Science & Technology Facilities Council
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RooUnfold
a history, scope, and status

Tim Adye
Rutherford Appleton Laboratory

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RooUnfold overview

- RooUnfold's purpose is to provide a framework for testing and using different binned unfolding methods, as far as possible maintaining a consistent view of each method to the user
  1. Iterative Bayes method was implemented for RooUnfold
     - Based on D'Agostini (1995), with corrected error calculation
     - This method seems to be used by the majority of RooUnfold users
  2. Iterative, Dynamically Stabilized (IDS) unfolding (Malaescu 2011)
     - Recently added to RooUnfold by Chris Meyer
  3. Singular Value Decomposition (SVD) method (Hoecker, Kartvelishvili 1995)
     - RooUnfold interface to enhanced version of TSVDUnfold ROOT class by Kerstin Tackmann et al
  4. Regularised least square fit, implemented in TUnfold (Schmitt 2012)
     - RooUnfold interface to TUnfold class in ROOT
  5. unregularised matrix inversion with singular value removal (TDecompSVD)
  6. using bin-by-bin correction factors, with no inter-bin migration

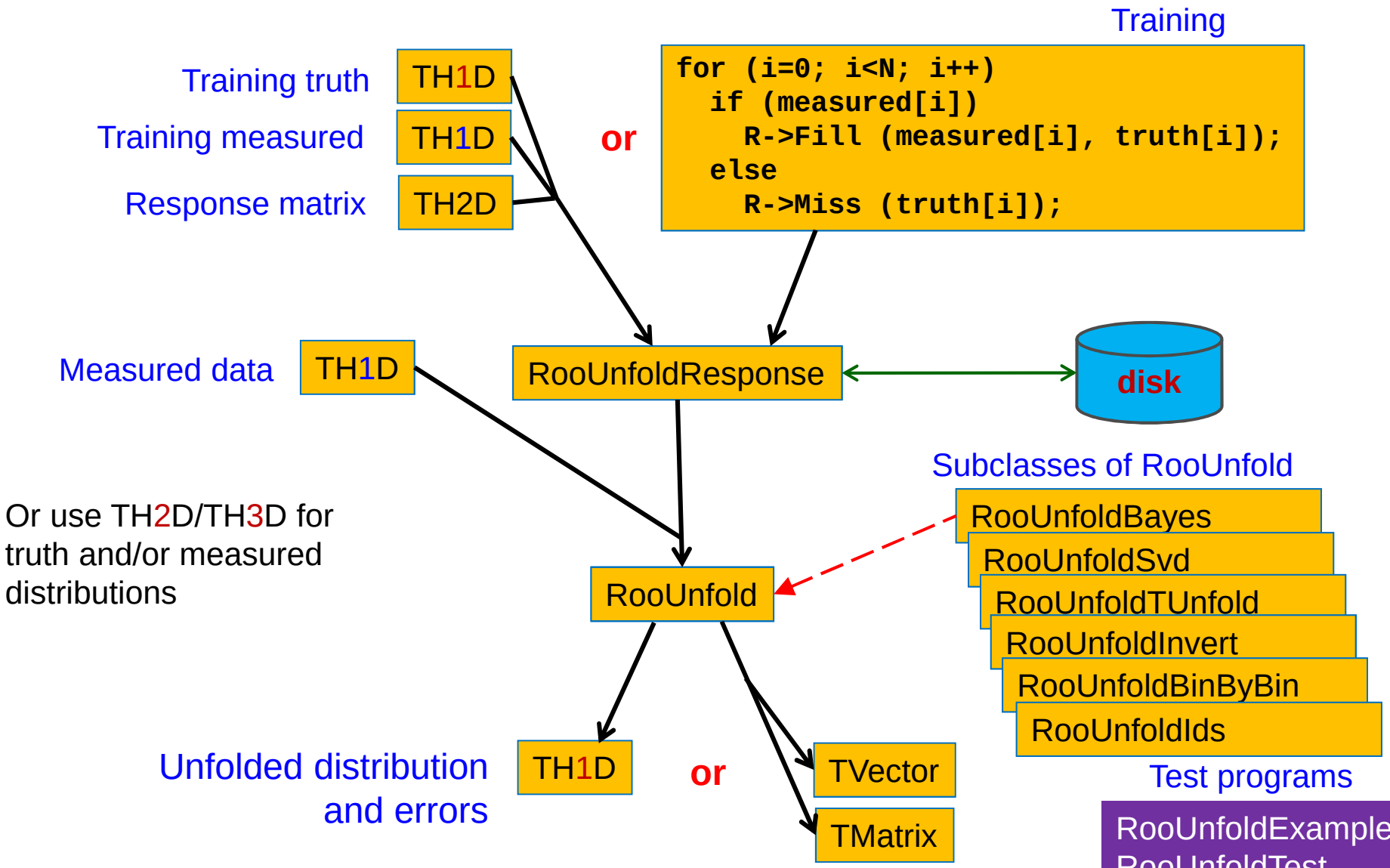
General features

- RooUnfold provides
  - Common features and interfaces to the different algorithms
  - Convenience methods for providing the inputs in different forms
    - response matrix can be given as histograms, matrices, or filled directly
    - 1D, 2D, 3D truth and/or measured distributions
    - Different binning in measured and truth
  - Support for inefficiency and fakes
    - even when not directly supported by underlying algorithm
  - Propagation of errors or automatic calculation using toys
    - Toys used to validate linear error propagation
  - Simple examples of use by C++ and Python
  - Extensive test suite for comparing methods using various simple toy MC distributions
    - 1D, 2D, 3D; bias and smearing; inefficiency and fakes; correlated inputs
    - Simple testing – all from the command-line

