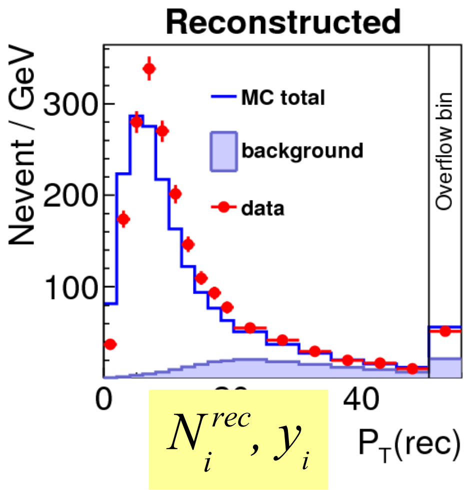
Example unfolding problem

- Toy example to illustrate basic properties of unfolding algorithms
- Decay of a heavy particle into two light particles
- Light particles smeared by spatial and energy resolution
- Trigger threshold causes reconstruction inefficiency
- Background important at high P_T
- Variable bin size, overflow bin
- Goal: reconstruct P_T distribution

- Two samples of toy events
  - "data" P_T distribution following Landau(6,1.8)
  - "MC" P_T distribution following Landau(5,2)
- Background mainly at high P_T



N_j^{gen}, x_j^{truth}



N_i^{rec}, y_i

Example unfolding problem

- Toy example to illustrate basic properties of unfolding algorithms
- Decay of a heavy particle into two light particle
- Light particles smeared by spatial and energy resolution
- Trigger threshold causes reconstruction inefficiency
- Background important at high P_T
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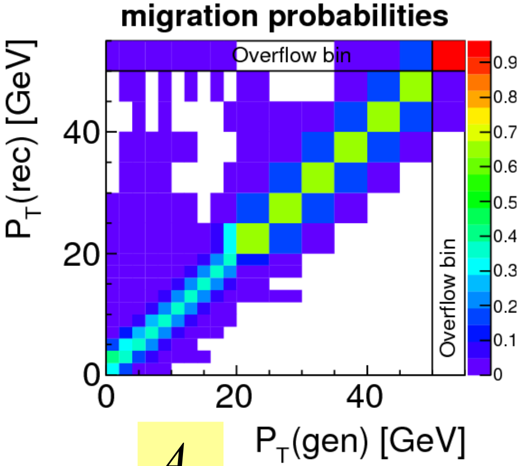
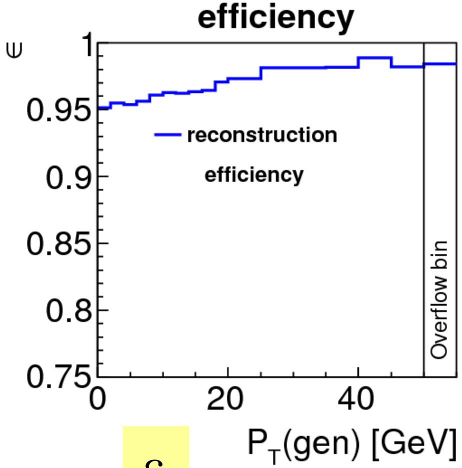
- Significant migrations at low P_T
- Change of bin size leads to change in bin purity
- Efficiency >95%, not important for this study


migration probabilities

A_{ij}


efficiency

ε_j

How to test unfolding results?

- Tests with real data
  - Look at (global) correlation coefficients
  - Trivial test: fold back unfolding result and compare to data

unfolding result: x_j^{unf}

fold back and compare to data:

$$y_i^{\mathrm{data}} \simeq \sum_j A_{ij} x_j^{\mathrm{unf}} + b_i$$

- Test with Monte Carlo
  - Trivial test: response matrix and MC using the same truth
  - Non-trivial test: use different truth for response matrix and

unfold alternative MC (here: "data"): x_j^{unf}

compare to alternative MC truth:

$$x_j^{\mathrm{truth}} \simeq x_j^{\mathrm{unf}}$$

Quantitative comparison: χ^2

This talk:

Look at average global correlation coefficients
Compare folded result with data
Compare result to “data” truth
Extract “data” truth parameters using a fit

… plus many other things not discussed here, e.g. eigenvalue analysis

Unfolding methods investigated in this talk

- Bin-by-bin correction factors
- Matrix inversion
- Template fit
- Tikhonov regularisation: [Tikhonov 1963]

  implementation: e.g. RUN [Blobel 1984], TUnfold [S.S. 2012]
- Iterative method: [Shepp/Vardi 1982, Mülthei/Schorr 1986, D'Agostini 1995]
- IDS method: [Malaescu 2011]

Bin-by-bin correction factors

- Very simple method:

$$x_i = (y_i - b_i)\frac{N_i^{\mathrm{gen}}}{N_i^{\mathrm{rec}}}$$

Correction factor

y_i : observed in bin i

b_i : expected backround in bin i

N_i^{gen} : MC truth in bin i

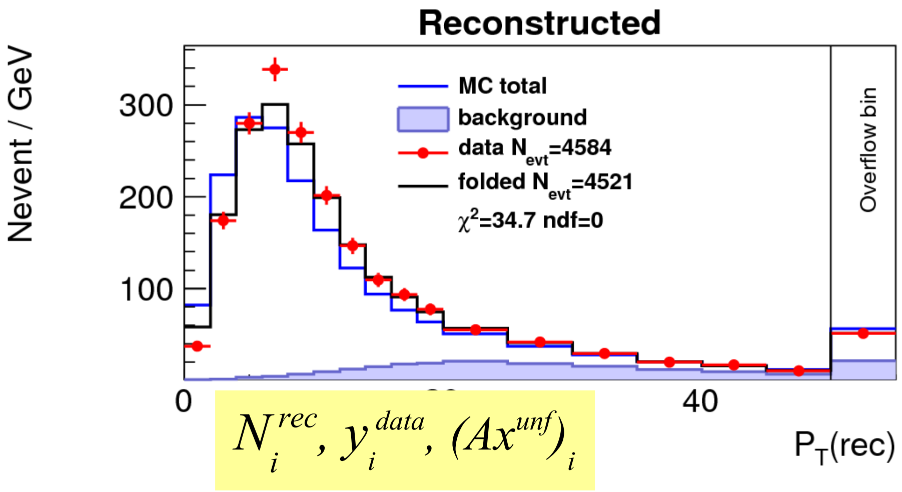
$N_i^{\mathrm{rec}} = \sum_j A_{ij} N_i^{\mathrm{gen}}$: MC reconstructed in bin i

Results “looks nice”

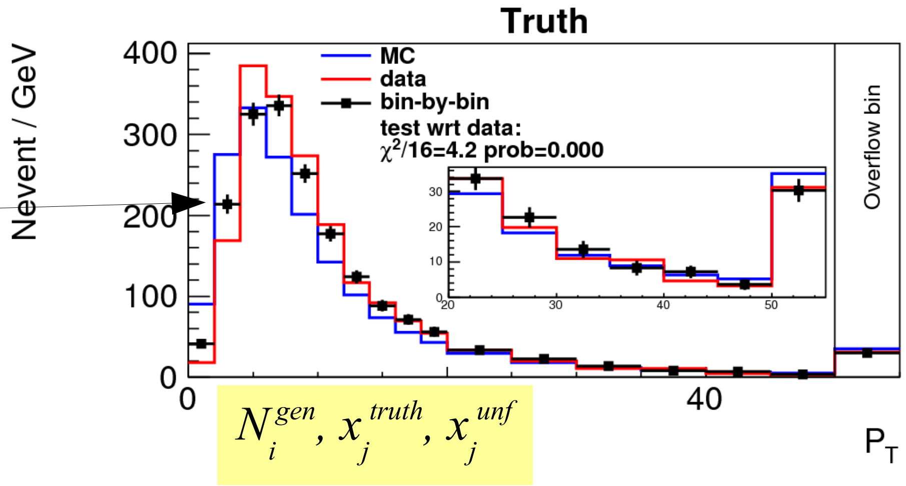
No statistical bin-to-bin correlations

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}

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- Bin-by-bin correction factors
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Matrix inversion

