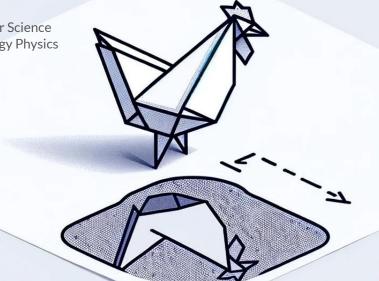
Vincent Croft

- ¹ LIACS, Leiden Institute of Advanced Computer Science
- ² Nikhef, Dutch National Institute for High Energy Physics
- ³ RooUnfold Development Team



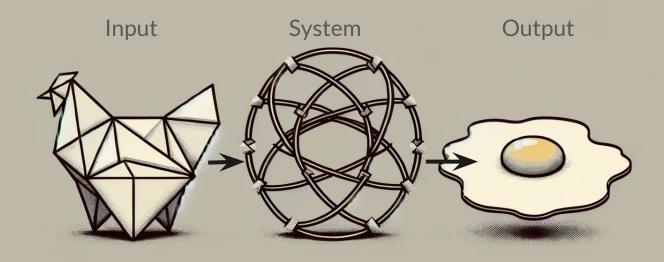
Unfolding In High Energy

Physics An introduction uncertainties,

An introduction, application to analyses, treatment of uncertainties,

and the choice of algorithm and regularisation

The problem with unfolding



A well defined problem

Existence

The problem must have a solution

Uniqueness

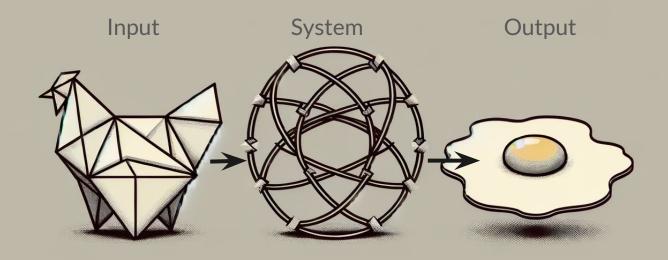
 There must be only one solution to the problem

Stability

 The solution must depend continuously on the data

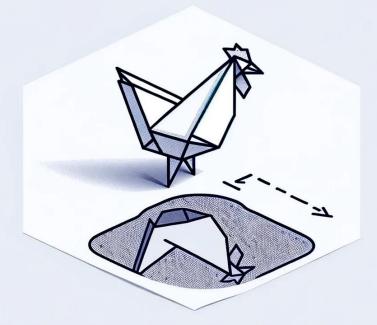


The problem with unfolding

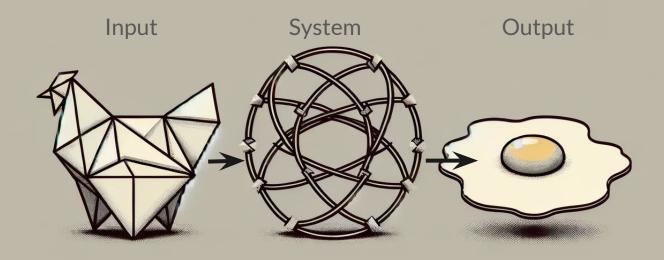


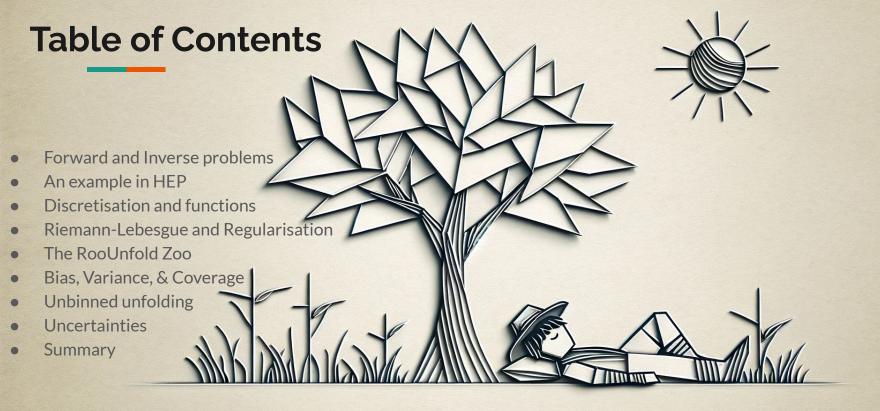
Simplest ill-posed problem

$$x_1 + x_2 = 1$$



The problem with unfolding





The Unfolding Problem

- Medical imaging CT scanning, electro-cardiography, etc.
- **Geophysical prospecting -** search for oil, land-mines, etc
- **Image deblurring -** astronomy, crime scene investigations, etc.
- Deconvolution of a measurement instruments response.



Users of RooUnfold

























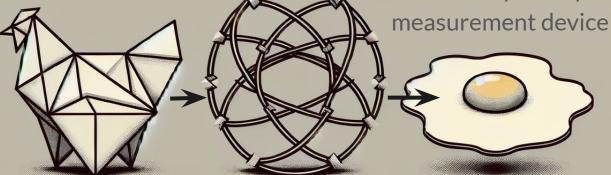


ALICE



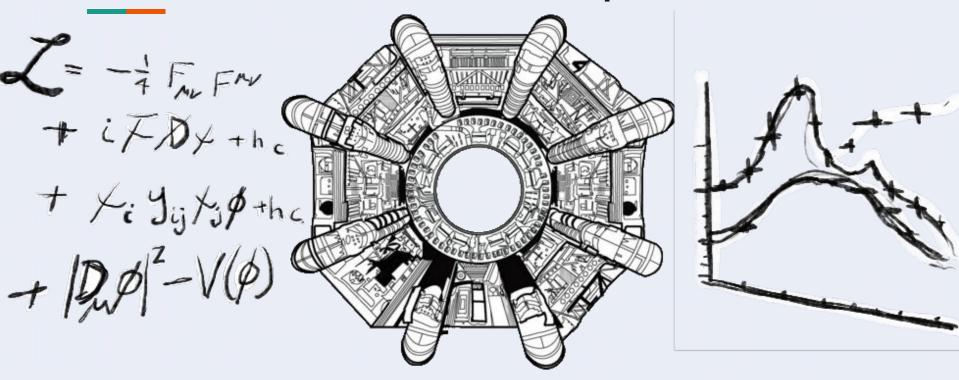
The Unfolding Problem

- Estimating the particle-level spectrum
 - Some physical quantity of interest
 - Some basis of observations
 - Smeared by an imperfect measurement device