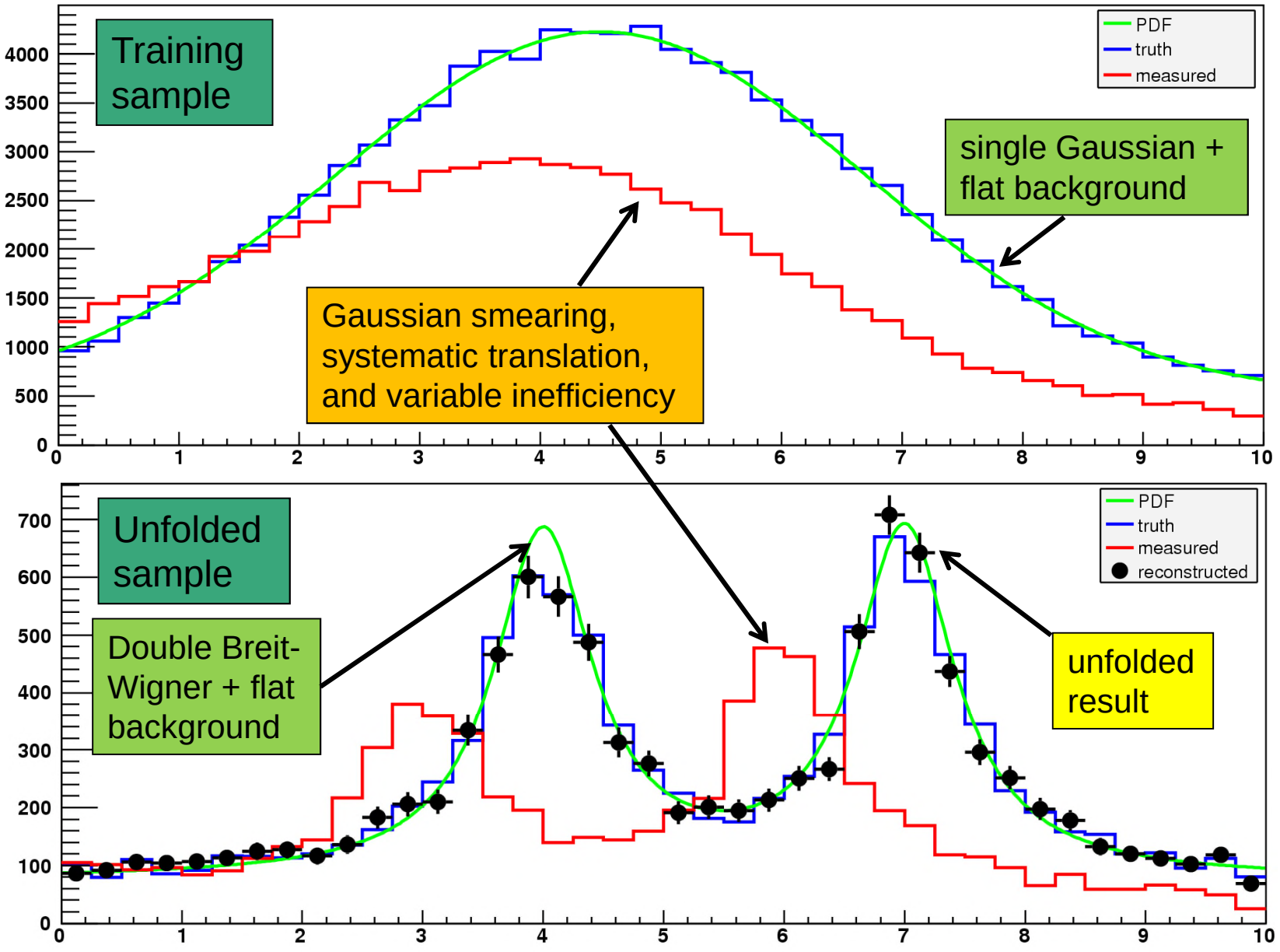
- Overview and class documentation, running instructions, download, and references:

  http://hepunx.rl.ac.uk/~adye/software/unfold/RooUnfold.html

RooUnfold classes



Example from the test suite



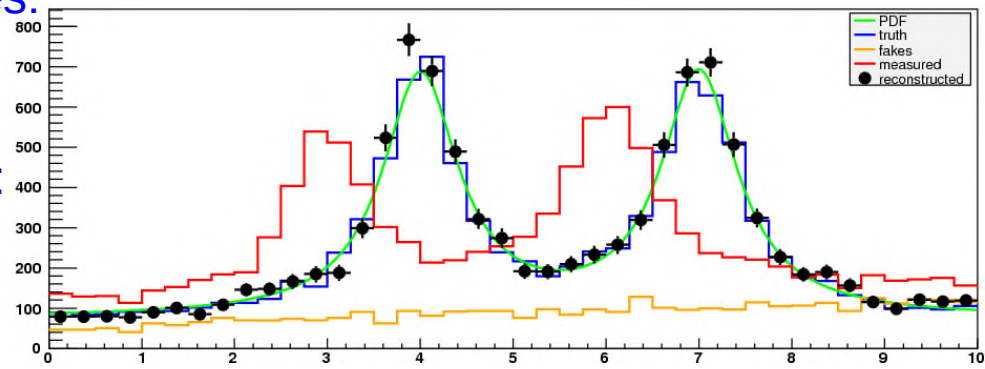
Binning

- 1D, 2D, 3D truth and/or measured distributions
  - Internally unpacked into 1D distributions
    - Multi-dimensional smoothing automatically selected for TUnfold
    - Only 1D smoothing implemented for SVD method
    - Other methods don't require smoothing
  - Choose binning with care, eg. response matrix for 2D distributions has N^4 bins
    - can require lots of MC for reasonable statistics

- Different binning in truth and measured distributions
  - TUnfold method requires 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 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 and bin-by-bin methods do not work well unless $N_{\text{measured}} = N_{\text{true}}$

Inefficiencies and fakes

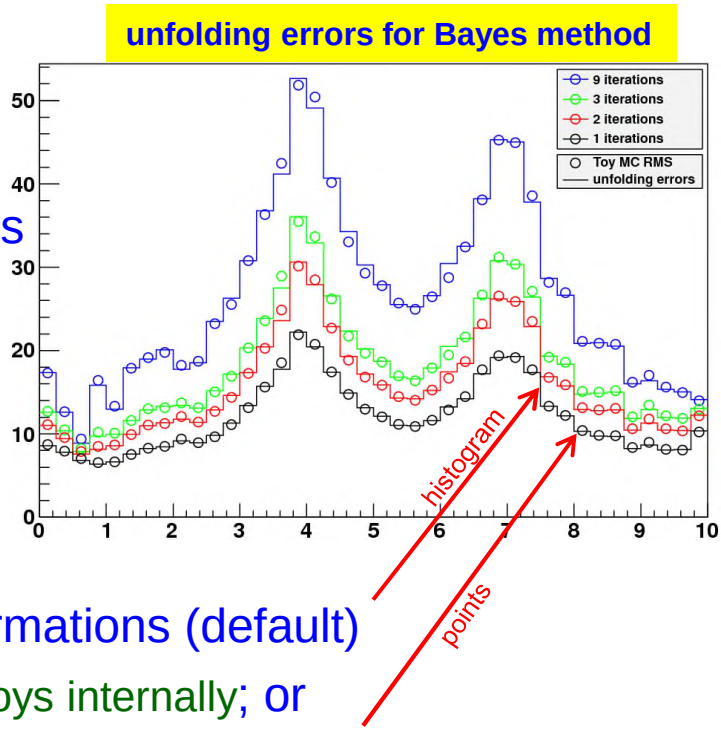
- As well as migration between bins, unfolding can also model
  - misses, inefficiencies, effectless-causes:
    - truth entries with no corresponding measurement
  - fakes, backgrounds, causeless-effects:
    - measurements with no corresponding truth entry



- RooUnfold allows misses and fakes to be specified when filling the response matrix
  - or inferred from the 1D truth/measured histograms given when creating the response matrix from a 2D histogram
  - Dealt with differently for each unfolding method, but generally misses are treated as a multiplicative efficiency and fakes as an additive background.
    eg. for the iterative Bayes method
    - Misses: The response matrix is scaled by the efficiency of each truth bin
    - Fakes: an extra truth bin for background is added to the response matrix
- Alternatively, can be handled outside RooUnfold by adjusting input and output
  - RooUnfoldResponse should then exclude misses and fakes
    - or in TH2 constructor, pass null histogram for TH1 measured/truth histograms

