Enabling Specialized Unfolding Methods with Modern Machine Learning (ML)

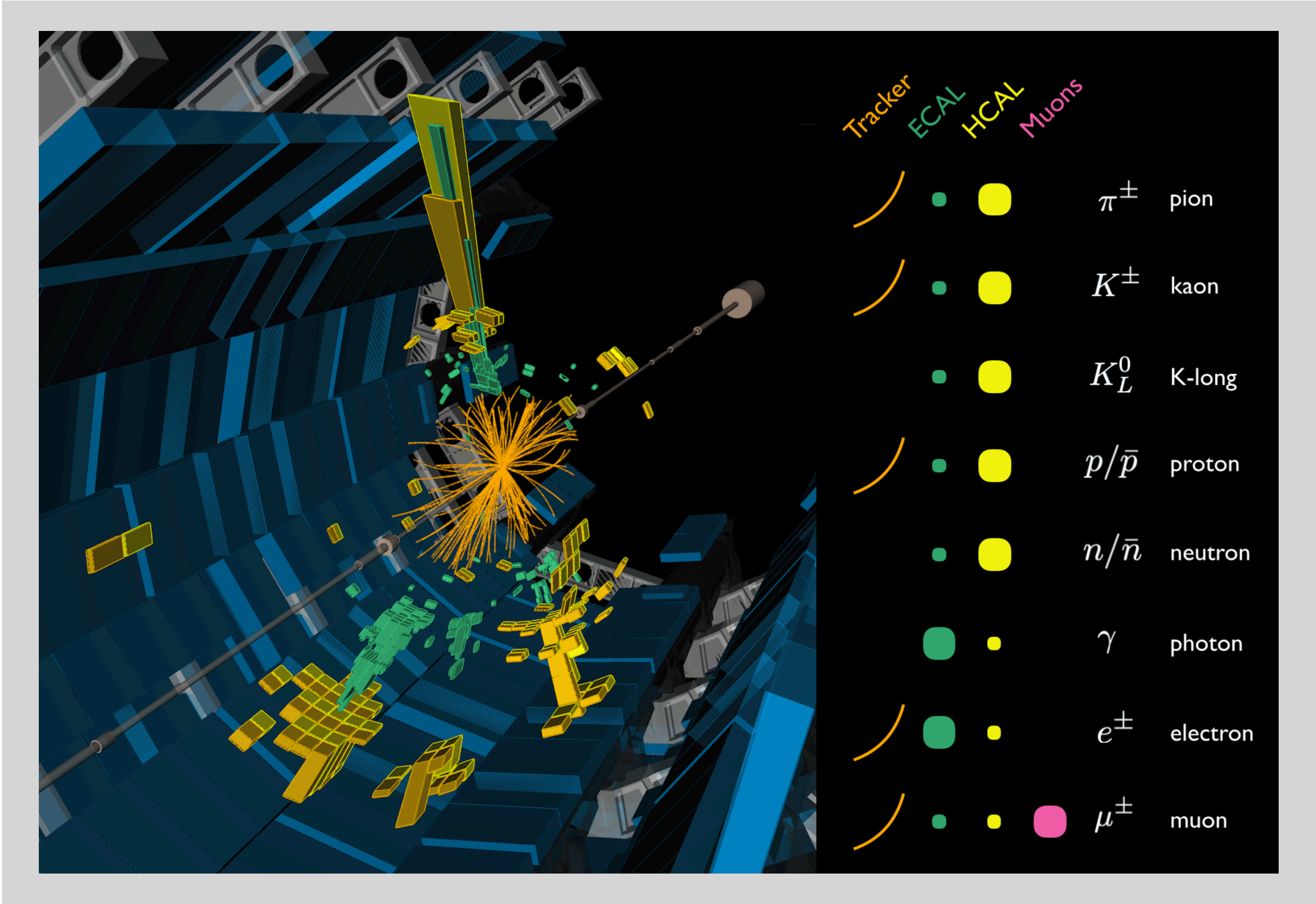