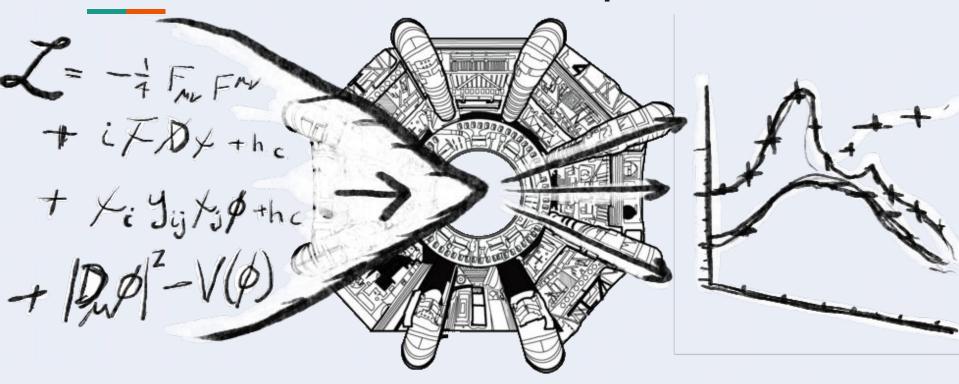


Estimating the true distribution when you measure a smeared spectrum

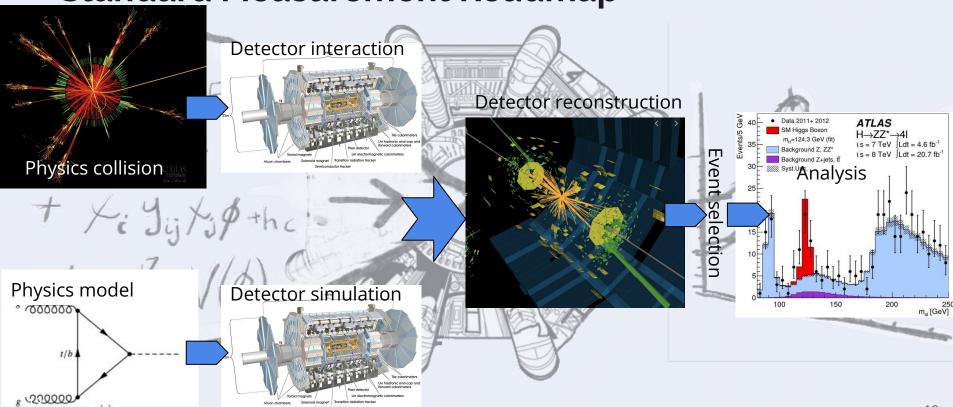
Standard Measurement Roadmap



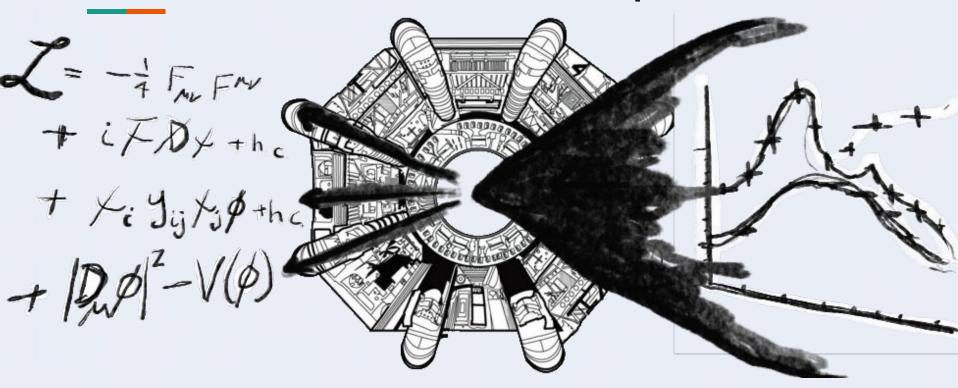
Standard Measurement Roadmap



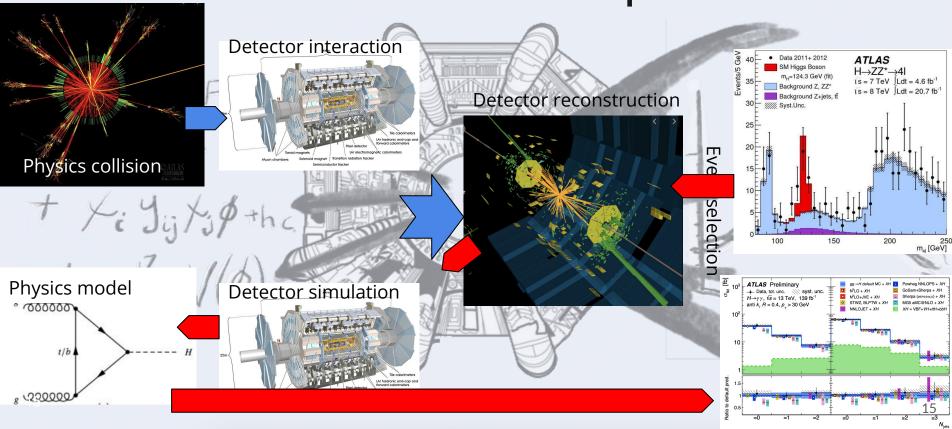
Standard Measurement Roadmap



Alternative Measurement Roadmap

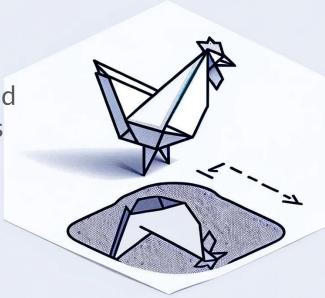


Alternative Measurement Roadmap



Why use the alternative?

- Multiple predictions differ within the uncertainties
- Ready for future reinterpretations and combinations with other experiments
- Learn about the physics model
 - Not just the likelihood
 - Physics parameters!



Fredholm integral equation

Consider a random variable y, the goal is to determine f(y)

$$\int_0^1 K(x,y)f(y)dy = g(x),$$

Here the kernel K and the right-hand side measured function g are considered known functions.

If f and K are known (as in the forward case) then we can simply compute g by evaluating the integral

Properties of the FIE
$$\int_0^1 K(x,y) f(y) dy = g(x)$$

Riemann-Lebesgue Lemma (aka Mercer's Theorem): mapping from f -> g has a dampening/smoothing effect for arbitrary kernels such that the information content of f diminishes with precision of g. As such, estimating f from a measurement of g means that arbitrary levels of noise in g can produce unbounded contributions to the prediction of f.

Smoothing: $K(x,y) = \sum_{i=1}^n \mu_i u_i(x) v_i(y)$ where μ_i are a decreasing sequence of singular values.

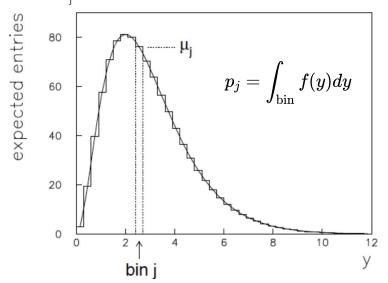
The "smoother" the kernel K, the faster the singular values decay to 0. The Picard condition states that for a solution to exist, coefficients singular functions describing the noise have to decay faster than the the singular values of the kernel.

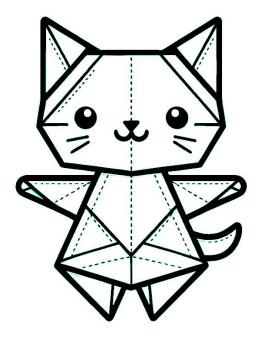
TL;DR: Lots can go wrong!

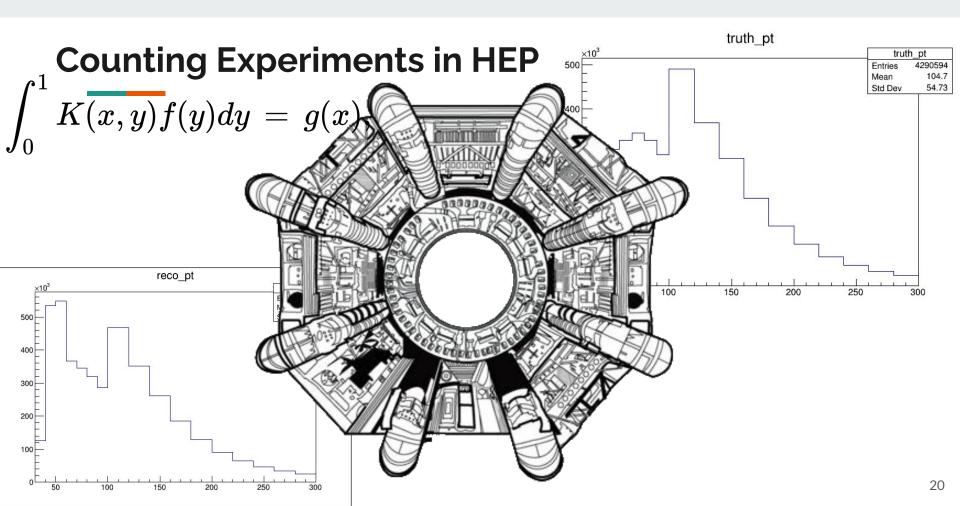
Counting Experiments in HEP

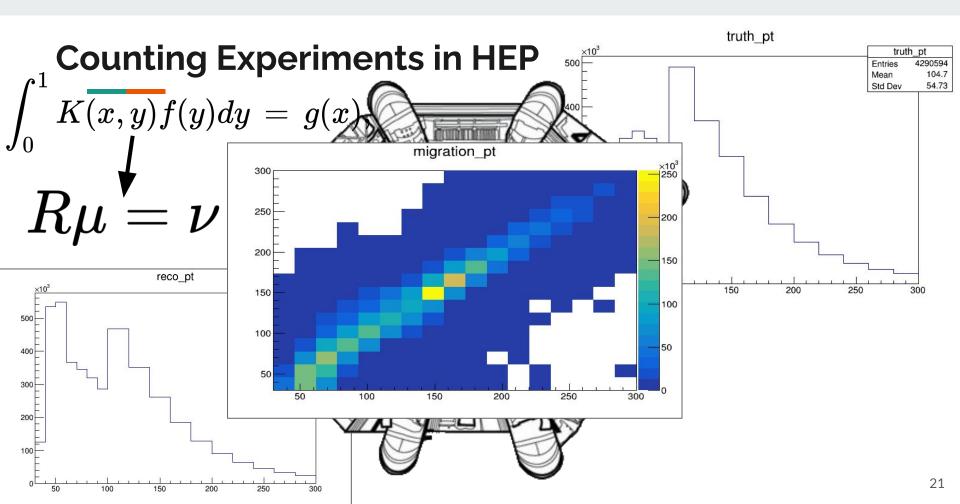
If parameterization $f(y;\theta)$ known, find Maximum Likelihood estimators $\hat{\theta}$

