Unfolding in the context of a CMS heavy ion analysis

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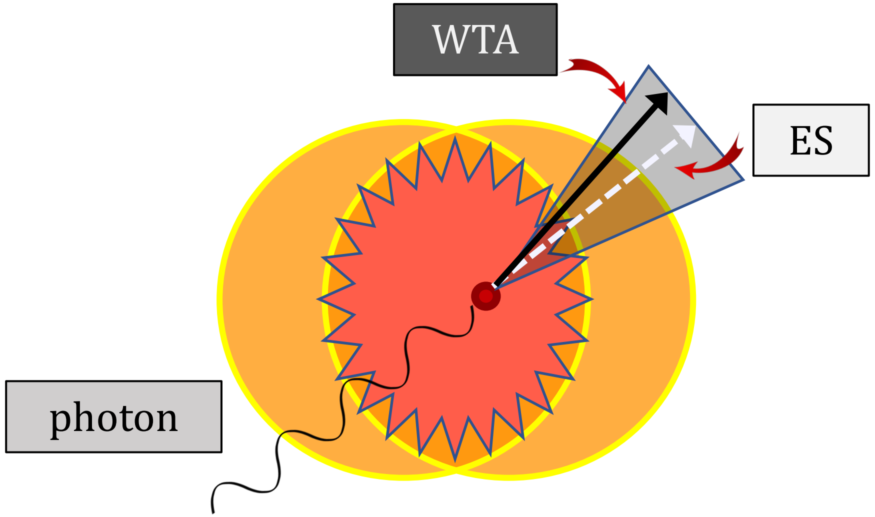
Observables

Studying the jet axis decorrelation, which is the angular difference between the WTA and E-Scheme jet axes

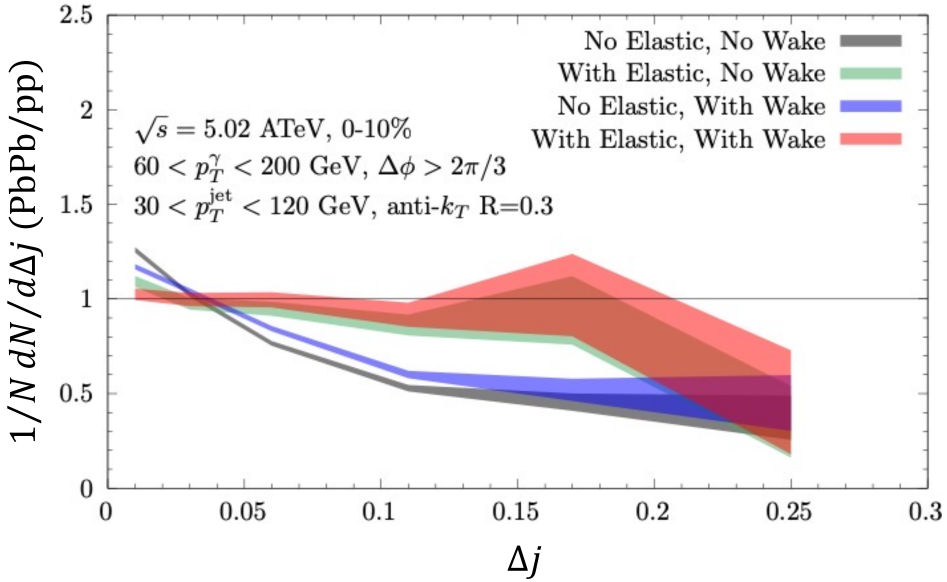
WTA axis = direction of leading energy flow in jet   **E-Scheme axis** = direction of average energy flow in jet

Potentially sensitive to elastic scattering effects in the QGP

Photon-Jet Schematic



Hybrid Model Prediction



$$\Delta j = \sqrt{(\eta^{E-Scheme} - \eta^{WTA})^2 + (\phi^{E-Scheme} - \phi^{WTA})^2}$$

Look at Δj of jets in photon-jet events with $60 < p_T^\gamma < 200$ GeV, $30 < p_T^{jet} < 120$, and $\Delta\phi_{\gamma jet} > 2\pi/3$

Observable unfolded in Δj and p_T^{jet} to allow comparison between pp, PbPb, and theoretical models

Analysis Methods

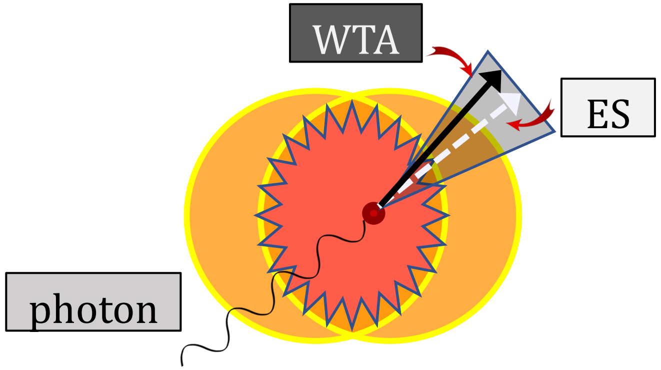
We study pp collisions and and PbPb 0-10%, 10-30%, 30-50%, and 50-90% centrality

Data is unfolded after several statistical background subtraction steps:

- **Mixed event background subtraction** – to remove the component of uncorrelated background jets from the underlying event in PbPb collisions
- **Photon purity subtraction** – to remove the component from jets correlated with decay photons vs isolated prompt photons

MC is used for all studies shown today, which is weighted in several ways to match data:

- **Underlying event density (ρ) weighting** – to match the underlying event density in MC to each centrality interval in data, since this is the primary variable affecting the jet energy resolution
- **Additional weights** – to match the v_z distribution, to weight different $\hat{p}_T$ samples, and, in PbPb collisions, to correct for excluded detector regions



Binning Scheme

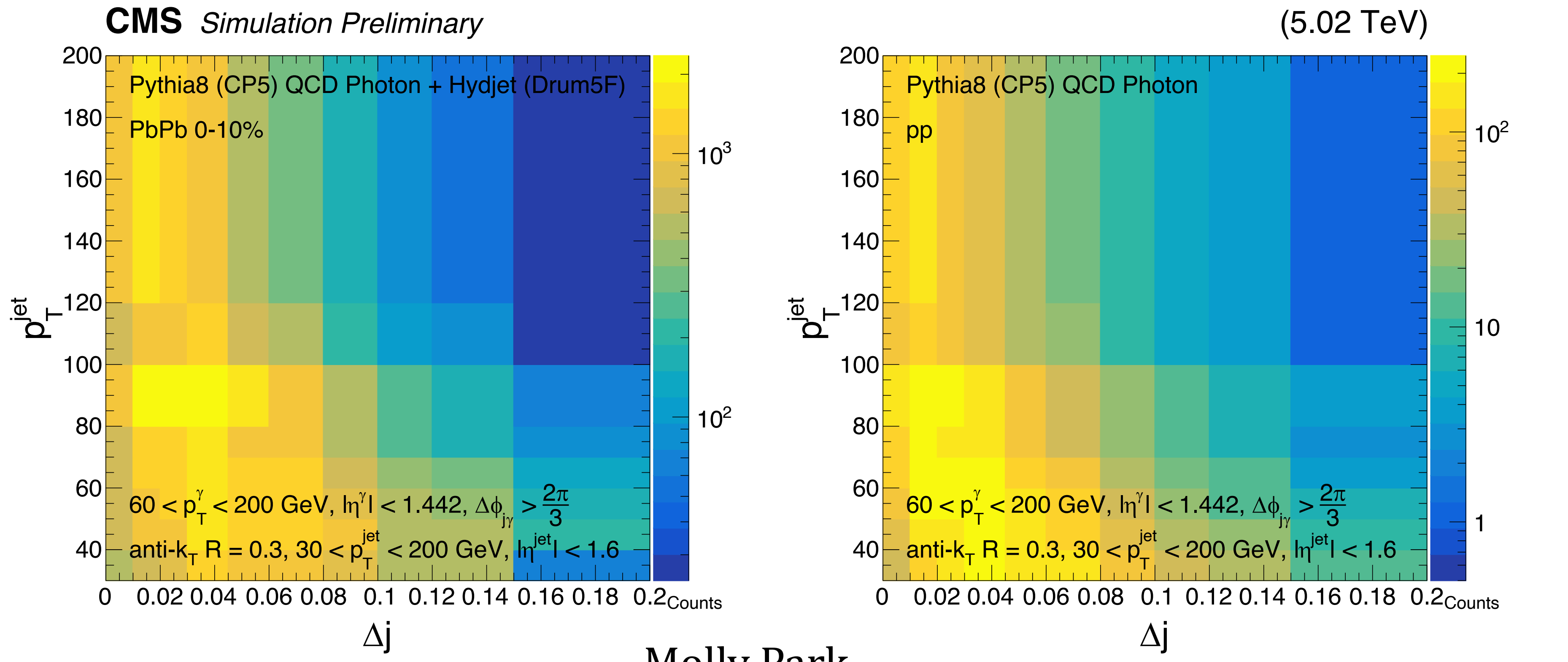
Same reconstruction and generator level binning schemes are used

$\boldsymbol{\Delta j}$: 0, 0.01, 0.02, 0.03, 0.045, 0.06, 0.08, 0.1, 0.12, 0.15, 0.2

$\boldsymbol{p_T^{jet}}$: 30, 40, 50, 60, 70, 80, 100, 120, 200 cut off after unfolding

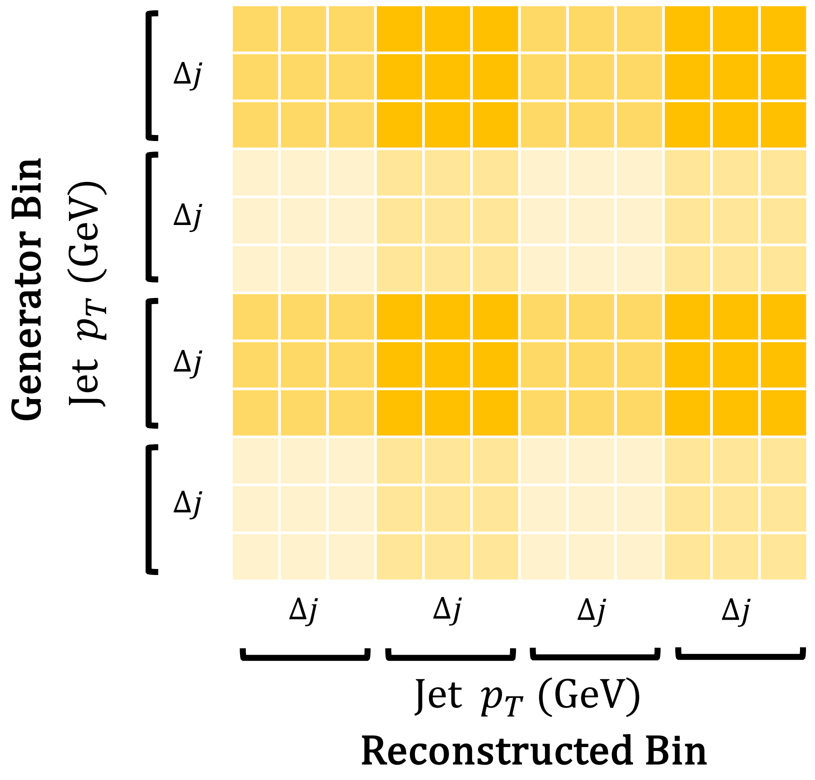
Plots show weighted counts after removing the jet background from underlying event fluctuations