Overview of Binned ML Unfolding Methods

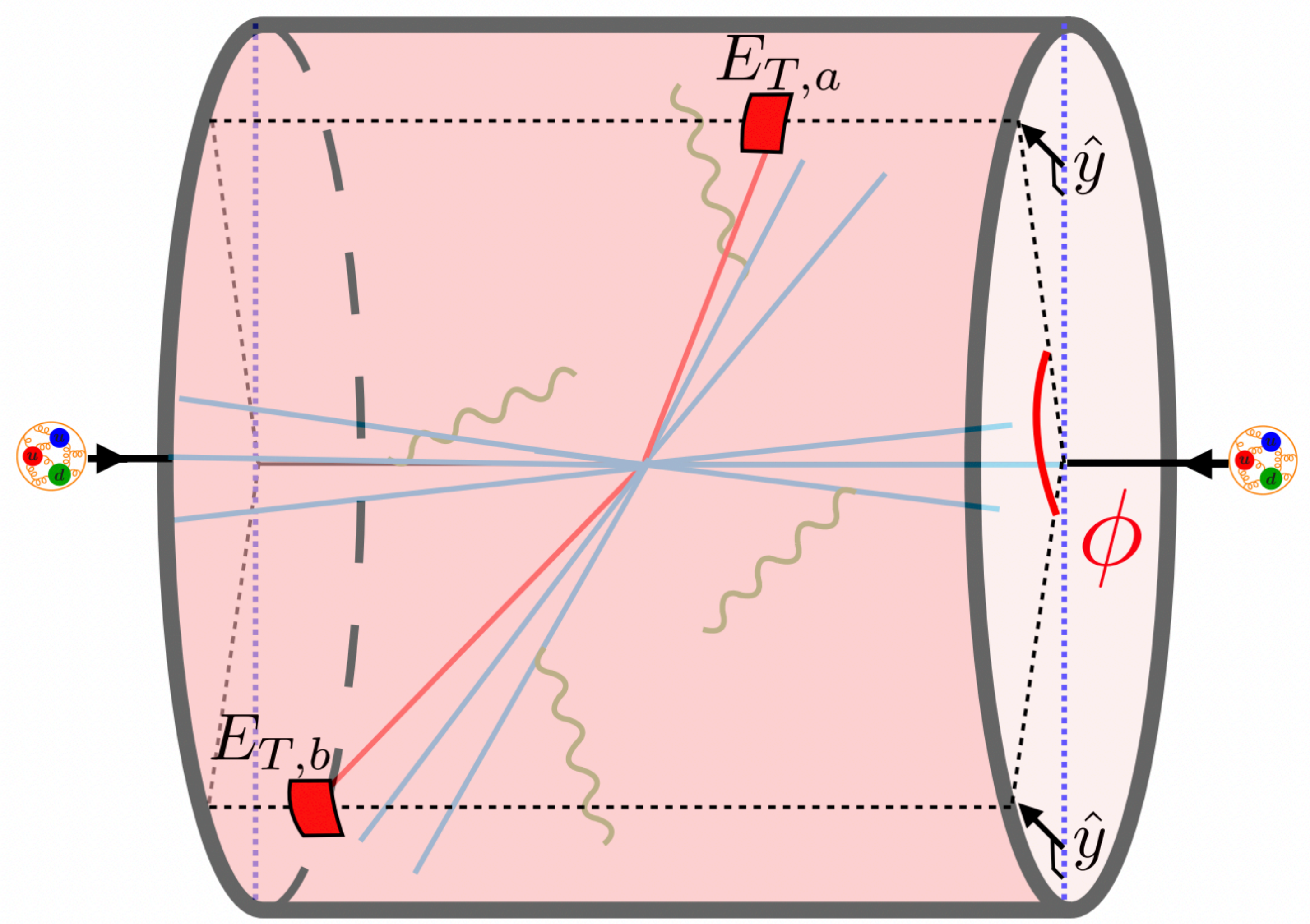
Jingjing Pan (Jing)

