Tools for unbinned unfolding and an application for jet measurements

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AI at the EIC Workshop 2025

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Overview

- Review of binned and unbinned unfolding
- Status of unbinned unfolding tools and application to jet measurements
- H1 unbinned unfolding
- Unbinned unfolding pipeline

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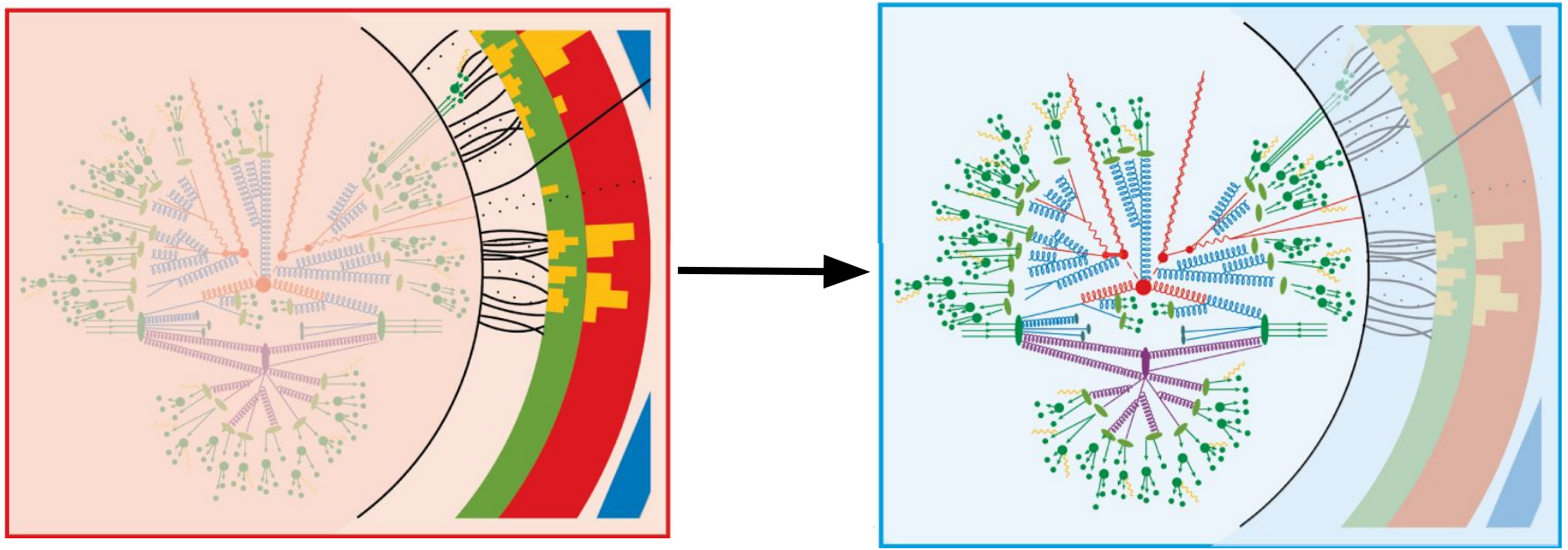
Overview of unfolding

- Objective: Remove detector distortions from experimental data



Experimental data

Physics information

Binned unfolding

$$m = Rt$$

Binned unfolding

$$m = Rt$$

Measured data

Binned unfolding

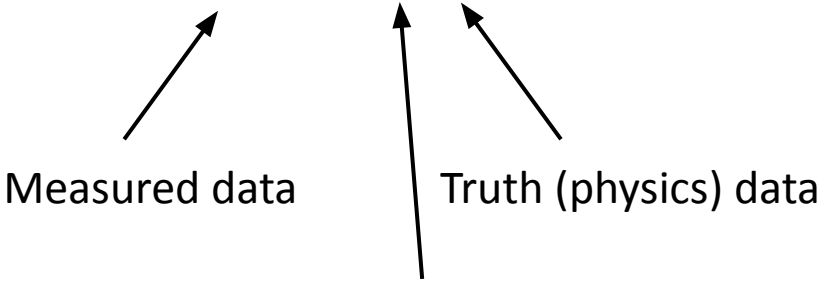
$$m = Rt$$

Measured data

Truth (physics) data

Binned unfolding

$$m = Rt$$



Measured data

Truth (physics) data

Response matrix

R_{ij} = Pr(measure in bin i | truth in bin j)

Made with simulation data

Binned unfolding

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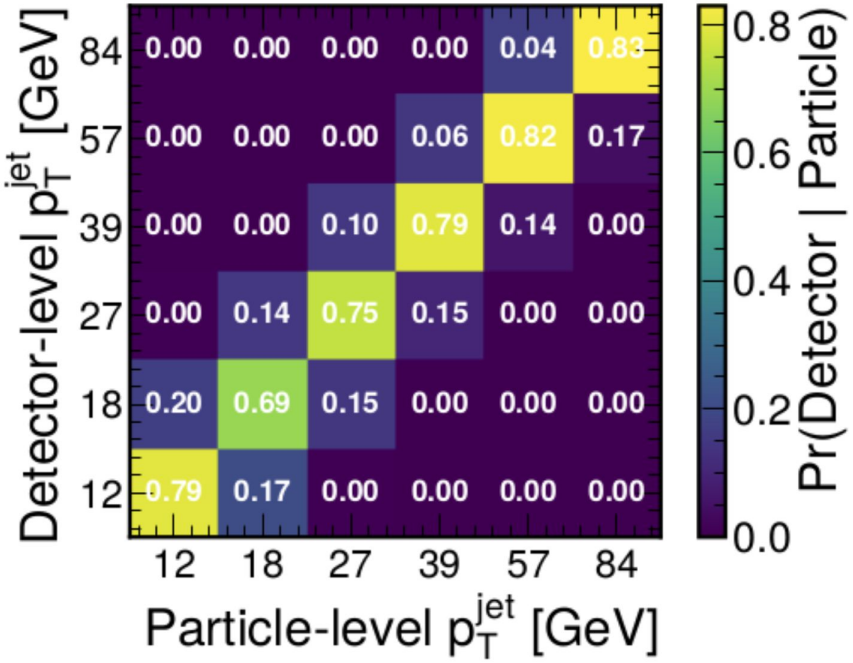
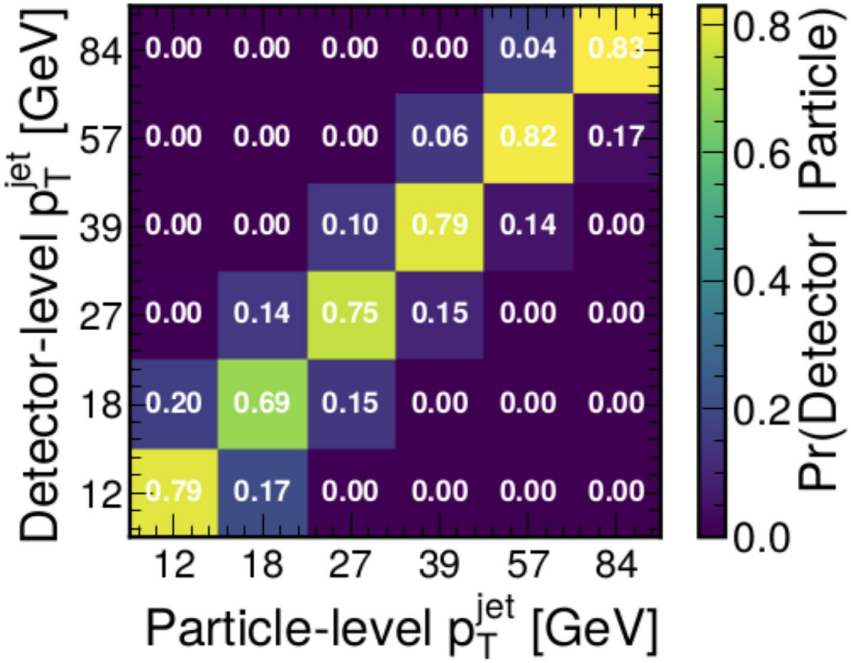