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

  → invert it

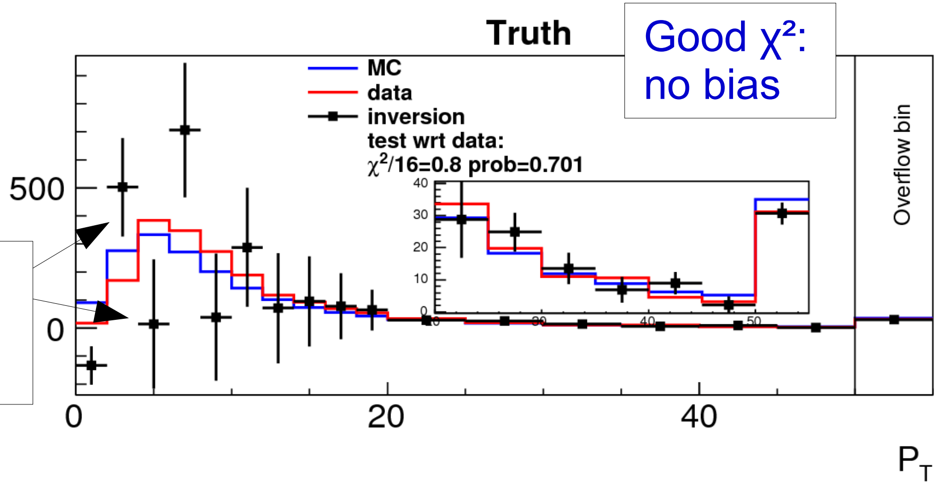
folding equation: $y = Ax + b$

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

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

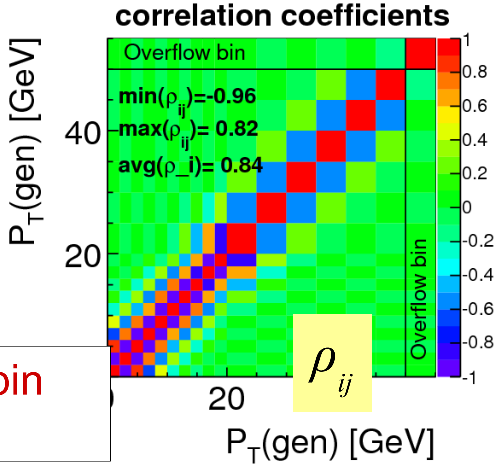
correlation coefficients: $\rho_{ij} = \dfrac{(V_{xx})_{ij}}{\sqrt{(V_{xx})_{ii} (V_{xx})_{jj}}}$

y : measurements
V_{yy} : covariance matrix of measurements
b : background
A : matrix of migrations