If no parameterization available, often construct histogram: construct estimators for the μ_j (or p_j) Where μ_i corresponds to the 'true' histogram





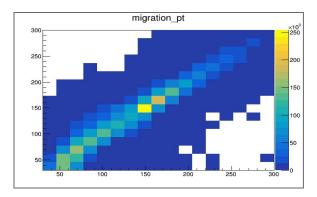




Counting Experiments in HEP (Notation)

Histogram data are $n=(n_1,n_2,\ldots,n_N)$

$$u_i = \mathit{E}[n_i] = \sum_{j=i}^M R_{ij} \mu_j \hspace{0.5cm} i = 1, \ldots, N$$



Where: $R_{ij} = P({
m observed \ in \ bin \ i \ | \ produced \ in \ bin \ j})}$ is called the response matrix

Note μ and ν are constant while n is subject to statistical fluctuations

Counting Experiments in HEP (Notation)

The 'true' histogram
$$\mu=(\mu_1,...,\mu_M)$$

Expectation values for observed histogram $\,
u=(
u_1,...,
u_N)\,$

Observed histogram
$$n=(n_1,...,n_N)$$

Expected backgrounc
$$eta=(eta_i,...,eta_N)$$

Response matrix $R_{ij} = P(\text{observed in bin i} \mid \text{produced in bin j})$

Related by
$$E[n] = \nu = R \, \mu + \beta$$

Maximum likelihood (ML) solution

Let us take the most obvious solution;

Assume that the problem $\nu = R \mu + \beta$ can be inverted

$$\mu = R^{-1}(\nu - \beta)$$

• But remember; v are the expectation values of the observed histogram, not the observed histogram (which is denoted by n).

Assume as well that the data can be considered as independent poisson distributions for each bin

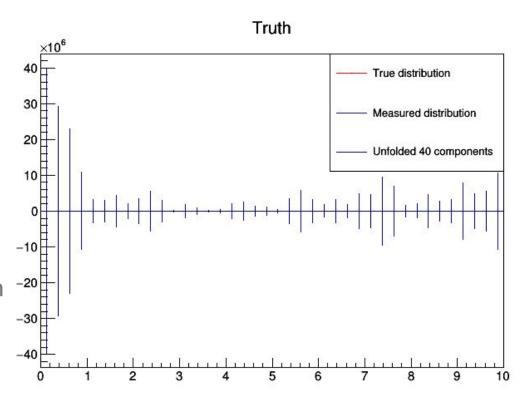
• Now the maximum likelihood estimator is $\hat{
u}=n$: so then

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

Example in practice

The problem: We don't have \mathbf{v} , only \mathbf{n} .

- R⁻¹ interprets fluctuations in n
 as the residual of original fine structure and puts this back into.
- Causes breakdown
 - In this example 40
 components corresponds to
 the matrix inversion solution



Bias, variance and coverage

Conclusion: In unfolding one must accept some bias in exchange for a (hopefully large) reduction in variance. So what do we need to consider?

- Bias: the difference between the estimator's expectation and the parameter's true value.
- ullet Variance: the diagonal elements of the covariance matrix of the estimators fo μ
- Coverage: the probability that the true value o μ_i falls between plus and minus one standard deviation about the estimator of μ_i

Note: the bias, variance and coverage are always defined with respect to the chosen true and expected data histograms.

Variance, Bias, and Coverage

Use a toy dataset with K events, the variance for bin i is then calculated as

$$\sigma_{\hat{\mu_i}}^2 = rac{1}{K-1} \sum_{k=1}^K \left((\hat{\mu_i})_k - rac{1}{K} \sum_{k=1}^K (\hat{\mu_i})_k
ight)$$

Use a toy dataset with K events, the bias for bin i is then calculated as

$$b_i^{ ext{das}} = rac{1}{K} \sum_{\mathbf{k}}^{\mathbf{K}} (\hat{\mu_i})_k - \mu_i$$

Under the assumption that $\hat{\vec{\mu}}$ are Gaussian distributed coverage probability can be calculated in closed form as

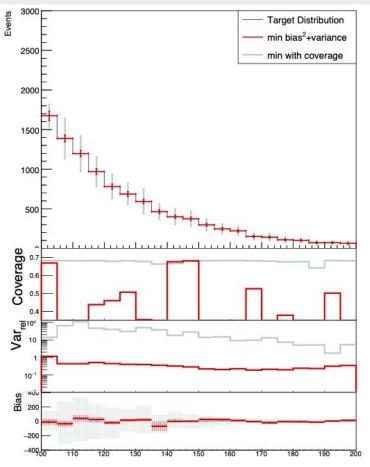
$$P_{\text{cov}} = \Phi\left(\frac{b_i}{\sigma_{\hat{\mu}_i}} + 1\right) - \Phi\left(\frac{b_i}{\sigma_{\hat{\mu}_i}} - 1\right)$$

Where Φ is the Standard Gaussian cumulative distribution function.

Choosing regularisation strength

So how do you take all these things into account in a smart way?

- Choose a regularisation strength that unconditionally minimises the bin-averaged MSE (the mean squared error, aka sum of bias squared and variance, averaged over the bins)
- Require the that the bin-averaged estimate of the coverage of the unfolded data reaches the target coverage of 68.3% within 1%.



Likelihood formalism and regularisation function.

The data are described with a given probability model that determines the likelihood functio $L(\vec{\mu}) = P(\vec{n}|\vec{\mu})$ Often the n_i are modelled as independent and Poisson distributed, so that the likelihood is

$$L(\vec{\mu}) = \prod_{i=1}^{N} \frac{\nu_i^{n_i}}{n_i!} e^{-\nu_i}$$

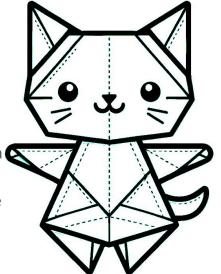
Where you can remember $v_i = \sum_{j=i}^M R_{ij} \mu_j + \beta_i$

To suppress the large variance of the maximum-likelihood estimator one chooses a μ that does not correspond to the maximum of the log-likelihood in L_{max} , but rather one considers a region of μ -space where ln $L(\mu)$ is within some threshold achieved by maximising not ln $L(\mu)$ but rather a linear combination of it and a regularisation function $S(\mu)$, which represents the smoothness of the histogram μ

 $\varphi(\vec{\mu}) = \ln L(\vec{\mu}) + \tau S(\vec{\mu})$

E.g Tikhonov regularisation

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



Study on smeared exponential distribution

We define as benchmark model an exponential decay distribution, smeared with a resolution function that is loosely inspired on a calorimeter response:

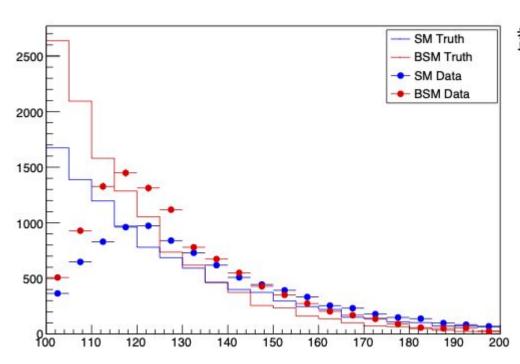
$$f(x|\alpha) = f_{\text{physics}}(x_{\text{true}}|\alpha) * f_{\text{detector}}(x_{\text{true}}, x)$$

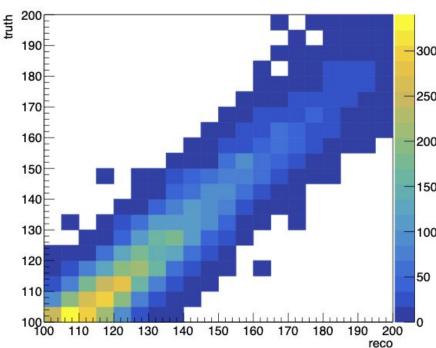
= $(\alpha \cdot \exp(-\alpha \cdot x_{\text{true}})) * \text{Gauss}(x - x_{\text{true}}, 7.5, 0.5 \cdot \sqrt{x_{\text{true}}} + 2.5)$

where the * symbol represents the convolution operator.