Example of response matrix

Binned unfolding

$$m = Rt$$

$$t = R^{-1}m$$



Example of response matrix

Binned unfolding

$$m = Rt$$

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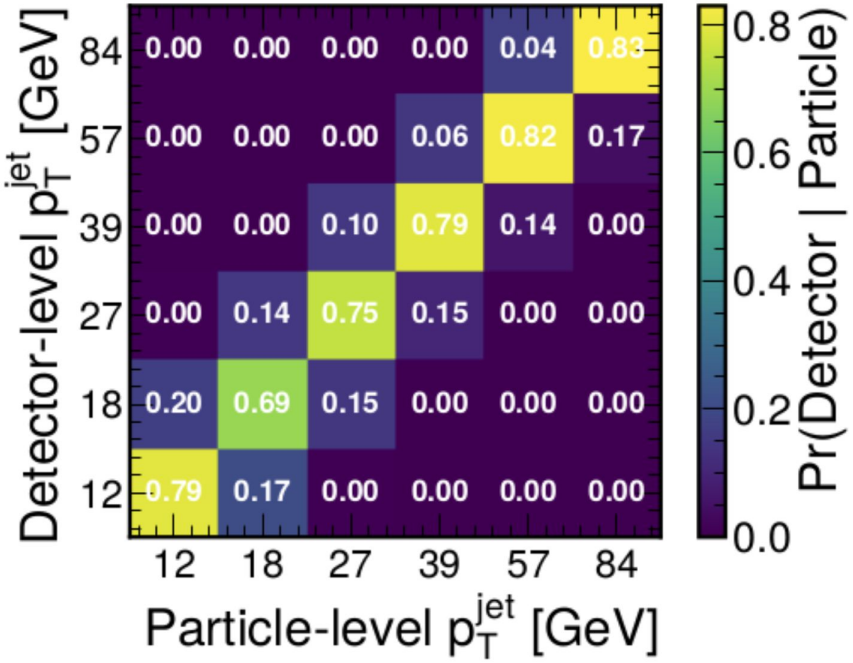
Main idea of binned unfolding is to ~invert the response matrix!



Example of response matrix

Binned unfolding

$$m = Rt$$

Examples:
Singular value decomposition,
Iterative Bayesian unfolding

$$t = R^{-1}m$$

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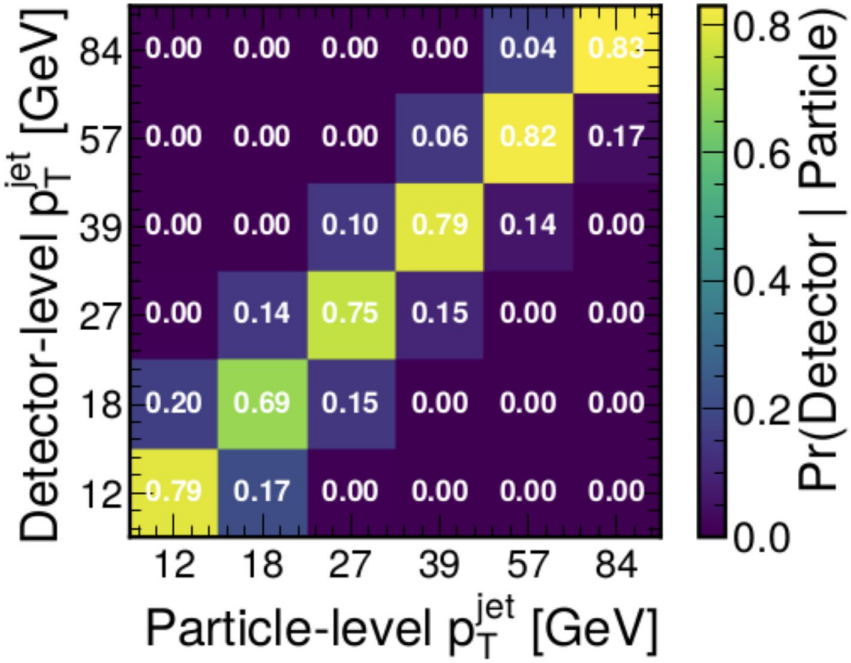

