Machine Learning-Assisted Unfolding for Neutrino Cross-section Measurements

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Measurements and Unfolding

Measure **selected number** of **events** in a **reconstructed variable** -- what the detector saw.

Efficiency

Background

Unfolding

Want the **total number** of **signal events** in a **true variable** -- what physically happened.

Assuming no background:

$$R_j = \sum_{i}^{N} S_{ij}\, T_i \longleftrightarrow T_j = \sum_{j}^{N} U_{ij}\, R_i$$

Unfolding is finding the unsmearing matrix **U** given the smearing matrix **S** and removing the detector effects from the measured data (**R** in *j* bins) to get the "true" distribution (**T** in *i* bins)

Simplest method would be to invert **S**, but this is usually regarded as a bad move

Unfolding is hard

The process of unfolding is to estimate (or infer) the true distribution using smeared (reconstructed) observations

Unfolding is an ill-posed problem with many methodological challenges

The main challenge is that the smearing (response) matrix S is an ill-conditioned matrix

As a result, **very different true histograms can map to very similar smeared (reconstructed) distributions** – distinguishing between true predictions based on noisy data is quite difficult

Slide entirely adapted from M. Kuusela

“Traditional” Unfolding

Several common unfolding techniques currently used for neutrino physics are:

- iterative Bayesian unfolding (aka D’Agostini)
- SVD unfolding (including Wiener SVD)
- template likelihood unfolding (e.g. recent T2K analyses)

These methods (generally) **require that the distributions are binned**, and work best with a **small set of variables** (around 1 to 4)

However many of the **corrections (e.g. efficiency) can have high-dimensional dependence**, and this is difficult to capture with only a few variables

In all cases the reconstructed MC distribution is reweighted to better match the data, and this is propagated to the truth MC distribution

Machine learning (ML) assistance

Neural networks **learn to approximate the likelihood ratio** when trained to distinguish between two datasets

(or something monotonically related to it in some known way)

This transforms the problem from **density estimation** (which is hard) to **classification** (which is ~~easy~~ less hard)

Neural nets are naturally unbinned and are well suited to high-dimensional datasets

Note: that other classifiers could be used for this, such as a boosted decision tree

Explained in detail in this paper: A. Andreassen, B. Nachman, PRD RC 101 (2020) 091901, arxiv:1907.08209

OmniFold concept: ML reweighting

Train a fully connected neural network to classify between two datasets A & B:

Using the **weighted cross-entropy loss** where each event **x** has a weight **w** and a true label **p** gets a prediction **q**

$$L(p_i, q_i) = -w_i \left(p_i \log(q_i) + (1 - p_i) \log(1 - q_i)\right)$$

The predictions from the network **q** then approximate the ratio of the two datasets and can be used to **reweight from one to the other**:

$$\mathcal{L} = p_A(x_i)/p_B(x_i) \approx q_i/(1 - q_i)$$

In practice this uses real (or fake) data and the MC prediction as inputs to the network ➔ this talk uses a public T2K MC dataset as input to OmniFold

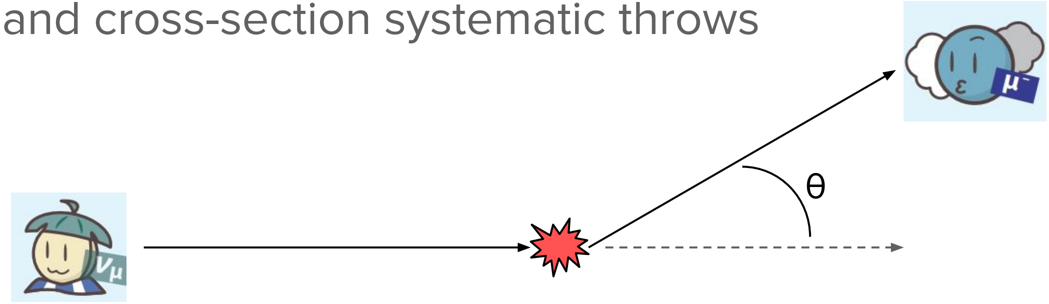
OmniFold paper: A. Andreassen, P. Komiske, E. Metodiev, B. Nachman, J. Thaler, PRL 124 (2020) 182001 | Ben's NuXtract Talk

T2K CC0pi event selection

CC0pi signal definition (neutrino mode): **one negatively charged muon**, **zero pions**, and **any number of hadrons** detected in the final state where the vertex was reconstructed in the FGD1 (scintillator) fiducial volume

Signal samples are categorized by the (sub-)detectors used in the event, and the analysis includes several control samples to constrain background events

Events in the data set are characterized by muon (proton) kinematics, and also include weights for detector, flux, and cross-section systematic throws



Corresponding paper:
https://doi.org/10.1103/PhysRevD.101.112001

(see also:
https://doi.org/10.1103/PhysRevD.108.112009 or
https://doi.org/10.1103/PhysRevD.101.112004)