Δj distribution depends strongly on p_T^{jet}

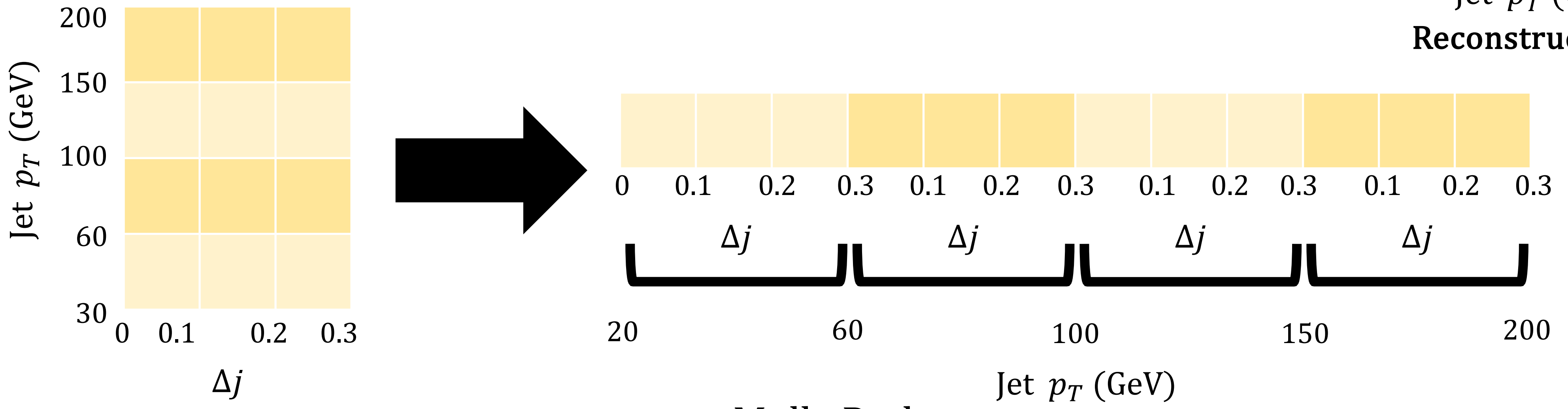


Unfolding Inputs

- Unfolding inputs are flattened two-dimensional histograms with R bins in p_T^{jet} and Δj
- Unfolding response matrices are flattened four-dimensional histograms with R bins x G bins
- Finer binning is in Δj and coarser binning is in p_T^{jet}



- Flattened two-dimensional histogram **example**:



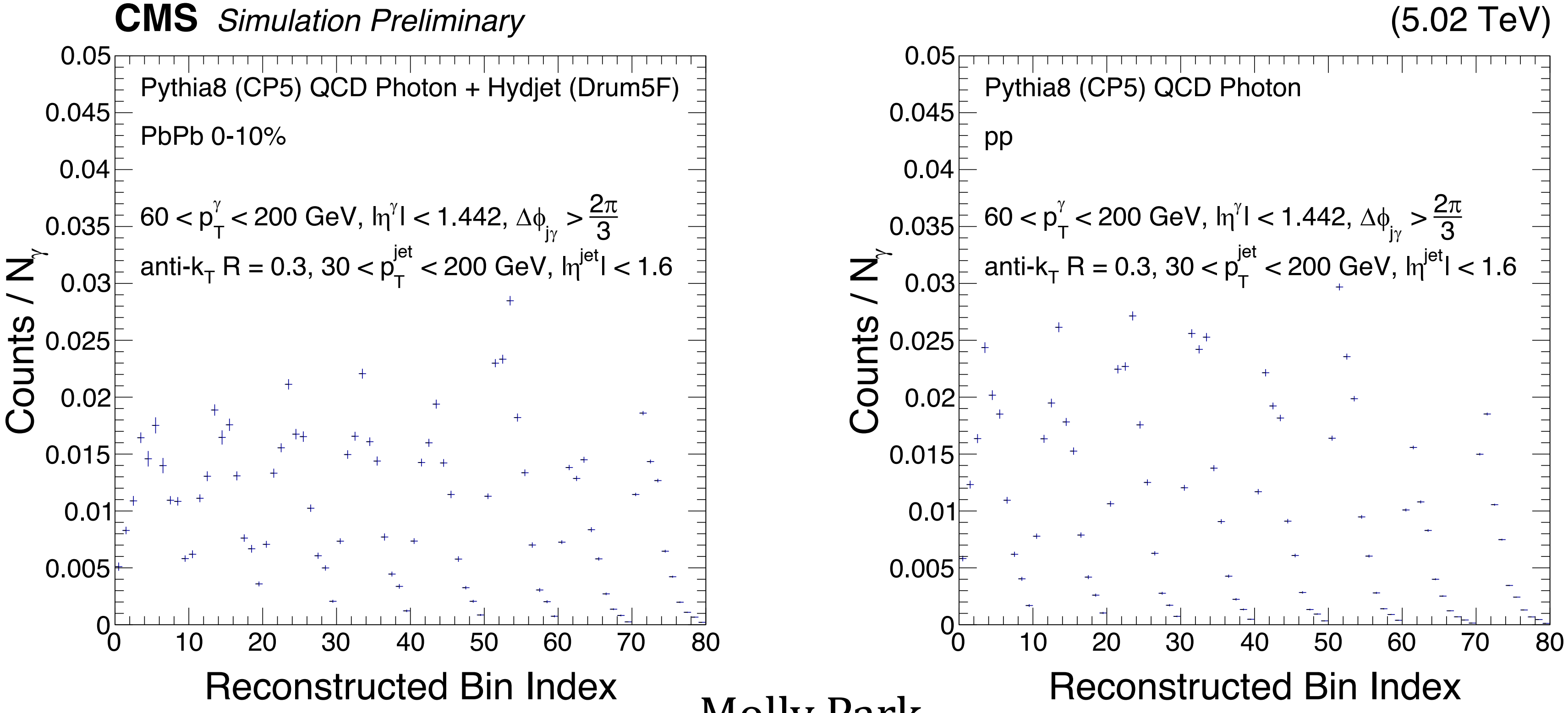
Unfolding Inputs: Flattened Δj-p_T^{jet}

Distributions are normalized per photon before photon purity subtraction

For MC unfolding tests:

- ½ statistics is used for the response matrices
- ½ statistics is run through the analysis chain

Finer binning is in Δj and coarser binning is in p_T^{jet}



Unfolding Inputs: Δj

Distributions are normalized per photon before photon purity subtraction

For MC unfolding tests:

½ statistics is used for the response matrices

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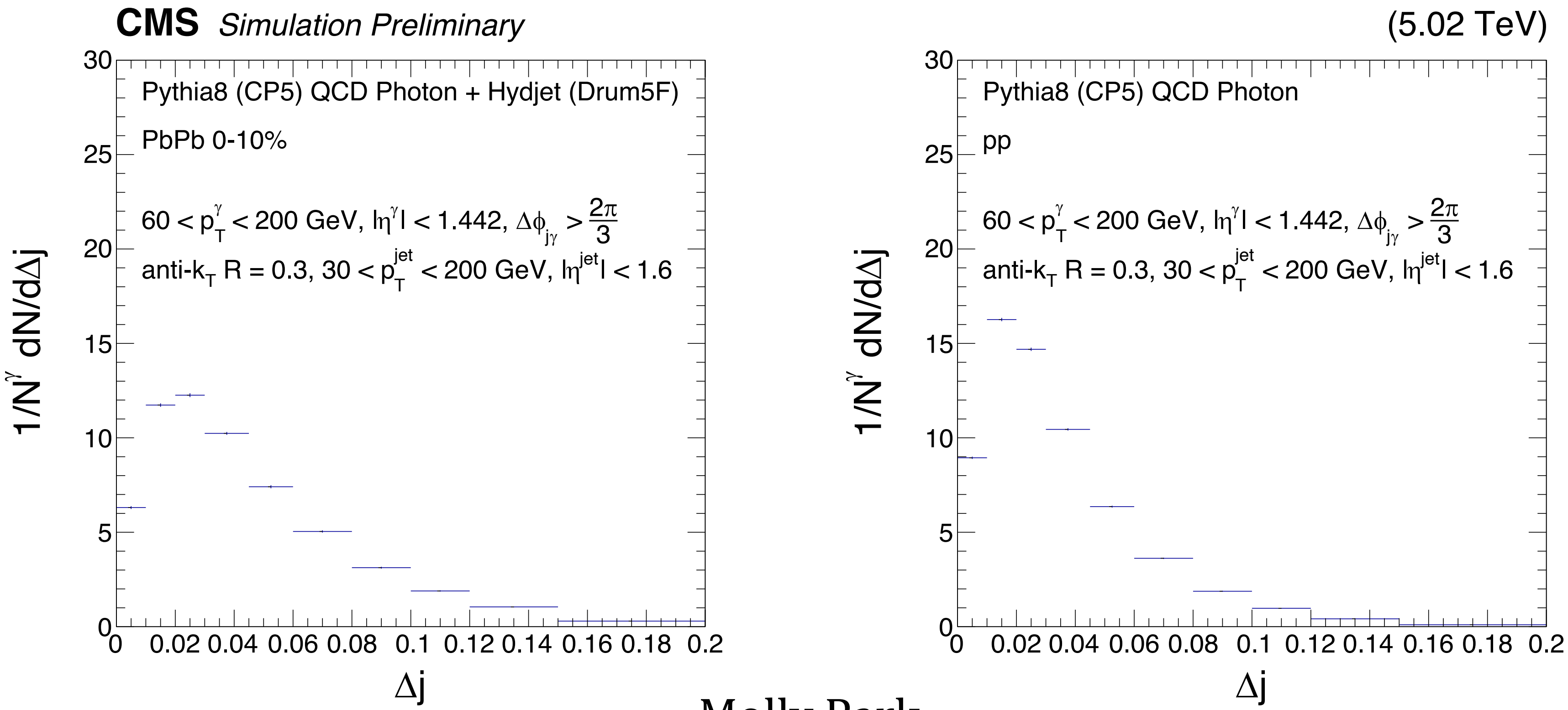
Difference between pp and PbPb in MC comes from smearing effects