Error calculations

- RooUnfold can calculate the errors on the unfolded distribution as
  - histogram bin errors
    - no bin-bin correlations, returned in **`unfold->Hreco()`** histogram; or
  - full covariance matrix
    - **`unfold->Ereco()`**, returning a **`TMatrixD`**
    - Regularisation and bin-bin migrations normally introduce significant bin-bin correlations
- Unfolding errors can be based on
  - input measurement errors
    - passed with input histogram or default $\sqrt{n}$; or
  - full covariance matrix of bin-bin measurement errors
    - **`unfold->SetMeasuredCov(TMatrixD)`**; and/or
  - errors on the response matrix
    - eg. due to finite MC stats
    - enable with **`unfold->IncludeSystematics()`**
- The error propagation can be calculated by
  - propagation of errors through the unfolding transformations (default)
    - SVD (response matrix errors) and IDS (all errors) use toys internally; or
  - toys generated internally by RooUnfold (**`RooUnfold::kCovToy`** flag)
- All these possibilities should work with all the unfolding algorithms



RooUnfold history

very brief summary of the history

- 10/2005: RooUnfold initially developed using an implementation of Bayes unfolding from Fergus Wilson (RAL) and then SVD unfolding from Kerstin Tackmann (LBNL)
- 2010–11: Development/discussion as part of the Helmholtz Alliance Unfolding Project, including:
  - 05/2010: DESY unfolding workshop
  - 01/2011: PHYSTAT unfolding workshop at CERN
- 08/2010: Added interface to TUnfold after discussion with Stefan Schmitt (DESY)
- 08/2010: Error calculation using toys
  - These two improvements implemented by RAL student, Richard Claridge
- 01/2011: Reimplement Bayes unfolding using matrix methods; fix error propagation
- 10/2011: last release version 1.1.1
  - Continuing development in SVN
- 10/2011: Add propagation of response matrix uncertainties
- 05/2015: RooUnfold included in ATLAS RootCore releases
- 07/2017: Chris Meyer (UPenn) adds IDS unfolding algorithm

- INSPIRE lists 110 paper (+158 other) citations to RooUnfold PHYSTAT note
- I've had email contact from 132 people from many different experiments in PP/PA/NP

RooUnfold status

- Last release 6 years ago: RooUnfold version 1.1.1
- There has been some continuing development and minor bug fixes that can be accessed from DESY SVN
  - Recommend that people use the development version until a new release is made
    - Main changes are now quite mature, and compatible with previous versions
    - Release version 1.1.1 no longer compiles with current versions of ROOT
      - Development version maintains compatibility with old and new versions of ROOT
- See the "Development" section of the web page to download, or browse the dev version's class documentation

Development version

- The main improvement in the dev version is to allow uncertainties on the response matrix (eg. due to finite MC stats) to be propagated to the unfolded errors
  - Can include the effect of measurement and response matrix errors together or separately
  - Can be calculated using error propagation or automatic toys

- The other main changes since version 1.1.1:
  - Addition of RooUnfoldIds, implementing IDS unfolding
  - Improvements in SVD method (and TSVDUnfold), especially the error propagation
    - requires updated TSVDUnfold not yet in ROOT
    - Local version included in RooUnfold package
  - Simplify interactive running with CINT, CLING, ACLiC, or PyROOT
  - Test alternatives to unfolding: parameterised fit with response matrix

(much-delayed) plans

- I have collected many interesting and useful suggestions for improvements
  - interface with new algorithms, new tests, convenience methods, API…
    - but had very little time to work on unfolding, which was always a spare-time job
    - see backup for unedited list

- The first priorities are:
  - Make a new release based on the dev version
    - Validate changes for all algorithms – so far concentrated on Bayes and SVD methods
  - Update and improve documentation, especially
    - Setup and examples for ROOT6 with CLING or PyROOT
    - Document different ways of creating and filling the response matrix
    - Errors: propagation of errors or toys, measurement or response matrix errors
  - Later, submit for inclusion in ROOT
    - agreed in principle, but discussion was a long time ago

- hope to get to it in the next few weeks/months – but I've said that before ☹

Summary

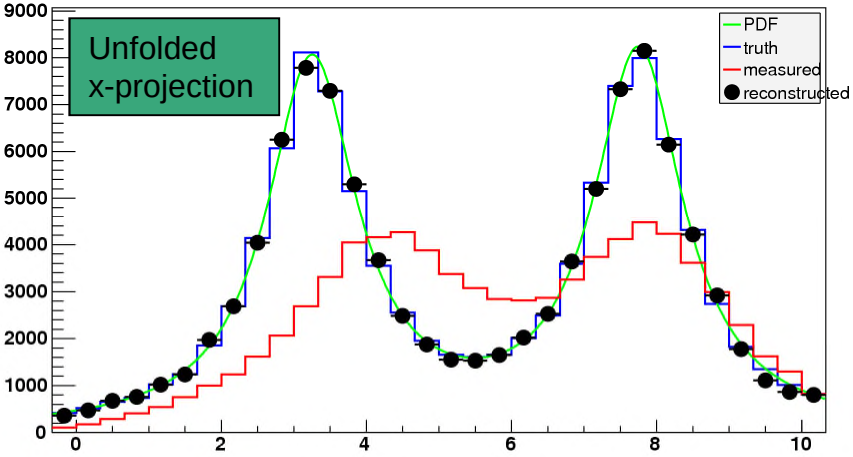
- RooUnfold is a widely-used framework for accessing different unfolding algorithms
  - in particular, implements D'Agostini's iterative Bayes method
- Implements many common requirements
  - multidimensional binning
  - inefficiencies, fakes
  - error calculations
  - algorithm tests using toy MC
- Missing a common framework for evaluating algorithms and their configuration for a specific physics distribution
  - See next talk → Chris Meyer

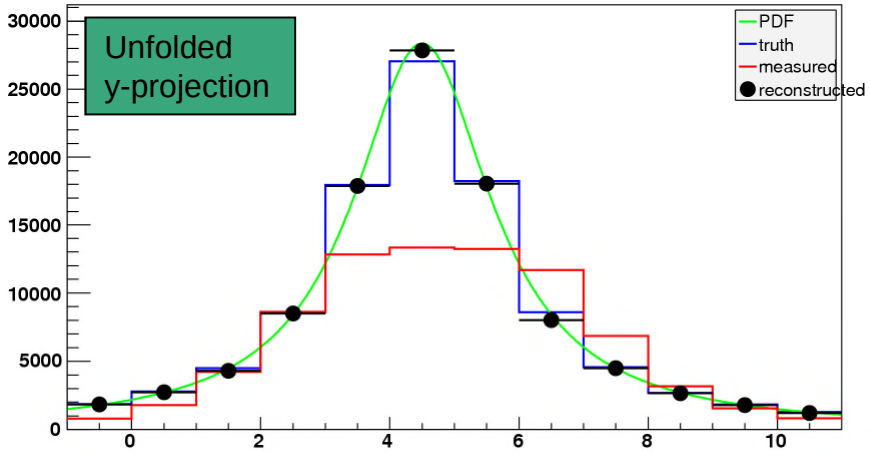
Backup

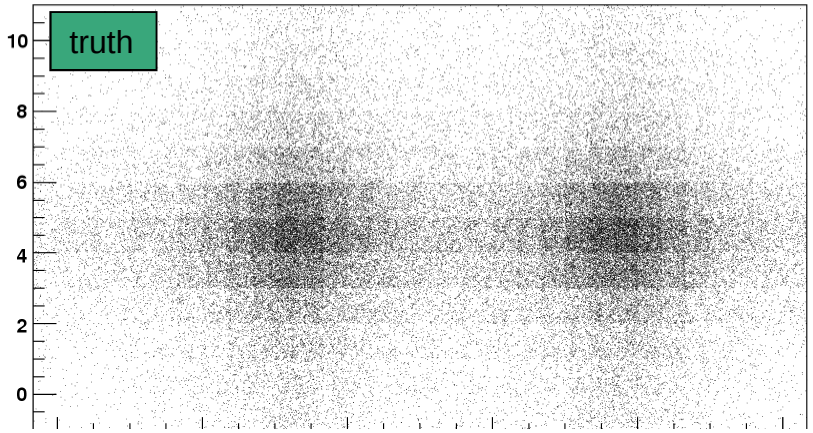
Possible tests and ideas for improvement