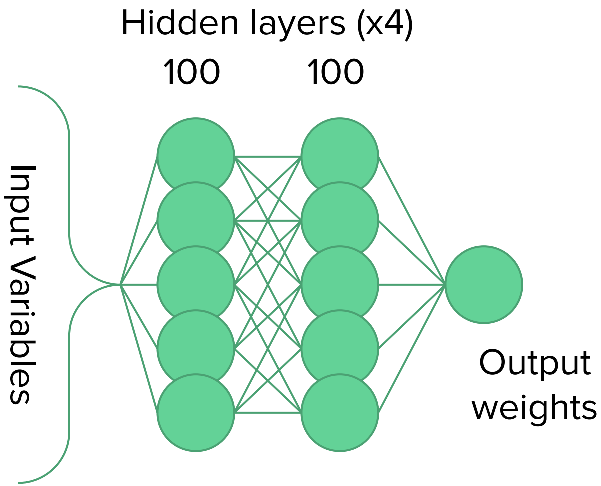
OmniFold Inputs & Network

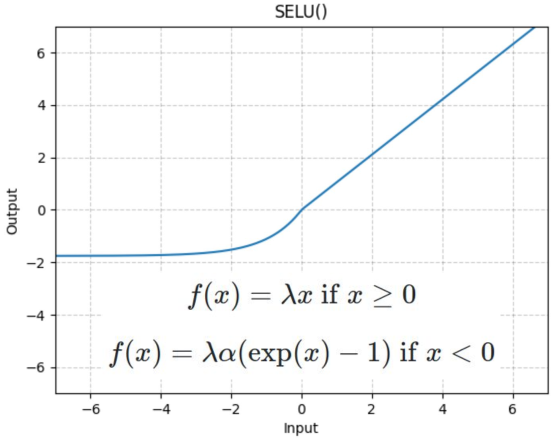
Network architecture is **four densely connected hidden layers** with **100 nodes each** (SeLU activation)

Input variables: **muon kinematics** and **leading proton kinematics** (if present) for each event parameterized as (log(|p|), cos(θ), φ), and **detector sample** (one-hot encoded)

Kinematic variables are normalized to have zero mean and unit variance

Not all background events are included due to missing information in the data release (e.g. NC events)





OmniFold procedure

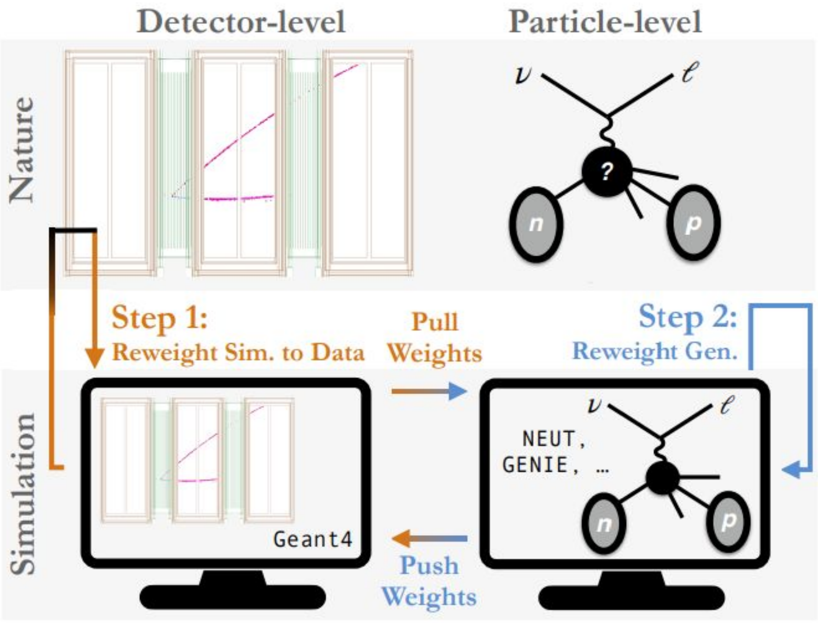
Running 15 iterations of OmniFold takes less than 30 minutes using a single NVidia A100 GPU on a NERSC Perlmutter node

OmniFold is an **iterative unfolding procedure** performed in two steps:

1. Reweight reconstructed MC distribution to (better) match data
2. Reweight nominal truth MC distribution to incorporate information from step 1

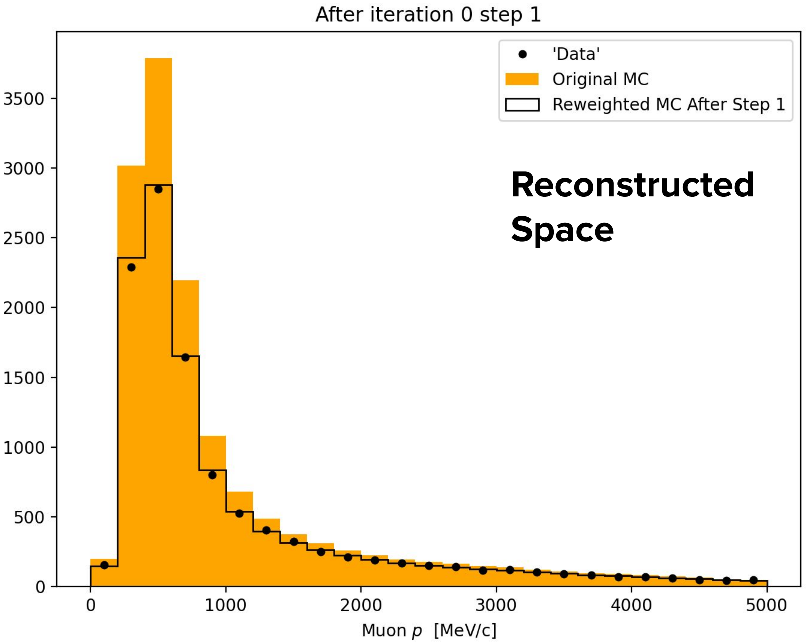
This is one iteration, and the method repeats until some convergence criteria is satisfied (or iteration limit is reached)

