New approaches to the problem of unfolding

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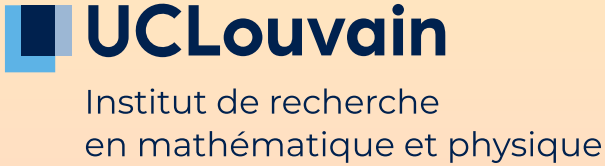

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Summary

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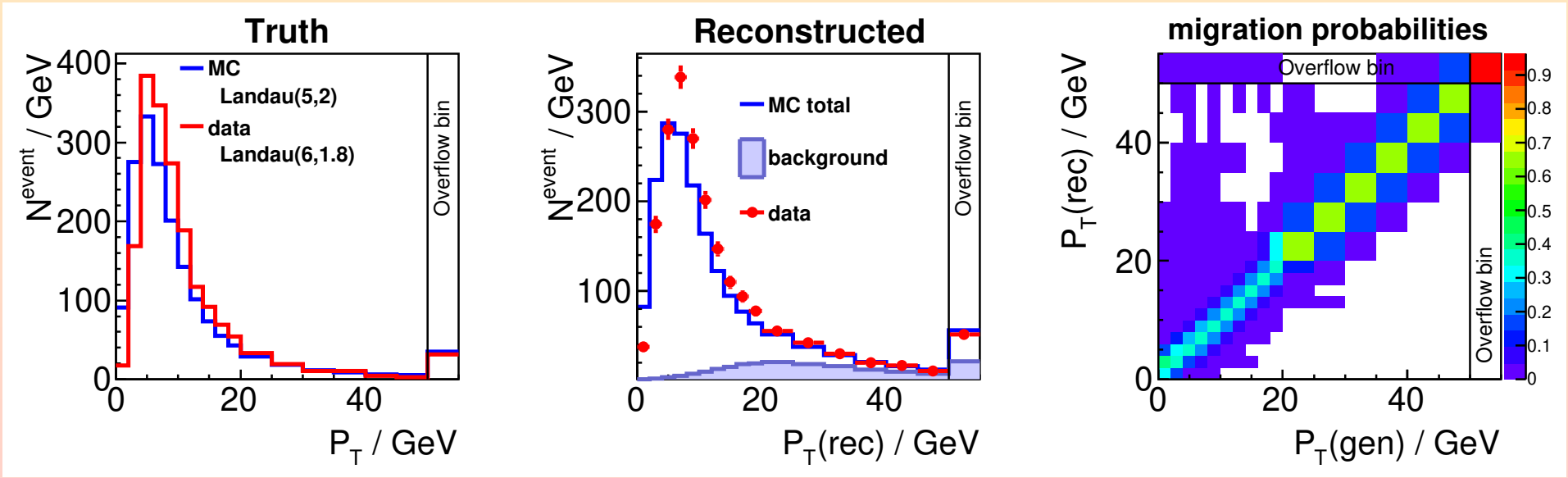
Unfolding: the problem

- Unfolding it's about how to invert a matrix that should not be inverted

$$\mathcal{L} = (\mathbf{y} - \mathbf{Ax})^T \mathbf{V_{yy}} (\mathbf{y} - \mathbf{Ax}),$$

- Observations y, to be transformed in the theory space into x
  - Model the detector as a response matrix
  - Invert the response to convert experimental data to theory space distributions
  - Usually to compare with models in the theory space
- The best solution is to fold any new theory and make comparisons in the experimental data space



Plot from ArXiv:1611.01927

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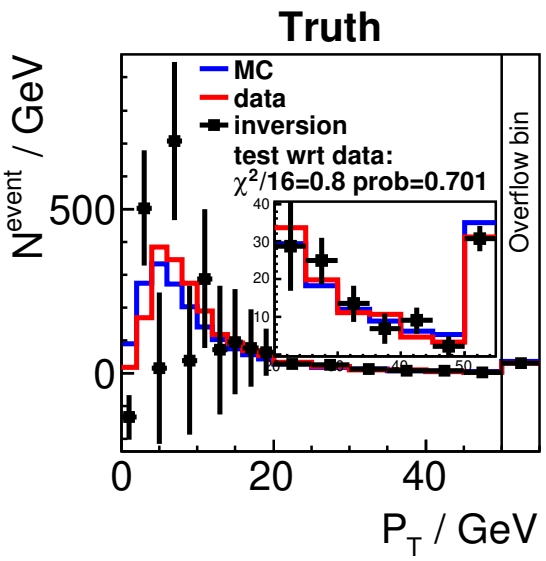
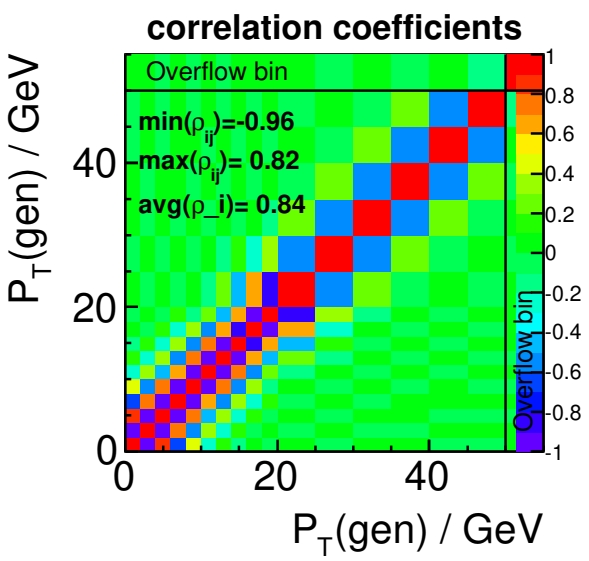
Unfolding: naïve solutions

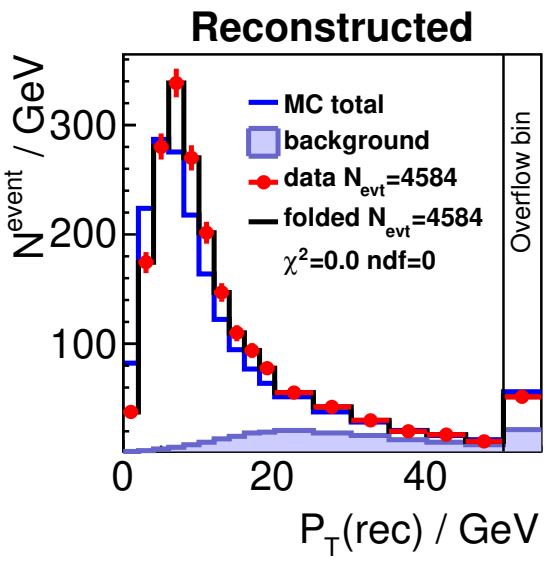
- Bin-by-bin correction factors $\hat{x}_i = (y_i - b_i)\frac{N_i^{\text{gen}}}{N_i^{\text{rec}}}$; disfavoured
  - Heavy biases due to the underlying MC truth
  - Yields the wrong normalization for the unfolded distribution
- Invert the response matrix $\hat{\boldsymbol{x}} = \boldsymbol{A}^{-1}(\boldsymbol{y} - \boldsymbol{b})$
  - Only for square matrices, but always unbiased
  - Oscillation patterns (small determinants in matrix inversion)
  - Patterns also seen as large negative $\rho_{ij} \sim -1$ near diagonal
  - Result is correct within uncertainty envelope given by $\boldsymbol{V}_{xx}$

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix}^{-1} = \frac{1}{ad-bc}\begin{bmatrix} d & -b \\ -c & a \end{bmatrix}$$

determinant







Cartoon from https://www.mathsisfun.com/algebra/matrix-inverse.html, plots from ArXiv:1611.01927