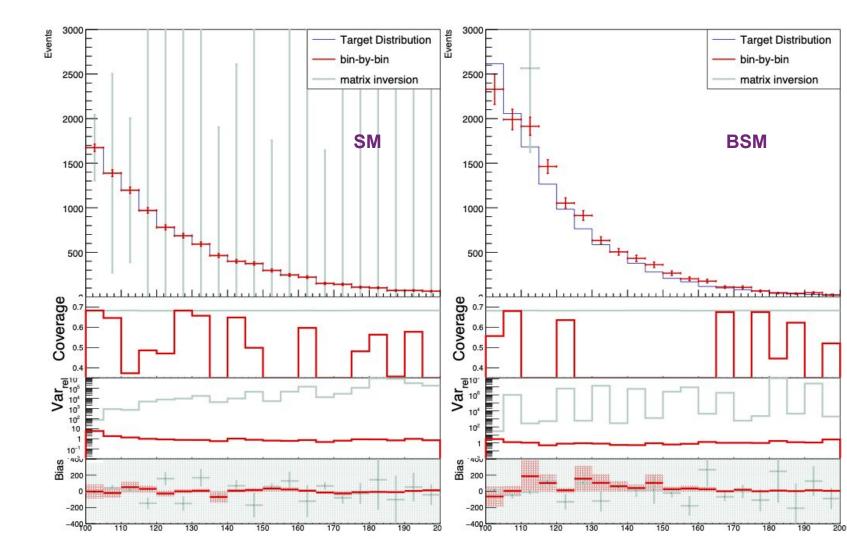
We define two models variants, labeled SM ('Standard Model') and BSM ('Beyond the Standard Model'), that correspond to an exponential distribution with a slope α of 0.035 and 0.05 respectively

Study distributions



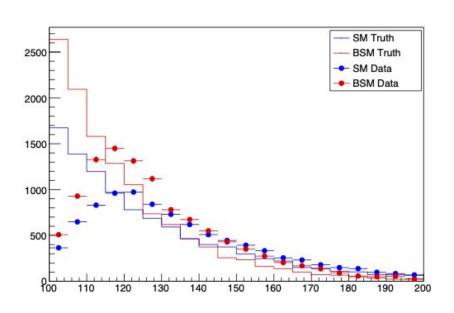


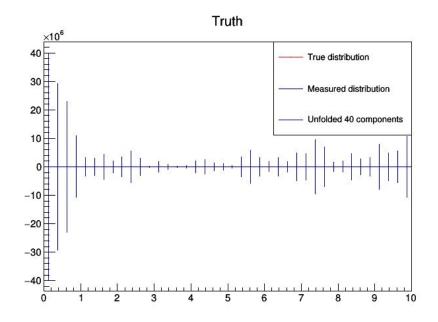
Methods that are not



Single Value Decomposition (SVD)

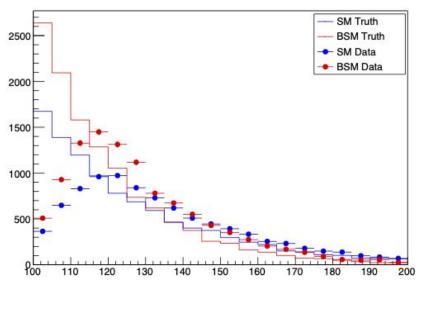
Remember

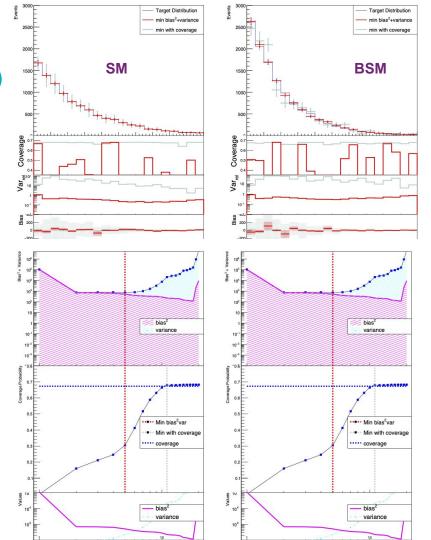




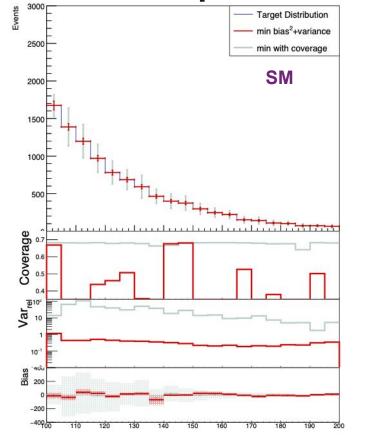
Single Value Decomposition (SVD)

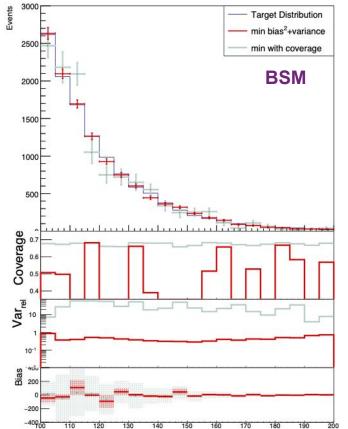
Looking at Coverage, Variance and Bias





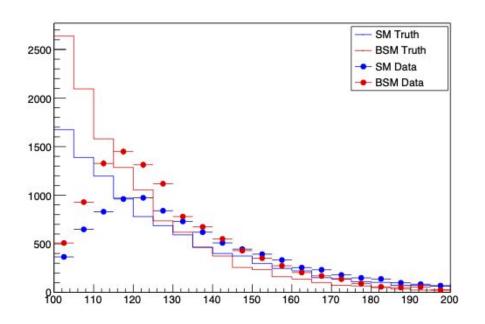
Single Value Decomposition (SVD)

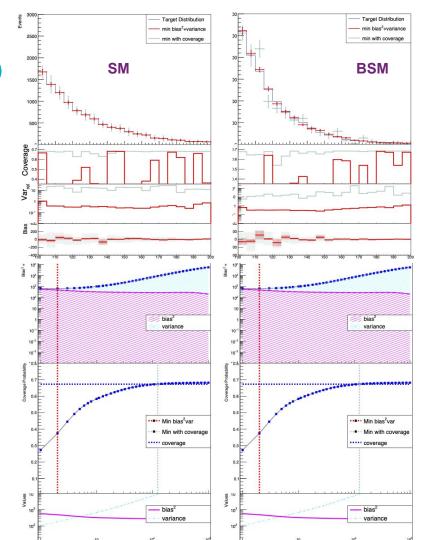




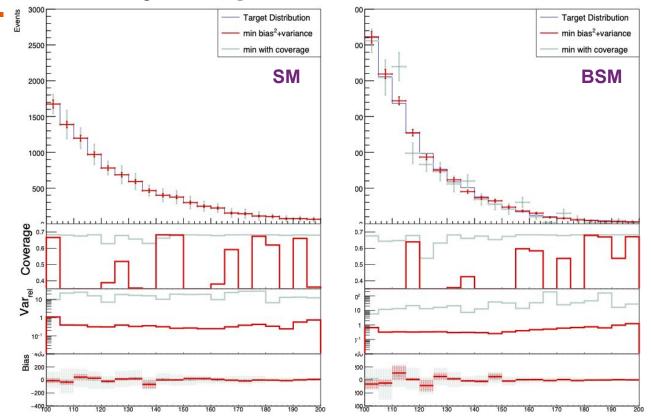
Richardson-Lucy (D'Agostini, IBU)

Looking at Coverage, Variance and Bias



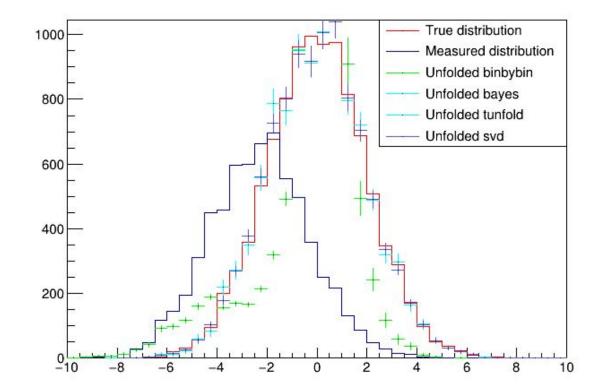


Richardson-Lucy (D'Agostini, IBU)



A Summary of Unfolding Methods in RooUnfold

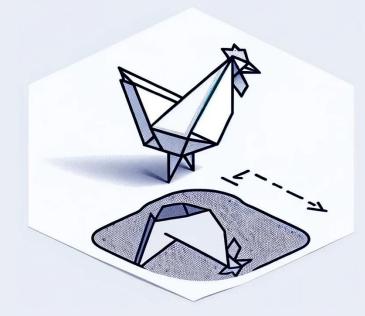
- Common interface to multiple methods
- Each with different error propagation
- Each with different responses to distributions
- Each with different regularisation parameters.