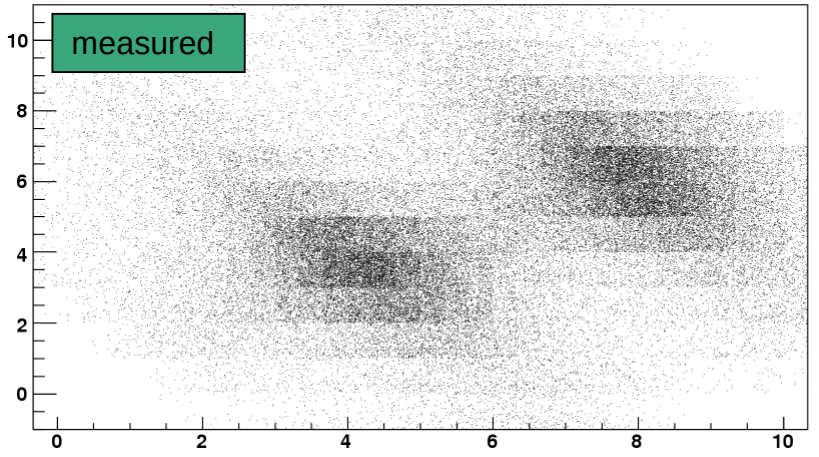
Unordered log of tests and ideas that could be investigated. No plan yet to implement any of them.

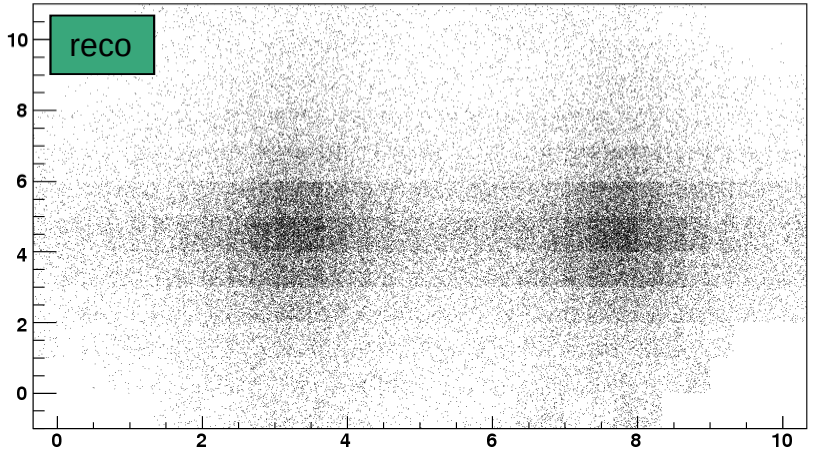
- RooUnfoldBayes option to allow to use flat (or other) prior (Jan Therhaag, Kolja Kauder 2/10/2017)
- Iterative bin-by-bin method: V. B. Anykeyev, A. A. Spiridonov, V. P. Zhigunov, *Correcting factors method as an unfolding technique*, NIM A322(1992)280-285
- Better figure of merit, eg. alternate chi^2 definition (Vato Kartvelishvili)
- Low statistics tests. Does toy MC handle bins where the fluctuation may go negative? Bayes toy MC has some funny effects
- RooUnfoldResponse convenience methods to created from a TMatrix and to plot directly the "Miss" data. Presumably can be done by subtracting the projection from the truth. (Andrii Chyzh, 22/6/2011)
- Fully Bayesian Unfolding method, https://arxiv.org/abs/1201.4612
- Use THn class for response matrix?
- RooUnfoldResponse::RunToy should probably update the measured and truth normalisations. How to handle the uncertainty in the efficiency and fakes? (Katharina Bierwagen, 18/7/2012)
- Consistent handling of fakes: add bin or adjust input? Currently (since 27/1/2012) add bin for Bayes, and subtract fakes for the others. Adding bin may not work well for SVD or TUnfold since the extra bin isn't continuous with the others. (Kerstin Tackmann 19/12/2012)
- Add GetEfficiency() (or GetMiss()?) to see unfolded efficiencies
- RooUnfoldBayes with 0 iterations could return the initial distribution - useful for debugging? (Sercan Sen, 28/3/2013)
- When errors aren't required (especially for toys), skip error propagation in Bayes (and other?) unfolding. This can be really slow for large number of bins. (Elzbieta Richter-Was 11/11/2013)
- Better name for IncludeSystematics() (IncludeResponseErrors?) This might be confused with the systematic effect from the unfolding procedure, which can't be evaluated directly by RooUnfold.
- API improvement suggestions from Gero Flucke. Must be upward-compatible.











2D unfolding

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

Algorithms – Iterative Bayes' theorem

- Uses the method of Giulio D'Agostini (1995), implemented by Fergus Wilson and myself
  - 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
  - Correctly account for propagation of errors through multiple iterations
    - D'Agostini's paper did not account for dependence on previous iterations in error propagation
  - Does not do smoothing
    - Did not find this helped, and can introduce additional bias

Algorithms – SVD

- Uses the method of Andreas Höcker and Vato Kartvelishvili (**GURU** Fortran program)
  - Implemented in C++/ROOT by Kerstin Tackmann and Heiko Lacker and subsequently included in ROOT as TSVDUnfold
    - RooUnfold includes an interface to this class
- 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 → result dominated by MC truth
    - k too large → 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)

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 $\log_{10}(\tau)$.