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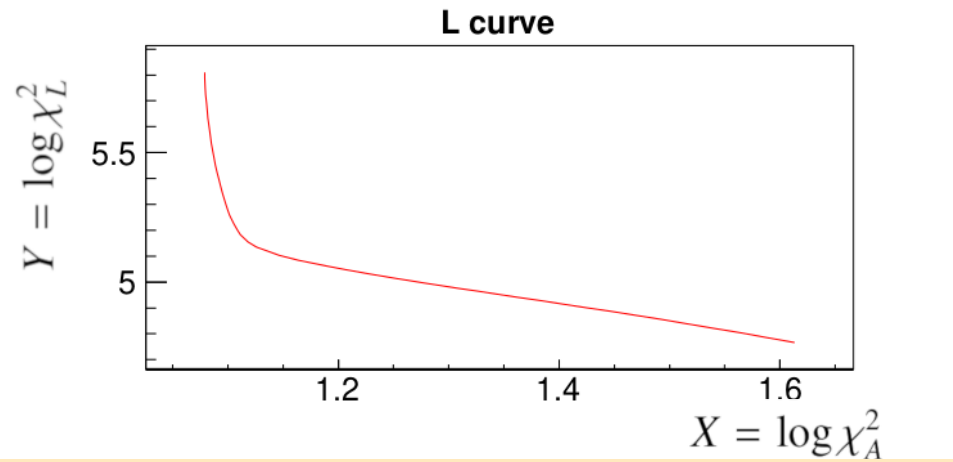
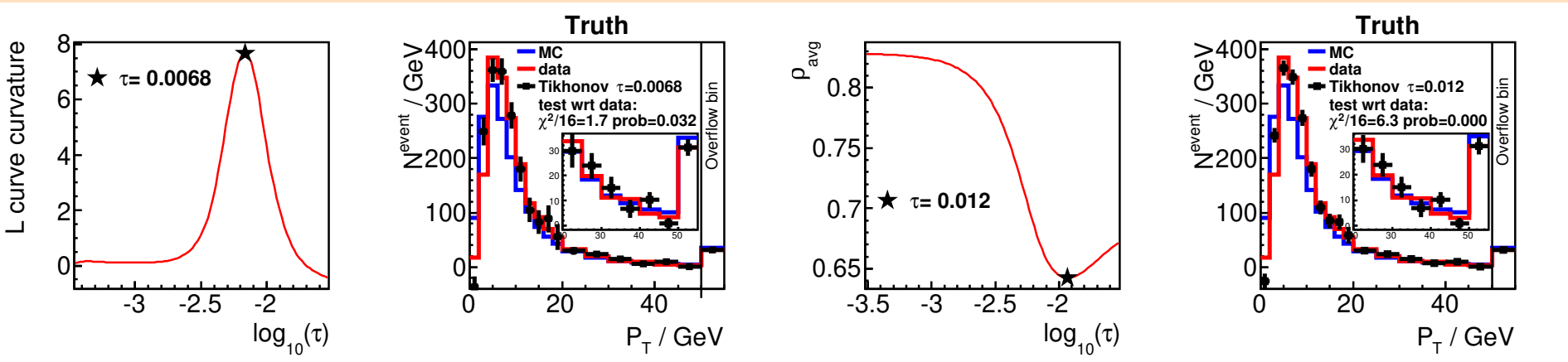
Unfolding: regularization 1/

$$\chi^2_{\text{TUnfold}} = \chi^2_A + \tau^2 \chi^2_L$$
$$\chi^2_A = (\boldsymbol{A}\hat{\boldsymbol{x}} + \boldsymbol{b} - \boldsymbol{y})^{\mathsf{T}} (\boldsymbol{V_{yy}})^{-1} (\boldsymbol{A}\hat{\boldsymbol{x}} + \boldsymbol{b} - \boldsymbol{y})$$
$$\chi^2_L = (\hat{\boldsymbol{x}} - \boldsymbol{x_B})^{\mathsf{T}} \boldsymbol{L}^{\mathsf{T}} \boldsymbol{L} (\hat{\boldsymbol{x}} - \boldsymbol{x_B})$$



- Choose τ corresponding to maximum curvature of L-curve
- Or minimize the global $\rho_{\text{avg}} = \frac{1}{M_x} \sum_{j=1}^{M_x} \rho_j$
  - Often results in stronger regularization than L-curve



Plots from ArXiv:1611.01927

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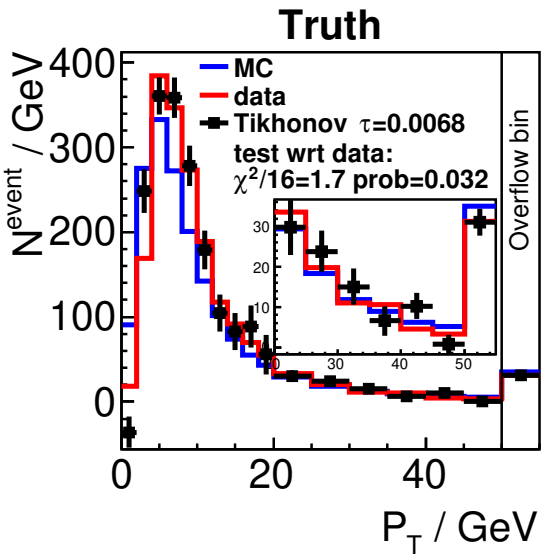
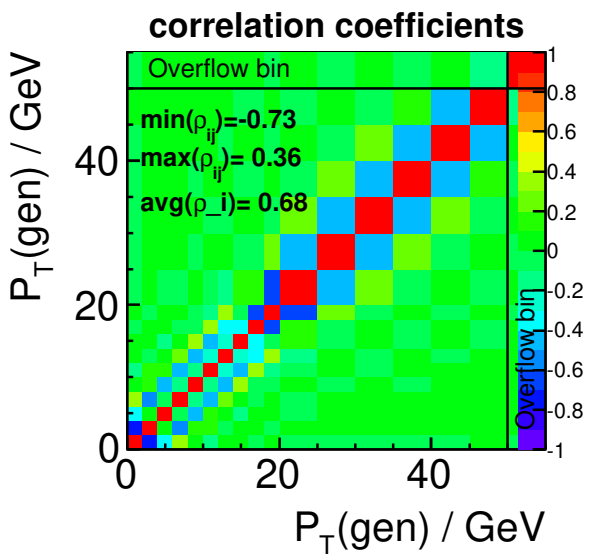
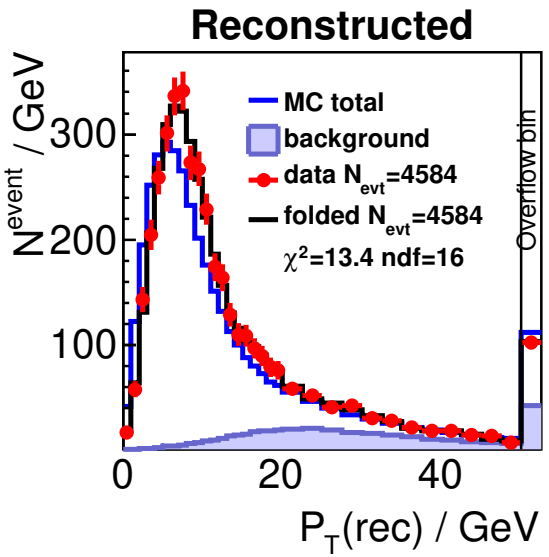
Unfolding: regularization 2/

$$\mathcal{L}(\mathbf{x},\lambda) = \mathcal{L}_1 + \mathcal{L}_2 + \mathcal{L}_3,$$
$$\mathcal{L}_1 = (\mathbf{y}-\mathbf{A}\mathbf{x})^T \mathbf{V}_{\mathbf{yy}} (\mathbf{y}-\mathbf{A}\mathbf{x}),$$
$$\mathcal{L}_2 = \tau^2 (\mathbf{x}-f_b\mathbf{x_0})^T (\mathbf{L}^T\mathbf{L})(\mathbf{x}-f_b\mathbf{x_0}),$$
$$\mathcal{L}_3 = \lambda(Y - \mathbf{e}^T\mathbf{x}),$$
$$Y = \sum_i y_i,$$
$$e_j = \sum_i A_{ij}.$$

- $\mathbf{y}$: observed yields
- $\mathbf{A}$: response matrix
- $\mathbf{x}$: the unfolded result
- $\mathcal{L}_1$: least-squares minimization ($V_{ij} = e_{ij}/e_{ii}e_{jj}$ correlation coefficients)
- $\mathcal{L}_2$: regularization with strength τ
- Bias vector $f_b\mathbf{x_0}$: reference with respect to which large deviations are suppressed
- $\mathcal{L}_3$; area constraint (bind unfolded normalization to the total yields in folded space)