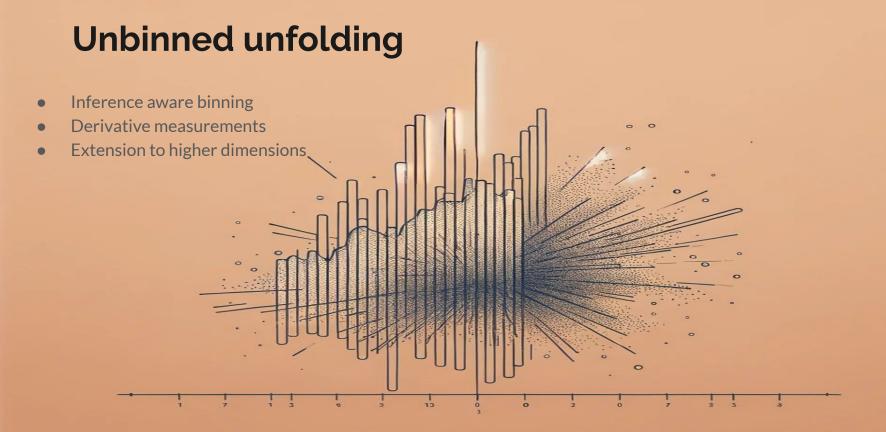
Detector uncertainties in the Likelihood

 $\mathcal{L}(\mu, \sigma \,|\, n)$



$$\mathcal{L}(\mu \mid \sigma, n)$$

$$\mathcal{L}(\mu \,|\, \hat{\sigma}, \bar{
u})$$



Function based unfolding

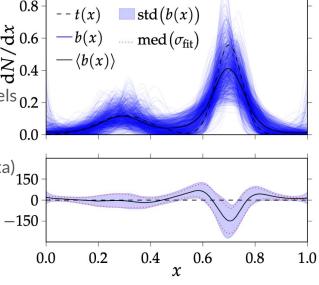
Goal: Train model to produce a function to approximate P(truth), evaluate conditional on data: P(truth|data)

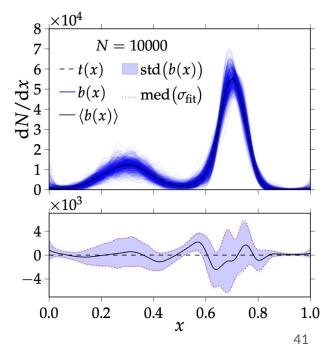
Three approaches:

• Fit a non-parametric density $\frac{\aleph}{N} 0.6 - \frac{1}{N}$ estimator.

• GAN/VAE learn implicit models $_{0.2}$ for \hat{P}

NF/DDIMs learn
 representation of P(truth|data)
 150





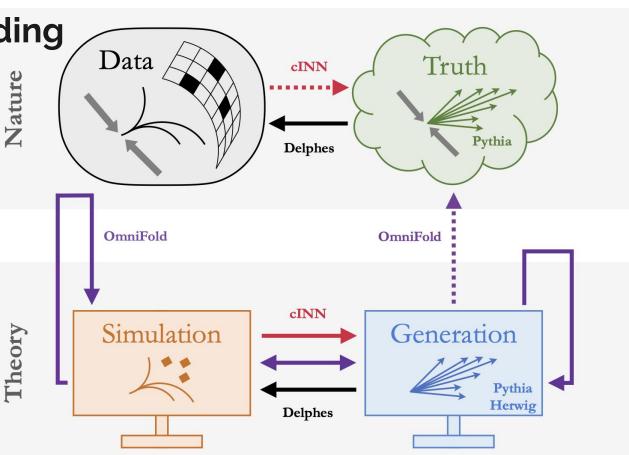
Detector-level

Particle-level

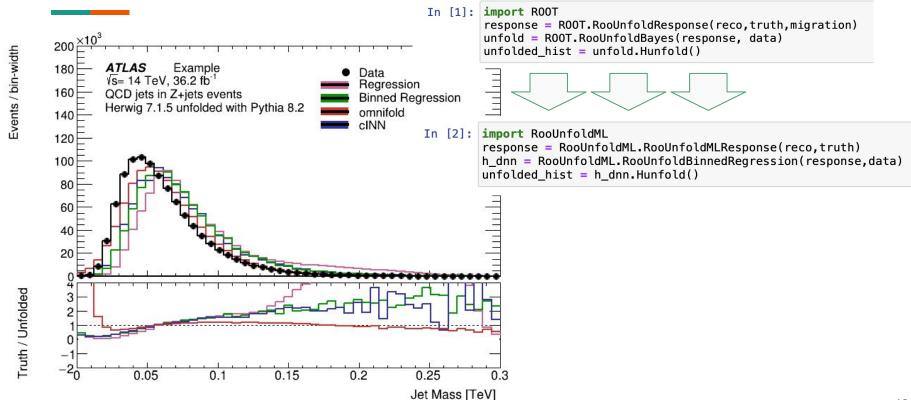
Classifier unfolding

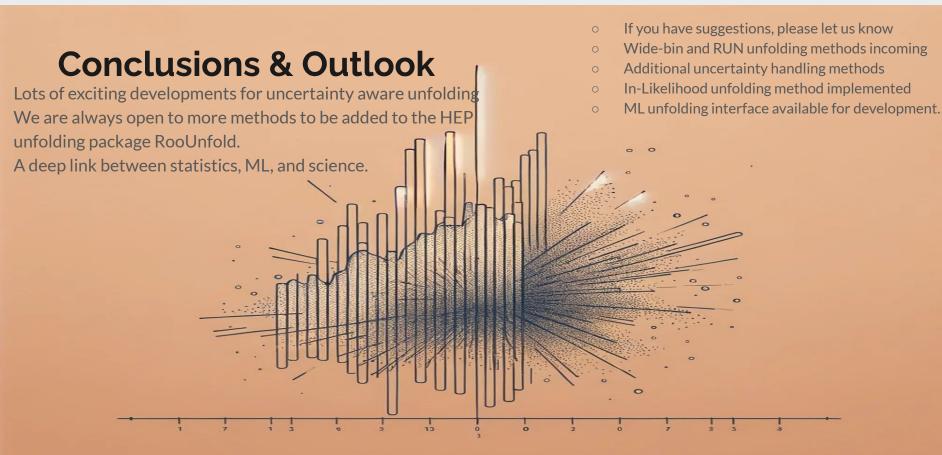
Goal: learn a function $\hat{\omega}$ that approximates the likelihood ratio

$$\omega(x) = rac{p(x)}{p_{ ext{MC}}(x)}$$



RooUnfoldML - https://gitlab.cern.ch/RooUnfold/RooUnfoldML/





Where do I find more information and code?

- RooUnfold; https://gitlab.cern.ch/RooUnfold (RooUnfold and RooUnfoldML)
- Paper; Comparison of unfolding methods using RooFitUnfold. International Journal of Modern Physics A, Vol. 35, No. 24, 2050145 (2020) https://arxiv.org/abs/1910.14654
- Paper; Publishing unbinned differential cross section results. JINST 17 (2022) 01, P01024
 https://arxiv.org/abs/2109.13243
- Paper; An algorithm for automatic unfolding of one-dimensional data distributions, Nuclear Instruments and Methods in Physics Research A 729 (2013) 410-416. PHYSTAT 2011

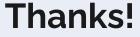
Per Christian Hansen: "Discrete Inverse Problems: Insight and Algorithms"

Discrete Inverse
Problems
Insight and Algorithms

Per Christian Hansen

Siam. On y = ATmult (

Issues or questions?