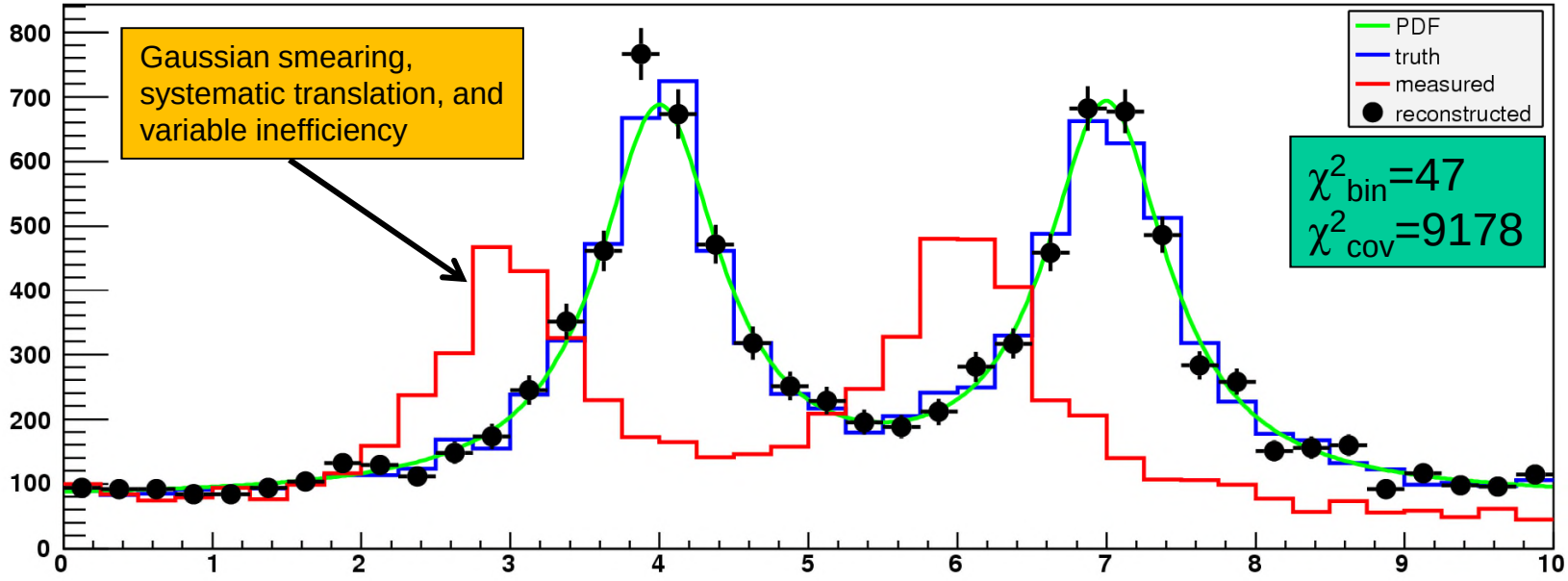
Unregularised Algorithms

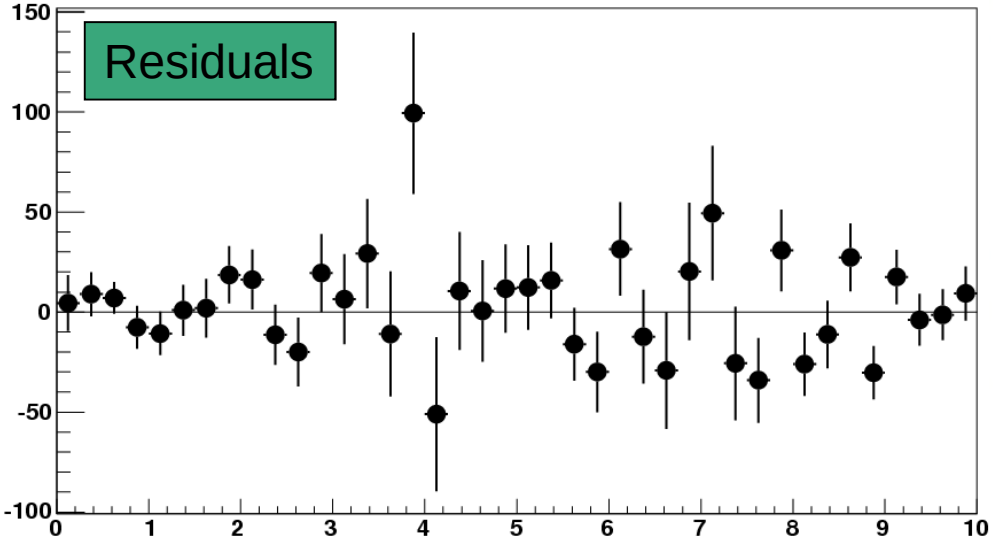
- Very simple algorithms
  - using bin-by-bin correction factors, with no inter-bin migration
  - using unregularised matrix inversion with singular value removal (TDecompSVD)

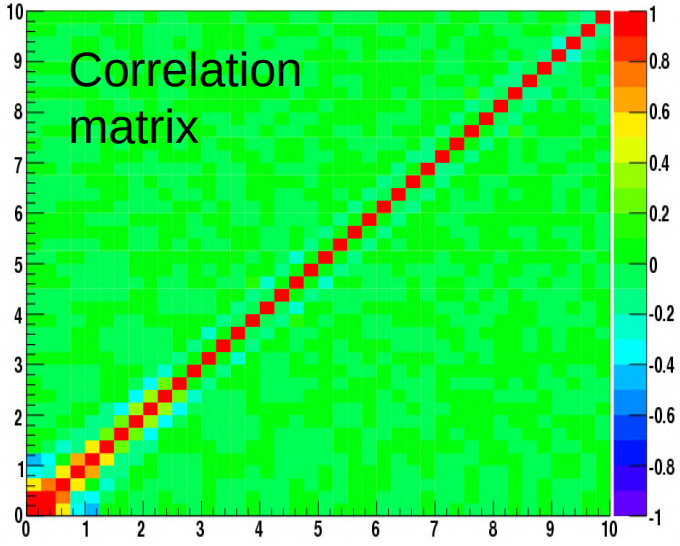
  are included for comparison – and to demonstrate why they should not be used in most cases!