Plots from ArXiv:1611.01927

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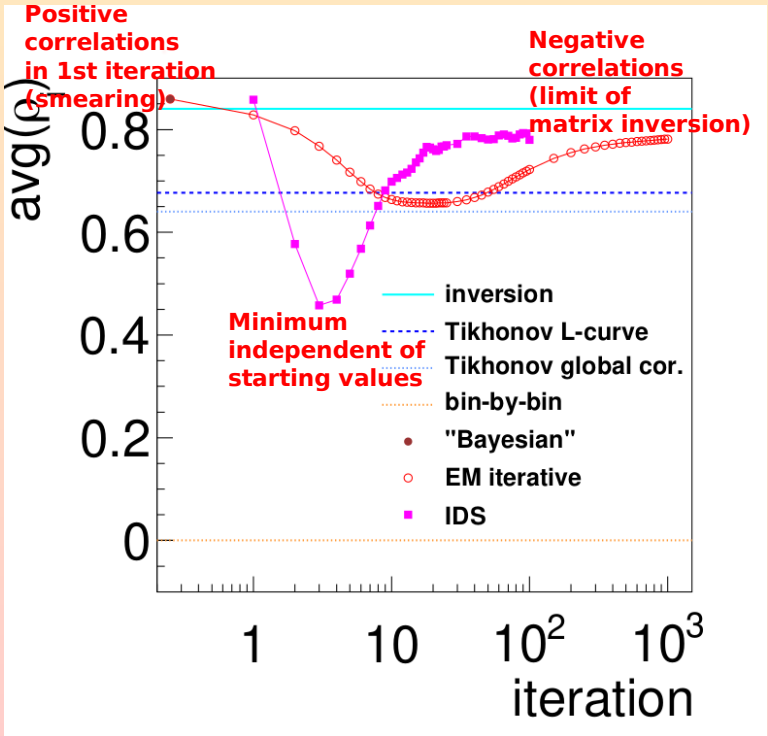
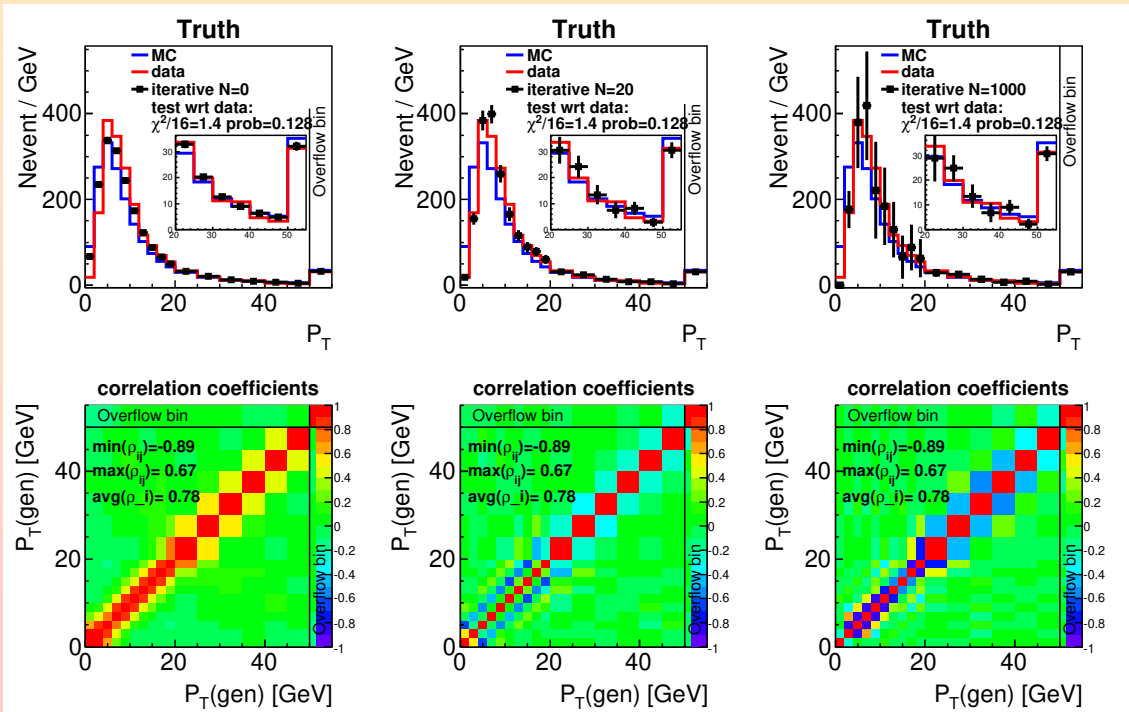
Unfolding: Iterative Unfolding

- Iterative improvement over the result of a previous iteration;

$$x_j^{(n+1)} = x_j^{(n)} \sum_{i=1}^{M} \frac{A_{ij}}{\epsilon_j} \frac{y_i}{\sum_{k=1}^{N} A_{ik} x_k^{(n)} + b_i}$$

  - It converges (slowly, $N_{iter} \sim N_{bins}^2$) to the MLE of the likelihood for independent Poisson-distributed y_i
  - Not necessarily unbiased for correlated data (does not make use of covariance of input data V_{yy})
- In HEP most people don't iterate until convergence
  - Fixed N_{iter} is often used; the dependence on starting values provides regularization
- Intrinsically frequentist method
  - for $N_{iter} \to \infty$ converges to matrix inversion, if all $\hat{x}_j$ from matrix inversion are positive
  - $N_{iter} = 0$ sometimes called improperly "Bayesian" unfolding (the author, D'Agostini, is Bayesian)
- Don't use software defaults!!! (e.g. some software has $N_{iter} = 4$)
  - Minimizing the global ρ is a good objective criterion, but there are others (Akaike information, etc)





Plots from arXiv:1611.01927

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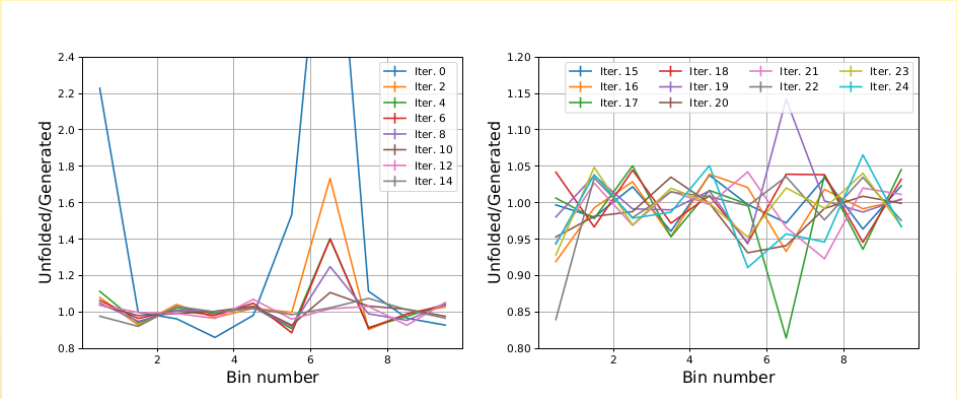
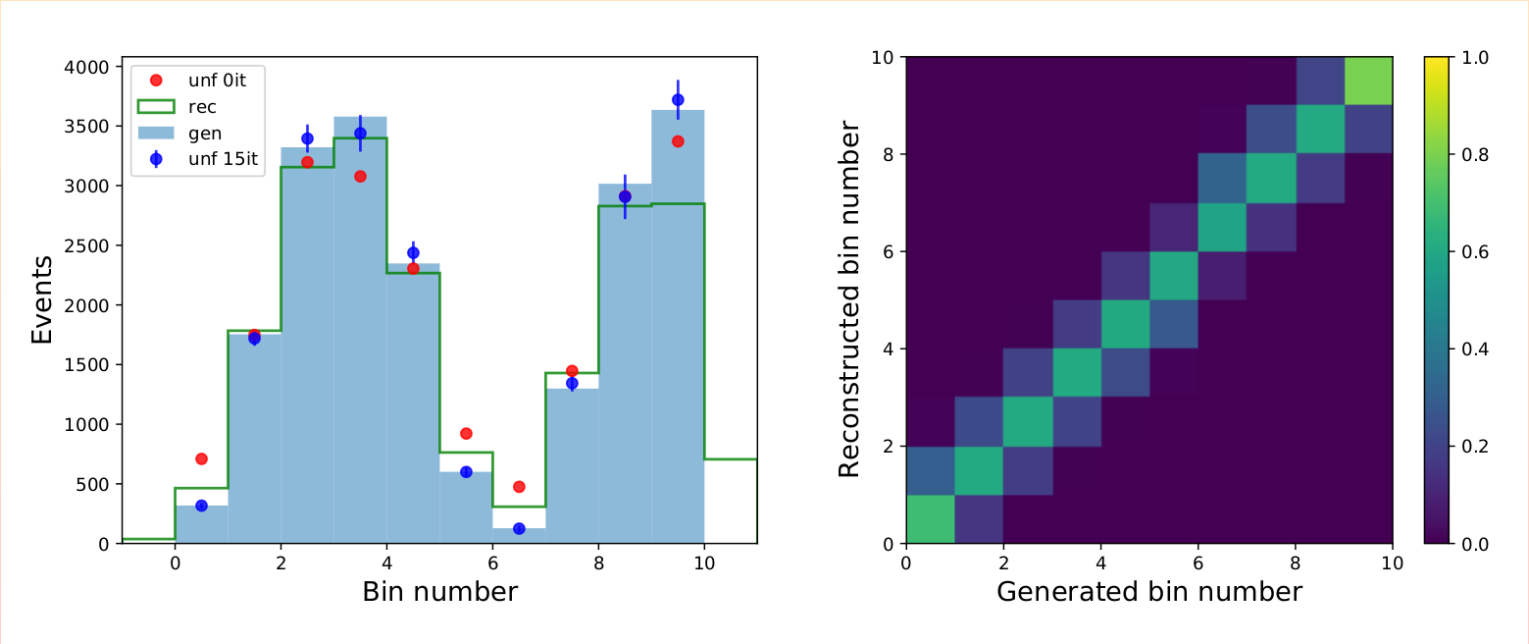
Unfolding with ML