The whole RooUnfold team

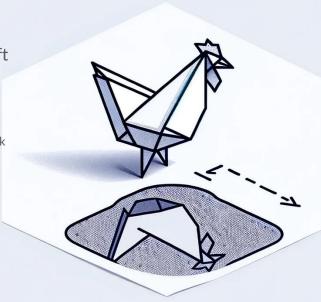
Lydia Brenner, Tim Adye, Carsten Burgard, Vincent Croft

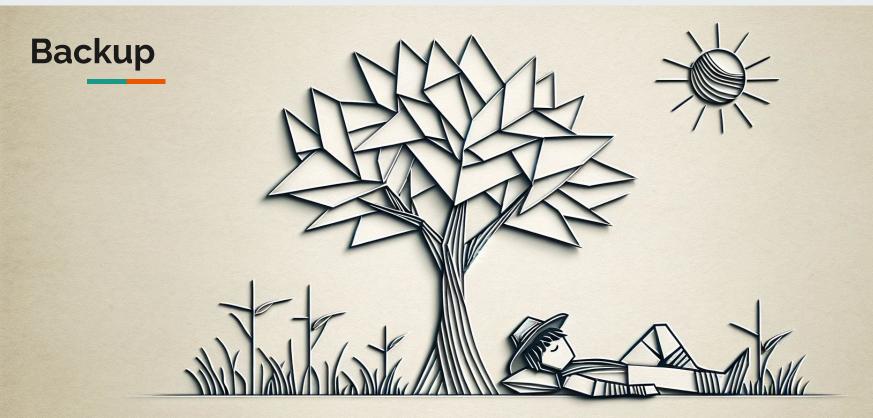
Les Houches PhysTeV workshop unfolding team:

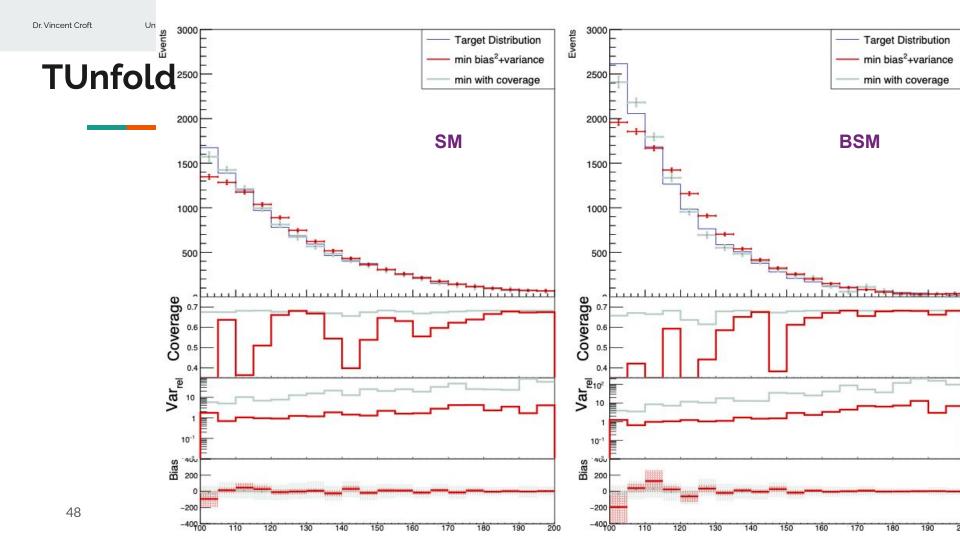
Miguel Arratia, Anja Butter, Mario Campanelli, Vincent Croft, Dag Gillberg, Aishik Ghosh, Kristin Lohwasser, Bogdan Malaescu, Vinicius Mikuni, Benjamin Nachman, Juan Rojo, Jesse Thaler, Ramon Winterhalder

Study collaborators

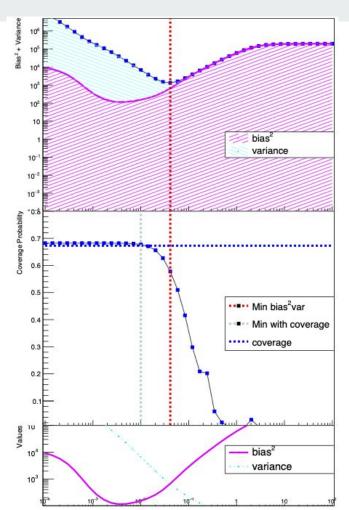
Pim Verschuuren, Glen Cowan, Wouter Verkerke



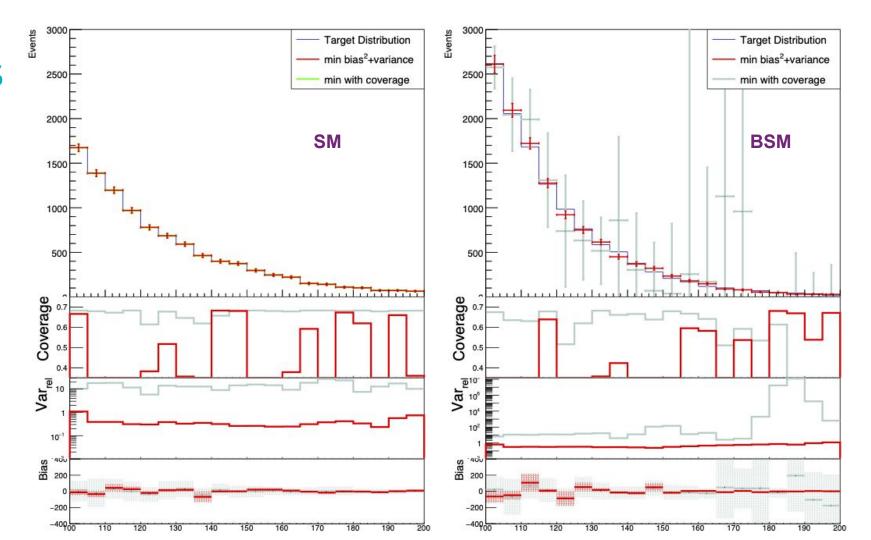




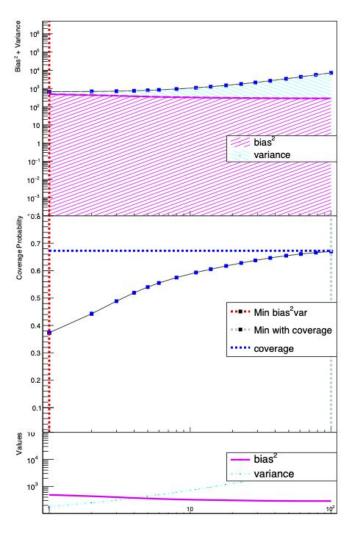
TUnfold



IBS



IBS



Look deeper into situations where the response matrix and the data are not sampled from the same model.

The bimodal model for this study is the sum of two Crystal Ball functions smeared by a a Gaussian resolution model

$$f(x|\alpha) = f_{\text{physics}}(x_{\text{true}}|\alpha) * f_{\text{detector}}(x_{\text{true}}, x)$$

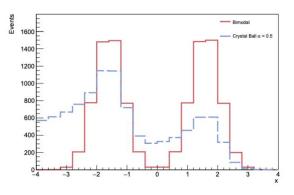
$$= (0.5 \cdot f_{CB}(x_{\text{true}}|\mu = 2.4, \sigma = 0.48, \alpha, n = 1) + 0.5 \cdot f_{CB}(x_{\text{true}}|\mu = 5.6, \sigma = 0.48, \alpha, n = 1))$$

$$* Gauss(x - x_{\text{true}}, 0, 0.4)$$

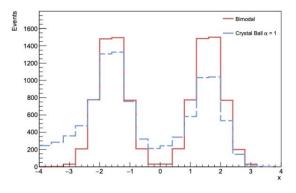
 $\alpha = 0.5$

 $\alpha = 1$

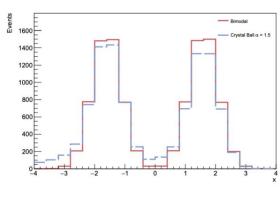
 $\alpha = 1.5$



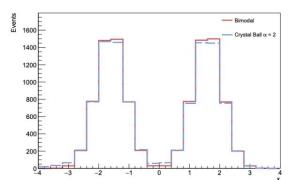


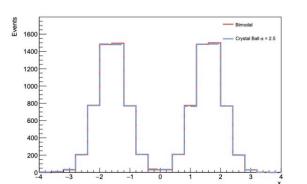


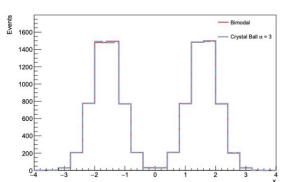
$$\alpha = 2.5$$



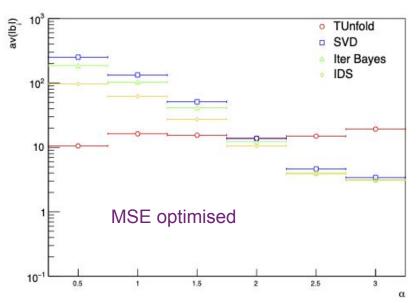


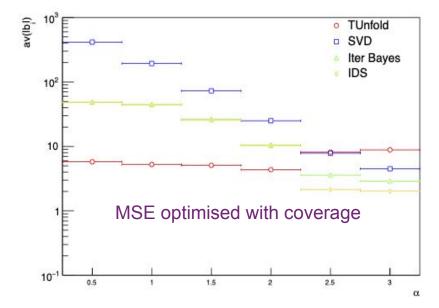




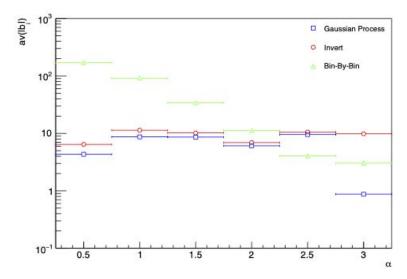


Bin-averaged unfolding bias for data from the distorted distribution unfolded with a response matrix for an undistorted distribution.