Unfolding Inputs: p_T^{jet}

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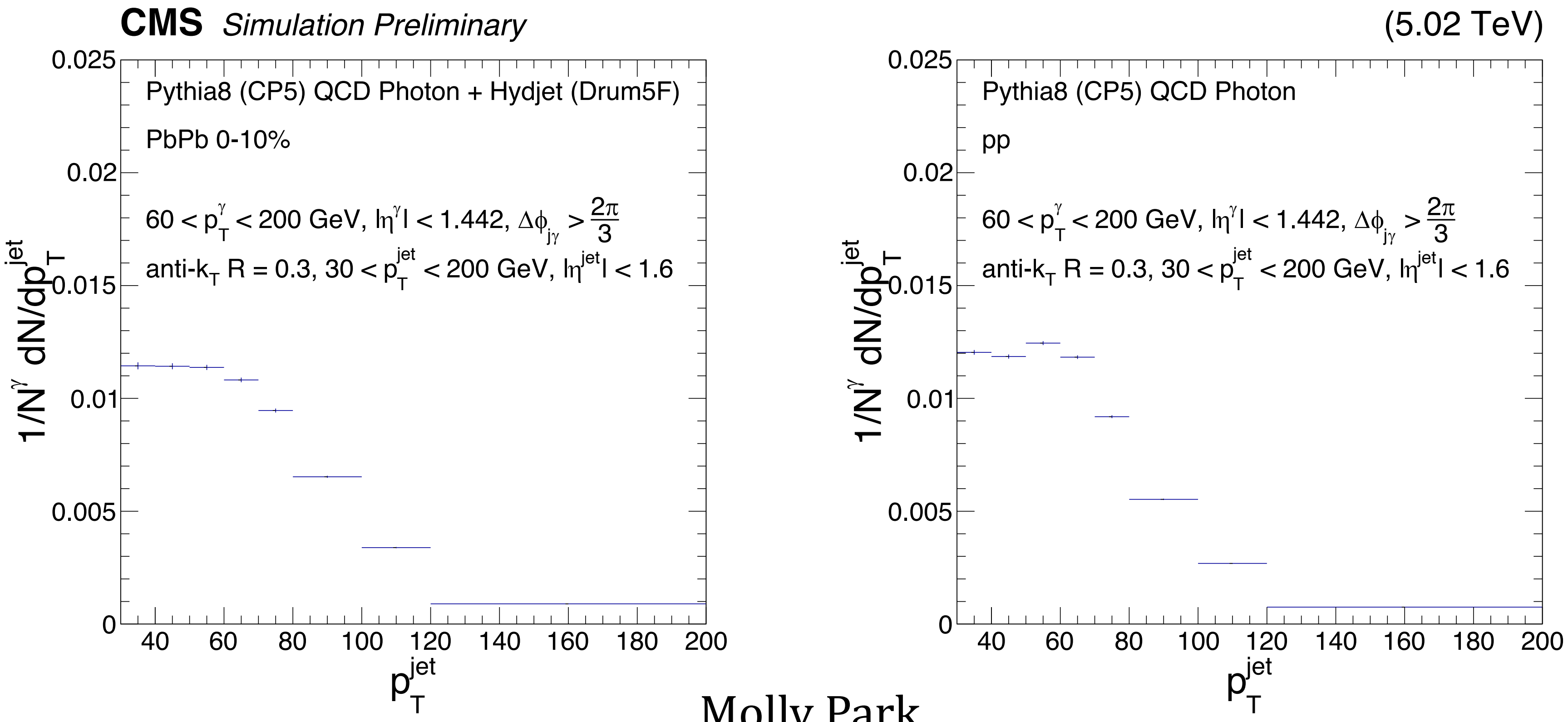
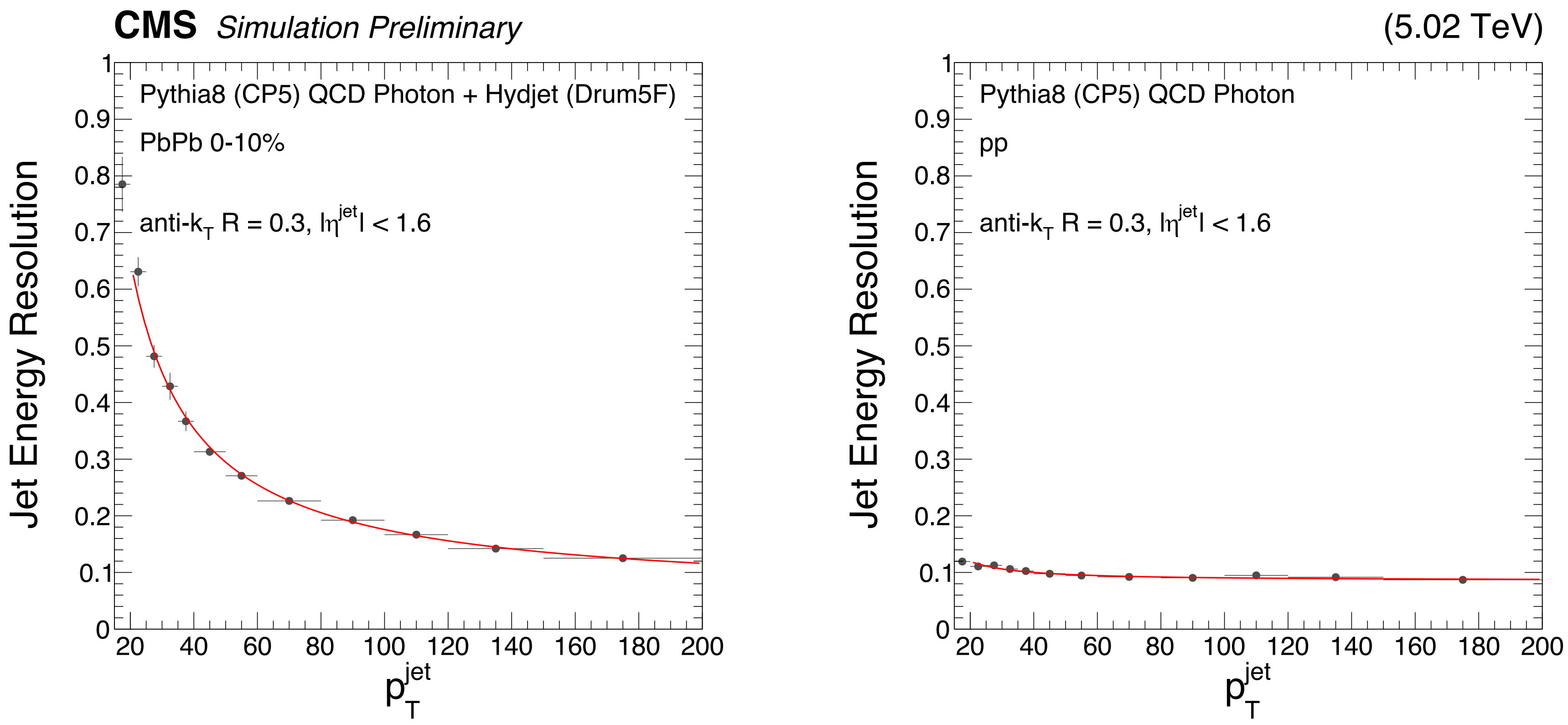


Jet Energy Resolution

p_T^{jet} and Δj resolution strongly affect the unfolding performance

Ratio of generator to reconstructed p_T^{jet} is fit to Gaussian to extract the jet energy resolution

PbPb 0-10% has much worse p_T^{jet} resolution than pp at low p_T^{jet}

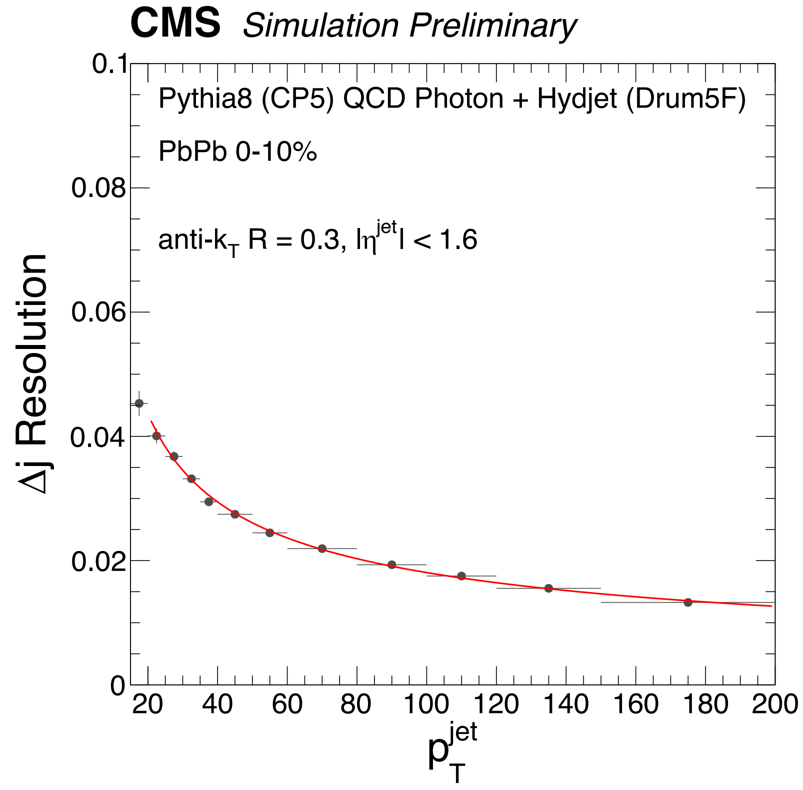


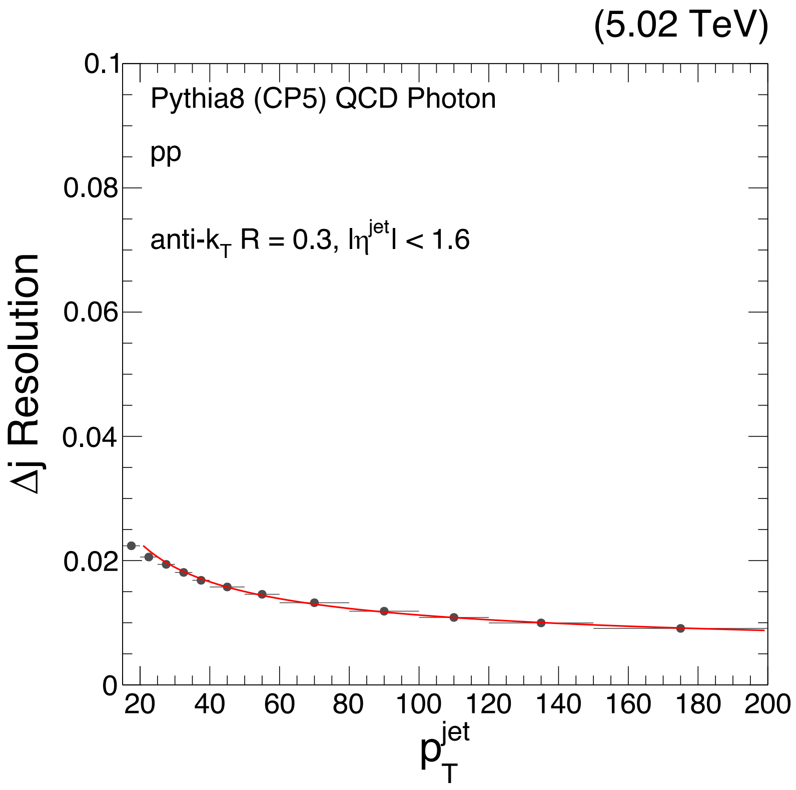
Δj Resolution

p_T^{jet} and Δj resolution strongly affect the unfolding performance

Difference between generator and reconstructed Δj is fit to Gaussian to extract the jet energy resolution