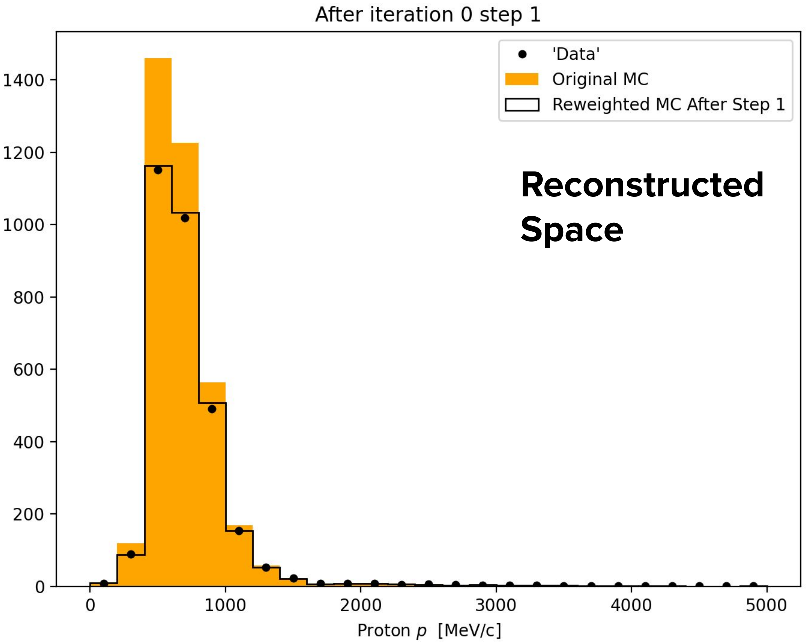
Each step uses its own network



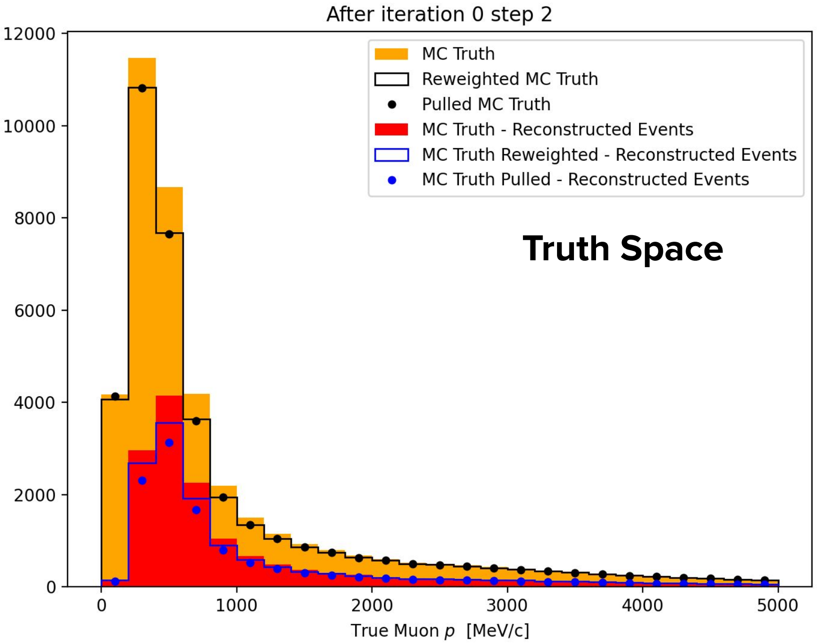
Reconstructed **Truth**

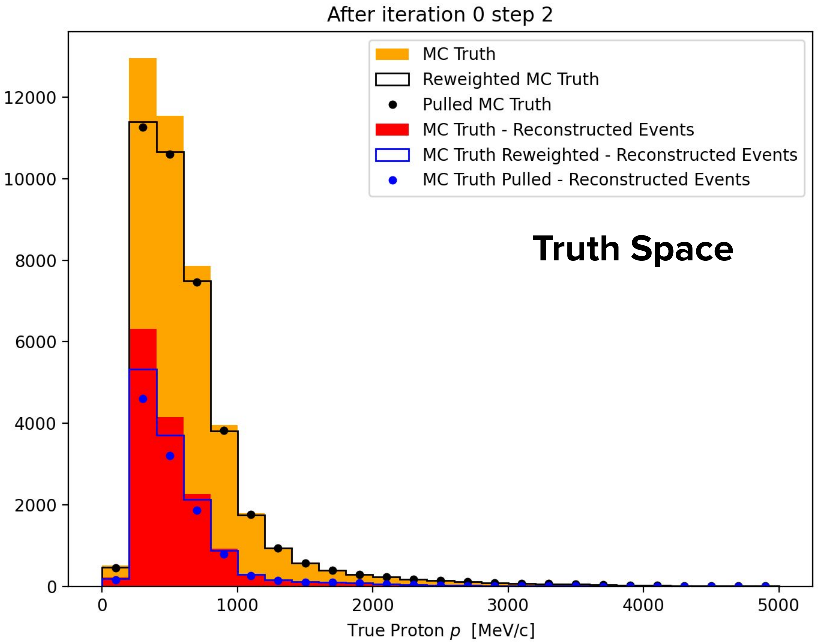
First Iteration – Step 1



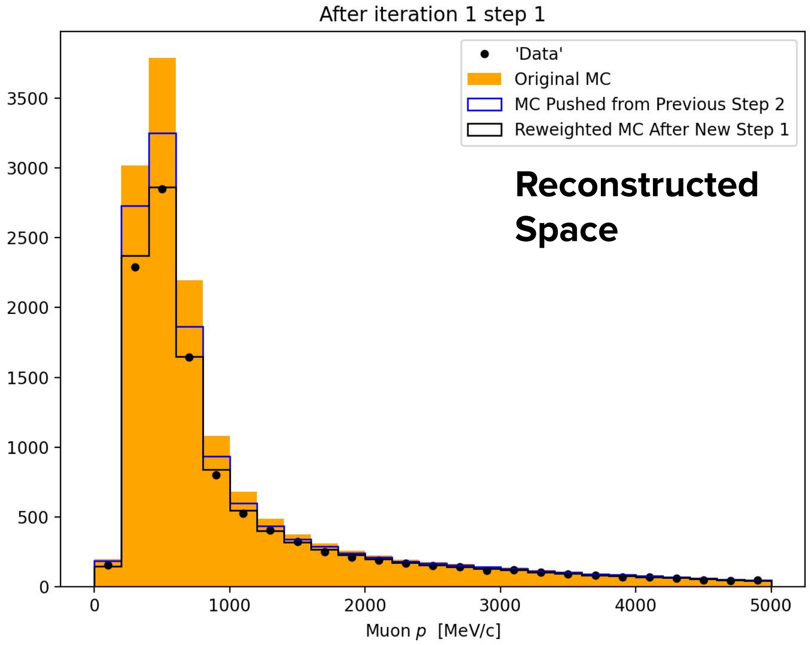


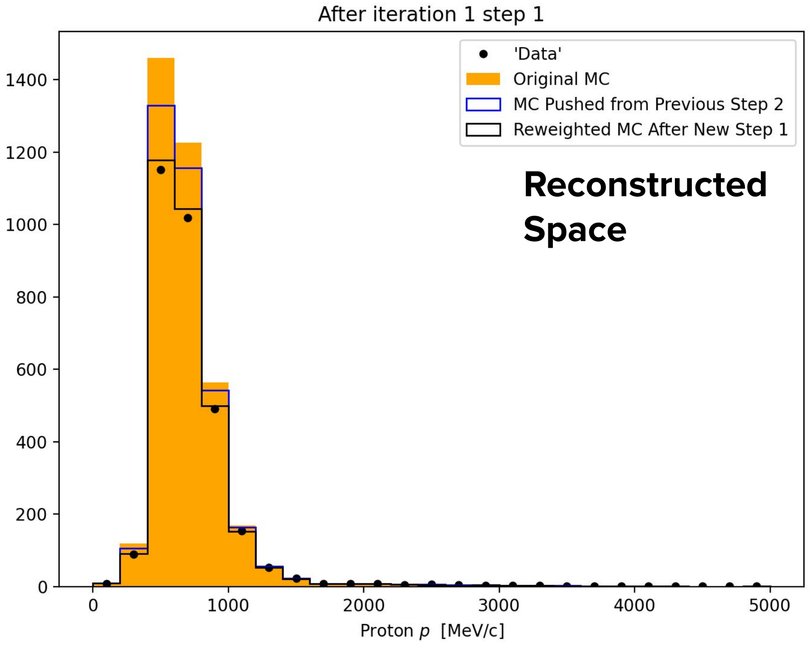
First Iteration – Step 2





Second Iteration – Step 1





Testing OmniFold

Comparing performance of unfolding using iterative Bayesian unfolding (aka D’Agostini or Lucy–Richardson unfolding)