Bin-averaged unfolding bias for data from the distorted distribution unfolded with a response matrix for an undistorted distribution.



RooUnfold update

- Many frameworks / implementations for unfolding exist
 - Most use RooUnfold as a backend internally
 - Main focus of many of these frameworks: uncertainty handling
- Updates to RooUnfold itself
 - Integration with RooFit
 - Easier uncertainty handling
 - Workspace handling
 - Easy for combination
- Make RooUnfold "future proof"
 - Ready for possible unbinned unfolding methods in the future
 - Improved user friendliness
- End product
 - Saved in a way to allow changing of method at later time

Unfolding and fitting

- Unfold taking systematic variations into account
 - Also done by other advanced frameworks
- Can unfold after fitting signal and background contributions
 - Need to bring fit results into a format suitable as unfolding input
 - Non-trivial to propagate uncertainties
- Why not do both at the same time?
 - Ideal solution: RooFit implementation of unfolding!

Introduction to RooFitUnfold

- Idea: Updated implementation of RooUnfold directly in RooFit
- Includes: Improved handling of uncertainties
 - Uses error propagation from any NPs to the unfolded distribution
 - Allows for inclusion of uncertainties coming from migration matrix
- Handels different input formats
 - Histograms (as already RooUnfold did)
 - o pdfs -> Means unbinned distributions can now be unfolded
 - Binned methods allow setting of internal binning
 - unbinned methods can technically be included in the future
- Lives in workspaces

Methods included

All RooUnfold methods included

- Iterative Bayes
- IDS
- SVD
- TUnfold
- Gaussian Processes unfolding (NEW)
- Poisson unfolding, a simple likelihood unfolding (NEW)
- Unregularised
 - Bin-by-bin
 - Matrix inversion
- Can easily include more methods

Documentation:

https://gitlab.cern.ch/roofitunfold-tutorial-2019/RooUnfold/blob/master/README.md

https://arxiv.org/pdf/1105.1160.pdf

Implementation

- RooUnfold uses TH1 objects as basis
 - Very user-friendly, but internally not ideal with RooFit
- Templated to use RooAbsReal as a base object
 - Can easily be plugged on top of an existing workspace
- Created RooUnfoldFunc
 - a RooAbsReal wrapper around RooUnfold

Implementation: Inputs

- Truth distristributions
 - Histograms (TH1) or pdf (RooFit/Workspace)
- Reco distributions
 - Histograms (TH1) or pdf (RooFit/Workspace)
- Response matrix
 - 2D Histogram (TH2) or pdf (RooFit/Workspace)
- Data: background subtracted if needed
 - binned (TH1 or RooDataHist) or unbinned (TTree or RooDataSet)

Implementation: Features

- RooUnfoldFunc can be imported into workspace
 - Can use any existing workspace as an input
 - Can update reco level workspace after unfolding
 - Can unfold and fit (on reco-level) simultaneously
 - Easy persistence
 - Extremely useful for combinations
- RooUnfoldSpec can be used to construct RooUnfoldFunc
 - Helper class similar to HistFactory
- Unfolding result is only cached
 - Can switch to a different unfolding method a-posteriori

Workspace write out

- Directly written out into a workspace
 - At any level of the analysis
 - Saves all information to be able to do a change of unfolding method on the fly
 - Includes error propagation
 - Writes out for ALL unfolding methods
 - So also for regularised methods

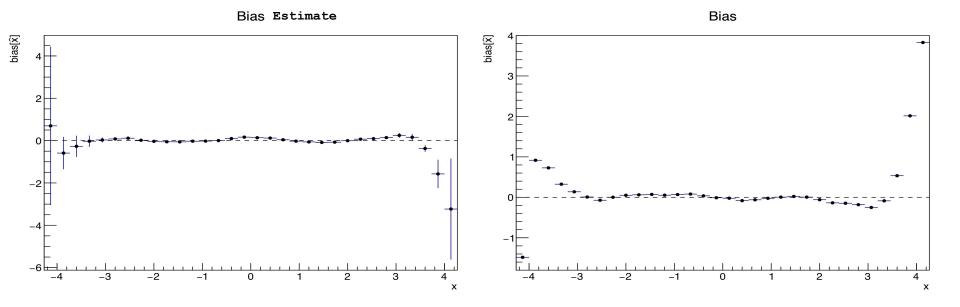
Error propagation

- Default RooUnfold can propagate simple uncertainties
 - Statistical uncertainties on Data
 - Bin-by-bin correlations
 - No handling of systematic uncertainties!
- RooFit functions (pdfs) can depend on arbitrarily many parameters
 - automatic error propagation from input parameters to all outputs by RooFit
 - ony requirement: the output needs to be a RooFit object
 - Nuisance parameter treatment comes "for free" with RooUnfold integration in RooFit
- No explicit handling of systematic uncertainties needed in RooUnfold
 - RooUnfold+RooFit handles uncertainties neatly :)
 - Some toy sampling methods required for bias calculation, but error bands on plots come directly from RooFit

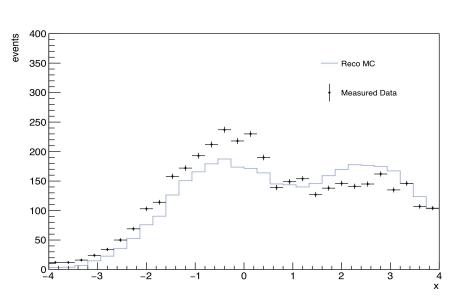
Bias

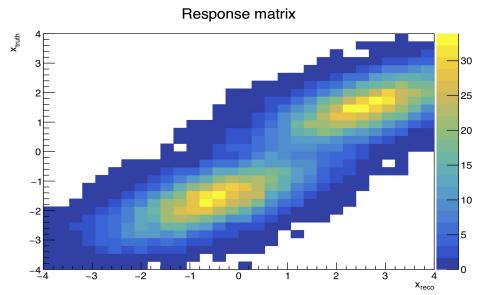
Two bias calculations included

Bias estimate without toys and a full bias calculation



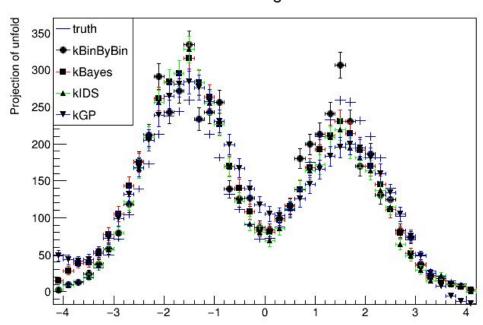
Reconstruction level plots



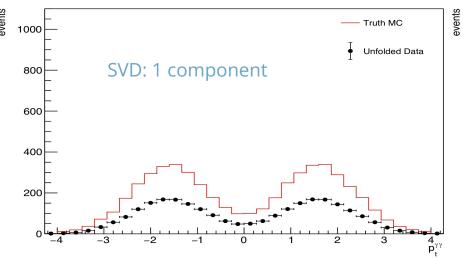


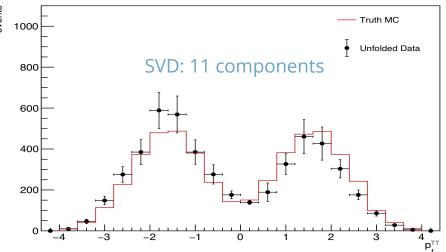
Compare different unfolding methods

Unfolding data



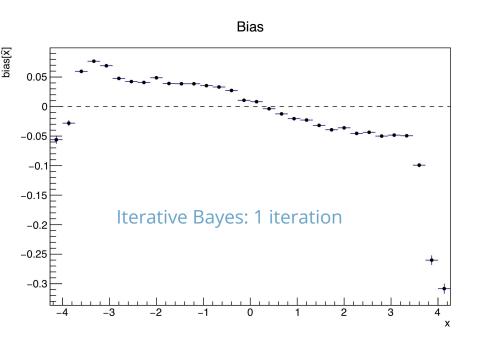
Compare different regularisation strengths

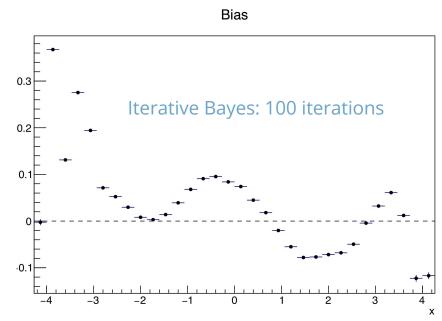




November 30th 2023

Compare different regularisation strengths: Don't forget the bias!