PbPb 0-10% has slightly worse Δj resolution than pp





Response Matrices

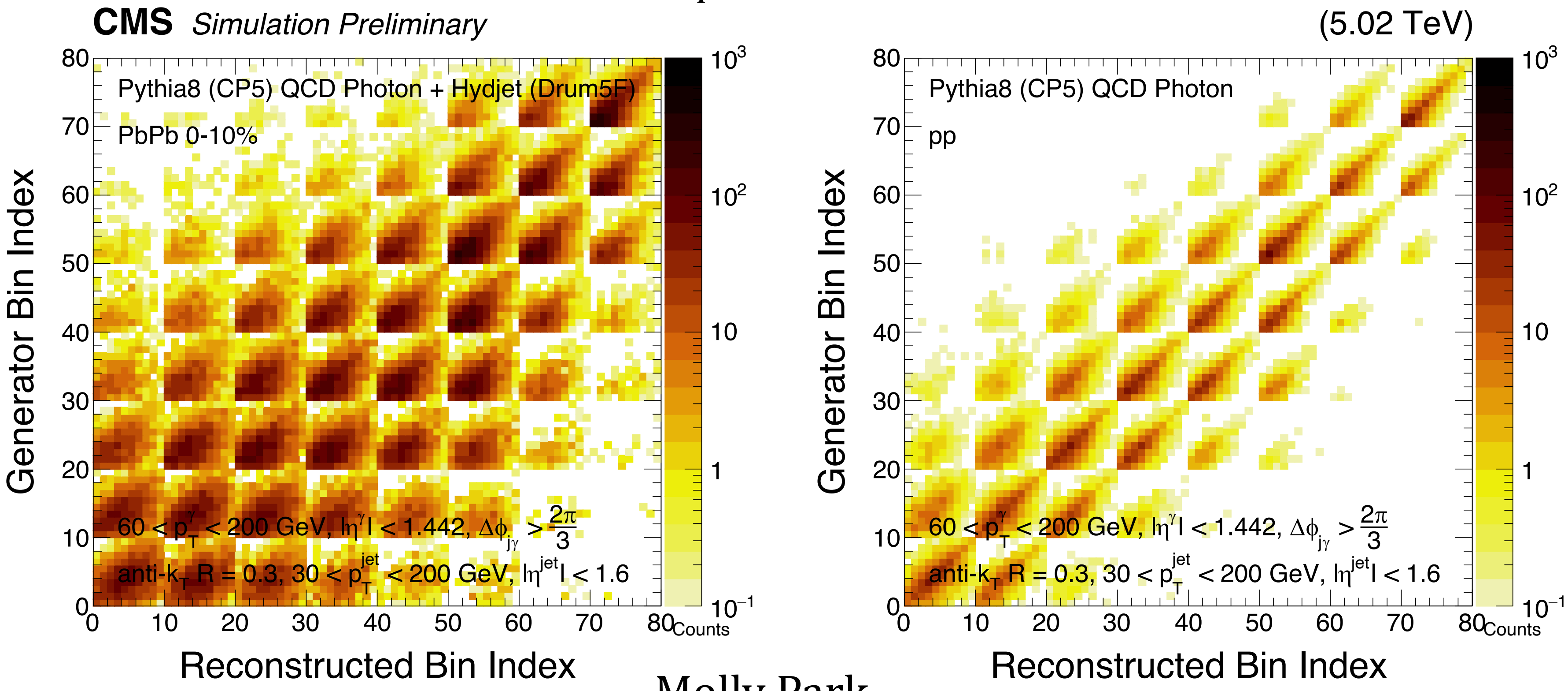
Response matrices filled with Pythia8 photon-jet MC

~ 1M events used in pp collisions

~ 7M events used in PbPb collisions, divided between four centrality classes

Can see by eye the degraded p_T^{jet} and Δj resolutions in PbPb 0-10% compared to pp

Finer binning is in Δj and coarser binning is in p_T^{jet}

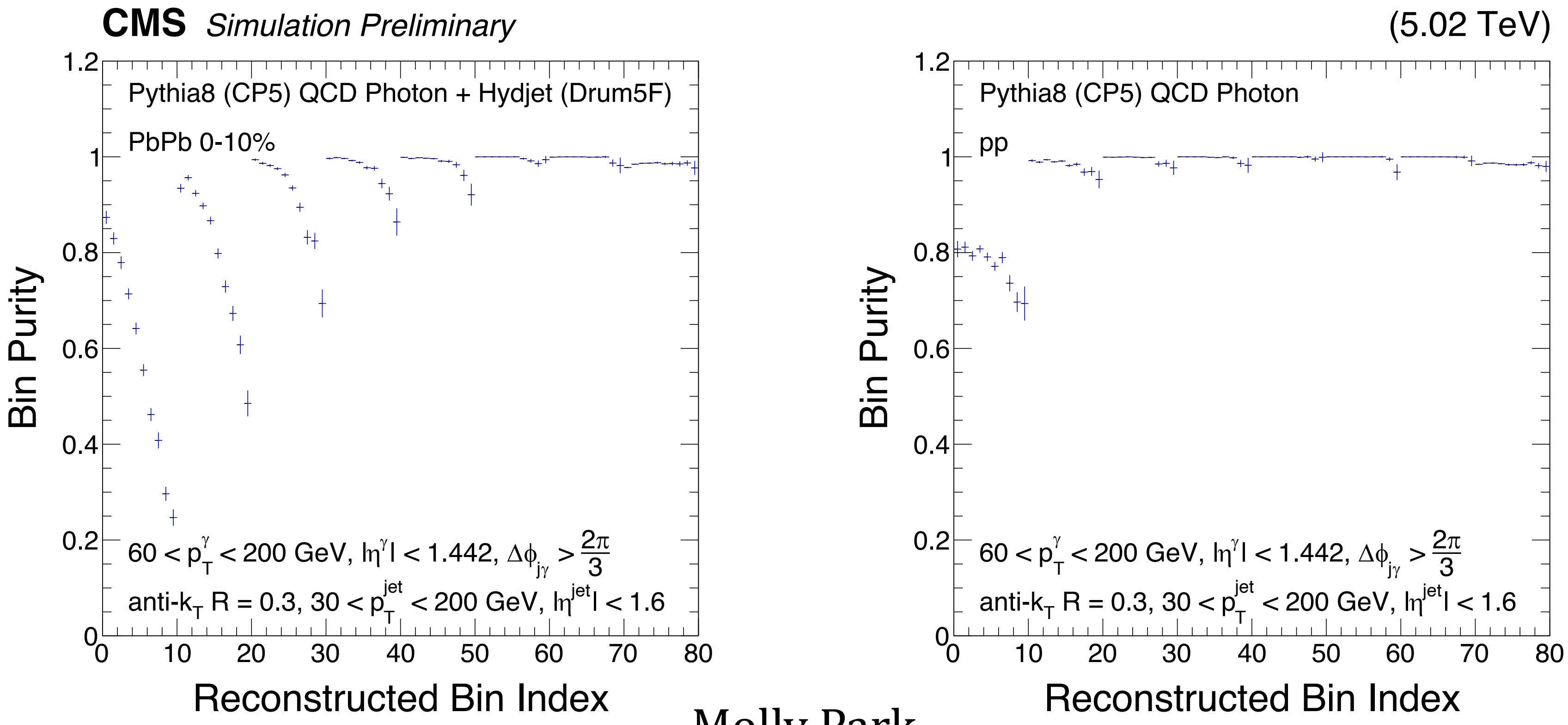


Reconstruction-Level Purity Correction

Bin-by-bin purity correction applied before unfolding

→ Corrects for detector-level jets between 30 – 200 GeV that are not matched to any truth-level jet between 30 – 200 GeV

Fake jets and fake photons are otherwise largely accounted for by the mixed-event background and photon purity subtractions

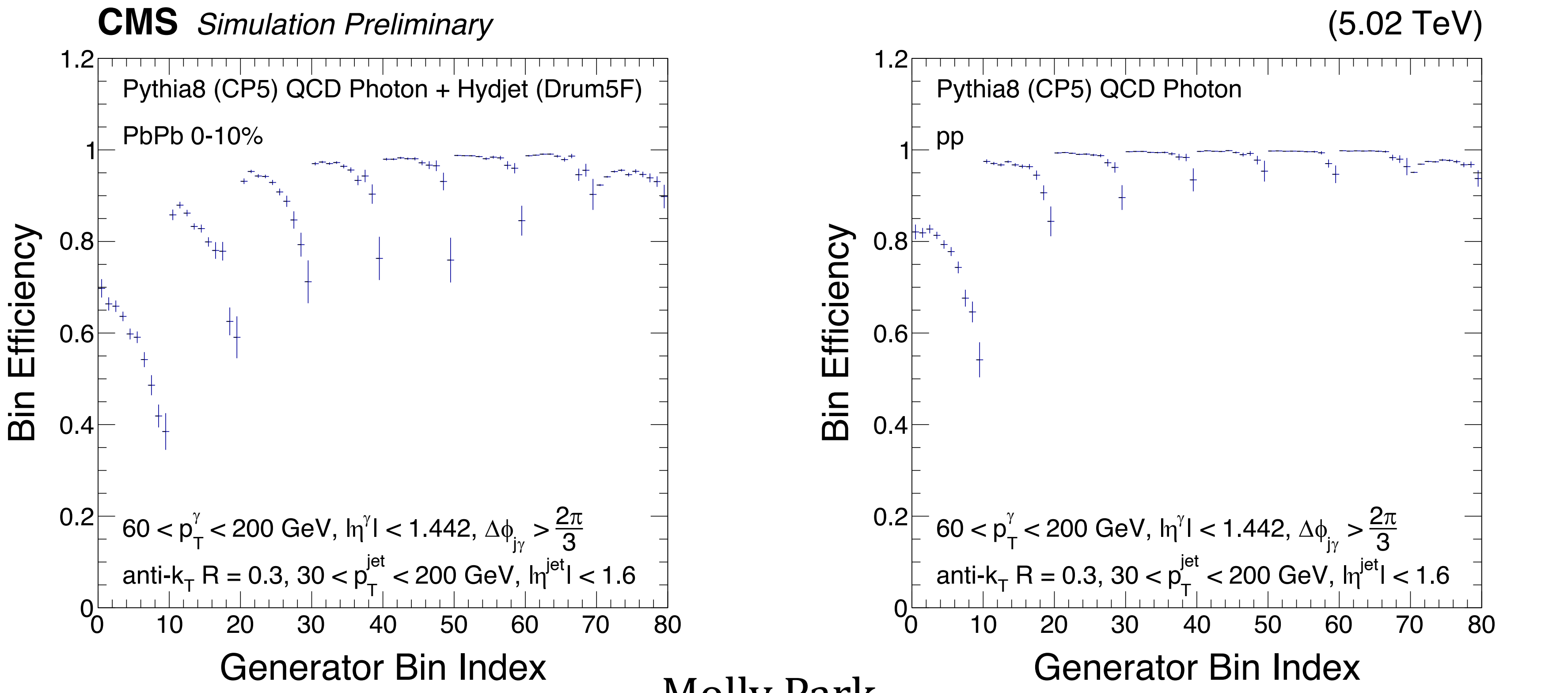


Generator-Level Efficiency Correction

Bin-by-bin efficiency correction applied after unfolding

→ Corrects for truth-level jets between 30 – 200 GeV that are not matched to any detector-level jet between 30 – 200 GeV