Using a series of mock data studies to assess the unfolding performance and network training / tuning

Example for this presentation uses an arbitrary function to change the event weights as a function of muon momentum

Additionally exploring more complicated or physics motivated mock data studies

Uncertainty, efficiency, and ensembling

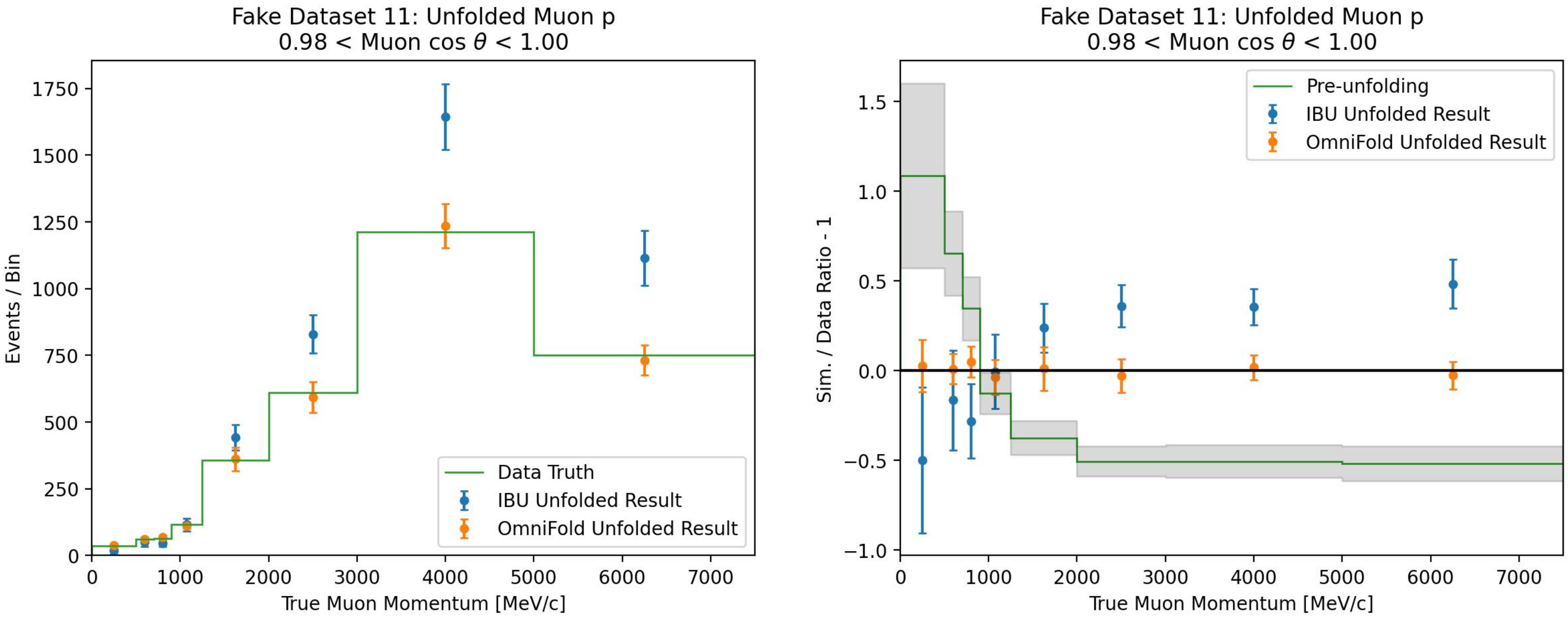
OmniFold naturally includes the efficiency correction when performing the unfolding (however this could be separated out and done as another step)