France-Berkeley PHYSTAT Workshop, June 11, 2024

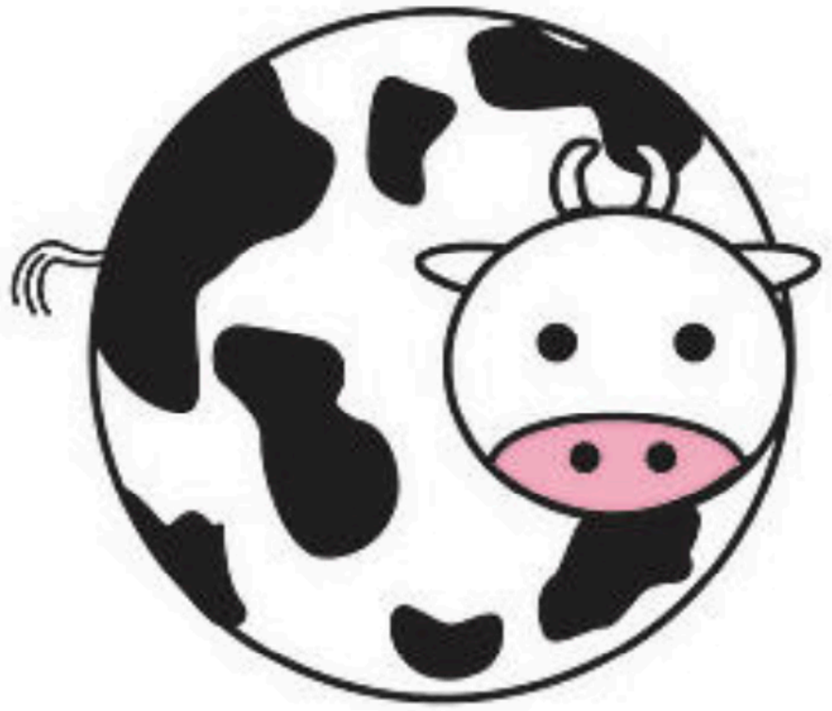
Unfolding: Bridging the Gap…

Necessary to compare data across different experiments / with theory





Experiment



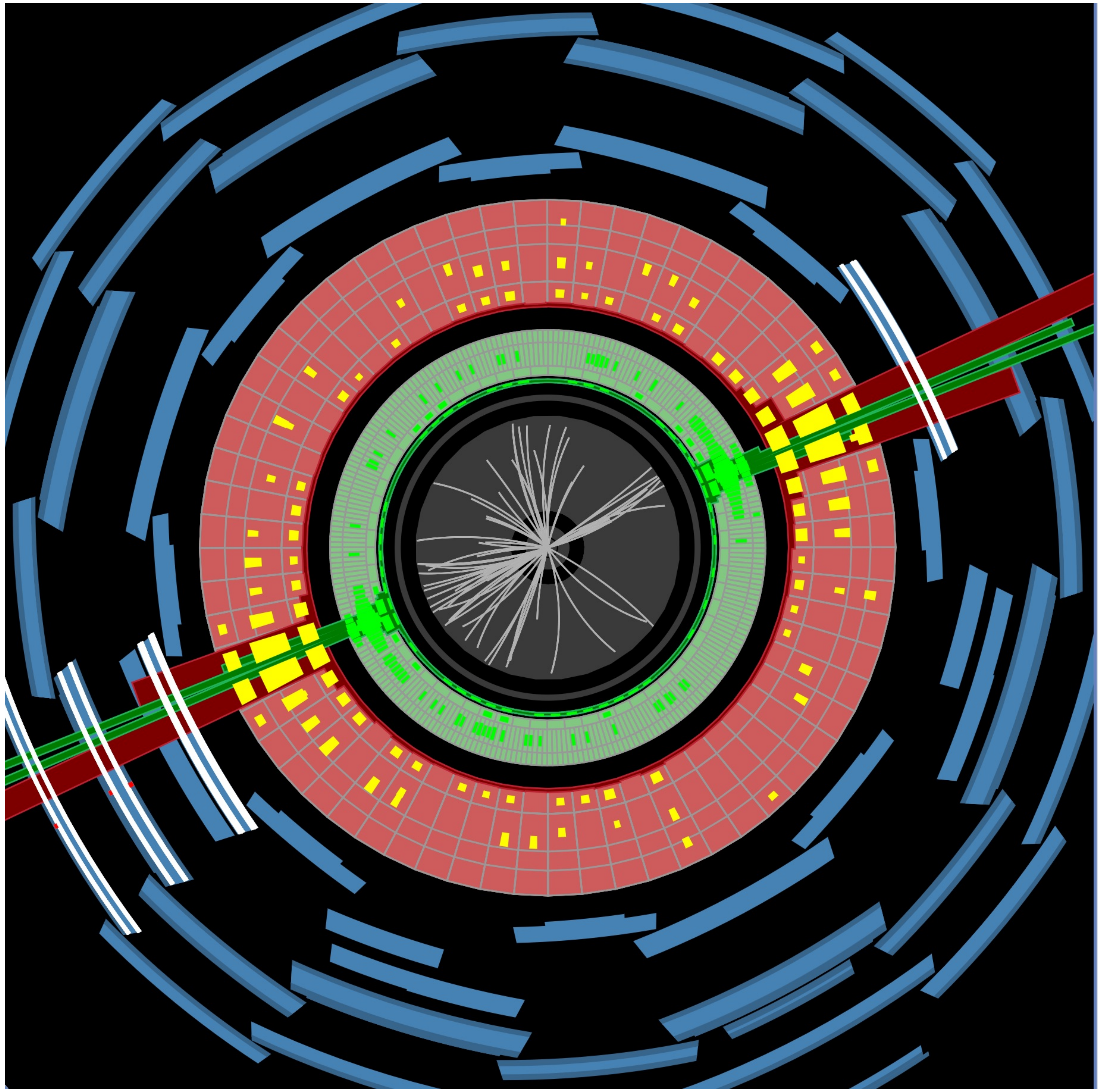
Theory

Better preserving data

Figure credit: Wouter Waalewijn (theory overview @BOOST 2020)