RooUnfold with Bayes algorithm

3 iterations

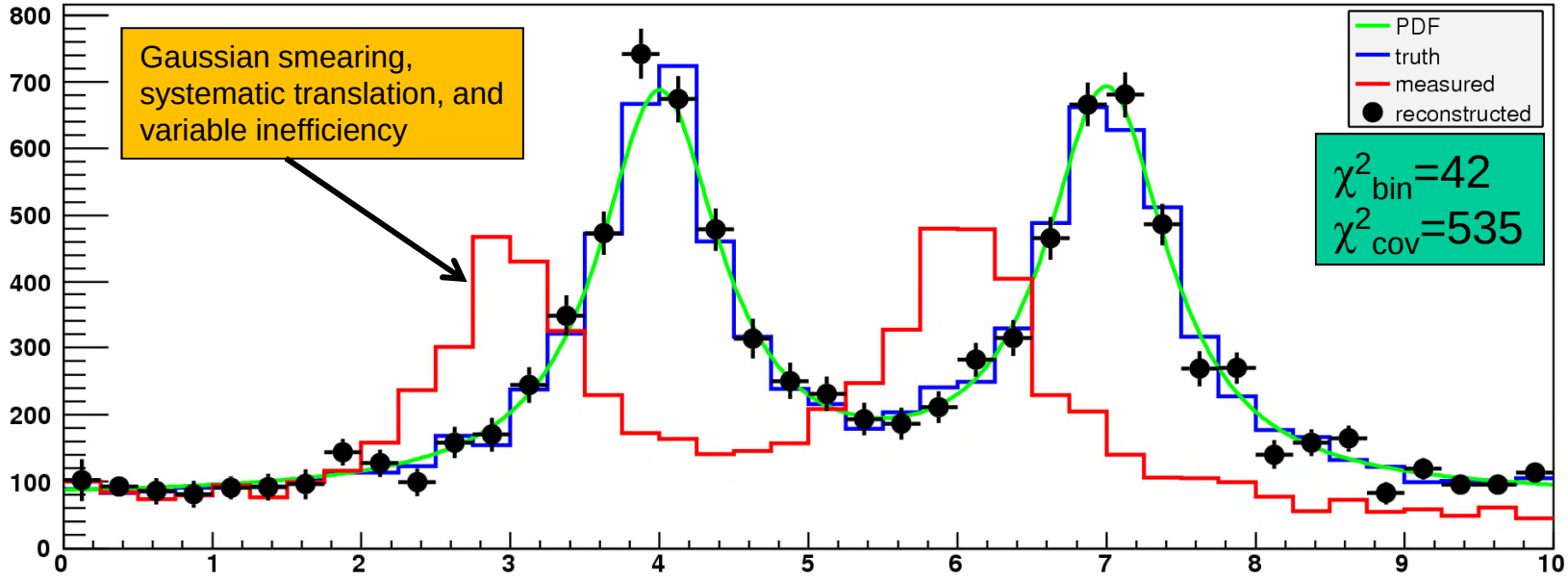


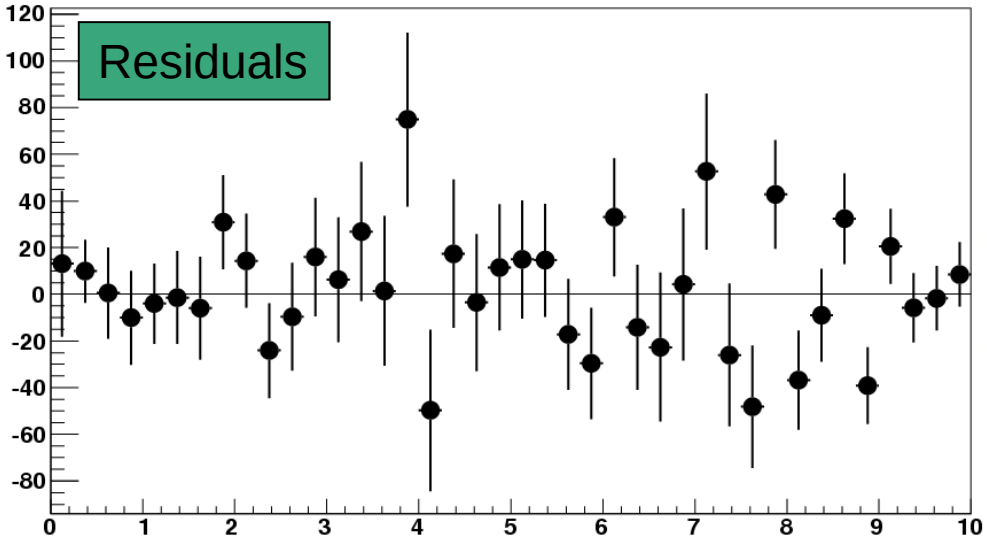


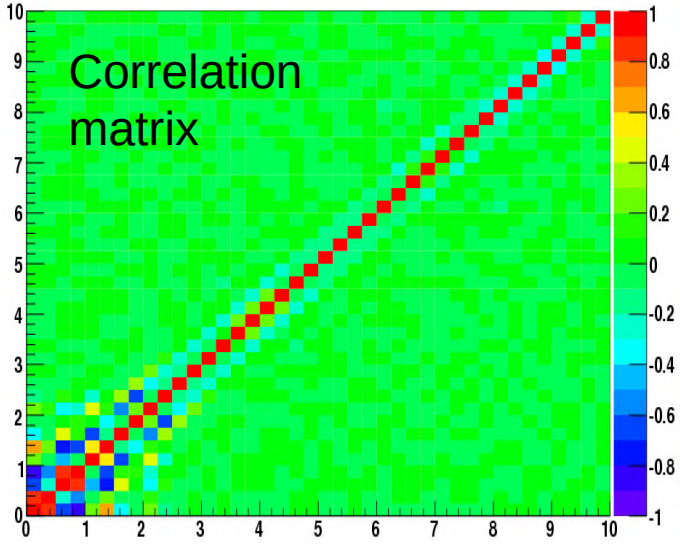


RooUnfold with SVD algorithm

$k = 30$