Systematic uncertainty is evaluated through a “universe” (toy throw) method where 500 different systematic variations are processed by OmniFold, and the spread in results gives an uncertainty band

Statistical uncertainty is evaluated by a bootstrap resampling with replacement where the “data” and MC event weights are varied for 500 throws / universes

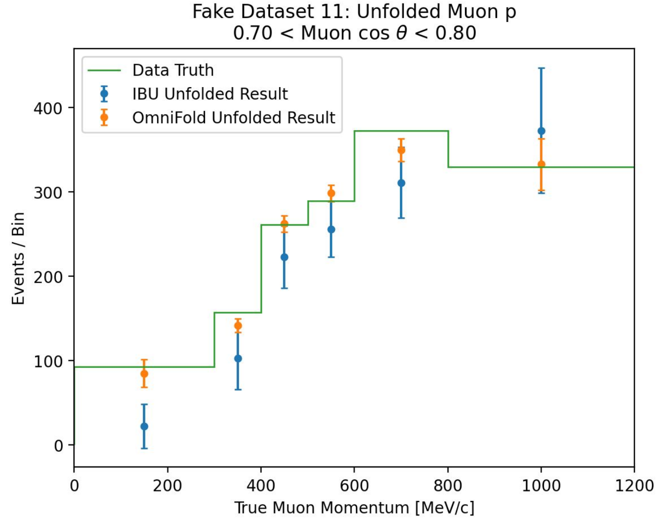
The inherent randomness of training neural networks is mitigated by ensembling using the average result of several trials

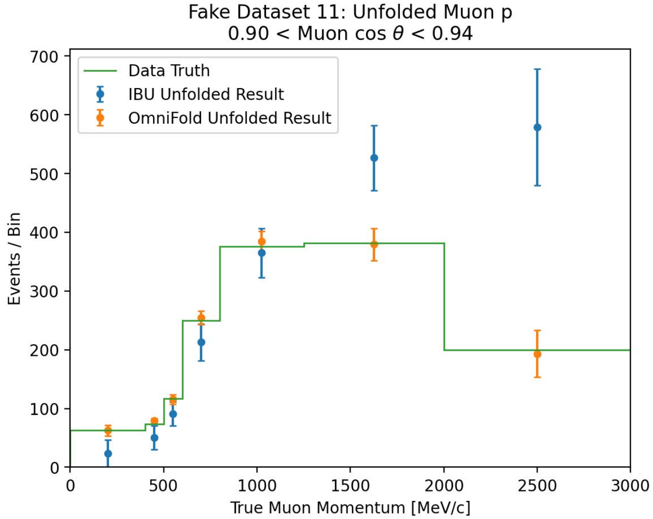
OmniFold results – muon momentum / angle

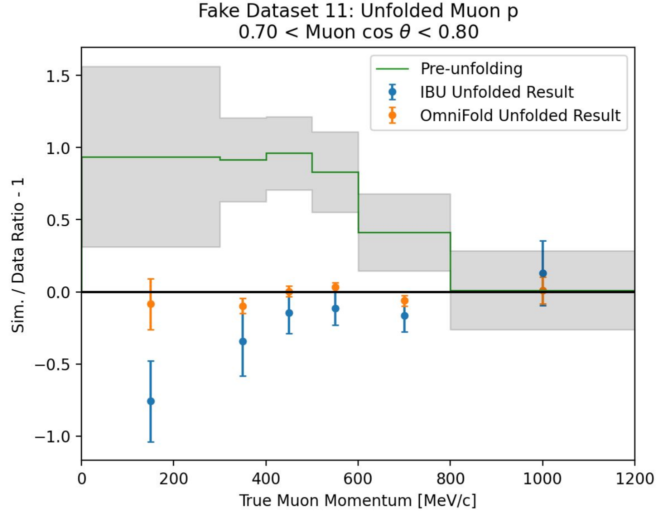


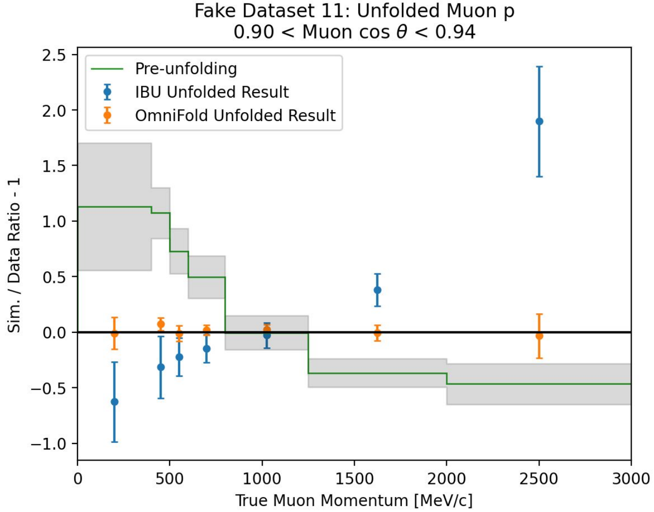
Slices of muon angle binned in momentum using T2K analysis binning (NB: OmniFold is unbinned)