Inefficiencies are almost entirely driven by the jet energy resolution



Unfolding Studies

In the following studies, compare different unfolding algorithms and prior choices

Unfolding algorithms:

- SVD unfolding: (using RooUnfold SVDUnfold method)
  - Uses a singular value decomposition of the response matrix
  - Regularization parameter is the rank of the singular value decomposition (k_{reg})
- D'Agostini unfolding: (using RooUnfold BayesUnfold method)
  - Starts with a prior and successively updates the solution based on Bayes' Theorem
  - Regularization parameter is the number of iterations

Prior choices:

- MC prior:
  - From the response matrix truth (Pythia8)
- Flat prior:
  - Flat versus Δj and p_T^{jet} when normalized by bin width
  - Helps understand prior bias effects

Regularization Determination

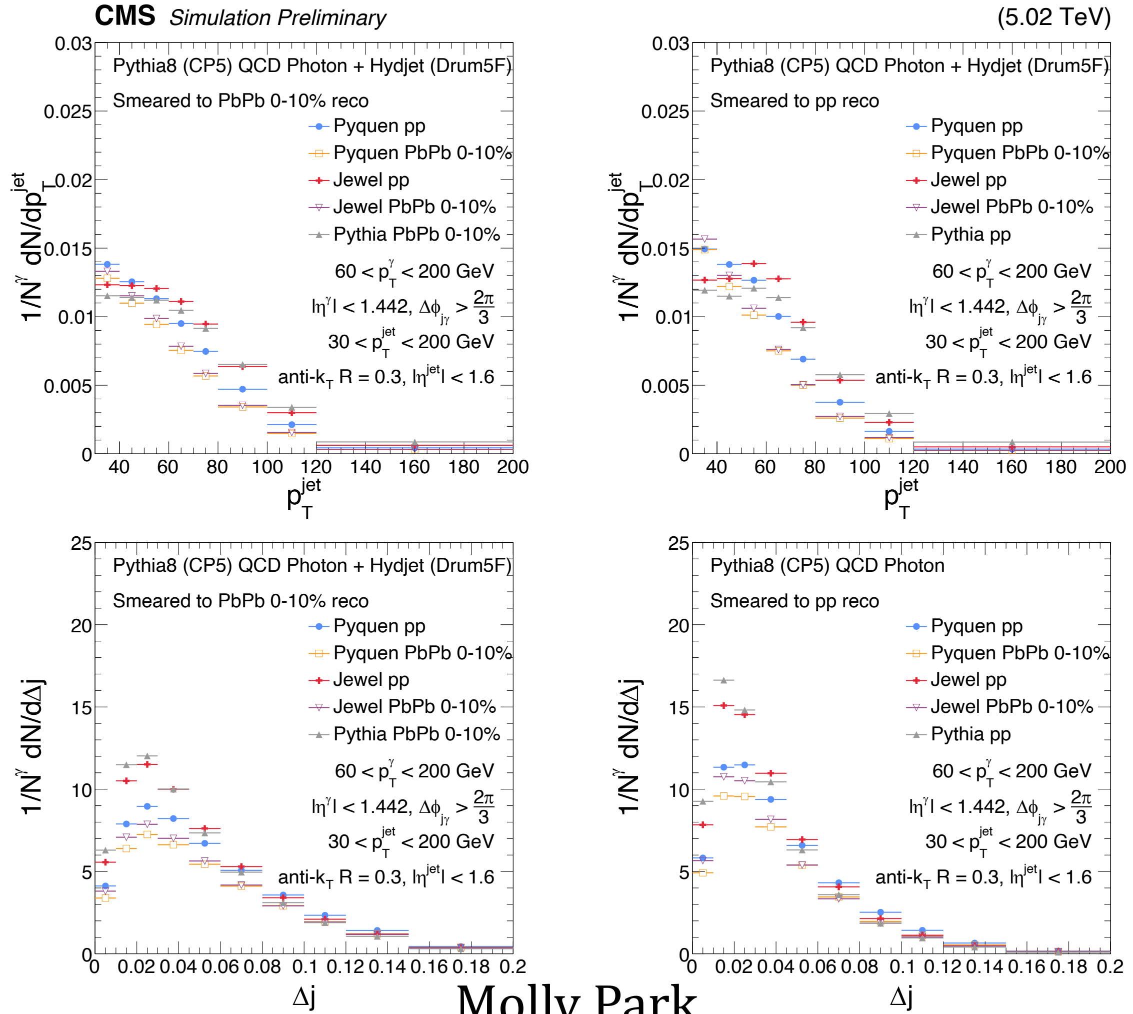
- Regularization parameter determines the trade-off between bias and statistical variance
- Minimize mean squared error (sum of bias squared and variance)
  - Method (link) taken from Fall 2023 PHYSTAT seminar by Lydia Brenner et al.

$$MSE = \frac{1}{M}\sum_{i=1}^{M} V[\hat{\mu}_i] + b_i^2$$

  - $b_i = E[\hat{\mu}_i] - \mu_i$ where $E[\hat{\mu}_i]$ is the expectation of the estimator, μ_i is the true value
  - $V[\hat{\mu}_i]$ is the variance of the estimator
- Method outline:
  1. Start with some theoretical input or toy unrelated to both data and the PYTHIA8 prior
  2. Apply efficiency correction, forward fold with the response matrix, and apply the purity correction
  3. Throw 200 – 1000 toys from the forward-folded input by varying each bin with a **Gaussian**, where the mean is the nominal bin value and the standard deviation is the uncertainty in **data**
  4. Unfold each toy, and use the unfolded toy sample to calculate the bin-averaged bias, variance, and MSE
  5. Choose the regularization choice that minimizes the MSE
- Can't use **Poisson** because we normalize per photon, have background subtraction, and use weights → alters variance from $\frac{1}{\sqrt{N}}$
- Instead use **Gaussian** with standard deviation equal to error in **data**

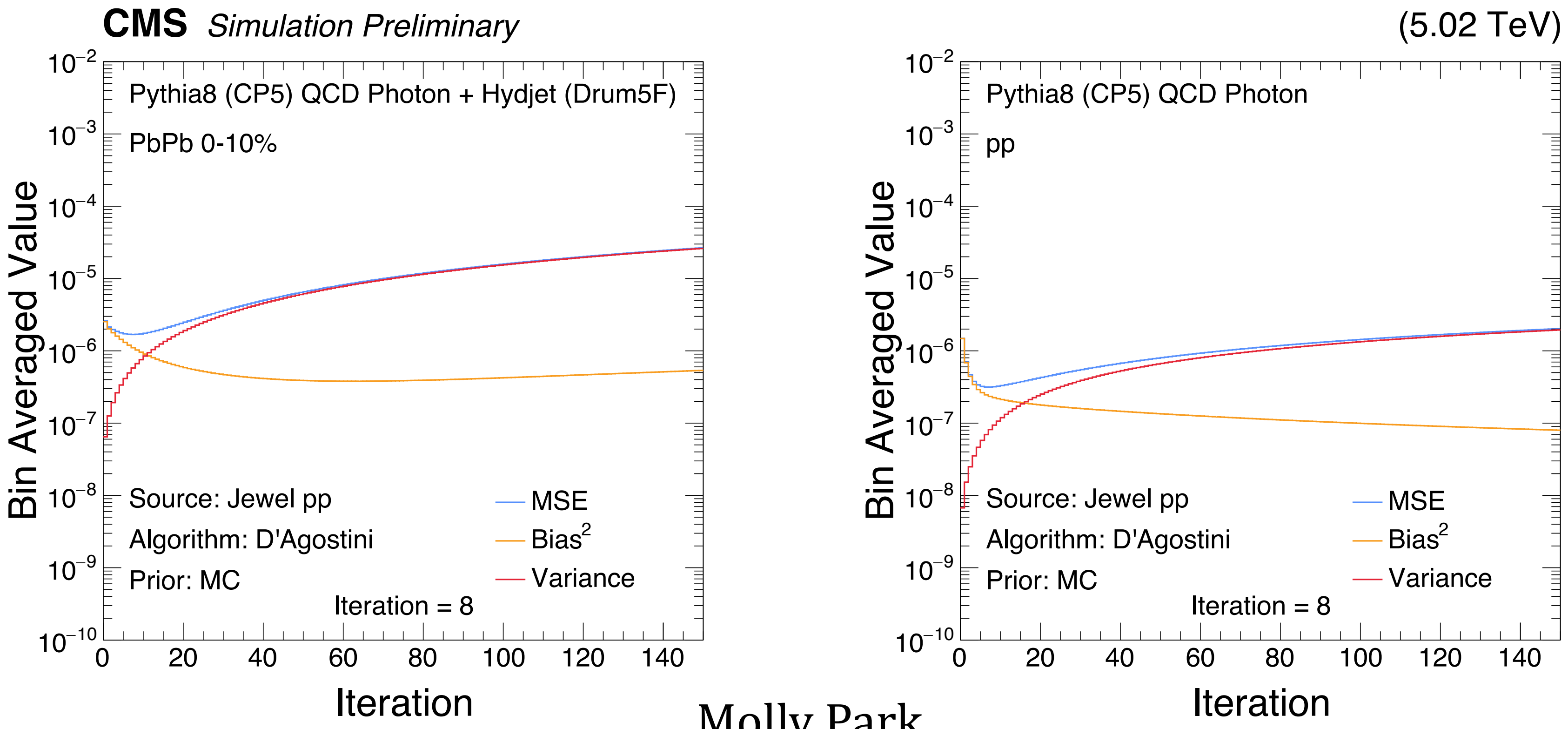
Folded Theory Comparison

- Use several different theory inputs to generate the Asimov dataset and determine MSE
- Can use theory for any collision and centrality interval and forward-fold with relevant response matrix
- Inputs cover a wide range of possibilities => increases robustness of regularization determination



MSE: D'Agostini, MC Prior

- Unfolding performed with the D'Agostini iteration with early stopping method
  - RooUnfold used for unfolding
  - Regularization parameter is the iteration choice
  - Reweight response matrix truth to prior
- MSE determined with 1000 toys starting from JEWEL pp theory