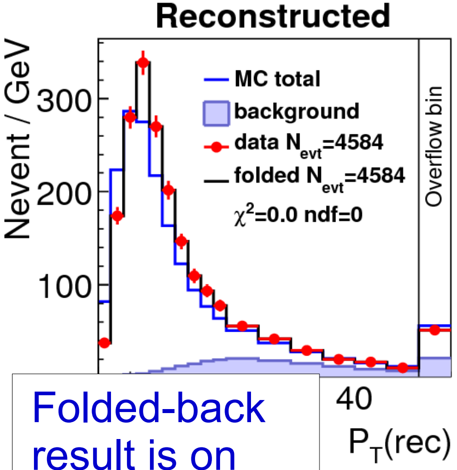
Good χ²: no bias

Unfolded result exhibits bin-to-bin oscillations



ρ_{ij}

Large bin-to-bin correlations



Folded-back result is on the data

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

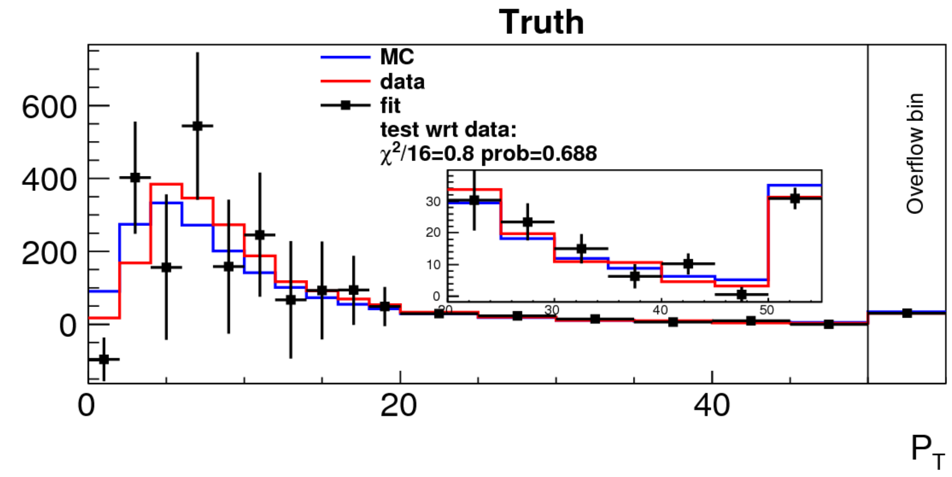
b : background

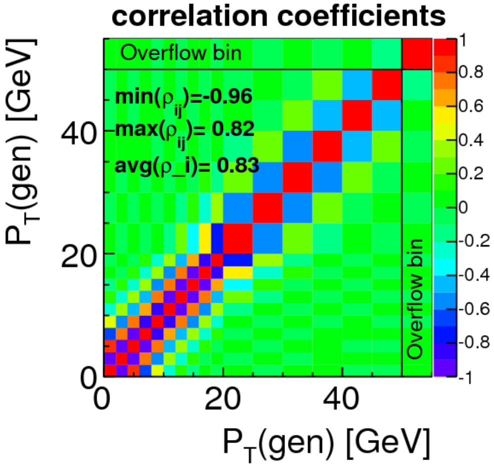
A : matrix of migrations

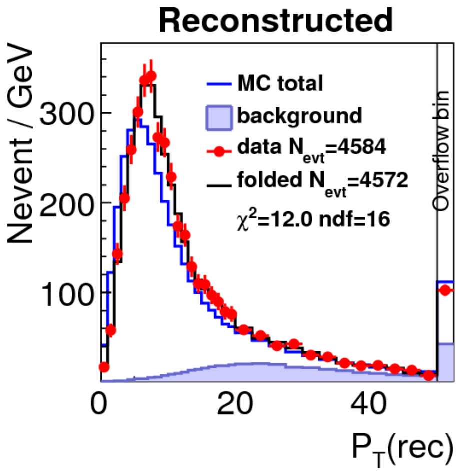
A_{ij} : MC template for truth bin j

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

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







Template fit

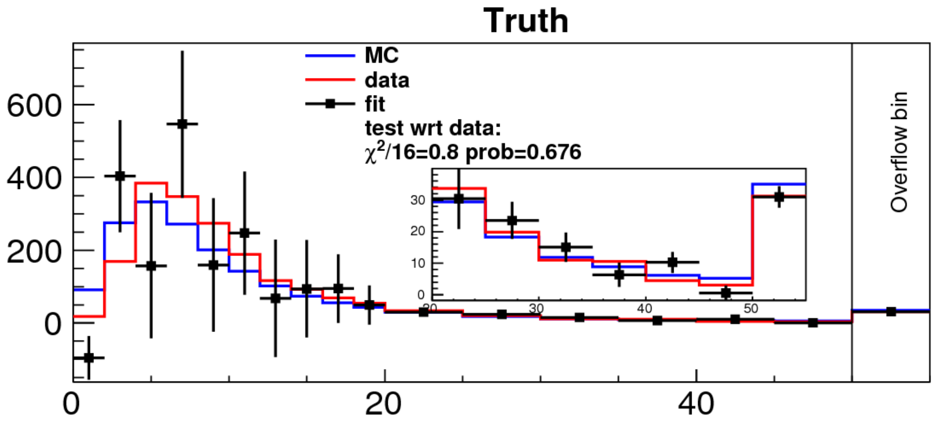
- Choose larger number of reconstructed bins than truth bins → least-square fit
- Idea: use more information → obtain better result

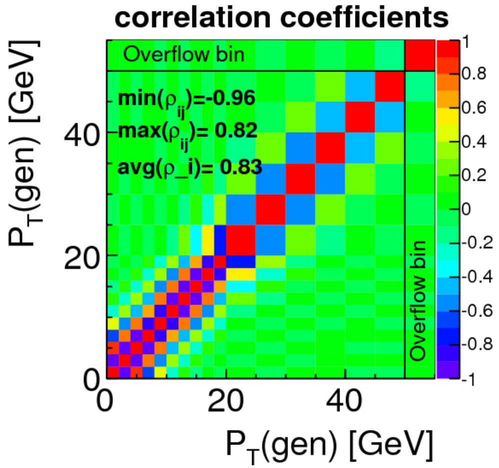
→ Result does not improve much over matrix inversion in this example

New problem: normalisation is not preserved [$N_{data}=4584$, $N_{fold}=4572$]

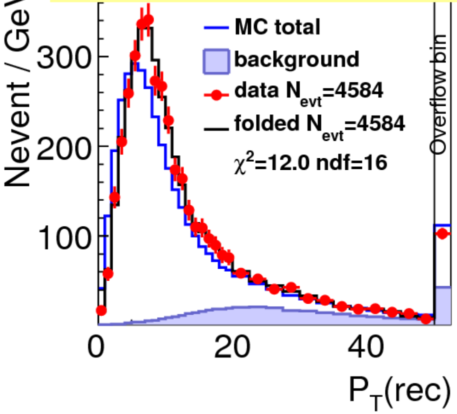
Well-known problem with least-square fits to Poisson-distributed data if sqrt(N) uncertainties are used

Can be improved by adding a constraint to the fit





2x more (finer) bins for reconstructed quantities



Template fit with area constaint

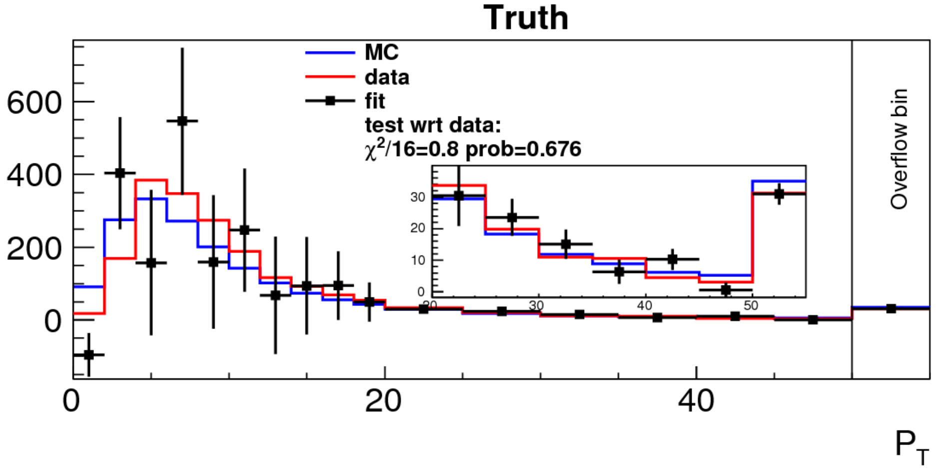
- Template with with constraint on the total number of events
- Basic idea: preserve normalisation for the folded-back result by adding the constraint

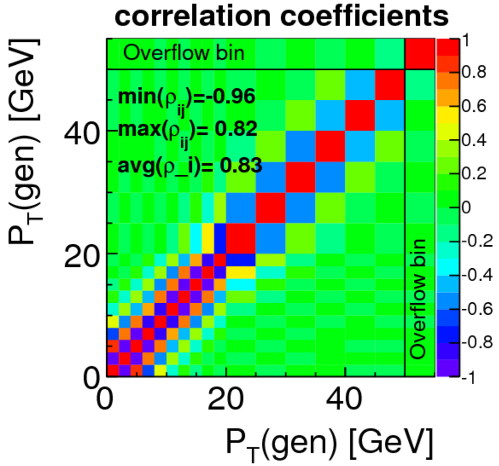
$$\sum (y_i - b_i) = \sum_{i,j} A_{ij} x_j$$

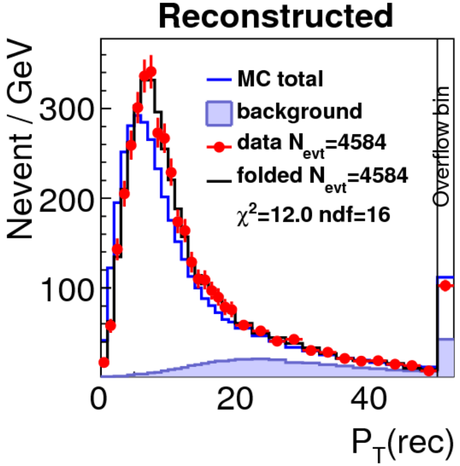
- Technical implementation: see TUnfold documentation