Example of response matrix

Drawbacks of binned unfolding

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- How to define optimal binning?
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- How to define optimal binning?
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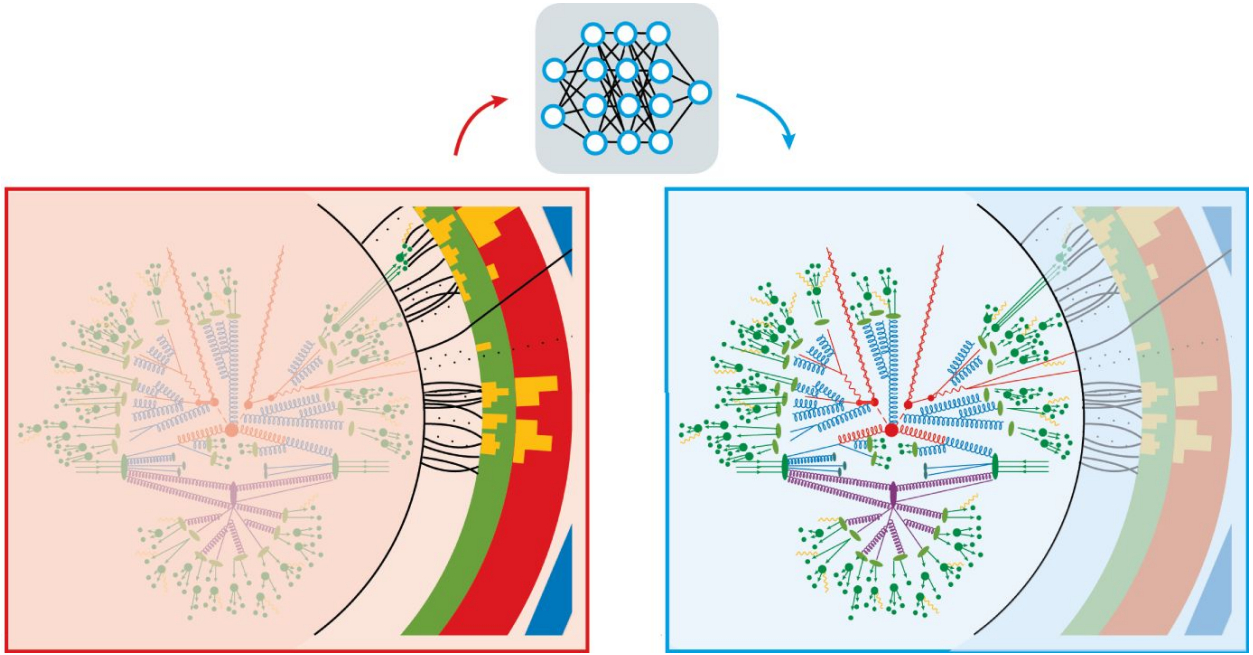
  - Binning choices makes it difficult to compare between experiments and to publish data
- Difficult to scale histograms to multiple dimensions by including multiple distributions
- Integrate over quantities thought to be irrelevant for a specific analysis
  - For other observables, like those motivated by future theoretical insight, may have to repeat analysis from scratch

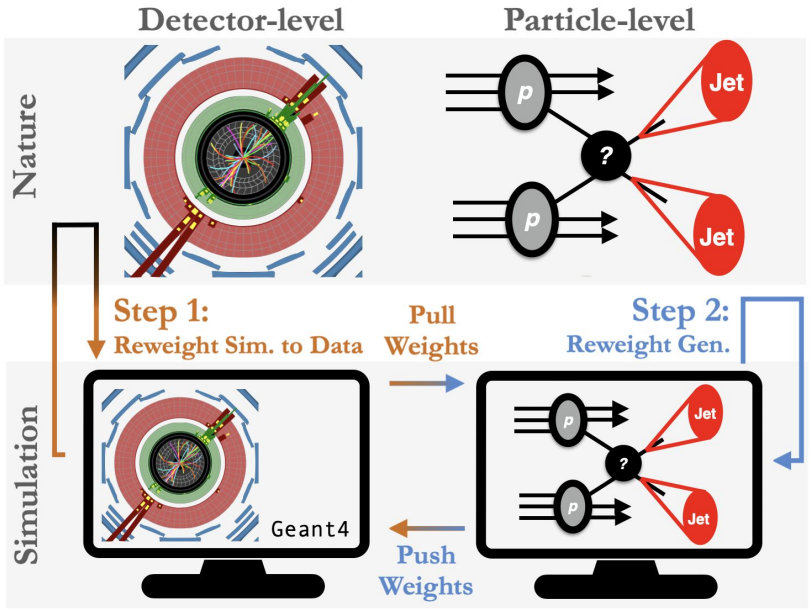
Unbinned unfolding motivation

- Motivates an unbinned unfolding method using machine learning
- Naturally unbinned and can handle high dimensions



Unbinned unfolding with OmniFold

- Iterative Bayesian Unfolding (IBU) is a popular binned unfolding algorithm
- Each iteration can be broken down into two steps
- In each step, a likelihood ratio is approximated
- Can estimate these two ratios using classifiers instead
- Use these likelihood ratios as unfolding weights!



A. Andreassen, et al., Phys. Rev. Lett. **124**, 18200

Applications of OmniFold

- OmniFold has been applied to many experimental analyses!

PHYSICAL REVIEW LETTERS **128,** 132002 (2022)

Measurement of Lepton-Jet Correlation in Deep-Inelastic Scattering with the H1 Detector Using Machine Learning for Unfolding

Measurement of event shapes in minimum bias events from pp collisions at 13 TeV

The CMS Collaboration

PHYSICAL REVIEW D **108,** L031103 (2023)

Multidifferential study of identified charged hadron distributions in Z-tagged jets in proton-proton collisions at $\sqrt{s} = 13$ TeV

R. Aaij *et al.*[*]
(LHCb Collaboration)

Measurement of CollinearDrop jet mass and its correlation with SoftDrop groomed jet substructure observables in $\sqrt{s} = 200$ GeV pp collisions by STAR

PHYSICAL REVIEW LETTERS **133,** 261803 (2024)

Simultaneous Unbinned Differential Cross-Section Measurement of Twenty-Four Z + jets Kinematic Observables with the ATLAS Detector