MSE: D'Agostini, Flat Prior

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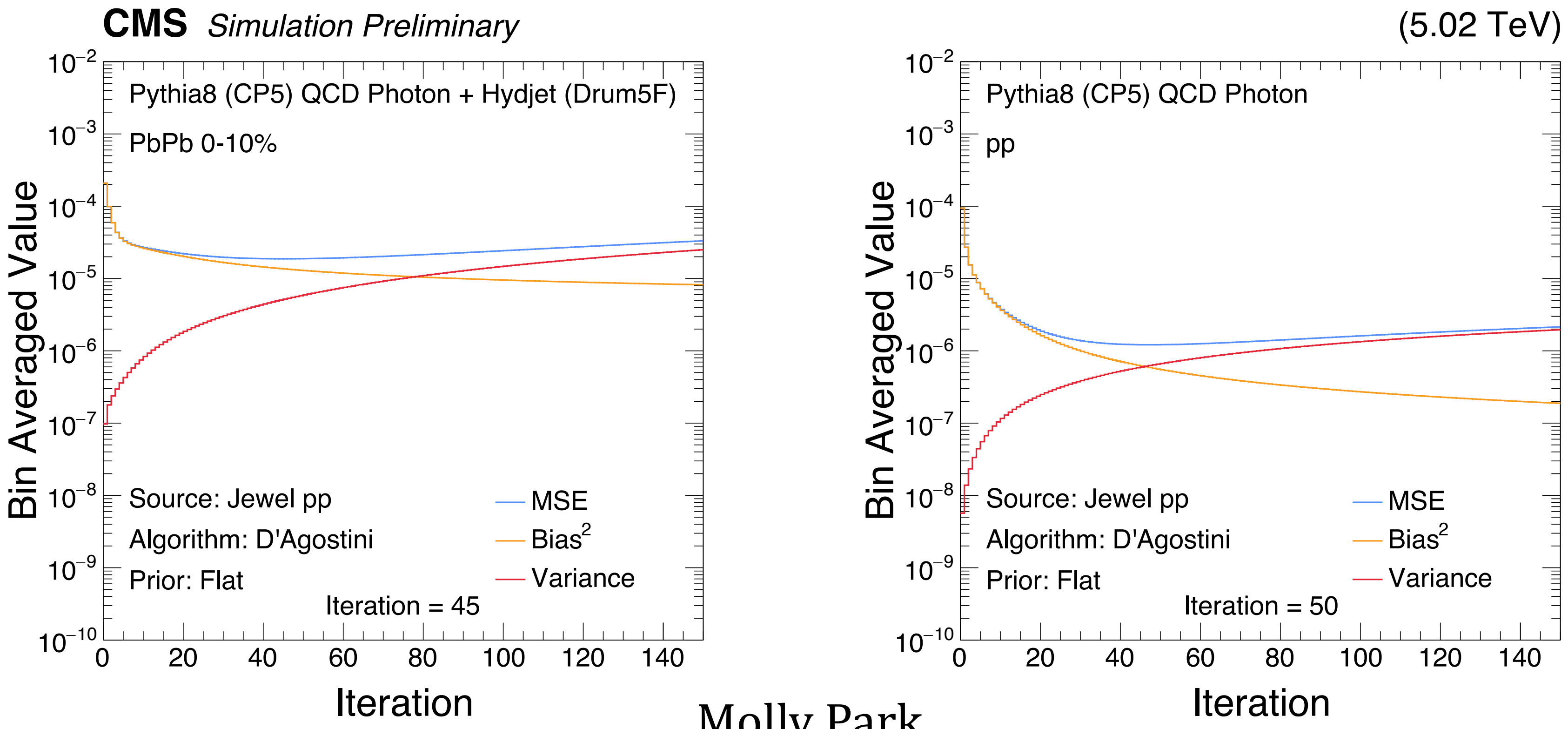
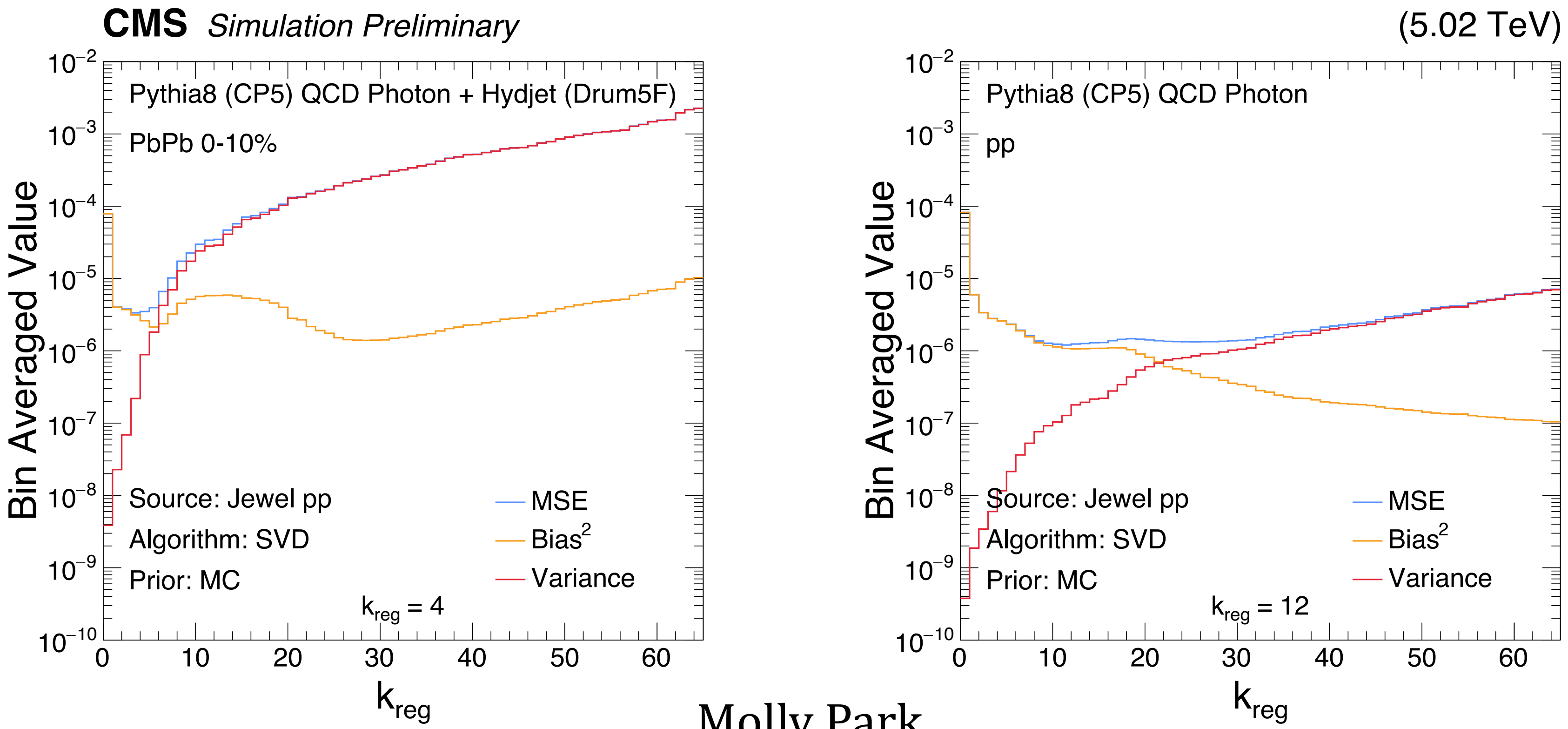
- MSE determined with 1000 toys starting from JEWEL pp theory
- **With a flat prior, the apparent bias is over 10x larger**



MSE: SVD, MC Prior

- Unfolding performed with the SVD method
  - RooUnfold used for unfolding
  - Regularization parameter is k_{reg}, which is the rank of the singular value decomposition
  - Reweight response matrix truth to prior
- MSE determined with 200 toys starting from JEWEL pp theory
- **Bias is ~2-3 times larger than D'Agostini with a MC prior**



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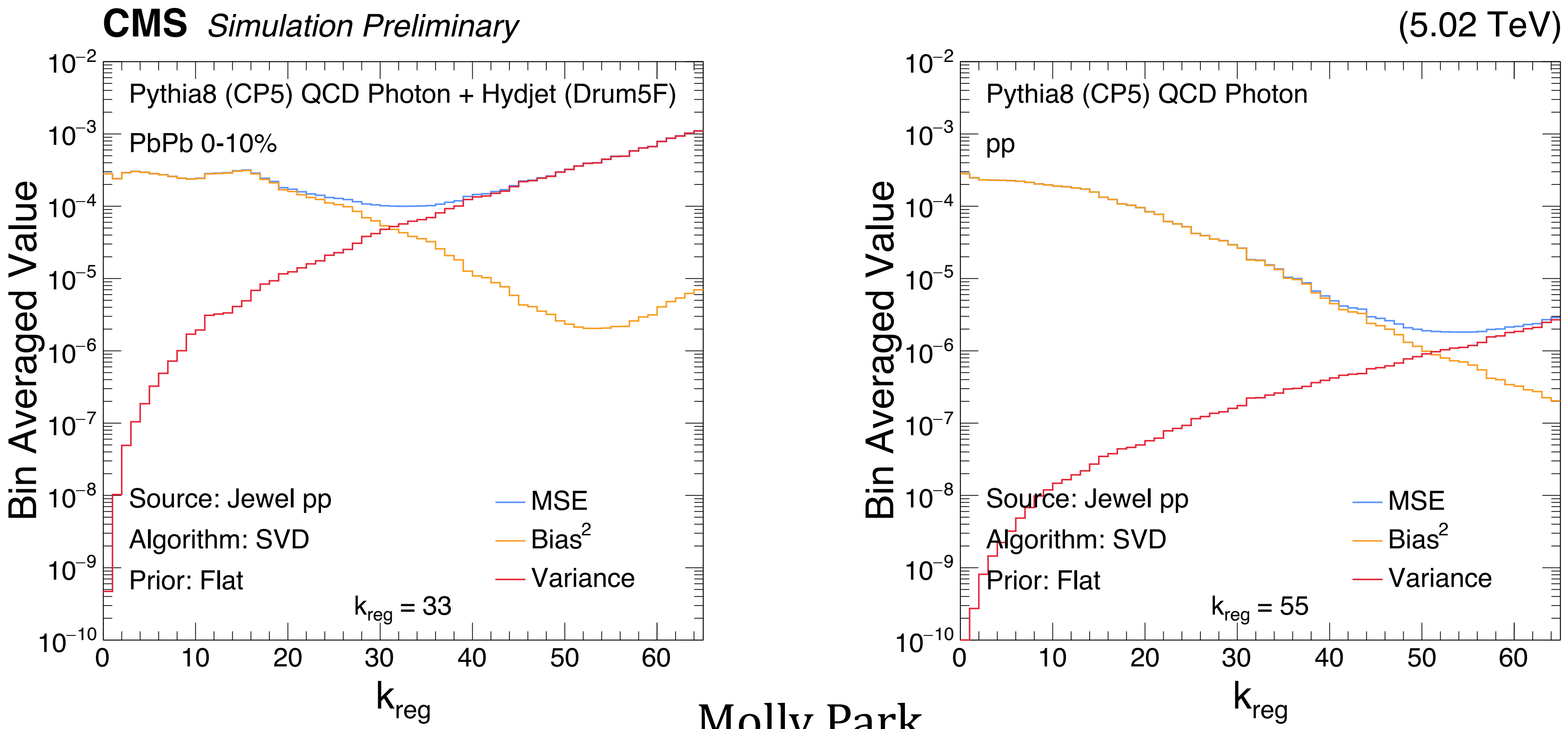