→ 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

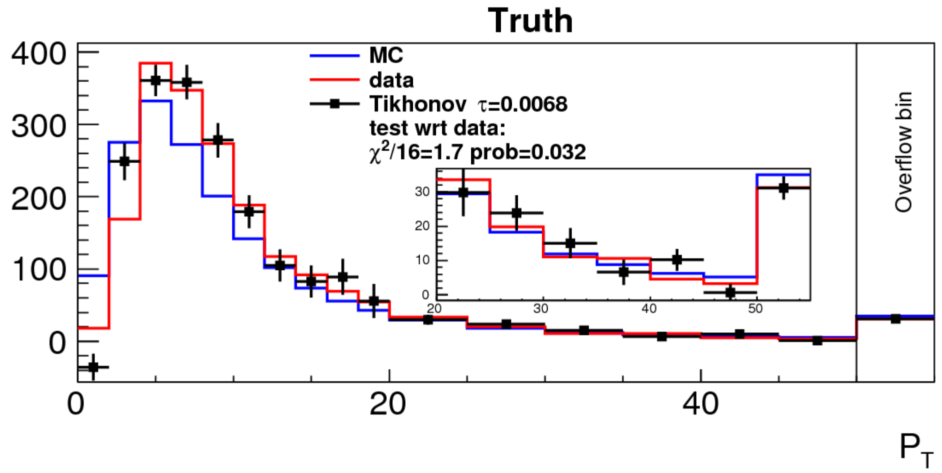
$$\tau \ll 1/\sigma$$

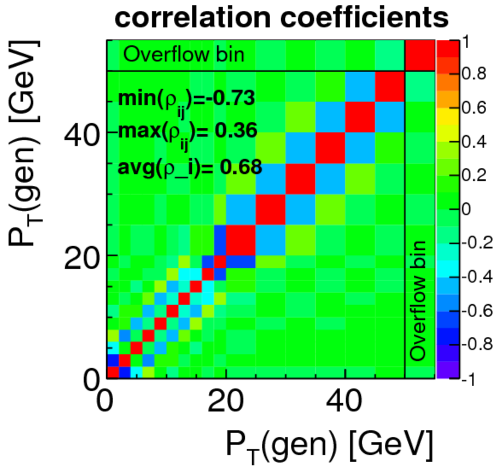
where σ~uncertainty after unfolding

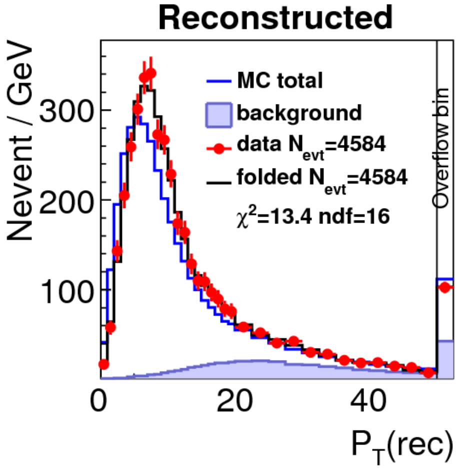
Tikhonov regularisation (e.g. TUnfold)

- 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







Choice of the regularisation parameter τ

- Eigenvalue analysis (SVD)

  → not discussed in this talk

- Scan of parameter τ
  - L-curve scan
  - Scan of global correlation coefficients

- Other data driven methods (e.g. compare stat and syst errors, define convergence criteria) → not discussed in this talk

L-curve scan

- Algorithm is often used in medical image processing

for each τ repeat the unfolding:

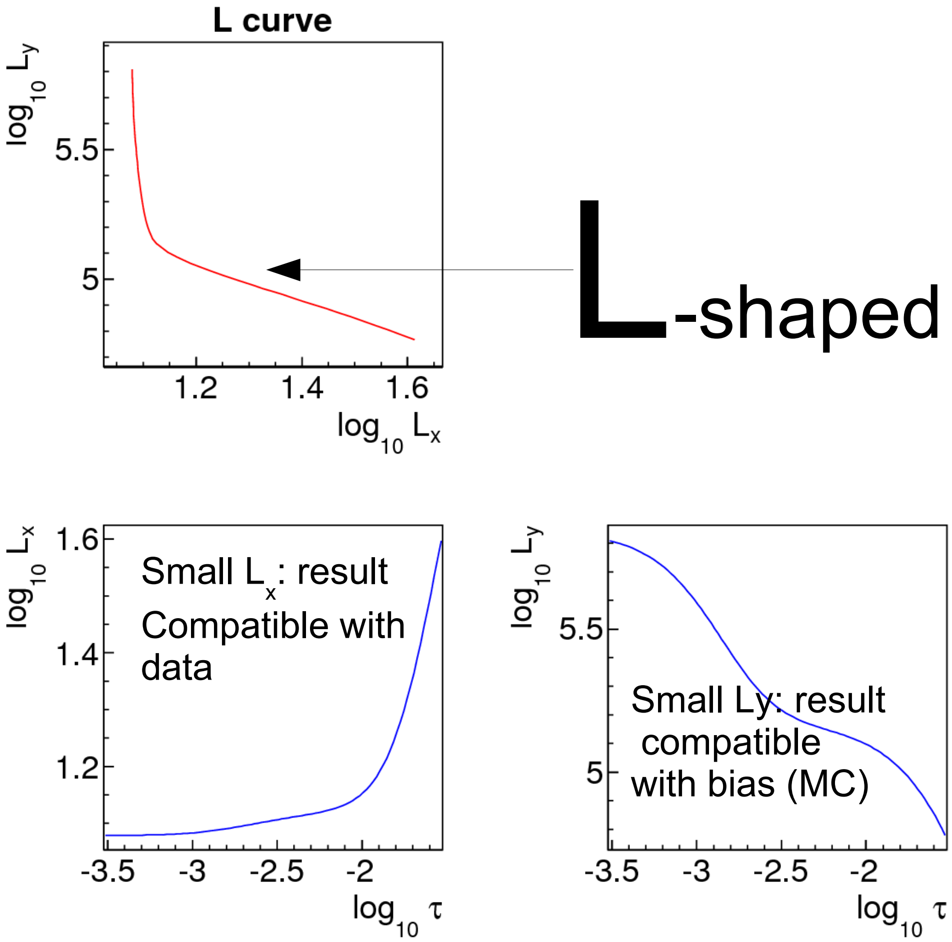
$$\chi^2=(y-b-Ax)^T V_{yy}^{-1}(y-b-Ax)$$
$$+\tau^2(L(x-x_B))^T L(x-x_B)$$
$$\equiv L_x+\tau^2 L_y$$

study parametric plot of: $\log L_x$ vs $\log L_y$

- Parametric plot is “L-shaped”

→ kink (largest curvature) defines τ

For a review, see: [P. C. Hansen 2000]



Scan of global correlation coefficients

- Global correlation coefficient (bin i)

$$\rho_i=\sqrt{1-\frac{1}{(V_{xx})_{ii}(V_{xx}^{-1})_{ii}}}$$

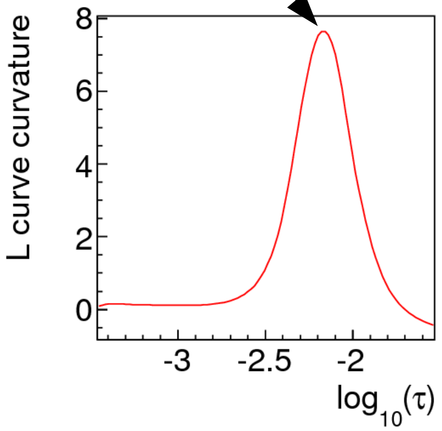
V_{xx} : result's covariance matrix

- Take average of all ρ_i and study dependence on τ → choose point with smallest avg(ρ_i)

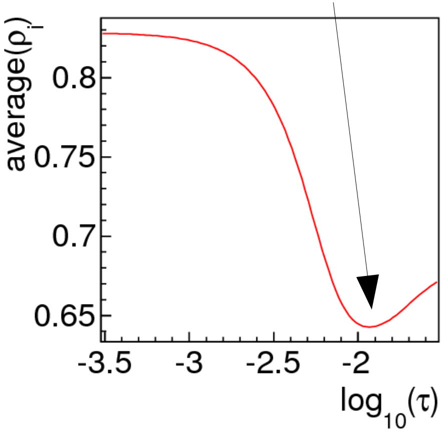
  (idea by V. Blobel/DESY)