- 1712.01814 frames the problem as a classification one
  - Assign to each reconstructed data event the most probable truth bin
- Iterative process: train using flat inputs, apply to data to obtain updated binned distribution, use result to resample, retrain
- True space discretization regularizes the problem even before performing unfolding
- Coverage studies not (yet?) performed





Two proposed methods (shipped with the next arXiv posting)

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- Density estimation with normalizing flows
  - Estimate the transformation from true to smeared space (i.e. the response matrix) with masked autoregressive flows
  - Obtain an invertible transformation that can be used to transform arbitrary distributions
  - Unbinned method! Binning is performed only for displaying purposes (can use unbinned, or study regularization induced by binning)
  - Can unfold many variables at the same time (under study)
- Unfold without unfolding
  - Start from a distribution in true space (either a simulation, or a flat distribution)
  - Create proposal by resampling according to the statistical uncertainty in each bin
  - Fold the proposal using the untouched response matrix
  - Stochastically travel by accepting proposals if their folded realization is closer to the data than the current proposal
  - Purely binned method, further regularization schemes shown to be necessary

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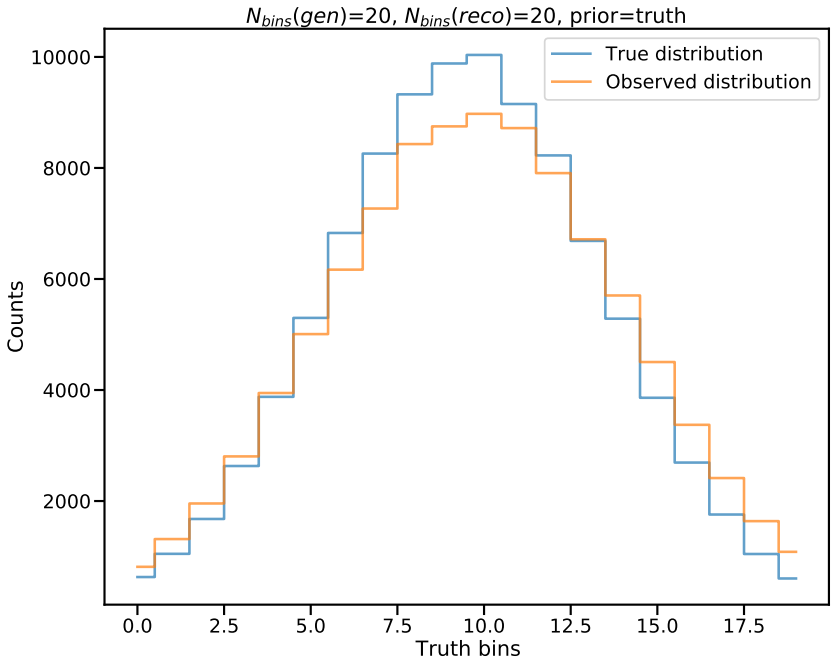
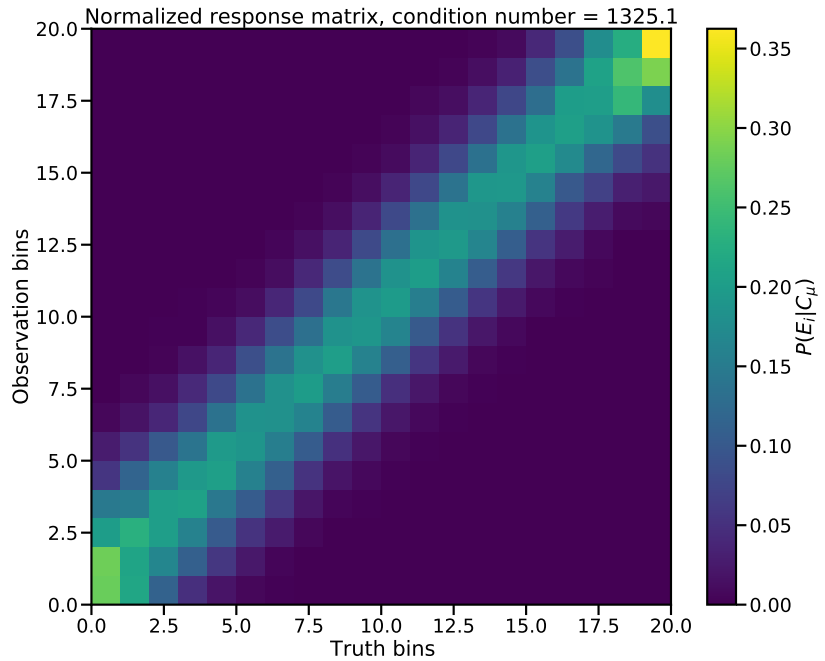
The scenarios

- Very simple scenarios based on Gaussian distributions smeared with random noise, 100k events per scenario
- Alternative data (representing scenarios where the data don't come from the assumed true distribution) generated by further smearing and shifting
- Different scenarios: less diagonal matrices will induce need for regularization)
  - Diagonality from max and min singular values in SVD decomposition of the response matrix $cond(R) := \frac{\sigma_{\max}}{max(0,\sigma_{\min})}$
- Different scenarios: $N_{bins}(gen)$ larger, smaller, or equal to $N_{bins}(reco)$





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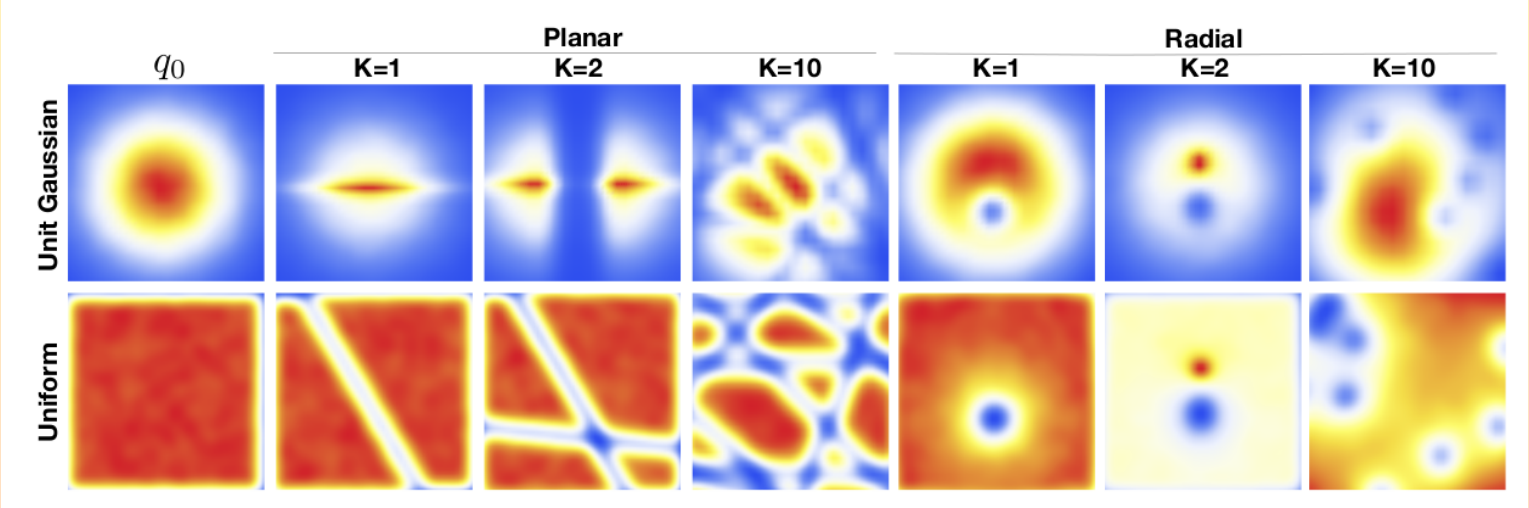
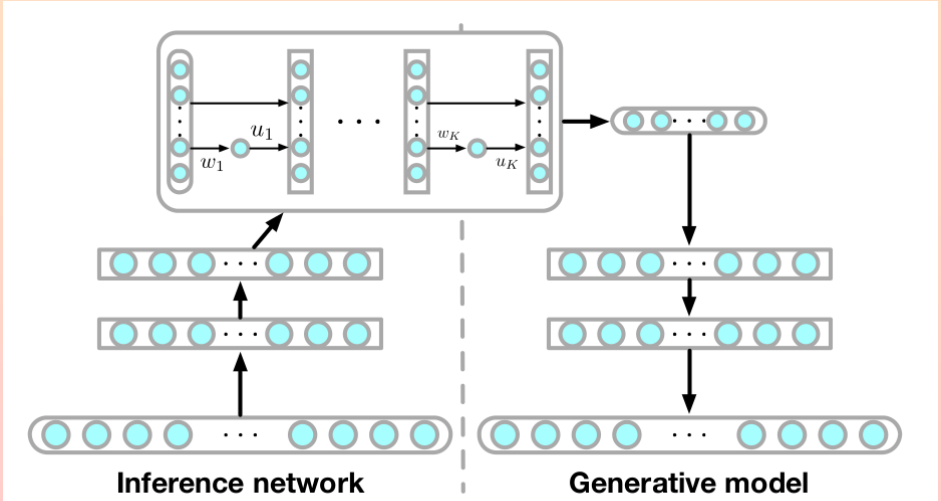
Normalizing flows