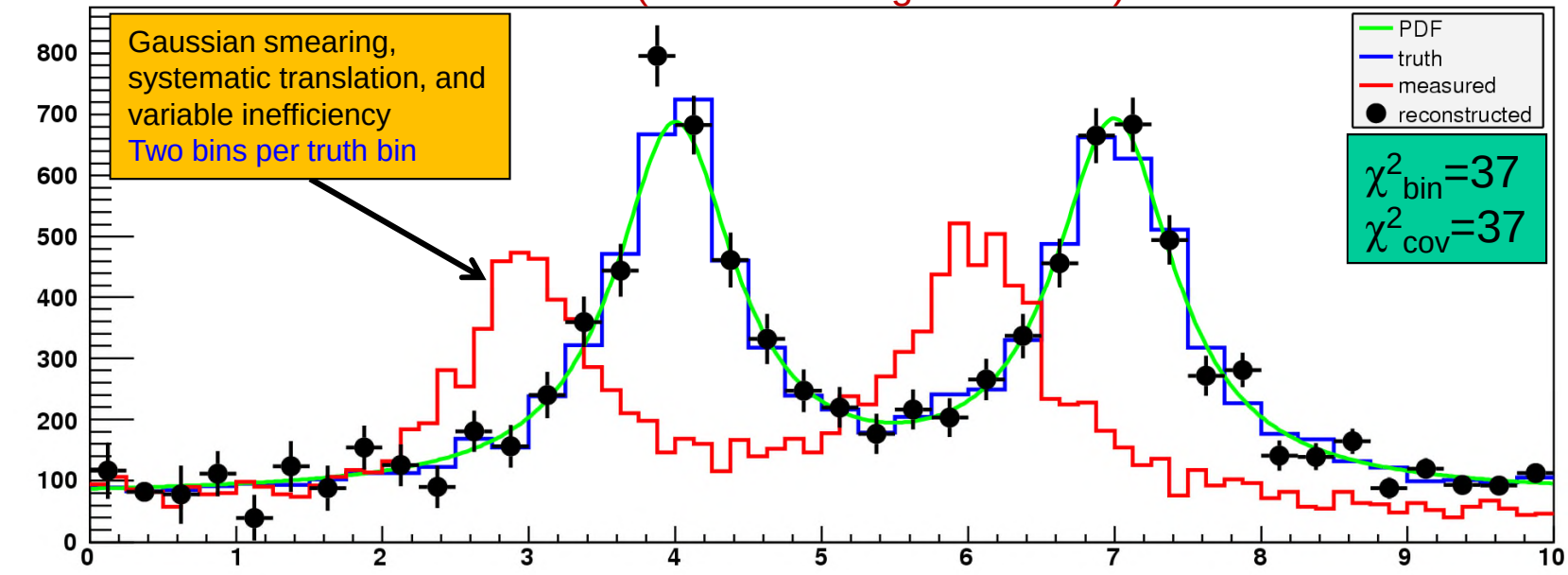


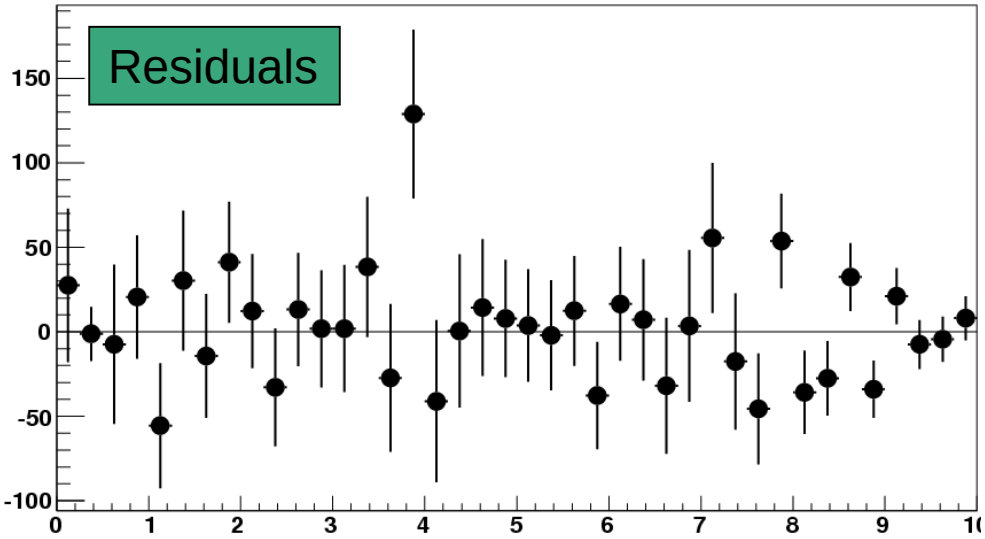


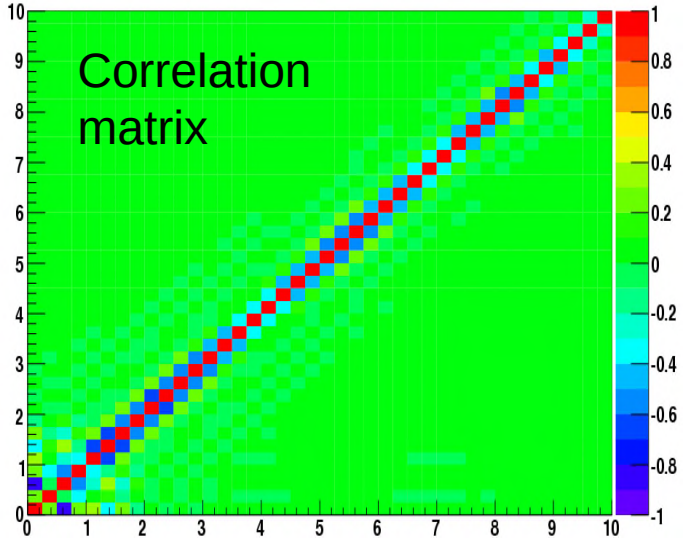


RooUnfold with TUnfold algorithm

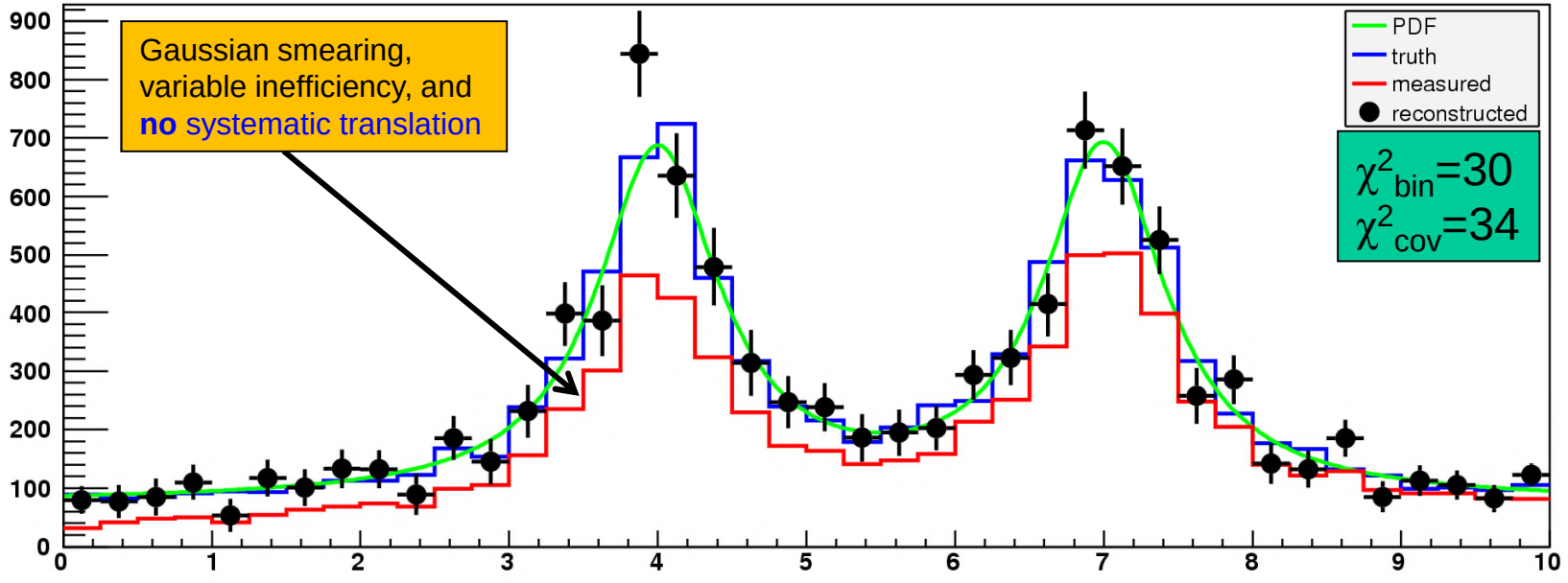
τ=0.004 (L-curve scan gave 0.0014)