G. Aad *et al.*[*]
(ATLAS Collaboration)

Youqi Song (Wright Laboratory, Yale University)

on behalf of the STAR Collaboration

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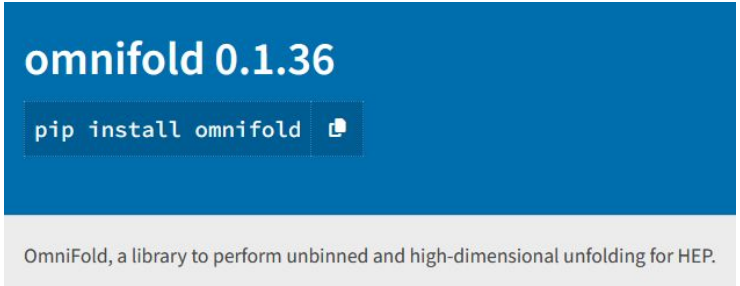
Status of unbinned unfolding tools

- PyPi omnifold:
  - Architectures: Multilayer perceptron (MLP) , point-edge transformer (PET)
  - Any number of dimensions
  - May need GPUs to train
- RooUnfold inspired omnifold:
  - Architecture: Boosted decision tree (BDT)
  - Low dimensional unfolding
  - Simple set-up: No data preprocessing, no GPUs needed



Application to jet measurements

- Test unfolding quality using closure test
  - Use two Monte Carlo simulations so we know what the truth looks like!
- Use Pythia as Monte Carlo (Gen/Sim), Herwig as pseudodata (“Truth”/“Data”) to get unfolded jet observables

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Method	ML type	Input	Unfolding type
OmniFold	PET	All particles	Unbinned

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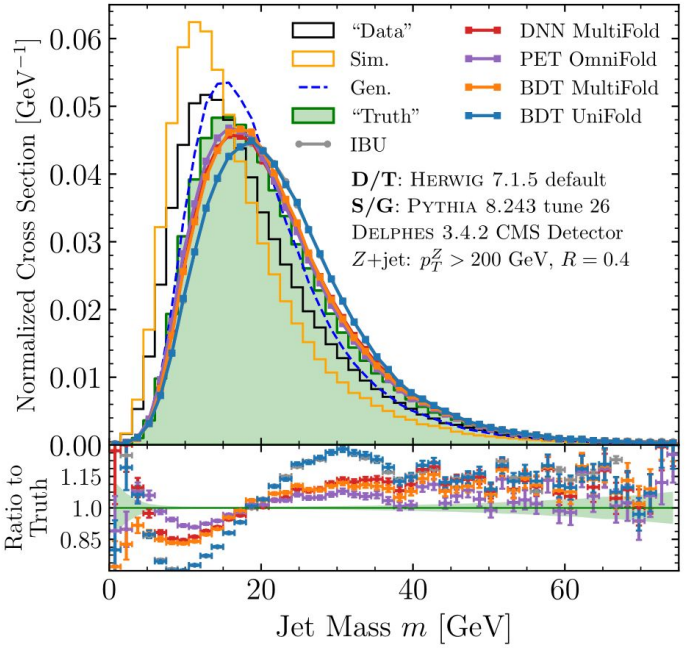
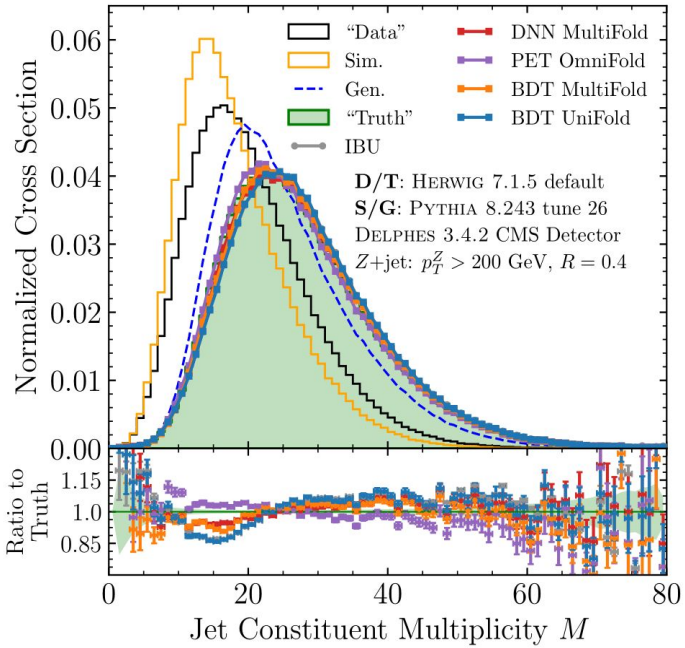
UniFold	BDT	Individual jet observables	Unbinned
IBU	N/A	Individual jet observables	Binned

Performance on jet observables

- Trying to match the “Truth” distributions by applying weights to Gen
- Other jet observables in paper: Width, Soft Drop mass, N-subjettiness ratio, groomed jet momentum fraction





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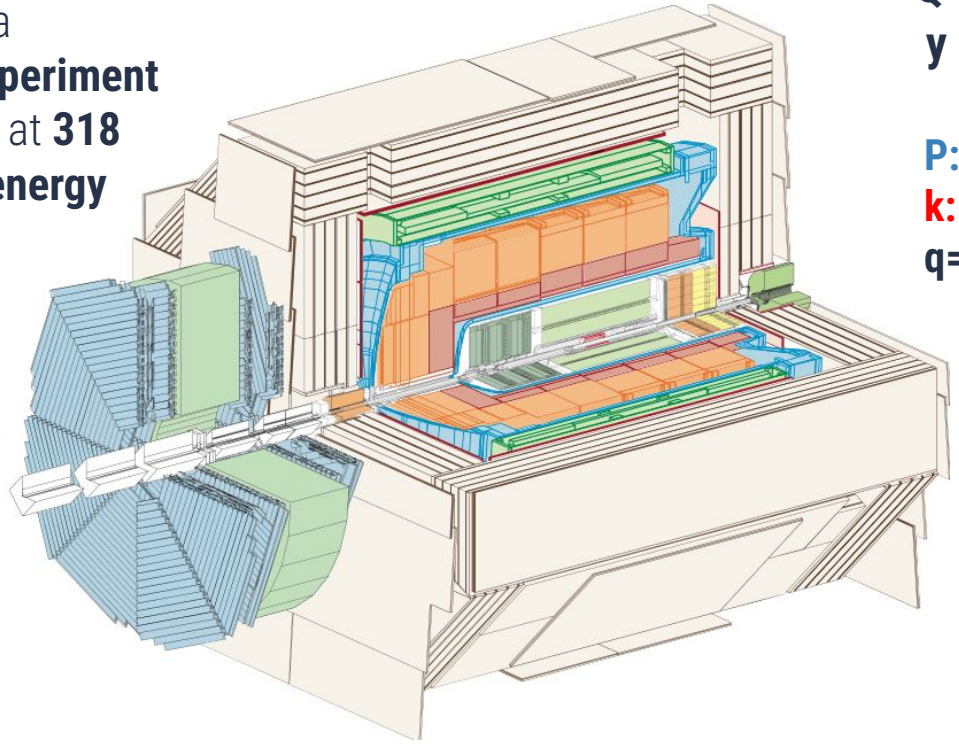
Application to H1