- Variational inference (Rezende and Mohamed, 1505.05770)
  - Start from a simple density
  - Apply a sequence of invertible transformations until the desired complexity is reached
- Combination of inference and generative model
  - Inference network maps observations to the parameters of the model
  - Generative model receives the posterior samples from the inference network at training time





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Gaussian autoregressive models

- Decompose a joint density into a product of conditional densities
  - Condition on *previous* variables (time series, or lower-index coordinates for some ordering
  - Predicted value of features depend on past values of the same feature, rather than on other predictors
- Used for density estimation
  - Take some variable with some implicit ordering (e.g. tensor)
  - Output a mean and standard deviation for each element of the input, conditioned on previous elements
- In a sense, a Bayesian network

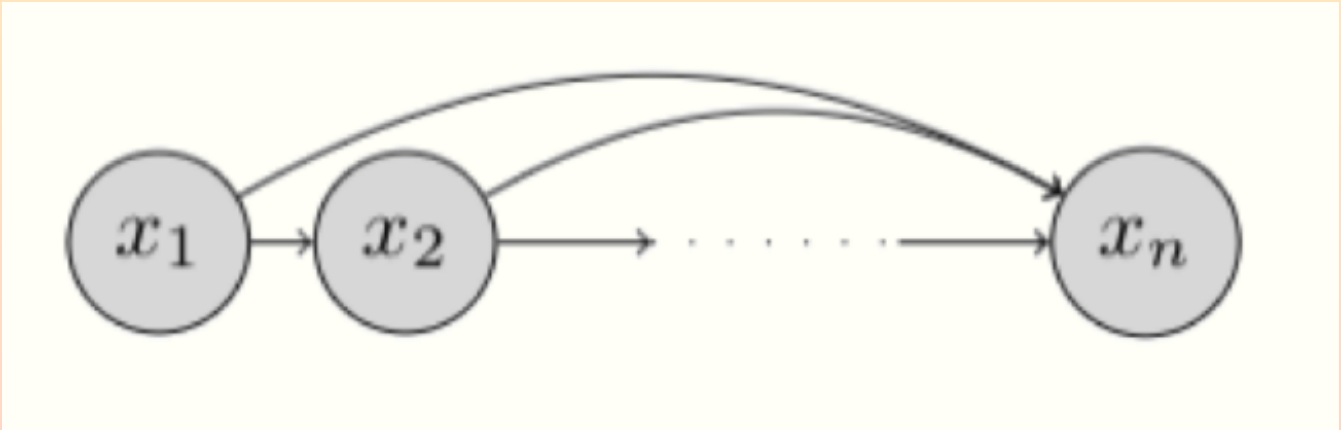

Image from https://deepgenerativemodels.github.io

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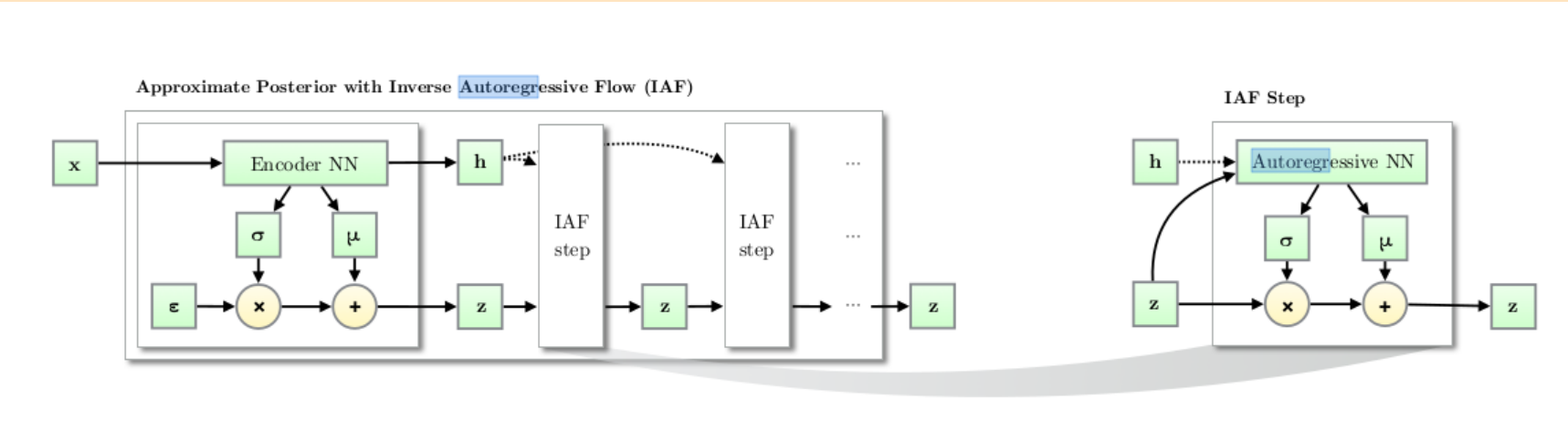
Autoregressive models are normalizing flows (if invertible)!

- Kingma and colleagues 1606.04934
  - Autoregressive models result in tranformations that by construction have a tractable Jacobian
  - If the transformation is also invertible, then the model is equivalent to a normalizing flow
- Can therefore be used for density estimation, e.g. Inverse Autoregressive Flow
- Decompose the operation of sampling from a posterior (typical Bayesian operation, e.g. in MCMC or ABC)
  - Sample from a very simple gaussian distribution
  - Apply chain of nonlinear invertible transformations
  - Obtain posterior sample



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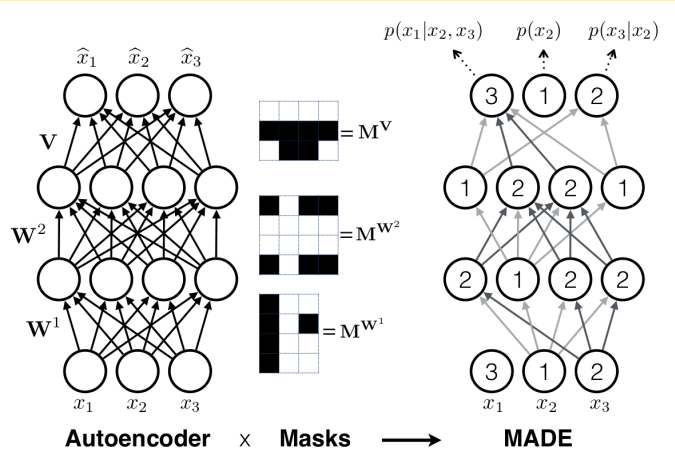
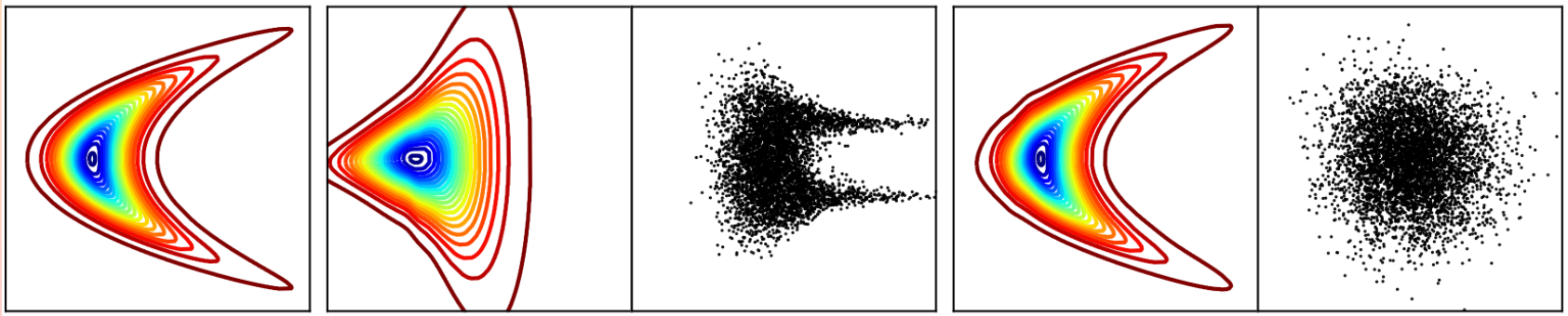
MADE and MAF

- MADE Germain and colleagues, 1502.03509
  - Masked Autoencoders for Distribution Estimation
  - Vectorized architecture for density estimation based on autoencoders
  - Fast and reliable
  - *Masked*: deactivate inputs to enforce autoregressive model!
- Masked Autoregressive Flows (MAF), Papamakarios and colleagues, 1705.07057
  - If you stack several autoregressive models that each learn a conditional density, you obtain a normalizing flow!