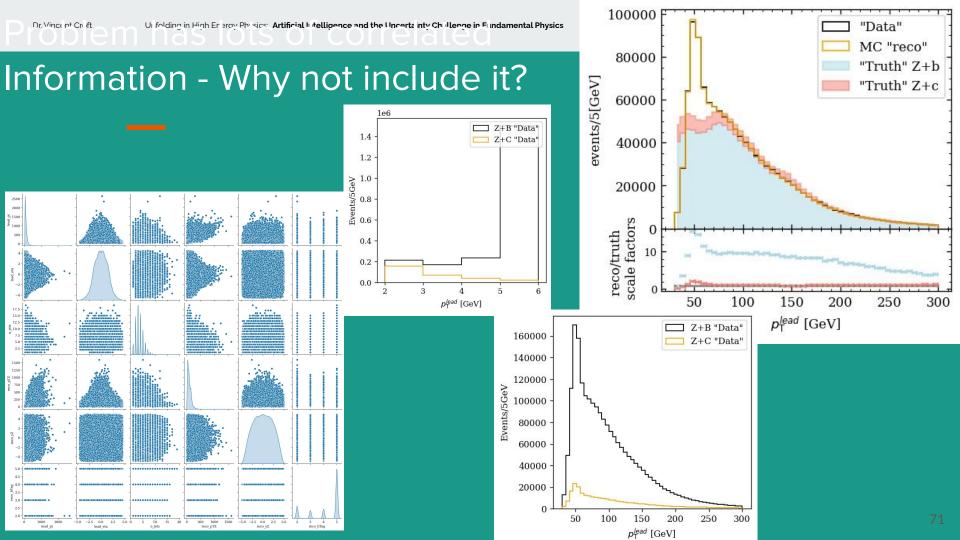
Bias calculation

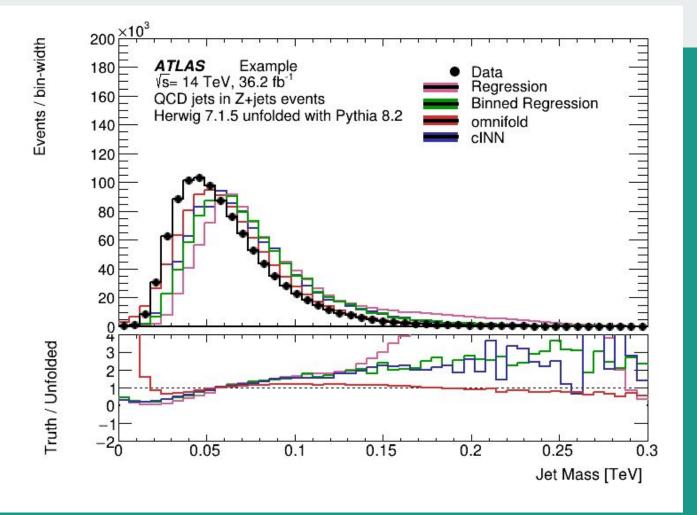
(Asimov) data-driven

First the uncertainties are taken truth level from the unfolded Asimov dataset. Toys are thrown in each bin around the Asimov truth values based on the full uncertainty. These toys are called level 1 toys. For each level 1 toy further toys are thrown, called level 2 toys. Each of the level 2 toys is folded and then unfolded with the chosen unfolding method. The bias for each level 2 toy is calculated as

biasl2 = $(\sigma refold - \sigma truth)/\sigma truth$,

where the truth refers to the value of the level 1 toy at truth level from which the level 2 toy is thrown and refold refers to the value of the level 2 toy after folding and unfolding. The bias of each bin in the distribution that is being unfolding is the average over all bias 12.





Lots of possibilities!

```
In [1]: import ROOT
    response = ROOT.RooUnfoldResponse(reco,truth,migration)
    unfold = ROOT.RooUnfoldBayes(response, data)
    unfolded_hist = unfold.Hunfold()
```



```
In [2]: import RooUnfoldML
response = RooUnfoldML.RooUnfoldMLResponse(reco,truth)
h_dnn = RooUnfoldML.RooUnfoldBinnedRegression(response,data)
unfolded_hist = h_dnn.Hunfold()
```

Easy to use

Dr Vincent Croft

- Will Ship as a lightweight extension to RooUnfold
- Optional extra flag on compilation
- Minimal Dependencies
- Meaningful default settings

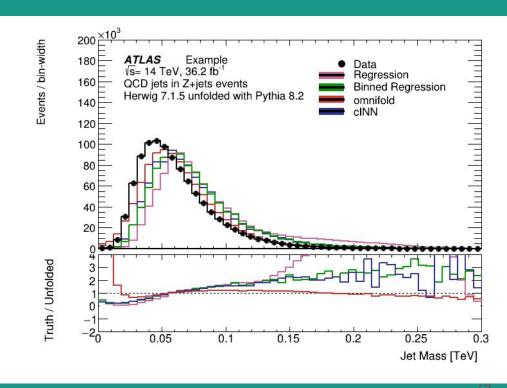
```
r = roounfoldml.RooUnfoldMLResponse(simobs, genobs)
cINN = roounfoldml.RooUnfoldCondition(r, dataobs)
cINN_data = cINN.Vunfold()
h_cINN = cINN.Hunfold("Mass",bin_edges)
```

Dr Vincent Croft

```
omnifold = roounfoldml.RooUnfoldReweight(r, dataobs)
omnifold_data,omnifold_weights = omnifold.Vunfold()
h_omni = omnifold.Hunfold("Mass",bin_edges)
```

```
reg = roounfoldml.RooUnfoldRegression(r, dataobs)
reg_data = reg.Vunfold()
h reg = reg.Hunfold("Mass",bin edges)
```

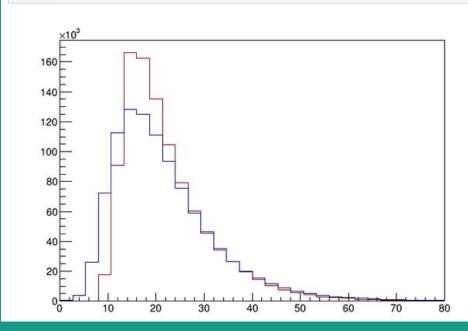
- Will Ship as a lightweight extension
- Optional extra flag on compilation
- Minimal Dependencies
- Meaningful default settings

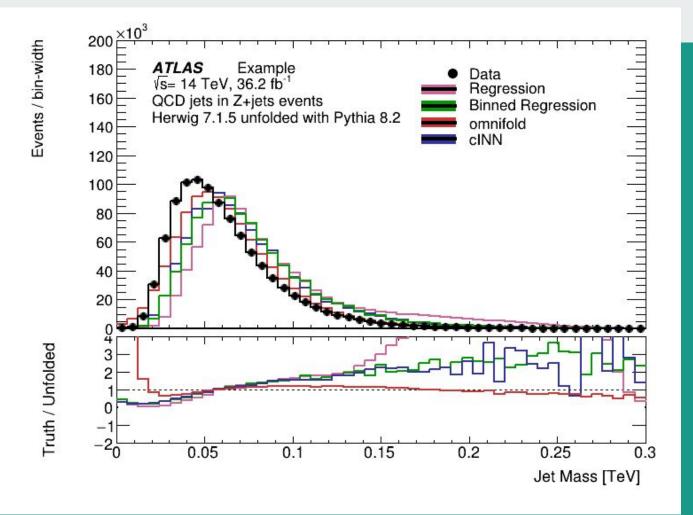


- Standard input is pandas dataframes
- Automatic conversion for:
 - TTree
 - **RDataFrame**
- Some internal conversions to tf.data.Datasets
- Might be inefficient.
- Easy integration with existing frameworks

```
dataobs = ROOT.RDF.MakeCsvDataFrame("/home/vcroft/dataobs.csv")
simobs = ROOT.RDF.MakeCsvDataFrame("/home/vcroft/simobs.csv")
genobs = ROOT.RDF.MakeCsvDataFrame("/home/vcroft/genobs.csv")
truthobs = ROOT.RDF.MakeCsvDataFrame("/home/vcroft/truthobs.csv")
```

```
roounfoldml.RooUnfoldMLResponse(simobs, genobs)
   roounfoldml.RooUnfoldRegression(r, dataobs)
data hist = truthobs.Histo1D(("","",30,0,80), 'Mass')
c = ROOT.TCanvas()
h = u.Hunfold("Mass", 30,0,80)
h.SetStats(0)
h.SetLineColor(ROOT.kRed+2)
h.Draw()
data hist.Draw("same")
c.Draw()
```





Lots of possibilities!