Error bars are from 500 stat+syst varied throws for both IBU and OmniFold





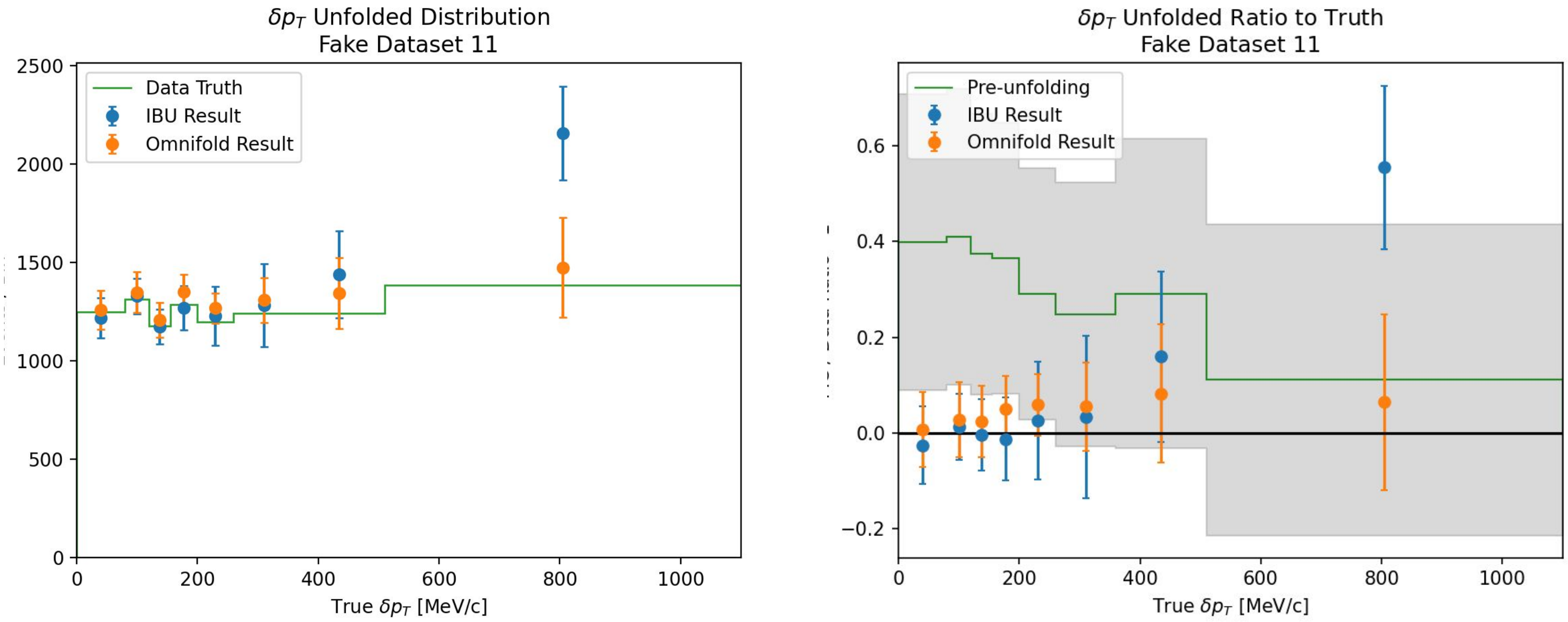




OmniFold does quite well recovering the mock data truth

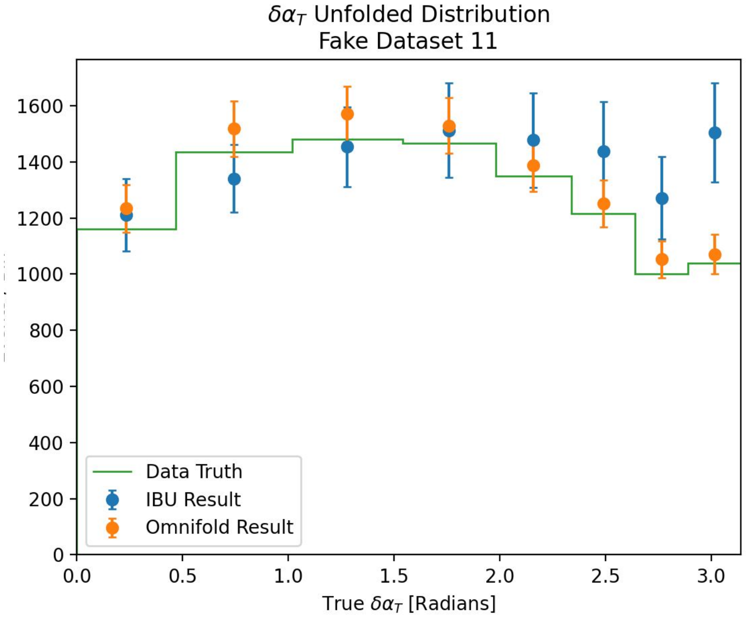
OmniFold achieves smaller bias and reduced uncertainties compared to IBU

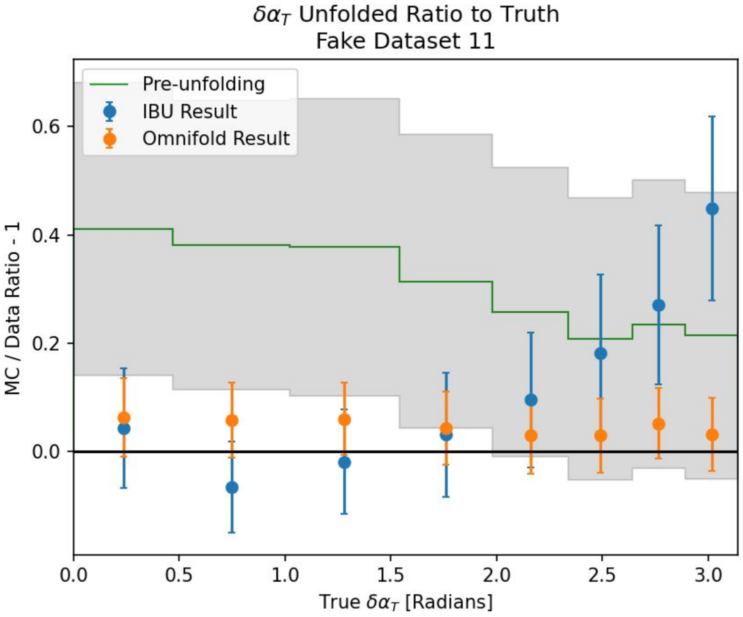
OmniFold results – transverse variables (pT)