(a) Target density (b) MADE with Gaussian conditionals (c) MAF with 5 layers

Learn response matrix with MAF

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- MAF composed of 10 MADE layers, with permutation after each one
  - Each model is essentially a copy of the first set of coordinates and a transformation of the second set of coordinates
  - Permutation ensures that in the next step the transformed coordinates are those that were simply copied at the previous step
- I use a simple Gaussian distribution as an input to the learning process

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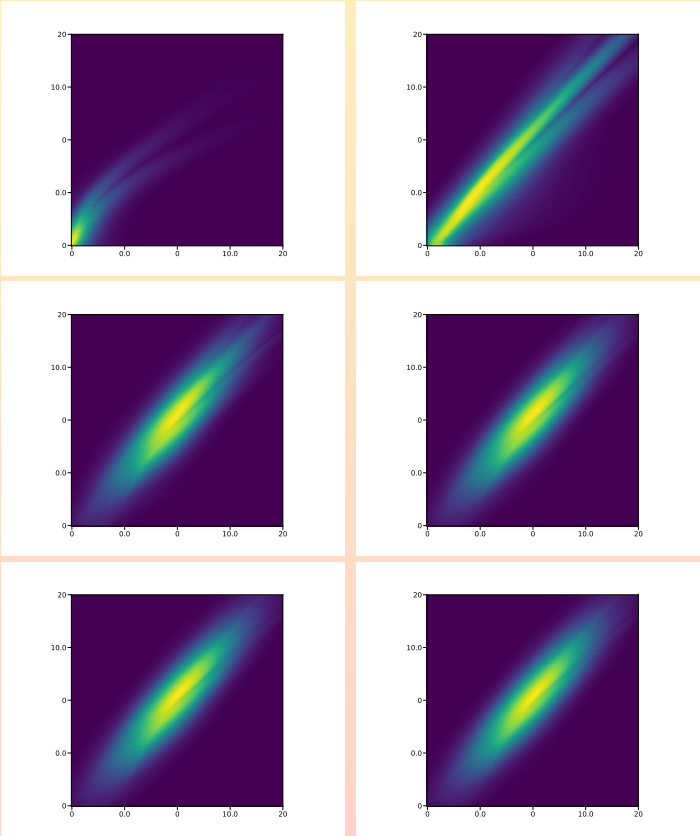
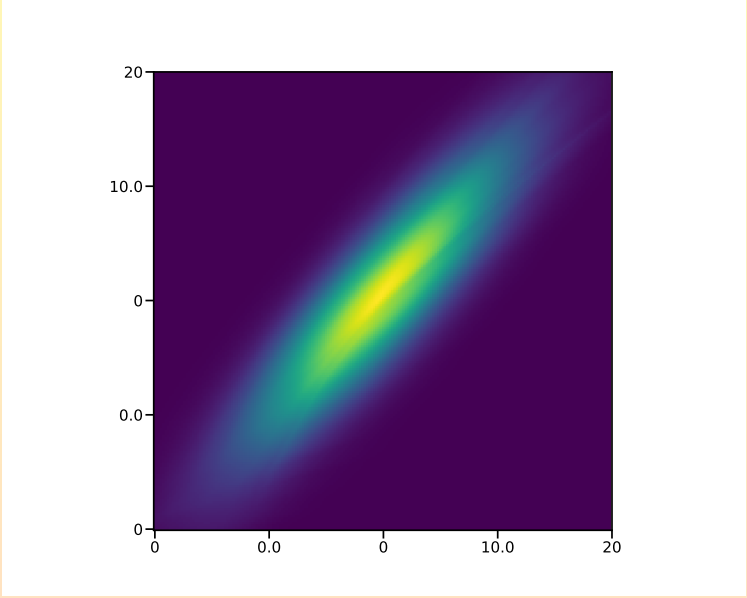
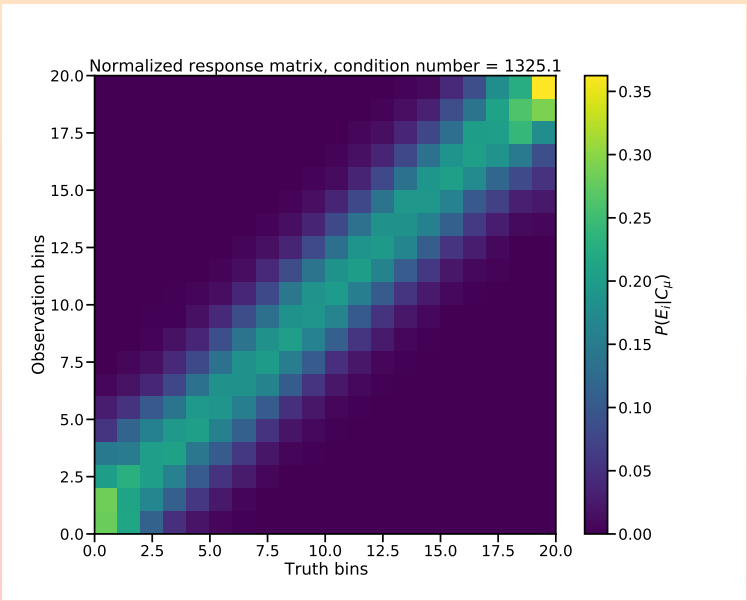
Learned response matrix

- 100 epochs (if early stopping, regularization)
- Density at epoch 0, 10,.. 50



- Final learned density: need to improve at boundaries





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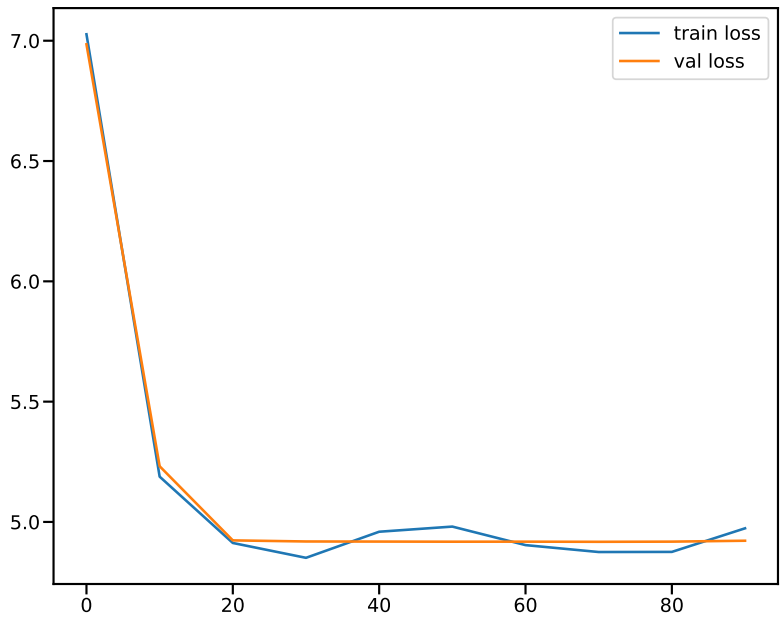
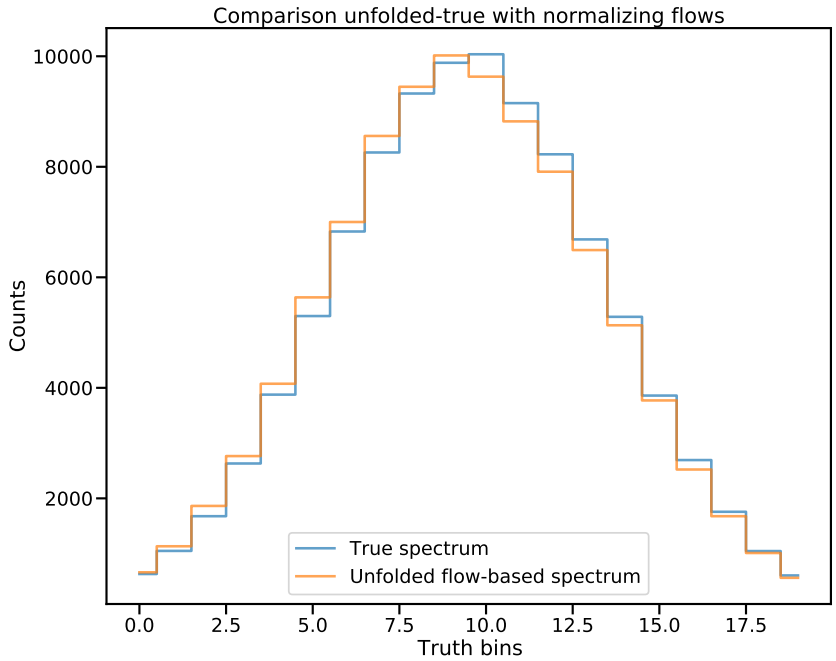
Use inverted MAF transformation as inverse of response matrix