(H1 slides courtesy of Vinicius Mikuni)

Using **228 pb^{-1}** of data collected by the **H1 Experiment** during **2006** and **2007** at **318 GeV center-of-mass energy**



$Q^2 = - q^2$

$y = Pq / pk$

P: incoming proton 4-vector
k: incoming electron 4-vector
q=k-k' : 4-momentum transfer

Reconstructed hadrons using combined detector information: **energy flow algorithm**

Experimental setup

Fiducial Phase space definition:

- $0.2 < y < 0.7$
- $Q^2 > 150\ \text{GeV}^2$

Particle selection:

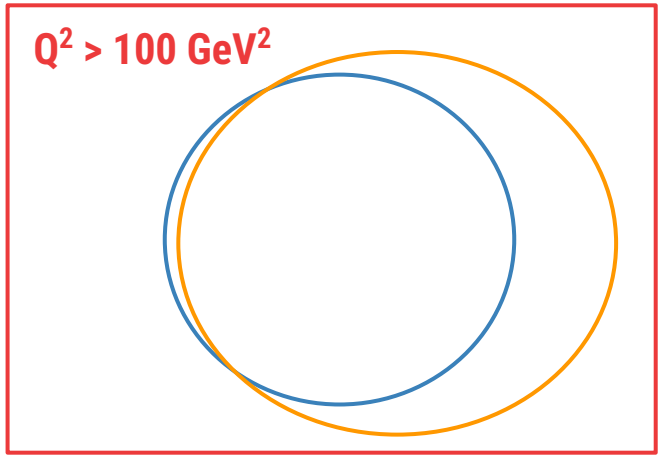
- $p_T > 0.1$ GeV
- $-1 < \eta_{lab} < 2.75$
- Charge information used if $\eta_{lab} < 2$

Reco Phase space definition:

- $0.08 < y < 0.7$
- $Q^2 > 150\ \text{GeV}^2$
- p_T miss < 10 GeV,
- $45 < \text{em}/p_z < 65$

Particle selection:

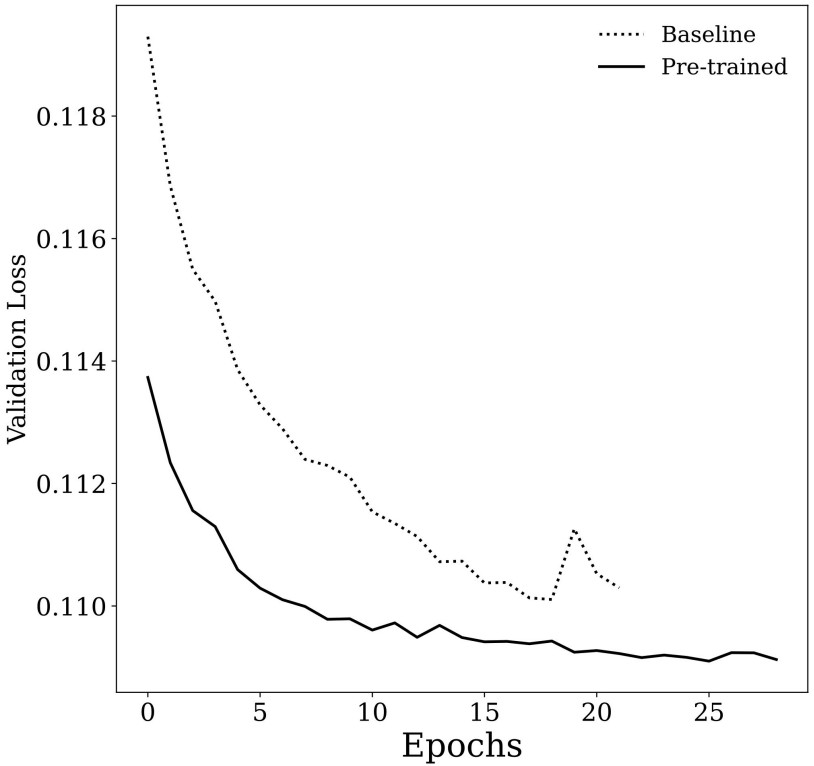
- $p_T > 0.1$ GeV
- $-1 < \eta_{lab} < 2.75$



Red box used during unfolding, but only fiducial results shown

- Pass reco selection: **Red -> Orange**: **77%**
- Pass fiducial selection: **Red -> Blue**: **58%**
- Pass fiducial and reco selection: **Blue -> Orange**: **96%**
- Don't pass fiducial but pass reco: **Red -> Orange** (without **blue**): **50%**

Pretraining



Pre-training:

- We use a smaller version of the OmniLearn model[1]
- We have around 20M simulated samples in Djangoh and Rapgap, but only around 200k data events
- We can improve the reweighting quality by **pre-training** the model first
- Train the model to **classify Rapgap from Djangoh** and use that as the initialization for the rest of the unfolding

1: **V. Mikuni**, B. Nachman, arXiv:2404.16091

Systematic uncertainties

Systematic uncertainties included in the results

- **HFS energy scale:** +- 1%
- **HFS azimuthal angle:** +- 20 mrad
- **Lepton energy:** +- 0.5%
- **Lepton azimuthal angle:** +- 1 mrad
- **Model uncertainty:** differences in unfolded results between Djangoh and Rapgap
- **Non-closure uncertainty:** Differences between the expected and obtained values of the closure test
- **Statistical uncertainty:** Standard deviation of 50 bootstrap samples with replacement (will increase to 100 when done running)

Uncertainties not yet added

- **QED uncertainty**: Use the variation of measured quantities when radiation is turned off in the simulation