Since OmniFold is unbinned, can extract results in many variables simultaneously, while IBU was run separately for each variable

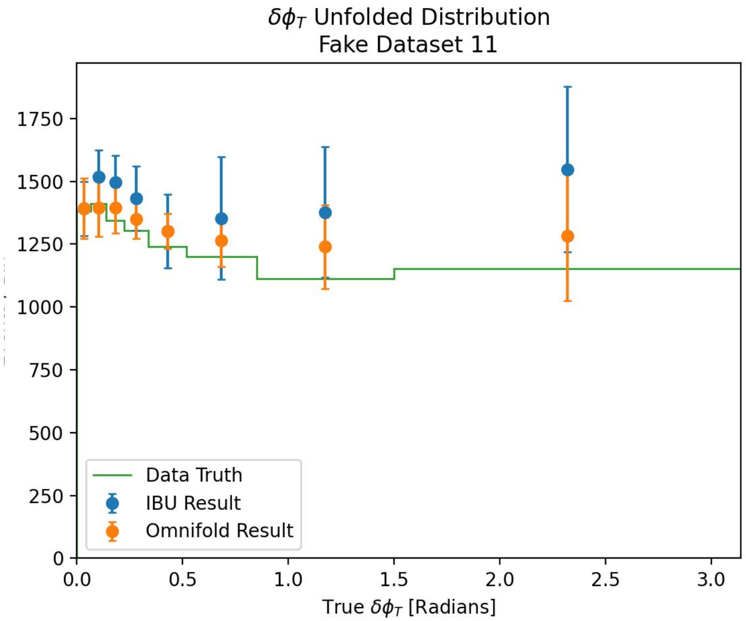
OmniFold results – transverse variables (αT)

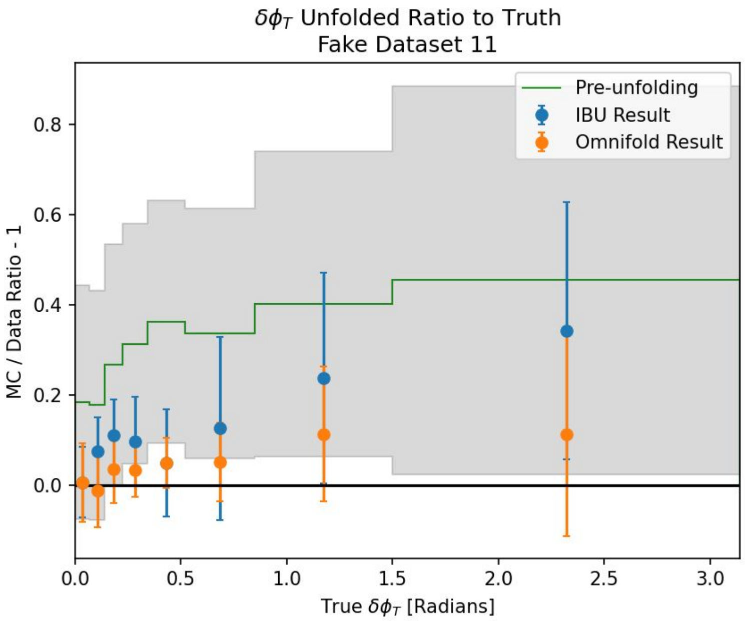




OmniFold still performs quite well, and overall better than IBU for the transverse variables

OmniFold results – transverse variables (φT)





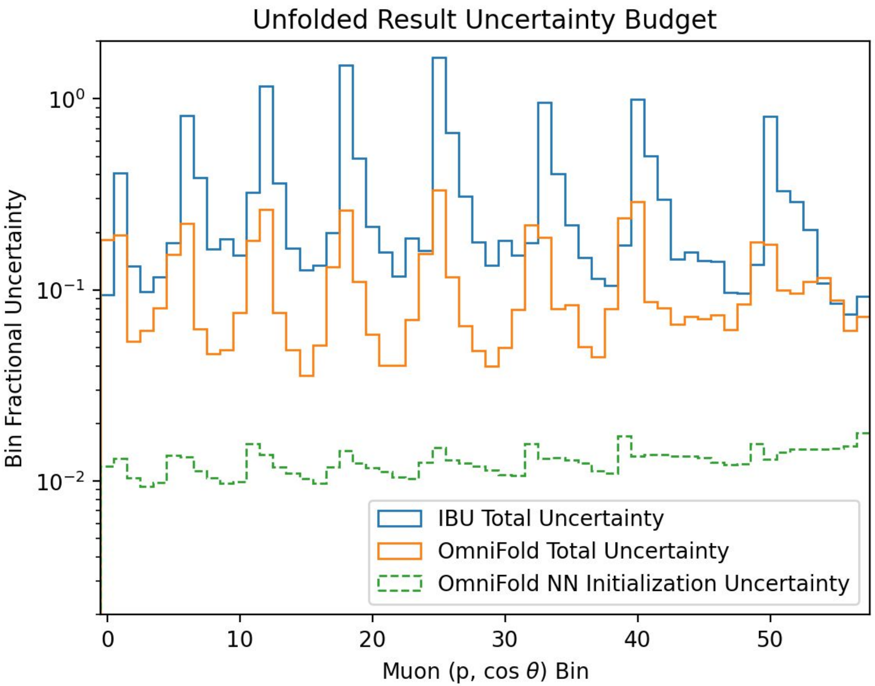
OmniFold still performs quite well, and overall better than IBU for the transverse variables