- Unfolding by transforming data using the MAF density suffers from the density not completely learned
- More studies ongoing with more complex models (gaussian-to-gaussian might be too simple) and using manifold learning





Unfolding by folding

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- Why should we invert the response matrix, when we can resample?
  - Start from binned distributions (but implicit regularization!)
  - We can resample as many times as we want in the true space
  - Assume a distribution, then resample assuming a Poisson pdf in each bin
  - Fold the resulting distribution, and compare it with data with a statistical test
  - If the test hints at better compatibility, accept proposal, otherwise keep the current one
- Turned out that the general idea was also developed by Landweber, 1951, but with gradient descent
- My proposal is then essentially a stochastic optimization version of the Landweber method

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Algorithm

- Can set threshold on the compatibility test for early stopping (regularization)
- Algorithm rather robust with respect to changes of statistical test
  - Pearson's χ^2 and its *minbin* modification by Porter, Bhattacharyya distance, Kullback-Leibler divergence, Wasserstein Distance etc
- Uncertainties from building a full distribution using best proposals (similar to ABC modification under study)

Algorithm 1: The algorithm to resample in the truth-level space until the folded distribution of the sample coincides with the data distribution. I have to put an early stopping and remove the maximum number of iterations.

input : A truth distribution $\boldsymbol{x}_s$;
the data distribution $\boldsymbol{y}$;
the response matrix R;
the number of iterations $N_{samples}$;
a statistical test *test* and an optional condition *oc* for similarity between histograms;
an optional early-stopping condition *sc*.

output: The random sample $\hat{\boldsymbol{x}}_{best}$ whose folded version matches the better with the data distribution.

$\hat{\boldsymbol{x}}_{best} \leftarrow \boldsymbol{x}_s$;
$TS_{best} \leftarrow 10^5$;
for $i \leftarrow 0$ **to** $N_{samples}$ **do**
  $\boldsymbol{x}_i \sim Pois(\boldsymbol{x}_{best})$;
  $\boldsymbol{y}_i \leftarrow R\boldsymbol{x}_i$;
  $TS \leftarrow test(\boldsymbol{y}_i, \boldsymbol{y})$;
  if $TS < TS_{best}$ *and* *oc* **then**
    $\hat{\boldsymbol{x}}_{best} \leftarrow \boldsymbol{x}_i$;
    $TS_{best} \leftarrow TS$;
  end
  if *sc* **then**
    return
  end
end

Dependence on parameters

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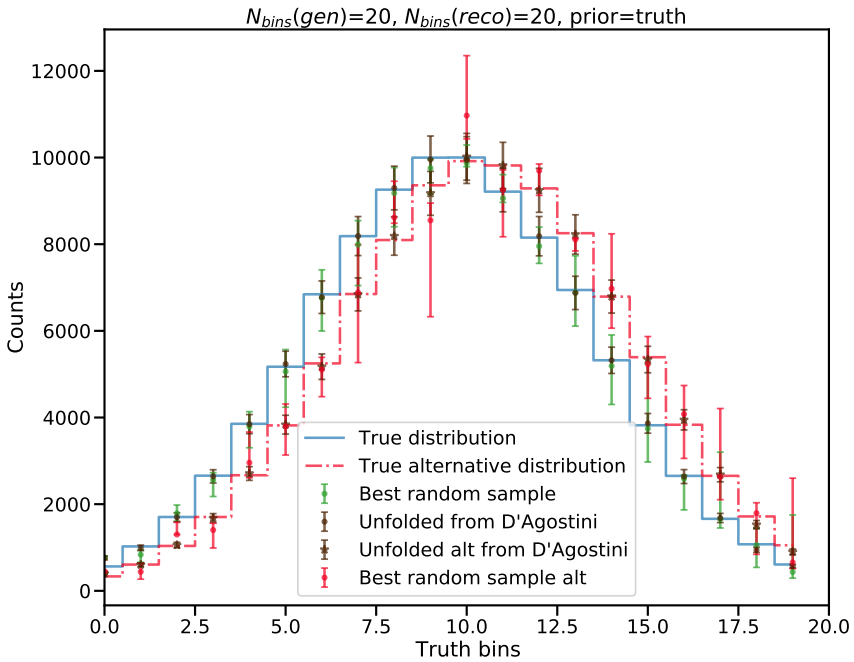
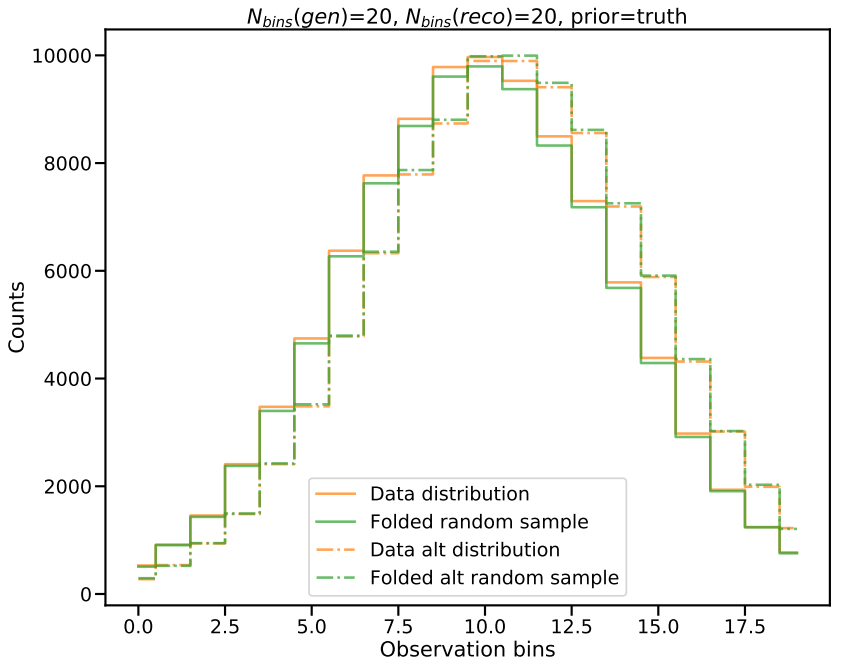
- Use d'Agostini unfolding as a reference for comparison
- The method performs very well for diagonal matrices...