Closure test

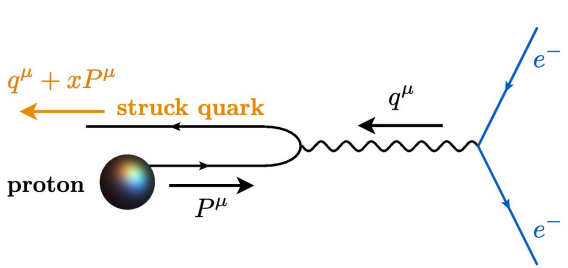
- Use Djangoh as the **pseudo-data** and unfold Rapgap
- Analysis is currently **preliminary** and **blinded**: Uncertainties shown use data information, but the plots will show only the closure results
- Although we **unfold everything,** we make a small number of observables public
  - Observables that reproduce previous results
  - Observables difficult to unfold classically

Results

	Lab k_T	Breit k_T	Centauro
$\Delta\phi^{\text{jet}}$	Y	N	N
$\ln(\lambda_1^1)$	Y	N	N
p_T^{jet}	Y	Y	Y
z^{jet}	Y	Y	Y

Jet Selections

- **Jet algorithm:** kT and Centauro both with R = 1
- **Jet pT cuts:**
  - Lab frame kT jets: $p_T > 10$ GeV
  - Breit frame kT jets: $p_T > 5$ GeV
  - Centauro jets: $z > 0.2$ (no pT cut)



Breit Frame provides a natural frame to study ep collisions, where the struck quark forms a jet opposite from the proton beam: useful for jet and TMD studies

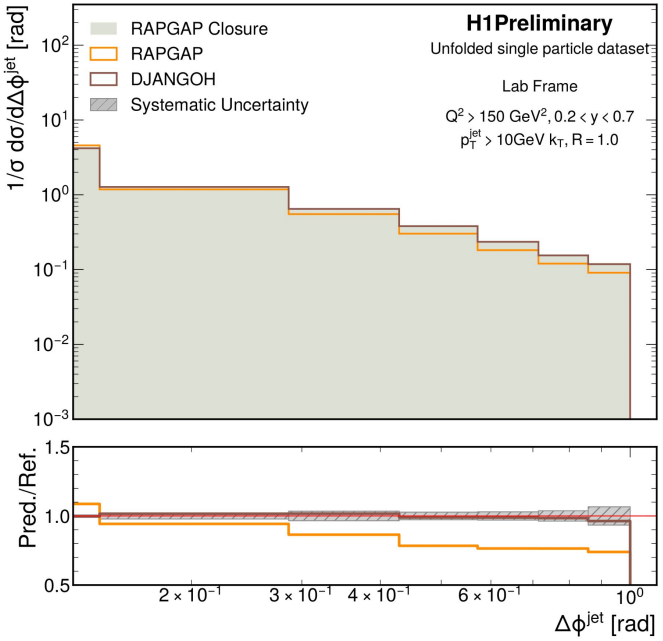
Centauro jet algorithm is a longitudinally invariant method designed for DIS studies

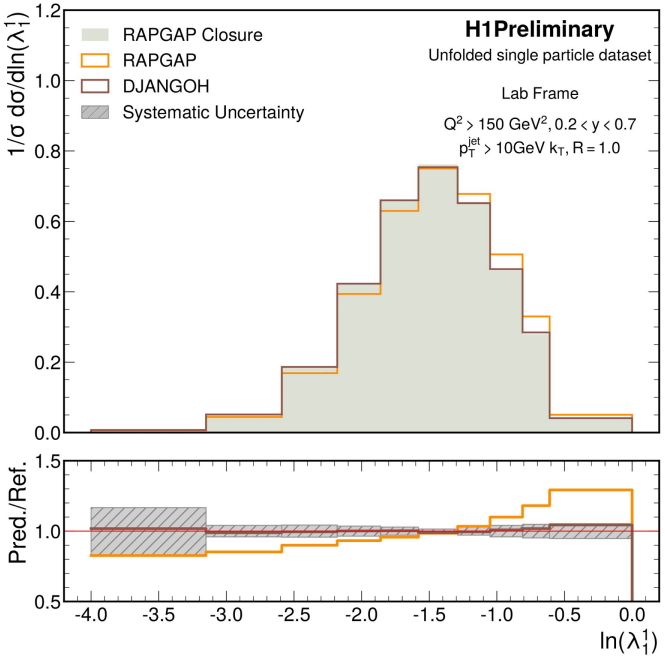
Δz and **Energy-Energy Correlator** are also measured in the Breit frame.

Asymmetric jet clustering in deep-inelastic scattering:
Arratia et al. Phys.Rev.D 104 (2021) 3, 034005

Results

Cluster jets using kT algorithm with radius of 1.0
Notice the analysis is **blind**: Plot shows the closure agreement, but uncertainties are calculated based on the data





	Lab k_T
$\Delta\phi^{\text{jet}}$	Y
$\ln(\lambda_1^1)$	Y

$$\lambda_\beta^\kappa = \sum_{i \in \text{jet}} z_i^\kappa \left(\frac{R_i}{R_0}\right)^\beta$$

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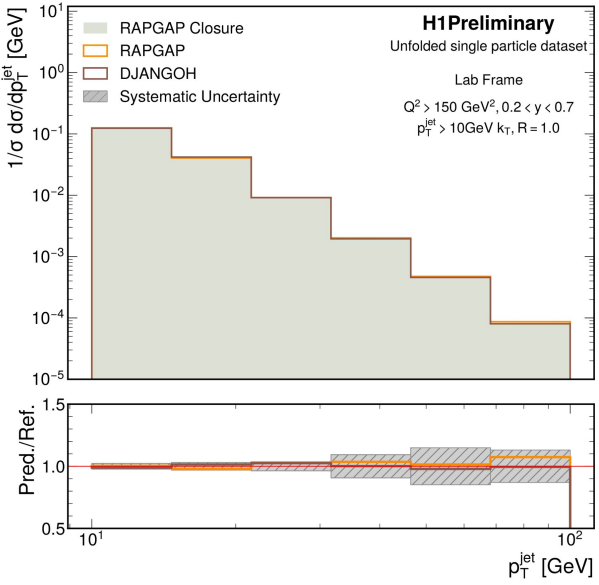