Optimal Regularization: MC Prior

D'Agostini	PbPb 50-90%	PbPb 30-50%	PbPb 10-30%	PbPb 0-10%	PP
Jewel pp	1	4	8	8	8
Jewel PbPb 0-10%	2	4	8	8	16
Pyquen pp	2	5	12	10	16
Pyquen PbPb 0-10%	2	4	7	6	18
Pythia (ind. stats)	1	1	1	1	1

SVD	PbPb 50-90%	PbPb 30-50%	PbPb 10-30%	PbPb 0-10%	PP
Jewel pp	4	4	6	4	12
Jewel PbPb 0-10%	4	4	4	4	9
Pyquen pp	6	7	7	3	30
Pyquen PbPb 0-10%	4	4	4	4	39
Pythia (ind. stats)	2	2	2	2	2

Regularization strength does not depend strongly on the model used to throw toys
Take difference in optimal regularization strength as systematic uncertainty

Bottom Line Test

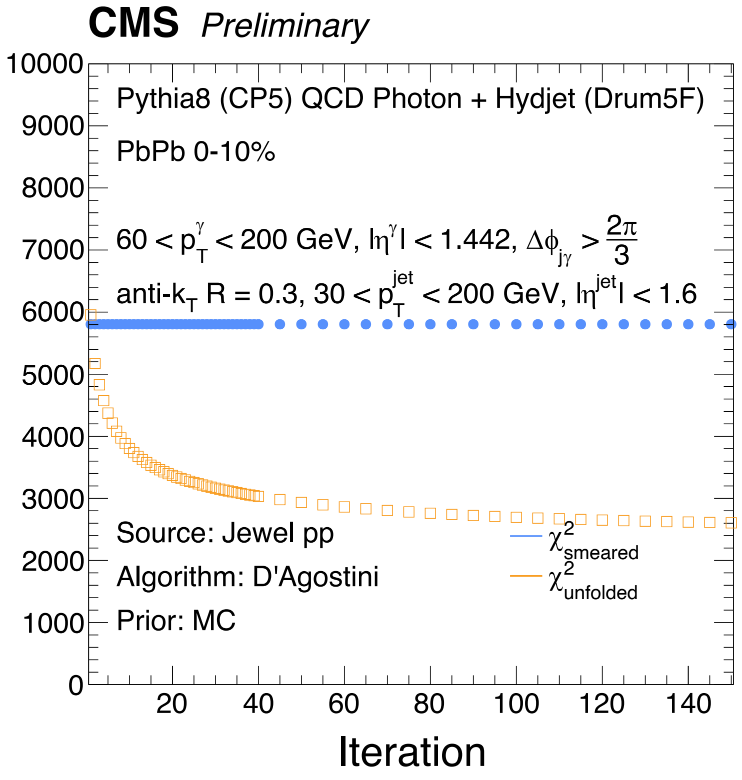
- After unfolding, we should have $\chi^2_{smeared} > \chi^2_{unfolded}$
- The unfolding procedure can only reduce or preserve the information about the model present in the data
- $\chi^2_{smeared} = (y - K\lambda)^T V_y^{-1} (y - K\lambda)$
  - $y =$ data before unfolding
  - $K =$ response matrix
  - $\lambda =$ model prediction
  - $V_y =$ covariance matrix of data before unfolding
    - Take to be a diagonal matrix, where each entry is the squared uncertainty in data
- $\chi^2_{unfolded} = (x - \lambda)^T V_x^{-1} (x - \lambda)$
  - $x =$ data before unfolding
  - $\lambda =$ model prediction
  - $V_x =$ covariance matrix of data after unfolding
    - Manually calculated with 2500 toys
- Performed bottom line test using covariance matrix from unfolding and theory from JEWEL, PYQUEN, or PYTHIA

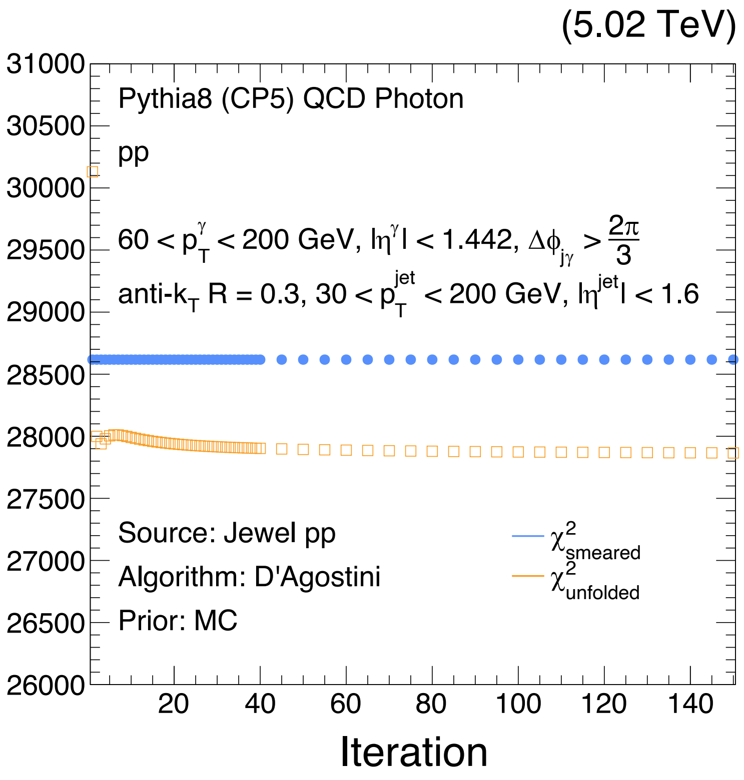
Bottom Line Test

Performed on unfolding outputs/inputs collapsed onto δj, since this is our observable of interest

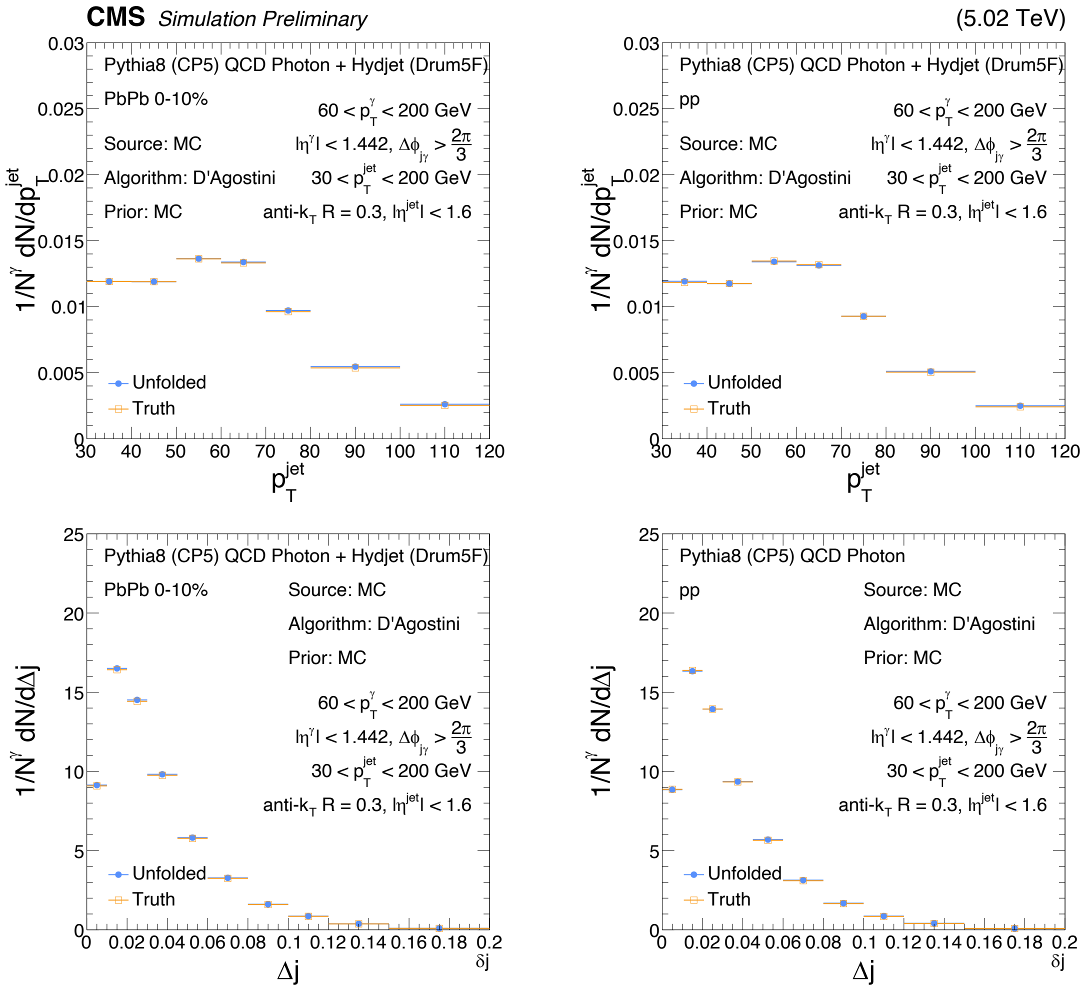
Data passes bottom-line test well before, or around the optimal iteration from the minimum MSE

Plateauing behavior appears to arise due to off-diagonal elements in the covariance matrix