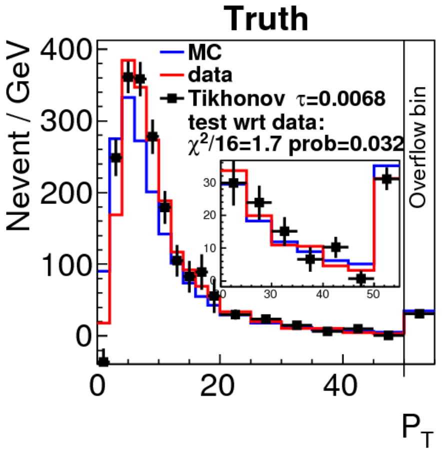
- Comparison to L-curve scan: stronger regulatisation, more bias, smaller uncertainties & correlations

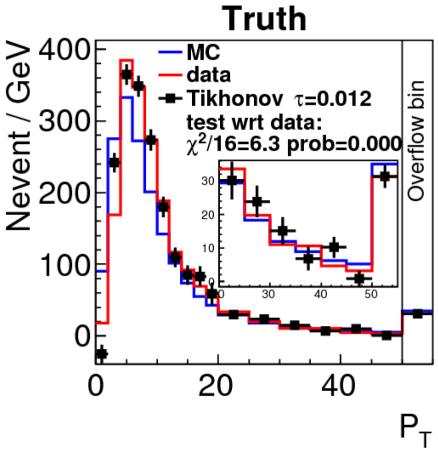
Maximum L-curve curvature



Minimum average global correlation







Unfolding methods investigated in this talk

- Bin-by-bin correction factors
- Matrix inversion
- Template fit
- Tikhonov regularisation: [Tikhonov 1963]
  - implementation: e.g. RUN [Blobel 1984], TUnfold [S.S. 2012]
- Iterative method: [Shepp/Vardi 1982, Mülthei/Schorr 1986, D'Agostini 1995]
- IDS method: [Malaescu 2011]

Iterative method

Ratio data to folded
→ iterate until ~1

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

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

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

$$\text{iterate until } N \text{ is sufficiently large}$$

- 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: $\tau \leftrightarrow$ 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 [used in this talk]
  - Apply statistical fluctuations on the data histogram

    → 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

  → test complete analysis chain

Iterative method: 0th iteration

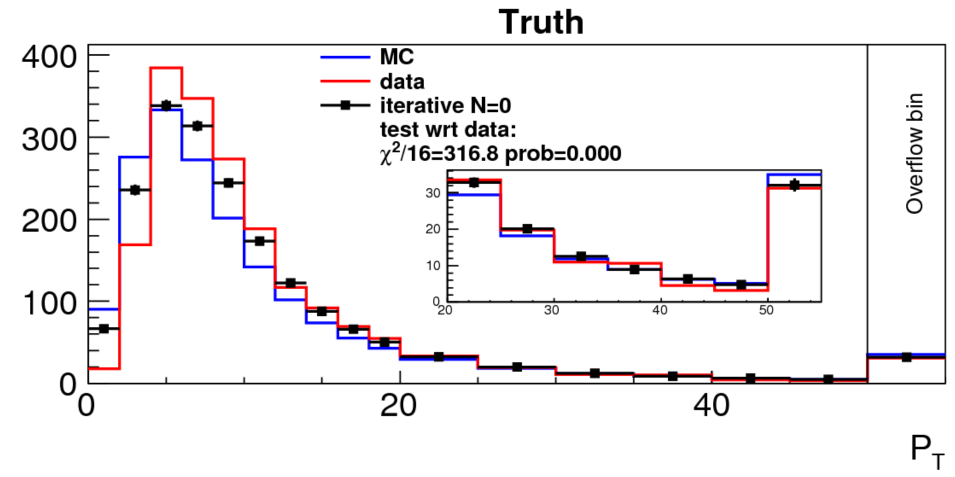
$$x_j^{(N+1)} = x_j^{(N)} \sum_i \frac{A_{ij}}{\epsilon_j} \frac{y_i}{\sum_k A_{ik} x_k^{(N)} + b_i}$$

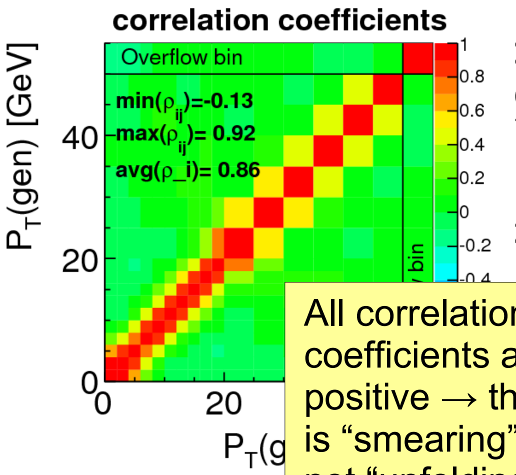
efficiency: $\epsilon_j = \sum_i A_{ij}$

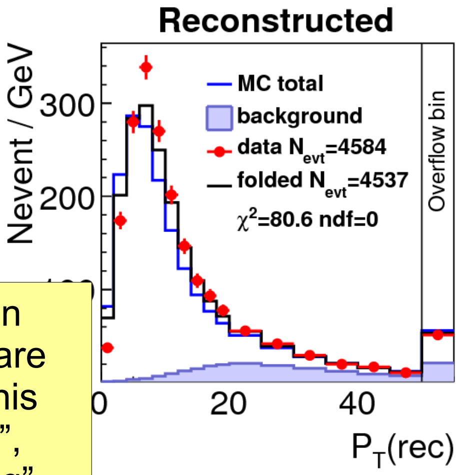
start values $x_j^{(-1)}$ set to MC truth

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

  → the method has to be iterated







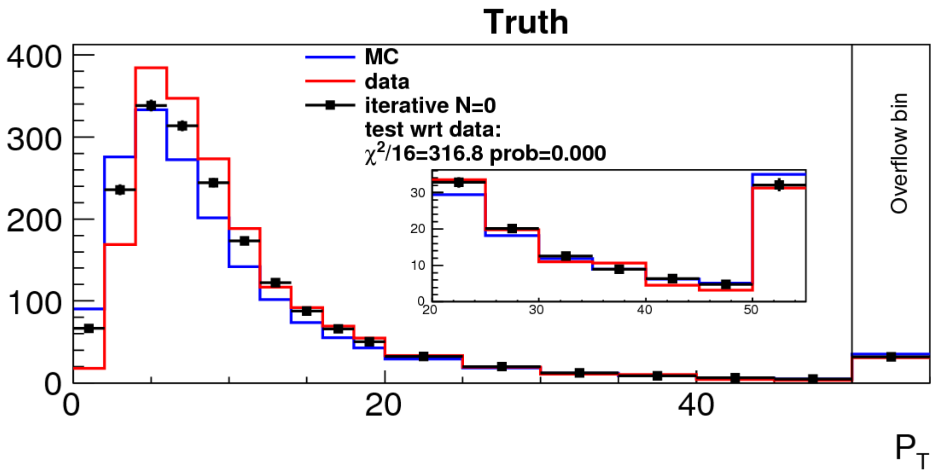
All correlation coefficients are positive → this is "smearing", not "unfolding"