Uncertainty budget

Total uncertainty is the combination of **500 statistical and systematic varied throws** of OmniFold

Uncertainty from the randomness from the neural network initialization and training is reduced by averaging the results of multiple trials

Results presented here use five trials of OmniFold for ensembling

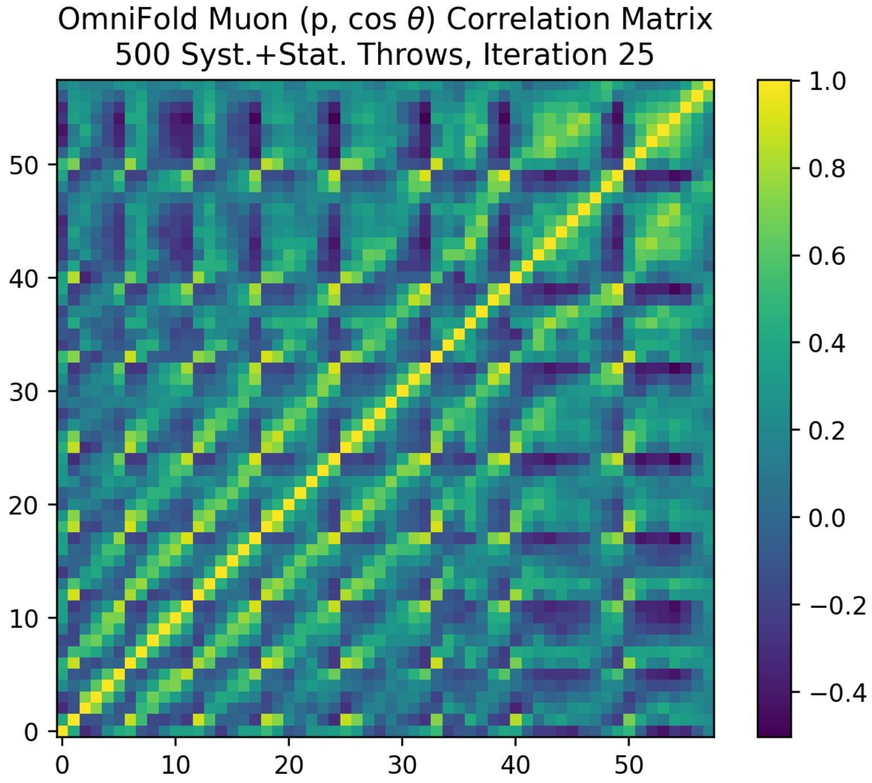


Correlation Matrix

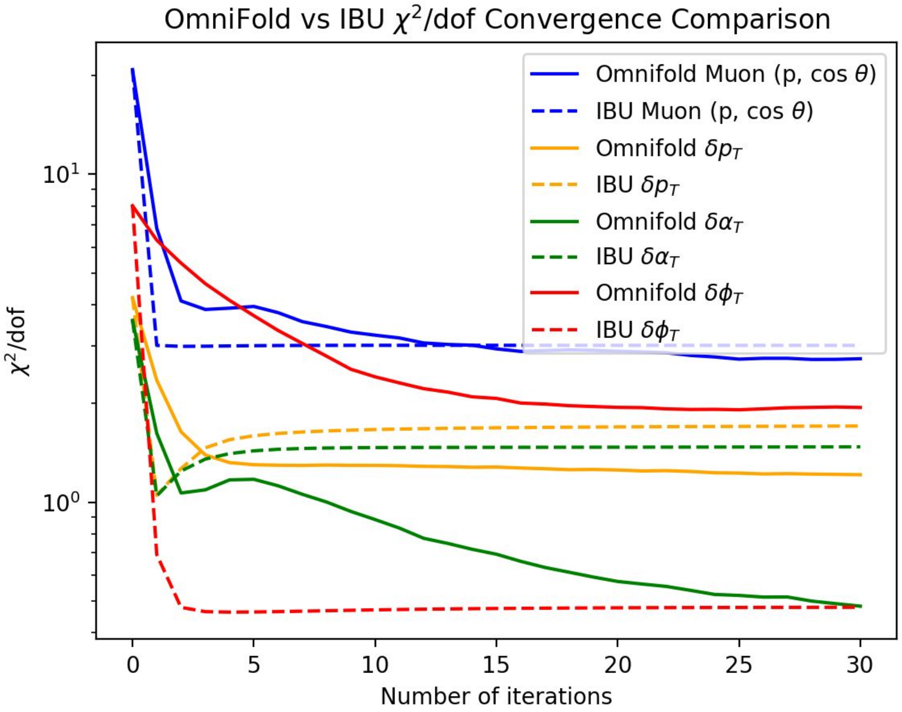
Covariance (and correlation) matrix can be calculated using the stat+syst varied throws

Calculated for muon kinematics for this example, but is available for every variable

Correlations also evolve with iterations in addition to the central value



Convergence Metric(s)



For recent tests, convergence is being monitored by calculating the chi-square for each iteration

Based on this, **OmniFold needs more iterations than IBU** and **can differ based on the variable / observable**

Requires knowing the observable and the kinematic binning, and only works when the truth is known

Other options being explored, particularly a way to do this unbinned

Summary & Future Work

OmniFold is an exciting technique for cross-section unfolding – naturally unbinned and high dimensional

OmniFold shows similar or better performance when compared to IBU, and automatically allows for unfolding in any number of variables

Several investigations are still ongoing on the performance for more complicated mock data studies and the impact of network architecture and hyperparameters

Looking forward, we want to test OmniFold on a more realistic analysis (e.g. T2K or even the 2x2) and are considering using a more sophisticated ML architecture or evolution of OmniFold