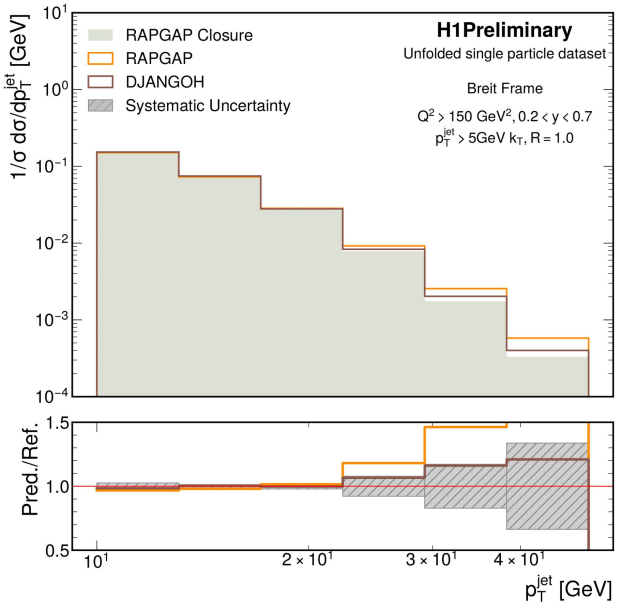

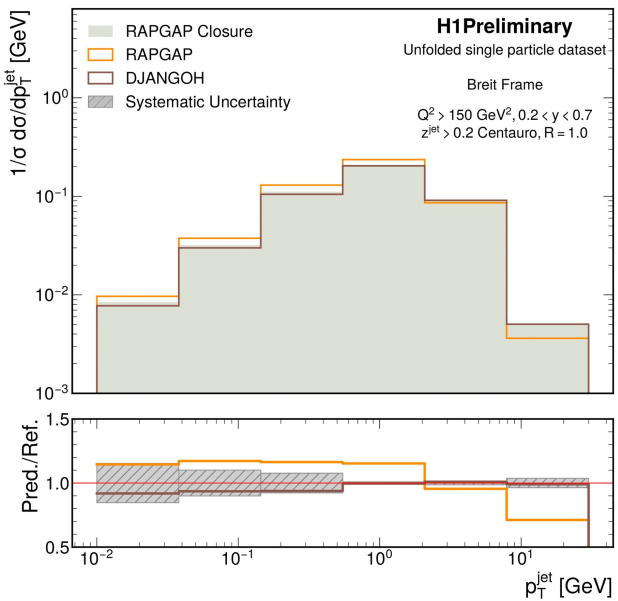

Lab Frame p_T **Breit Frame p_T** **Centauro p_T**

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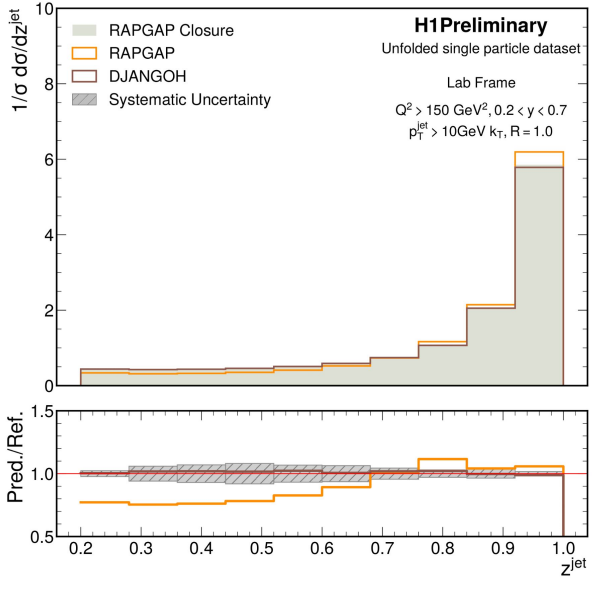

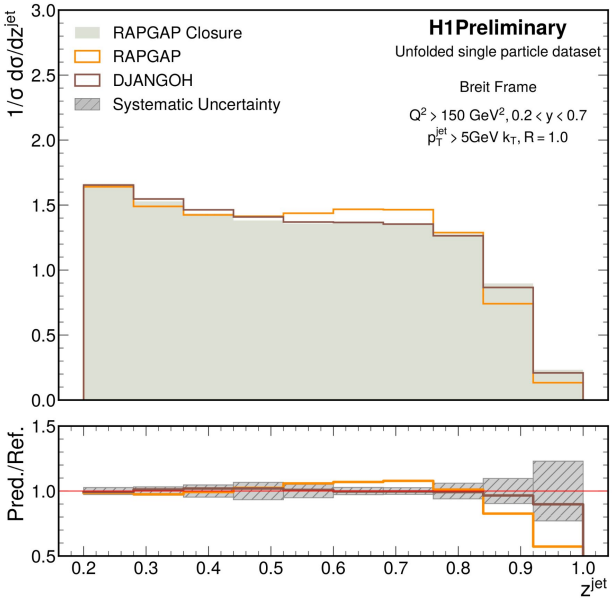

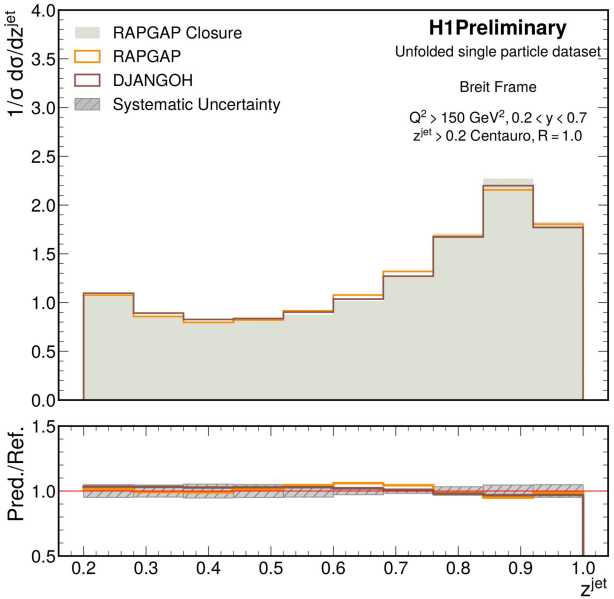

Lab Frame z

Breit Frame z

$$z_{\text{jet}} = \frac{P \cdot p_{\text{jet}}}{P \cdot q} \xrightarrow[\text{frame}]{\text{Breit}} z_{\text{jet}} = n \cdot p_{\text{jet}}/Q$$