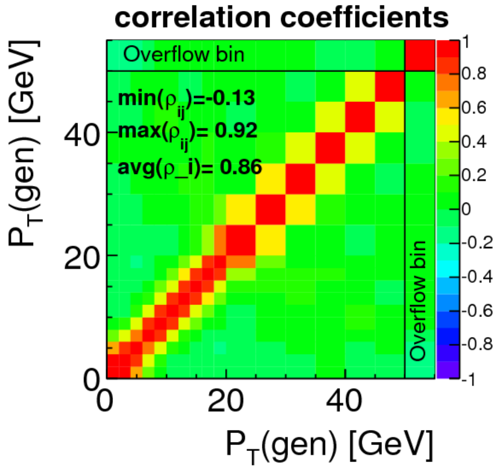
Iterative method: 1st iteration

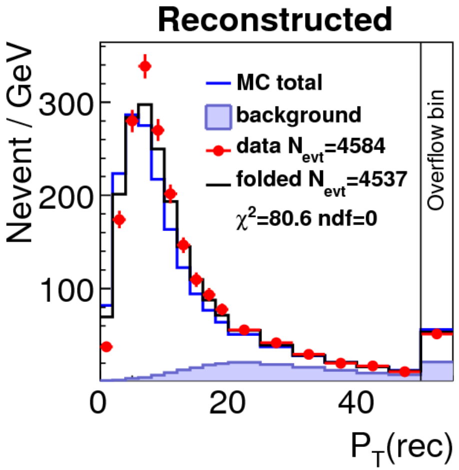
$$x_j^{(N+1)} = x_j^{(N)} \sum_i \frac{A_{ij}}{\epsilon_j} \frac{y_i}{\sum_k A_{ik} x_k^{(N)} + b_i}$$