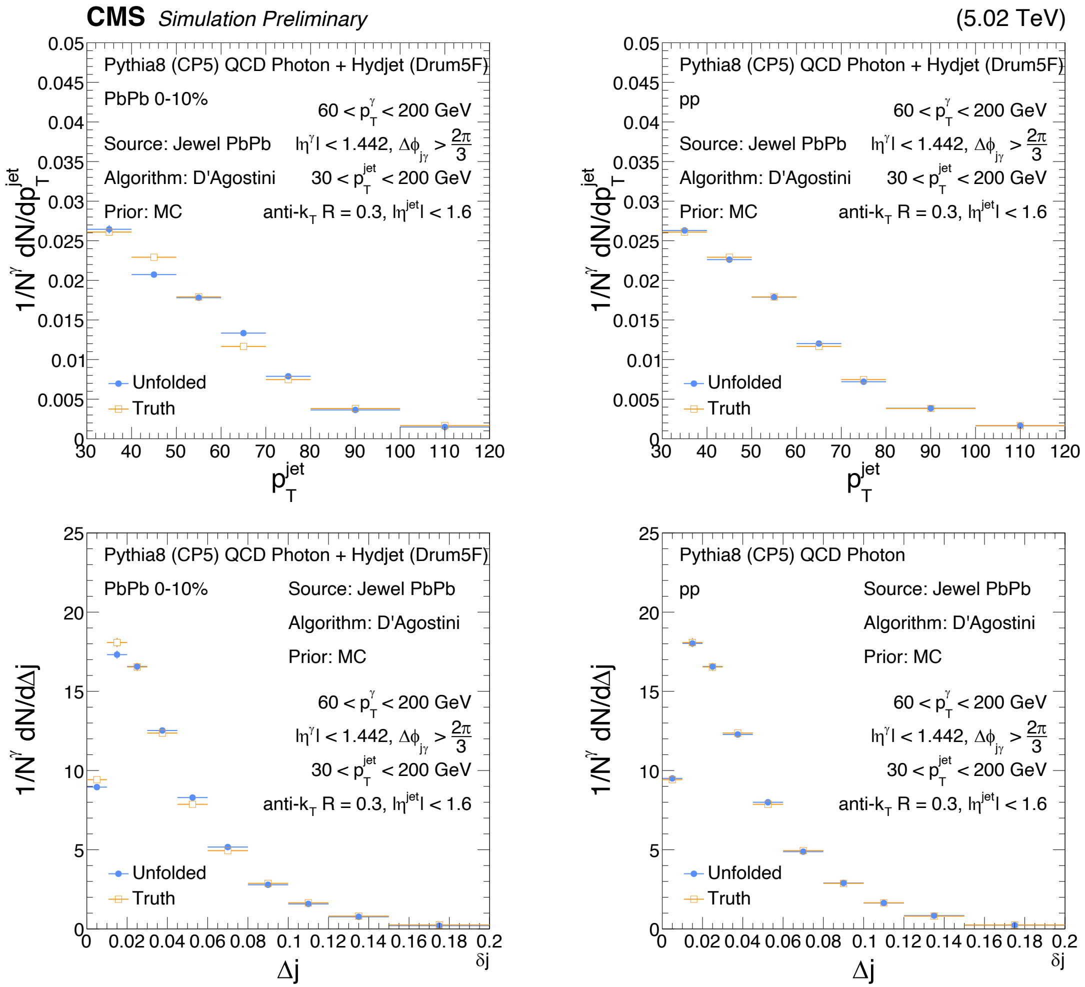


MC Closure: D'Agostini, MC Prior



Closure is very good for MC with independent statistics

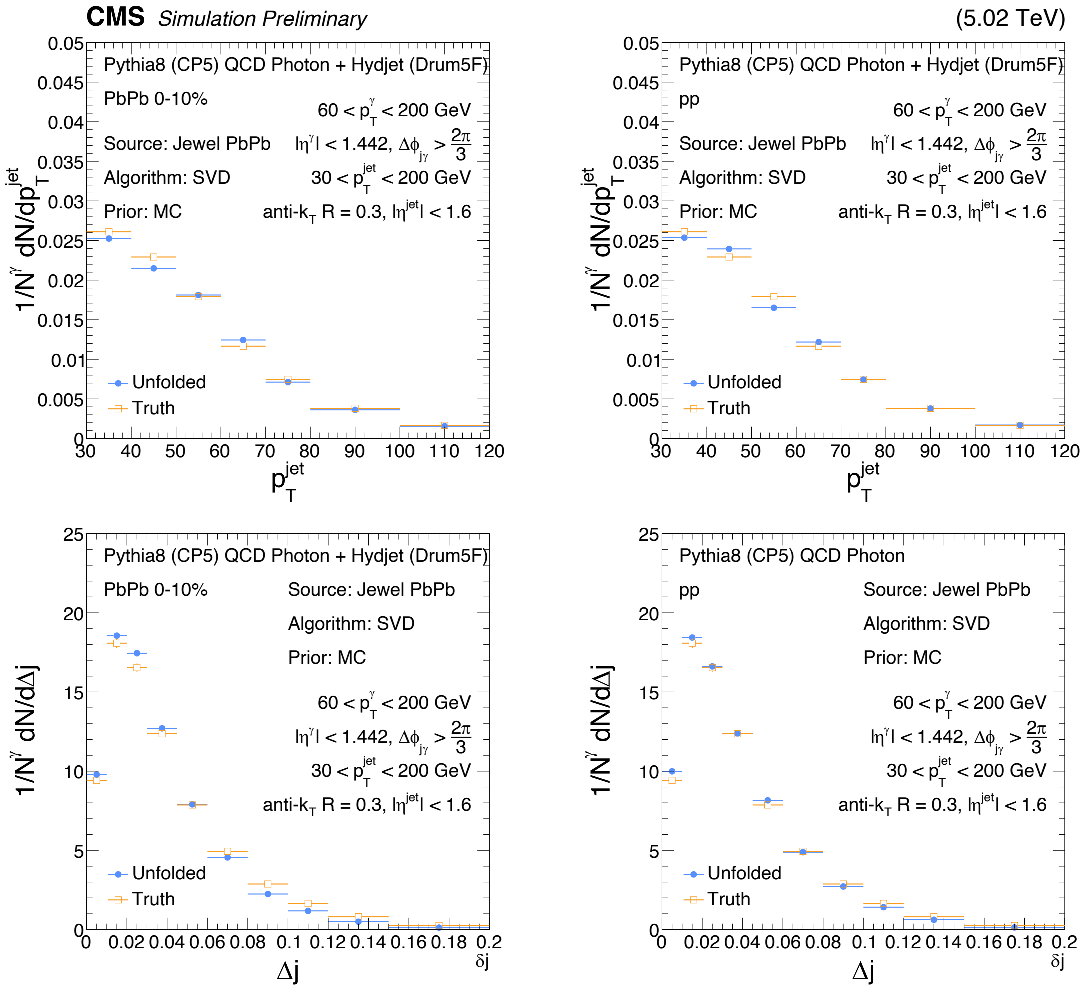
Jewel PbPb 0-10% Closure: D'Agostini, MC Prior



Jewel AA 0-10%, forward folded with each response matrix, and unfolded with MC prior

Closure is decent in Δj and jet p_T

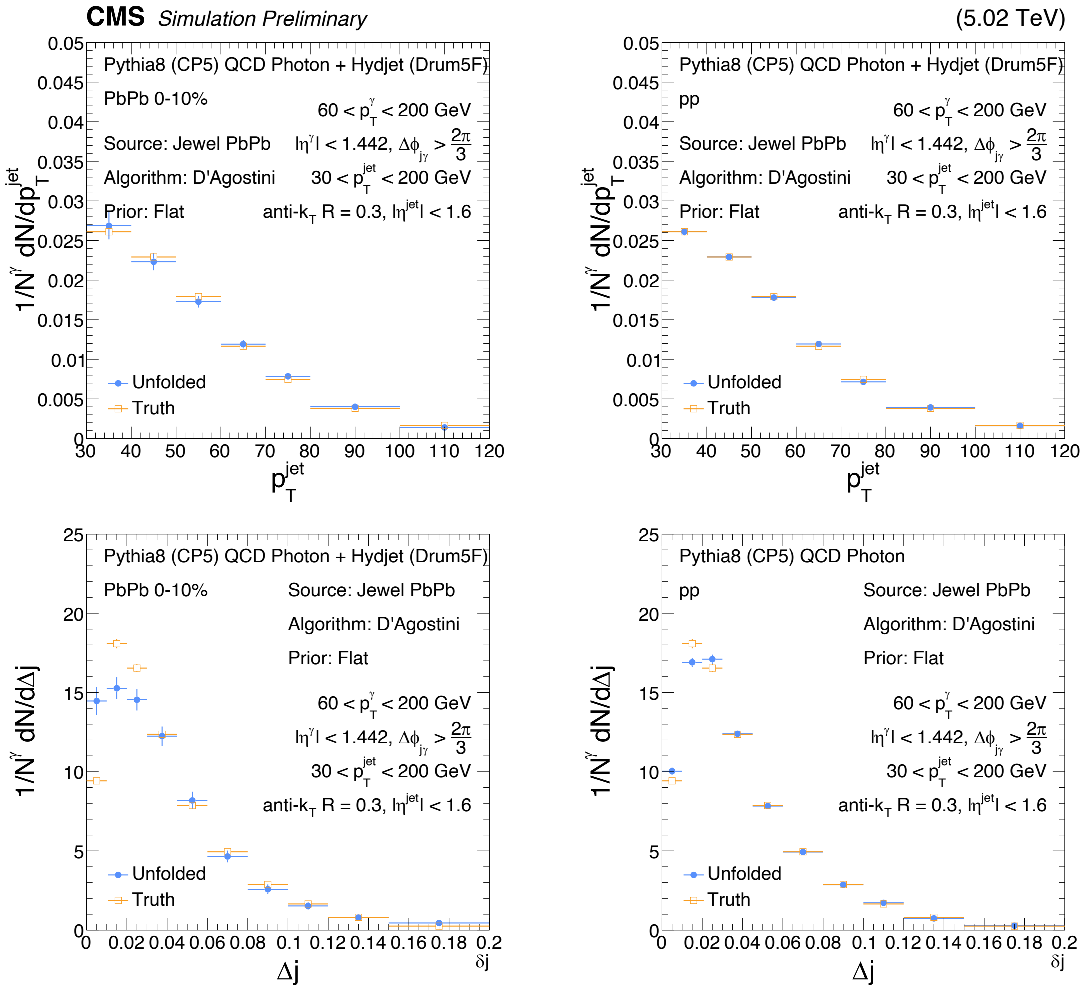
Jewel PbPb 0-10% Closure: SVD, MC Prior



Jewel AA 0-10%, forward folded with each response matrix, and unfolded with MC prior

Closure is decent in Δj and jet p_T

Jewel PbPb 0-10% Closure: D’Agostini, Flat Prior



Closure is ok for jet p_T, since it is relatively flat, but is extremely bad for Δj

Conclusions

- Large jet energy resolution in heavy ion collisions poses substantial challenge for unfolding
- Larger uncertainties in heavy ion collisions also pose a challenge for unfolding
  - Variance blows up very quickly as regularization strength is decreased
  - Minimum mean squared error occurs at much stronger regularization strength than in pp collisions
- Unfolding with a flat prior reveals large bias effects from prior choice
  - Using the flat prior for heavy ion analysis is not feasible due to very large nonclosure
  - Instead can account for uncertainty with a systematic by using a maximally different prior e.g. Jewel PbPb 0-10% for each collision system and centrality interval
- Using different theoretical models to determine the MSE yields very consistent regularization choice
  - Difference in choices can be used to determine the systematic uncertainty for regularization strength
- D'Agostini unfolding performs better in this analysis, but SVD also has good performance
  - Still works well despite background subtraction steps
  - However, need to manually determine the covariance matrix of unfolded data with ~ 2500 toys