Dependence on parameters

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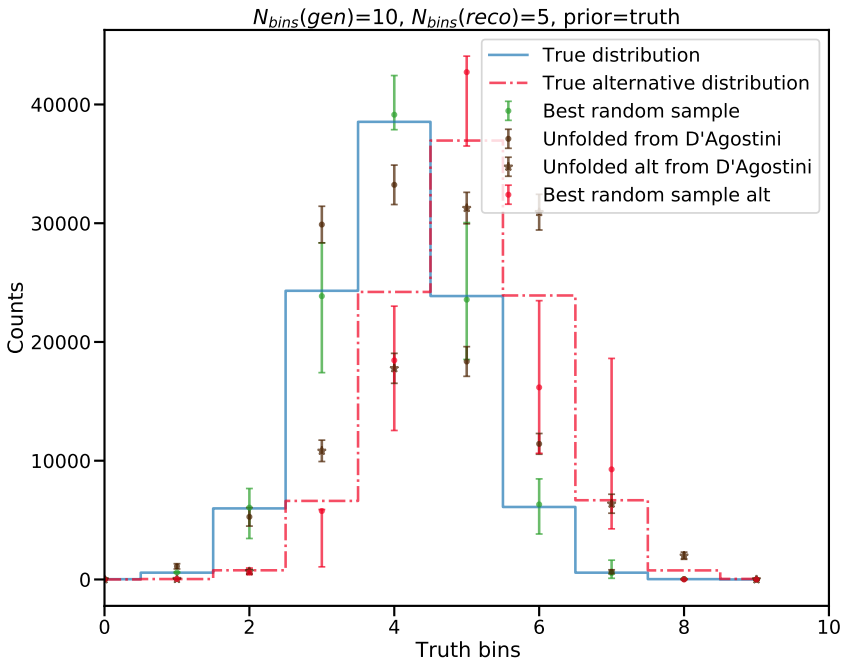
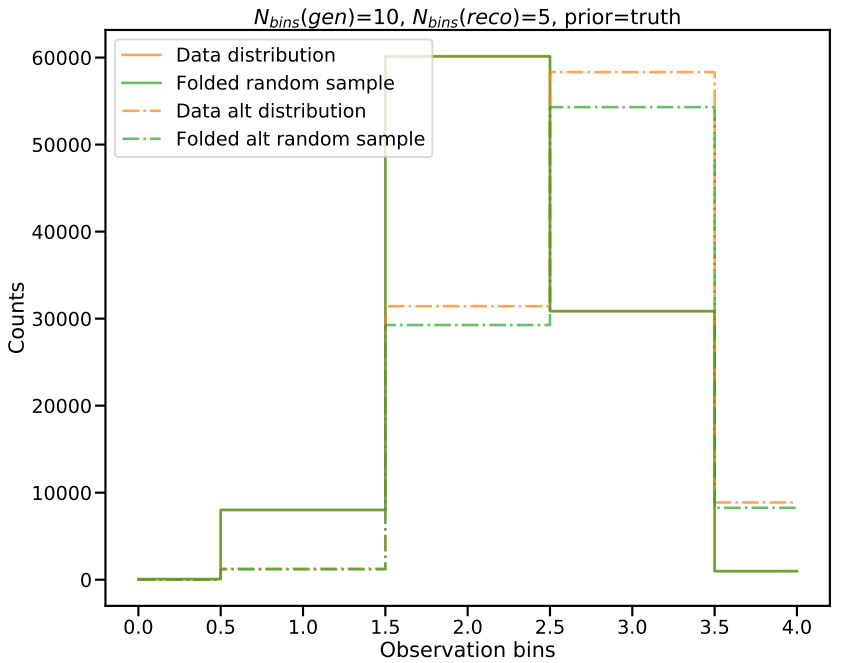
- ...and particularly well for usually ill-defined problems ($N_{bins}(gen) > N_{bins}(reco)$!!!





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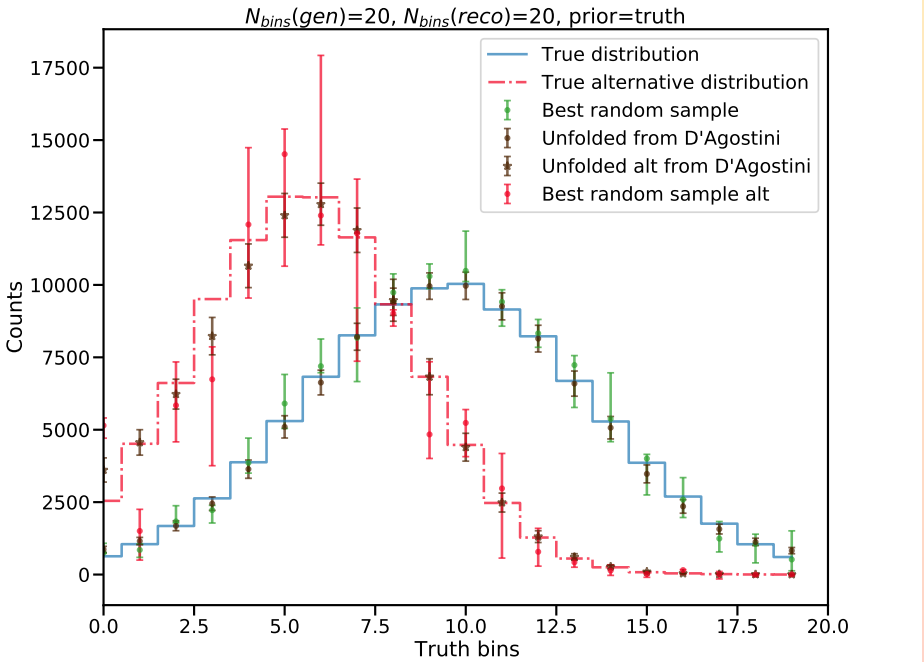
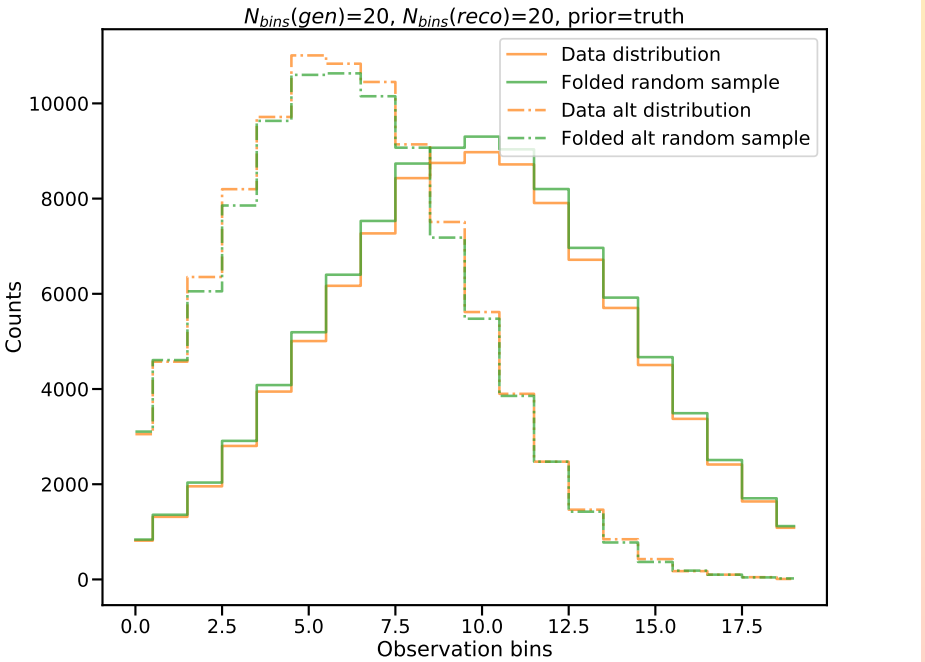
Dependence on parameters

- For less diagonal cases, further regularization is needed
  - More aggressive early stopping
  - Smoothness conditions on the proposals
  - Rebinning (unfold with finer bins, then rebin to larger bins)
- Coverage to be studied!





Bottom line test

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- Comparison between imperfect data and folded truth in folded space, and between best random from imperfect data and truth-level truth in unfolded space
- The idea is that the inference in the unfolded space should not be better than that in the folded space (Cousins and colleagues, 1607.07038
- Here using the Pearson χ^2, divided by $NDOF$
  - For the moment, the regular NDOF is used, its computation neglecting the covariance matrix.

Configuration	Algo1 $\chi^2/NDOF_{foldedSpace}$ $(altData, foldedTruth)$		Algo1 $\chi^2/NDOF_{unfoldedSpace}$ $(bestRandomFromAltData, truth)$		D'Agostini $\chi^2/NDOF_{unfoldedSpace}$ $(d'Agostiniunfolded, truth)$	
	init:truth	init:flat	init:truth	init:flat	init:truth	init:flat
$N_{bins}(gen) = 20, N_{bins}(reco) = 20$	280.753	280.753	306.196	322.679	307.210	307.210
$N_{bins}(gen) = 10, N_{bins}(reco) = 20$	285.260	285.260	592.488	596.413	603.189	603.189
$N_{bins}(gen) = 20, N_{bins}(reco) = 10$	542.366	542.366	302.102	358.552	304.772	304.772

Perspectives for uncertainties (ABC and MCMC)

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- Uncertainties in the response matrix dealt with as commonly in particle physics
  - Vary response matrix by applying systematic shifts to it (e.g. change jet energy scale, obtain new response matrix)
  - Re-unfold using the alternative matrix
  - Difference between the unfolded spectra is taken as the uncertainty
- Uncertainty of the method
  - Taking the samples that are better compatible (when folded) with the data is questionable
  - Switching to a full ABC implementation
  - Testing a full MCMC-based unfolding version

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Summary

- Briefly outlined the unfolding problem and the current standard methods
- Proposed two methods, which will appear on the arxiv in a couple days
- Unfolding with normalizing flows
  - Learn an invertible function representing the response matrix
  - Use it to convert smeared distributions to unfolded distributions
  - No binning needed
  - Can unfold multiple observables at the same time!
- Unfolding by folding
  - Build proposals by sampling in true space, folding them, and comparing with data
  - Stochastic optimization to find best solution
  - Build distribution to estimate uncertainty, or use full ABC/MCMC
  - Implicitly regularized (samples binned distributions), more regularization needed for non-diagonal cases
- Performing bias and coverage studies for both methods

Two Approaches to Unfolding: Invert the Problem using Normalizing Flows, or Stochastically Fold without Actually Inverting any Matrix

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