- 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



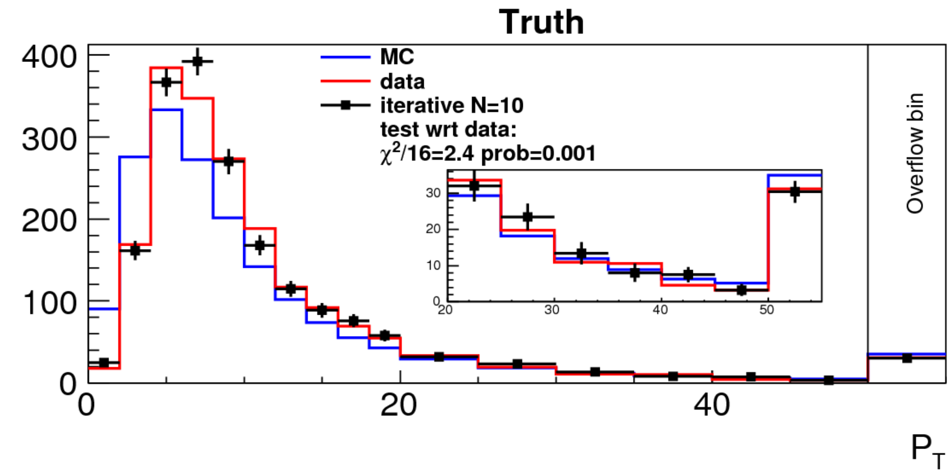


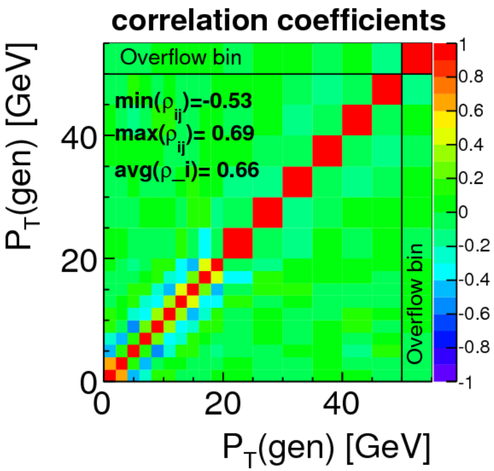


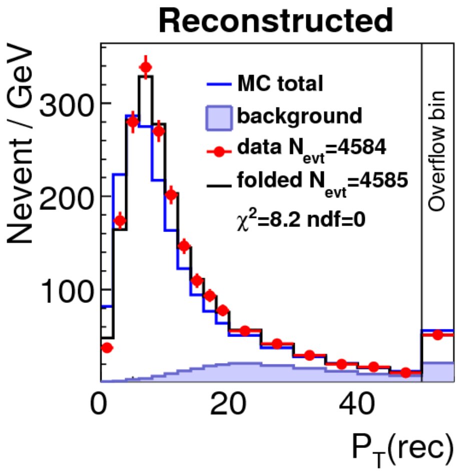
Iterative method: 10th iteration

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

- 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



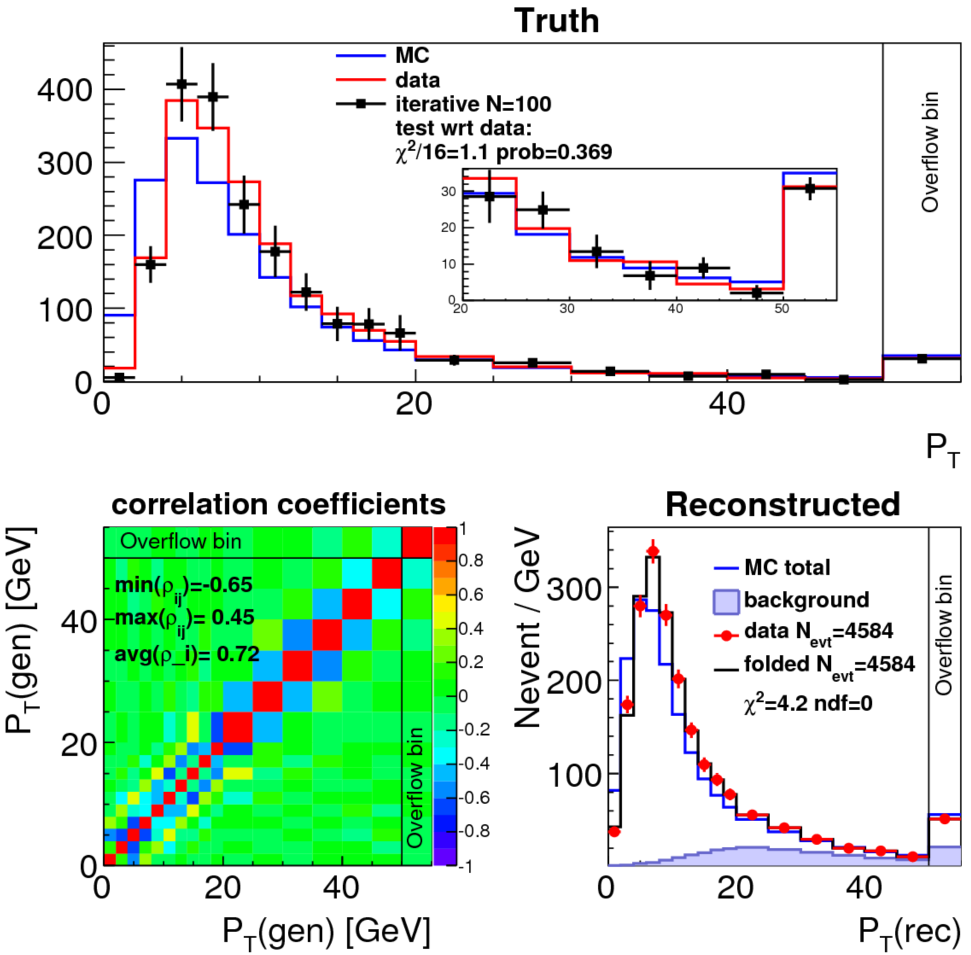




Iterative method: 100th iteration

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

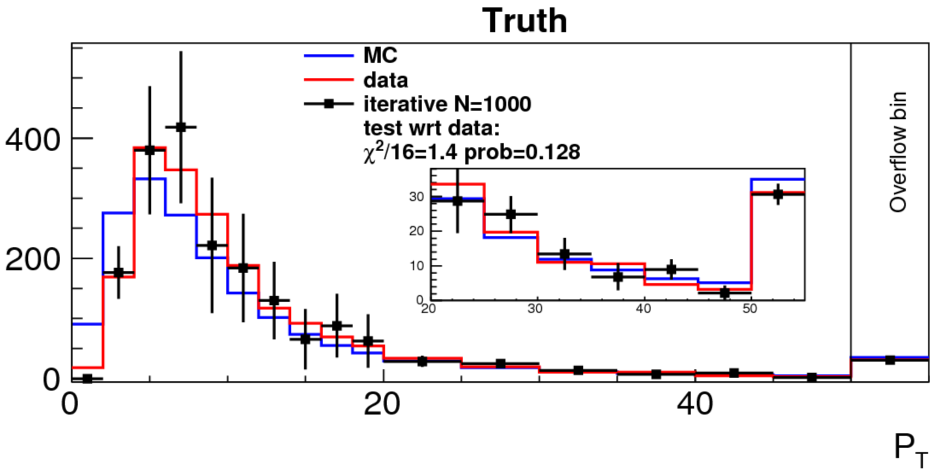
- Convergence rate is expected to grow quadratically with the number of bins [Mülthei/Schorr 1987]
- Look at 100th iteration
  - Similar to Tikhonov with weak regularisation

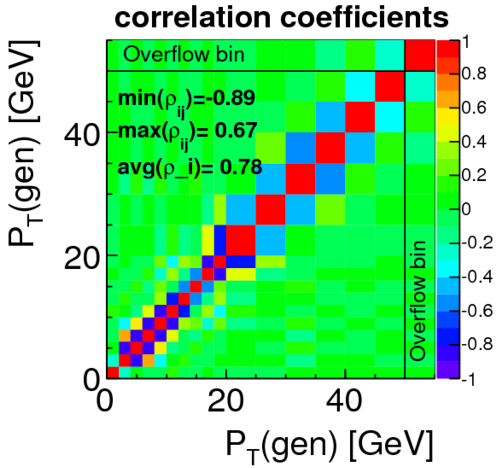


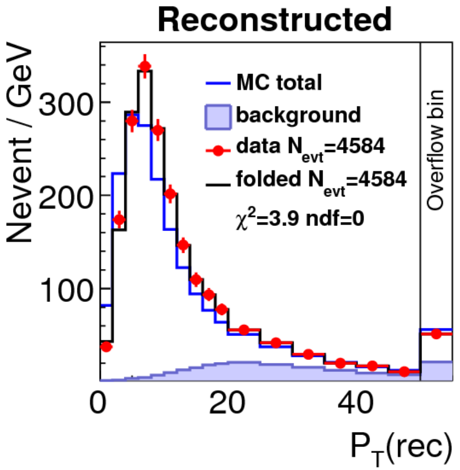
Iterative method: 1000th iteration

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

- 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?







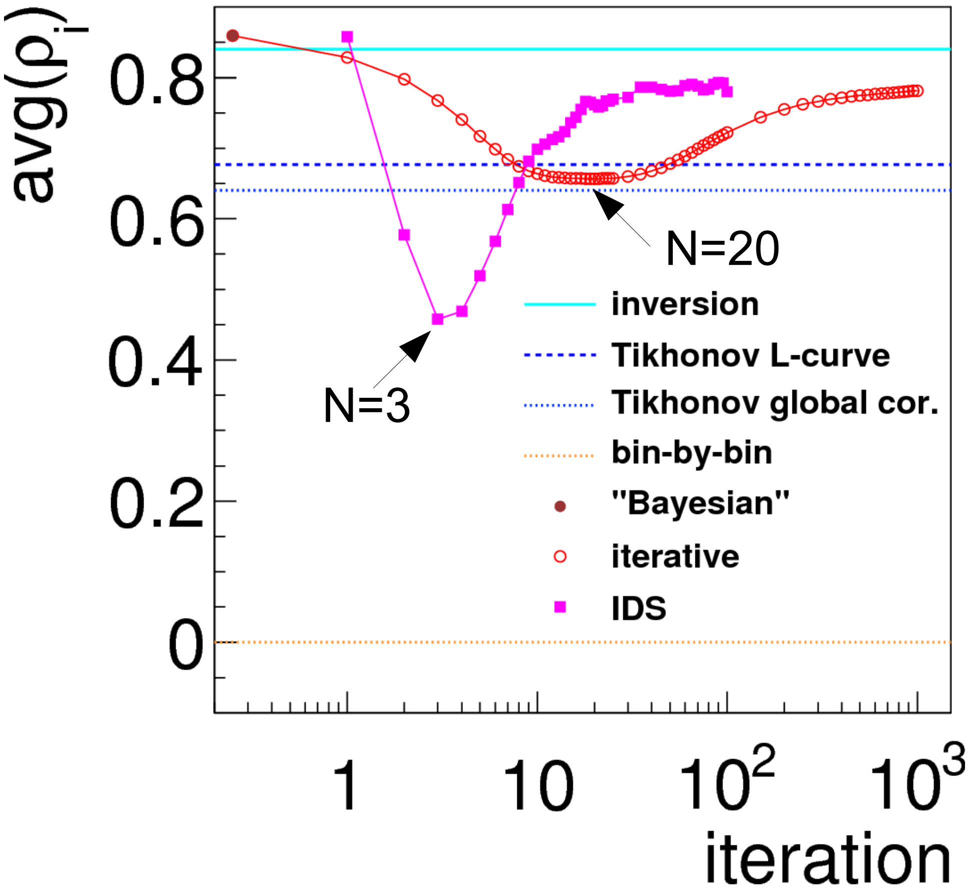
IDS method by B. Malaescu

- IDS: Iterative Dynamically Stabilized unfolding
- Based on iterative improvements of the matrix of (truth,reco) MC events
- Mathematics not discussed here in detail
- Method is using
  - Significance of data vs (iterated) MC in each bin
  - adjustment of the normalisation in each step
  - also includes a bin-by-bin correction-like contribution
- Method converges to the same result as the standard iterative method
- Speed of convergence is expected to be improved
- The bin-by-bin contributions may lead to reduced correlation coefficients

Iterative methods: scan of avg(ρ_i)

- Regularisation strength has to be chosen (τ for Tikhonov↔N_{iter} here)
- Try scan of global correlation coefficients

  [reminder: this yielded strong regularisation for Tikhonov method]
- Iterative minimum [N=20] is similar in amplitude to Tikhonov case
- IDS minimum [N=3] is much lower than other methods → scan of correlations is not expected to give optimal results for this method