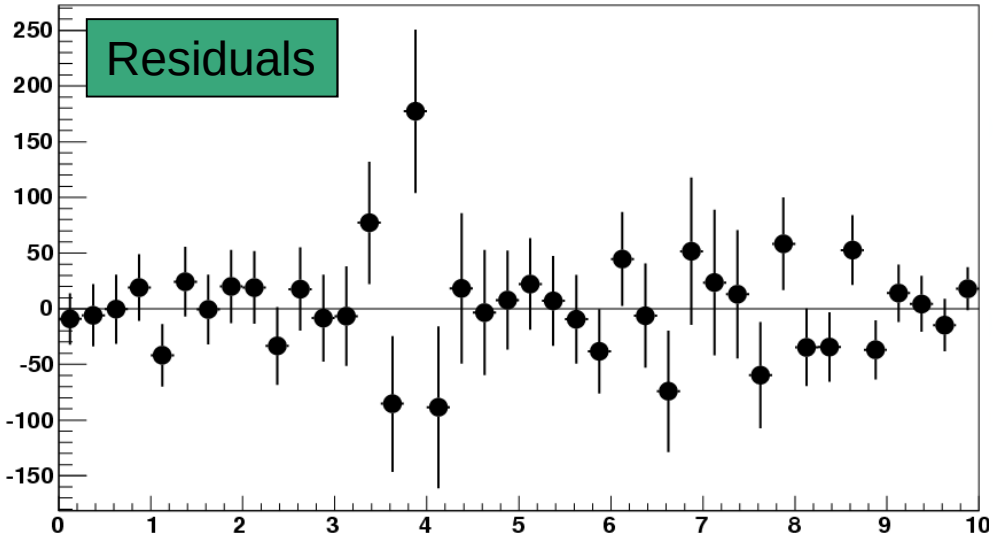


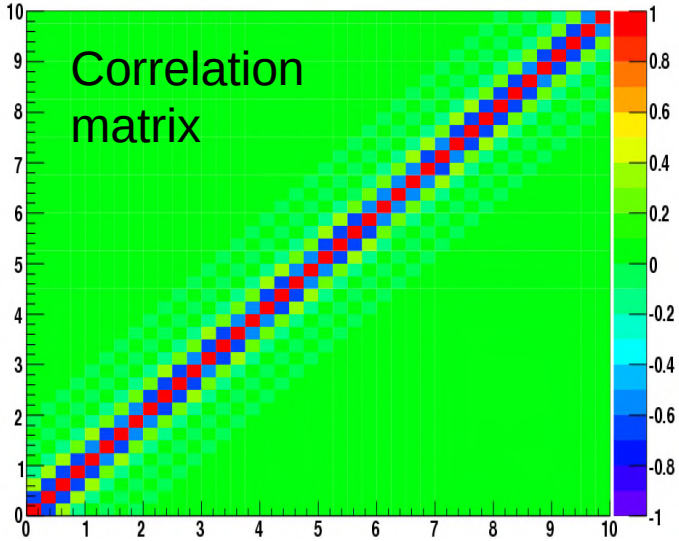




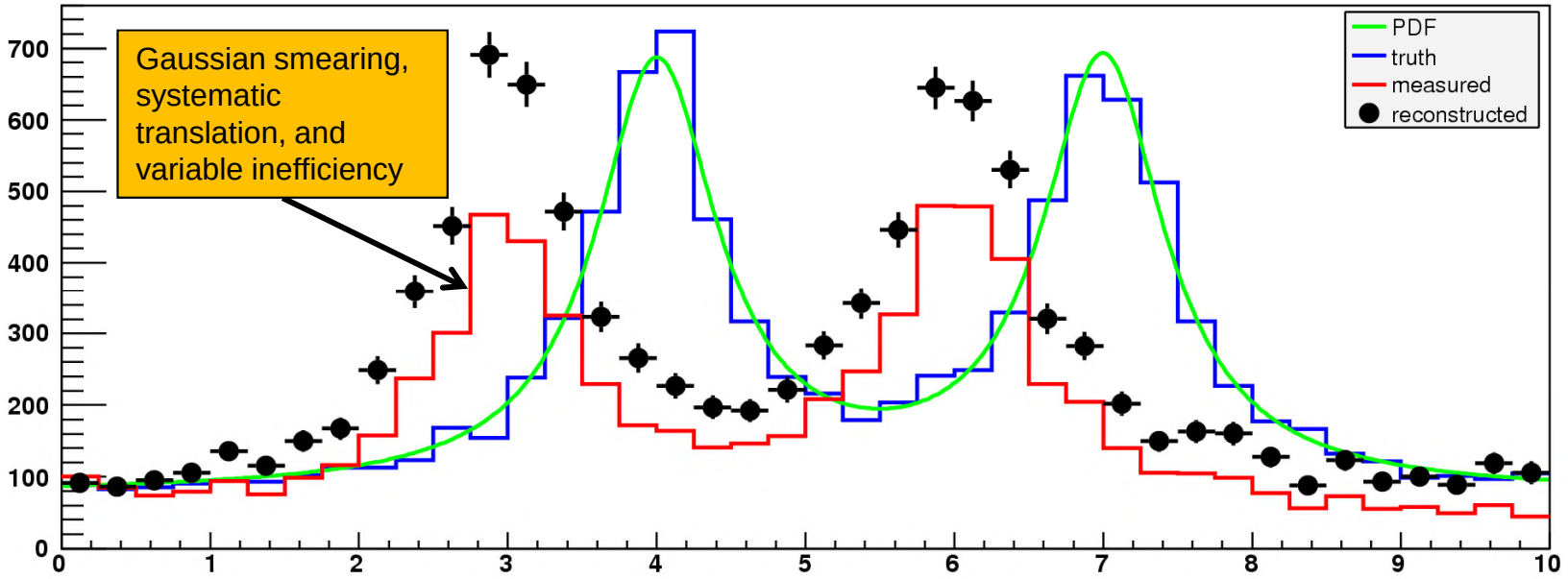
Unregularised matrix inversion

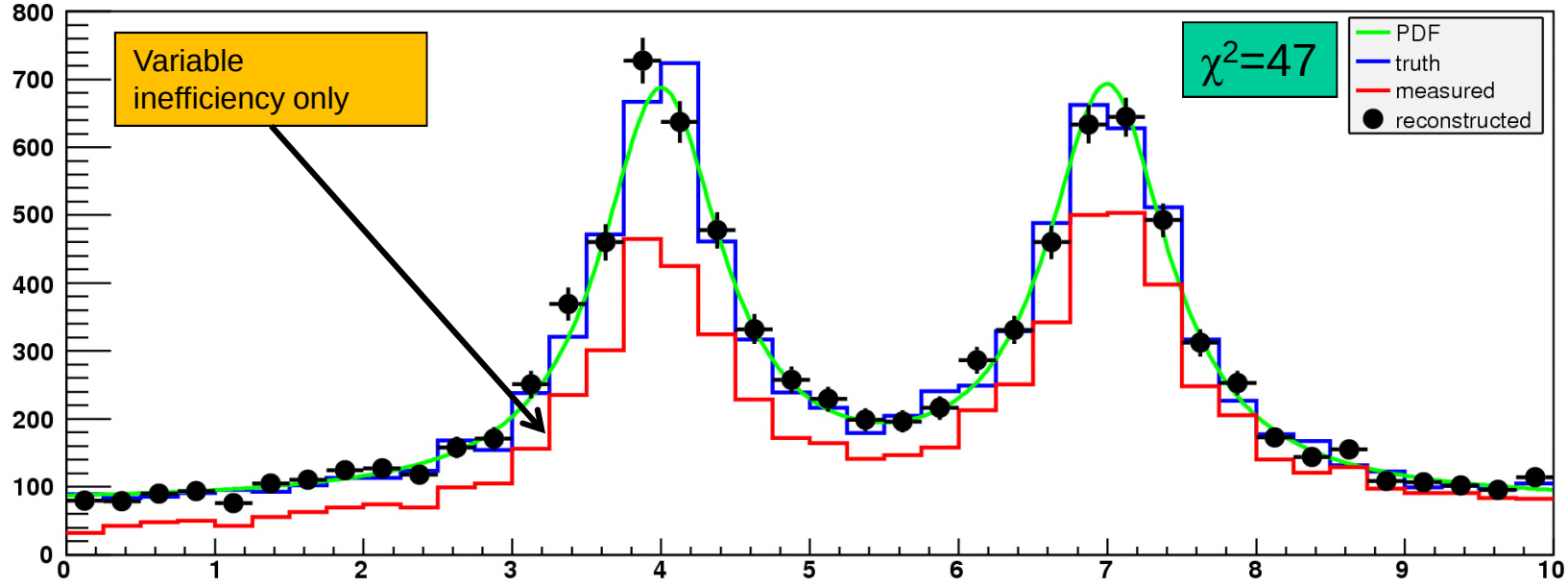






simple correction factors





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 ⟶ larger errors, but also larger residuals
  - Is there a better figure of merit?