Breit Frame z with Centauro

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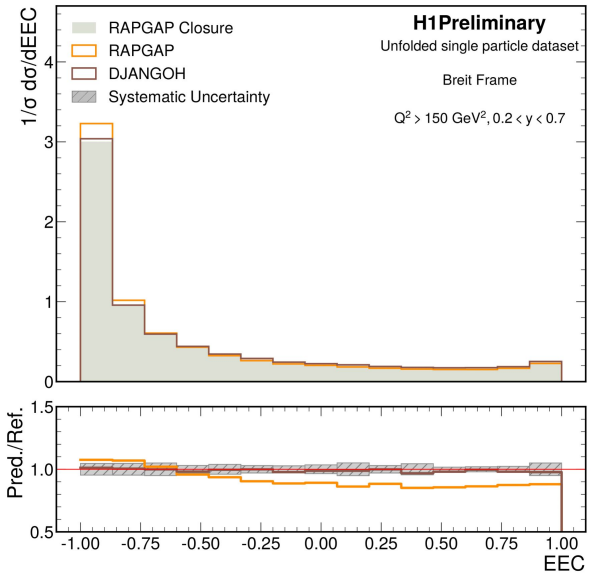

$$\mathrm{EEC_{DIS}} = \sum_a \int \frac{\mathrm{d}\sigma_{ep\to e+a+X}}{\sigma} z_a \, \delta(\cos\theta_{ap} - \cos\theta) \,,$$

$$z_a \equiv \frac{P \cdot p_q}{P \cdot (\sum_i p_i)} \,,$$

Energy-energy correlators in Deep Inelastic Scattering:
Li et al. Phys.Rev.D 103 (2021) 9, 094005

Energy-Energy Correlator (only defined) in Breit frame

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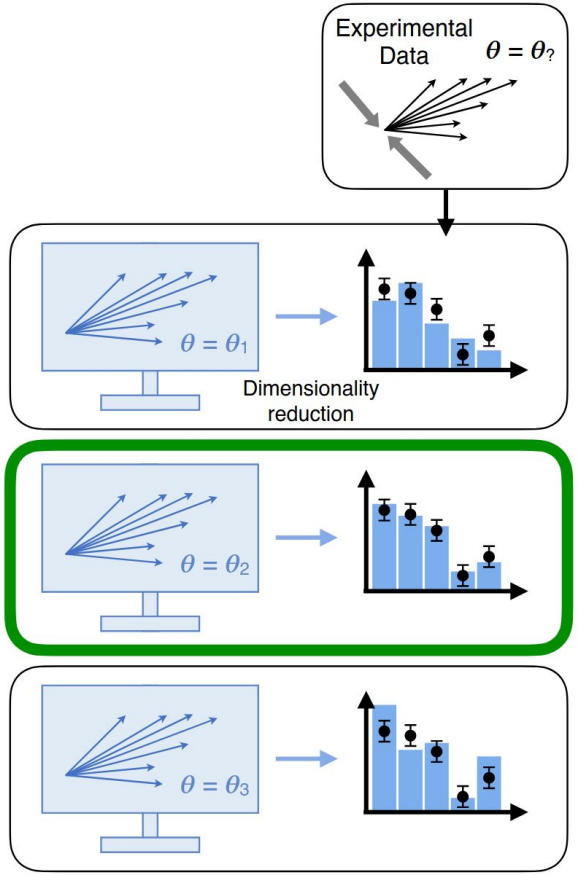
- **Unbinned unfolding pipeline**

Binned inference

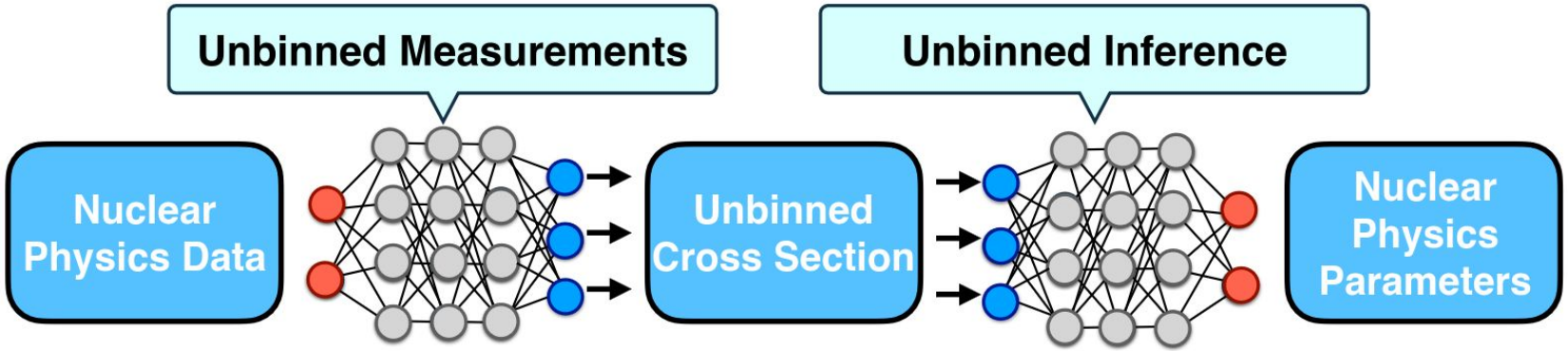
- To go from measurements to matching with theory, need to do inference
- Typically, a functional form is assumed and parameters are fit
  - Computationally expensive and depends on binning



Conventional inference

ML-based inference

- New approach: Train a model to output probability of data given parameters
- Use this model with unbinned unfolded data!



Summary and outlook

- Unfolding removes detector distortions from data
- Binned unfolding is limited, motivating an ML unbinned unfolding approach
  - With ML: Maintain correlations, high dimensional unfolding, no reliance on bin definitions
- We have developed powerful and easy to use tools to do unbinned unfolding
- BDT OmniFold is in a fork of RooUnfold and plans for including it into RooUnfold are ongoing
- Can apply OmniFold to H1 experimental analysis with good closure
- Can create a fully unbinned pipeline with unbinned inference

Thank you!