Comparison of results and truth

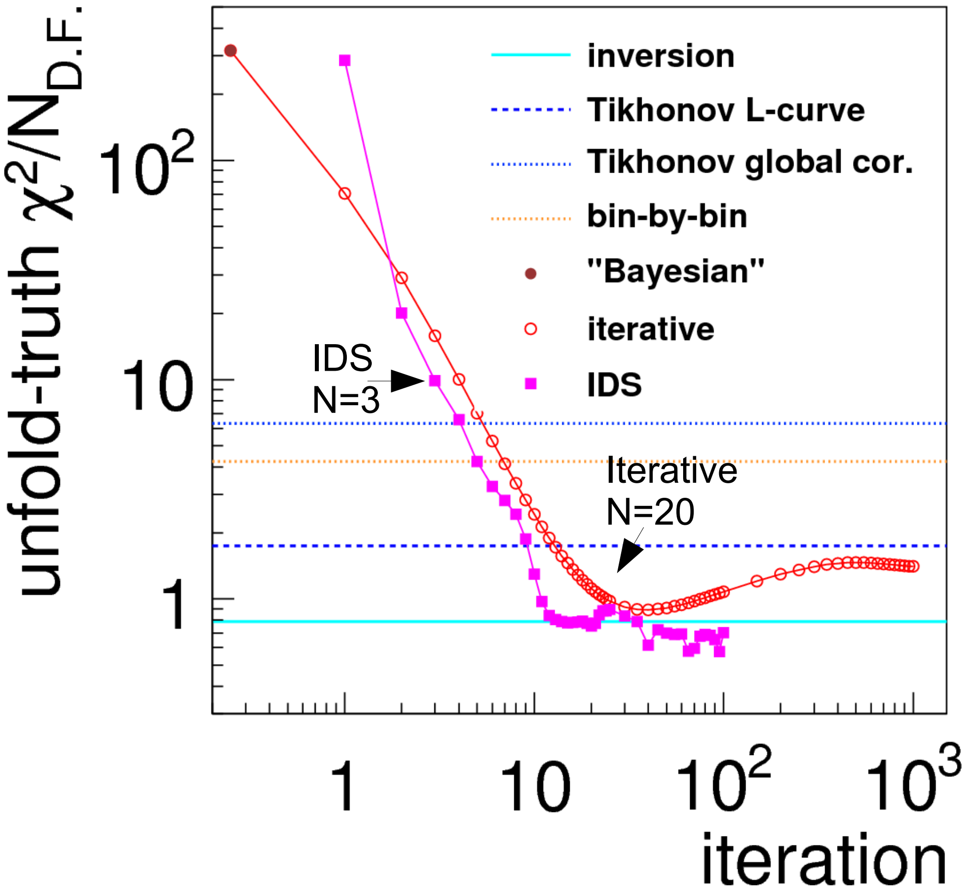
- Comparison (1): χ^2 test data against unfolded results
- Comparison (2): fit [known] parameterisation of data truth

Comparison (1) χ^2 wrt “data” truth

- Test χ^2 of unfolded results against “data” truth
- For real analyses, such tests can be done by unfolding alternative truth models

Method	$X^2 / N_{D.F.}$
Tikhonov L-curve	1.75
Tikhonov min(avg(ρ_i))	6.30
bin-by-bin	4.24
iterative, N=20 min(avg(ρ_i))	1.12
IDS, N=3 min(avg(ρ_i))	9.88
IDS, N=11	0.97

- For the example studied, iterative+min(avg(ρ_i)) performs best



- IDS does not work with the min(avg(ρ_i)) condition, N>10 seems appropriate

Comparison(2) wrt data truth parameters

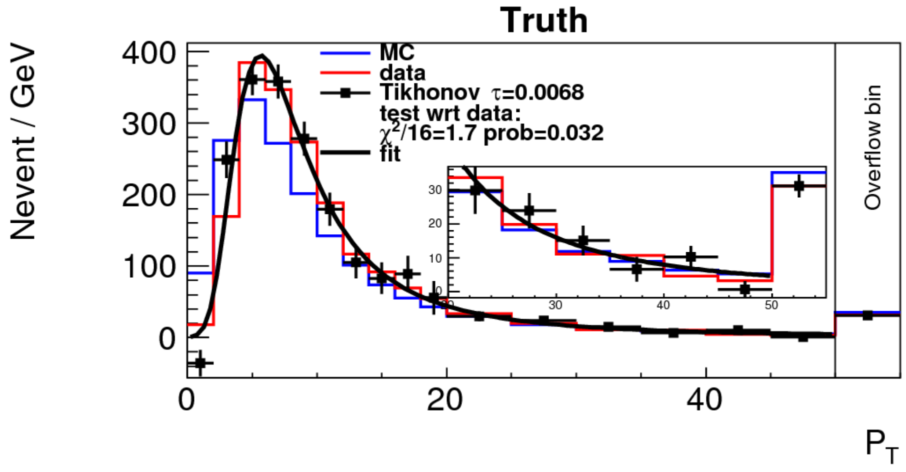
- Fit results by the analytic function use to generate the truth:

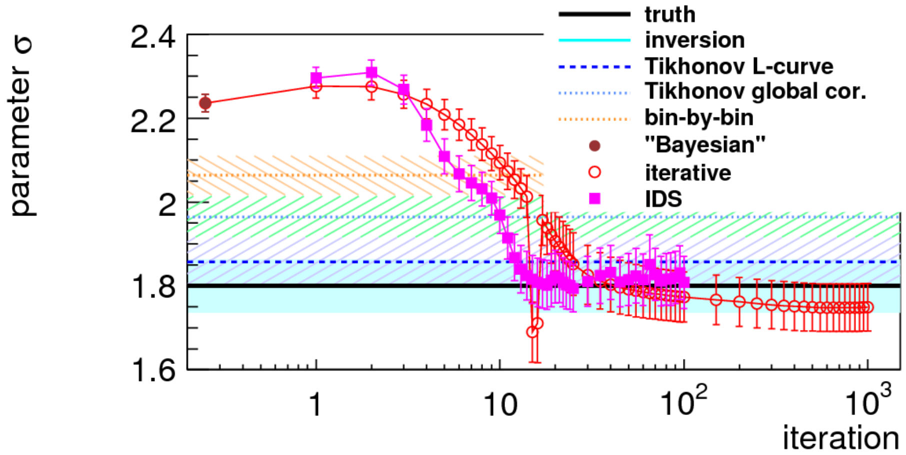
  Landau(μ,σ)

- Only the width σ is shown here (more difficult to fit)

Method	fit of width σ
Tikhonov L-curve	1.858 ± 0.057
Tikhonov min(avg(ρ_i))	1.965 ± 0.049
bin-by-bin	2.064 ± 0.046
iterative, N=20 min(avg(ρ_i))	1.906 ± 0.071
IDS, N=3 min(avg(ρ_i))	2.268 ± 0.034
IDS, N=11	1.915 ± 0.050
truth	1.800

- For this test Tikhonov with L-curve is doing better than the iterative method





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]

Plus many other methods
Please apologize for not listing them

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. Objectives studied in this talk: L-curve and scan of global correlation coefficients
- Tikhonov: L-curve scan is favored. Iterative: correlation scan seems to work
- Danger to obtain biased results if regularisation is too strong