Outline

1. Unfolding as a classification task
2. Optimizing reco-level observables with ML
3. Fast regularized neural posterior estimation with normalizing flows



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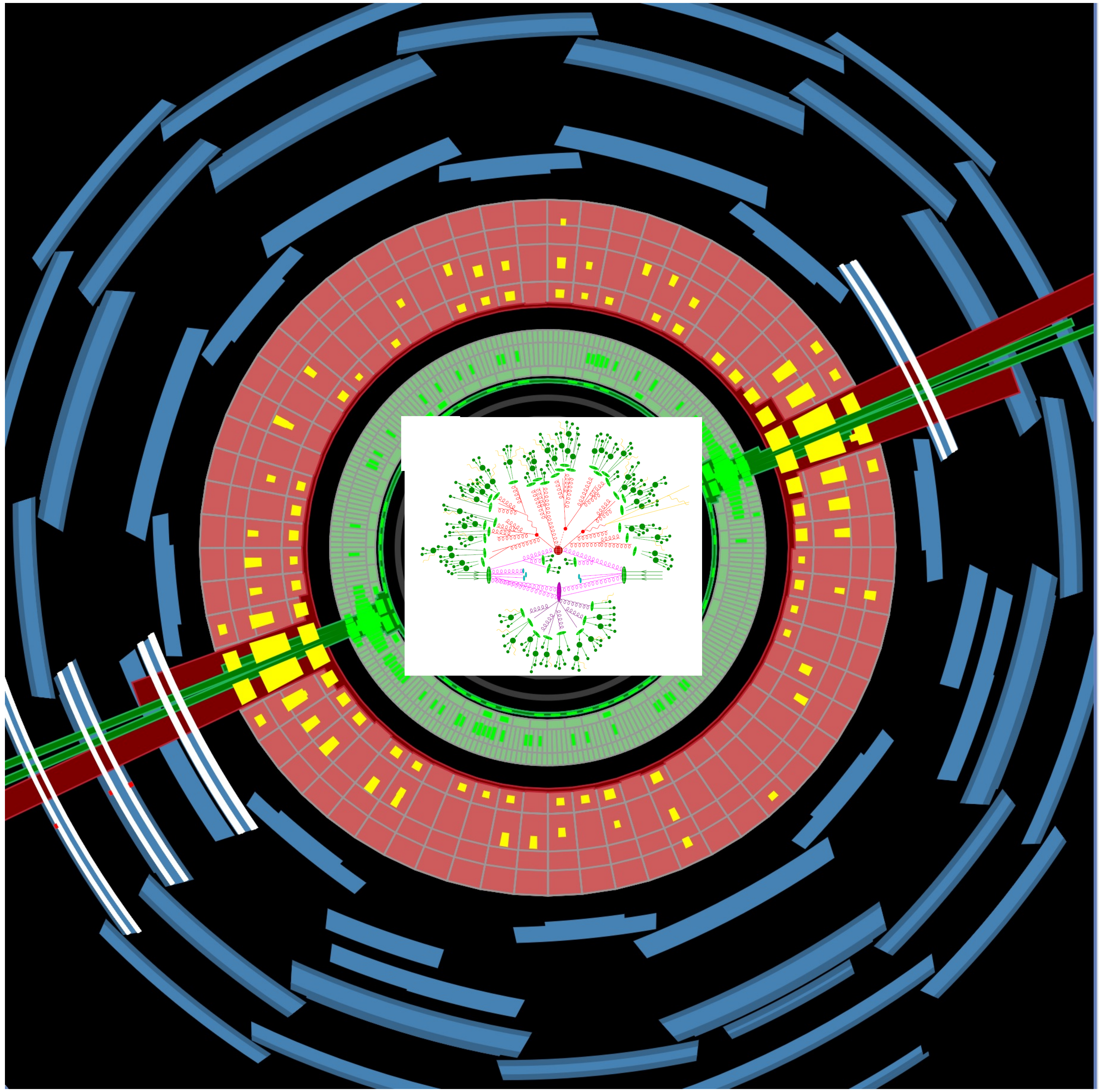

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1. Unfolding as a classification task

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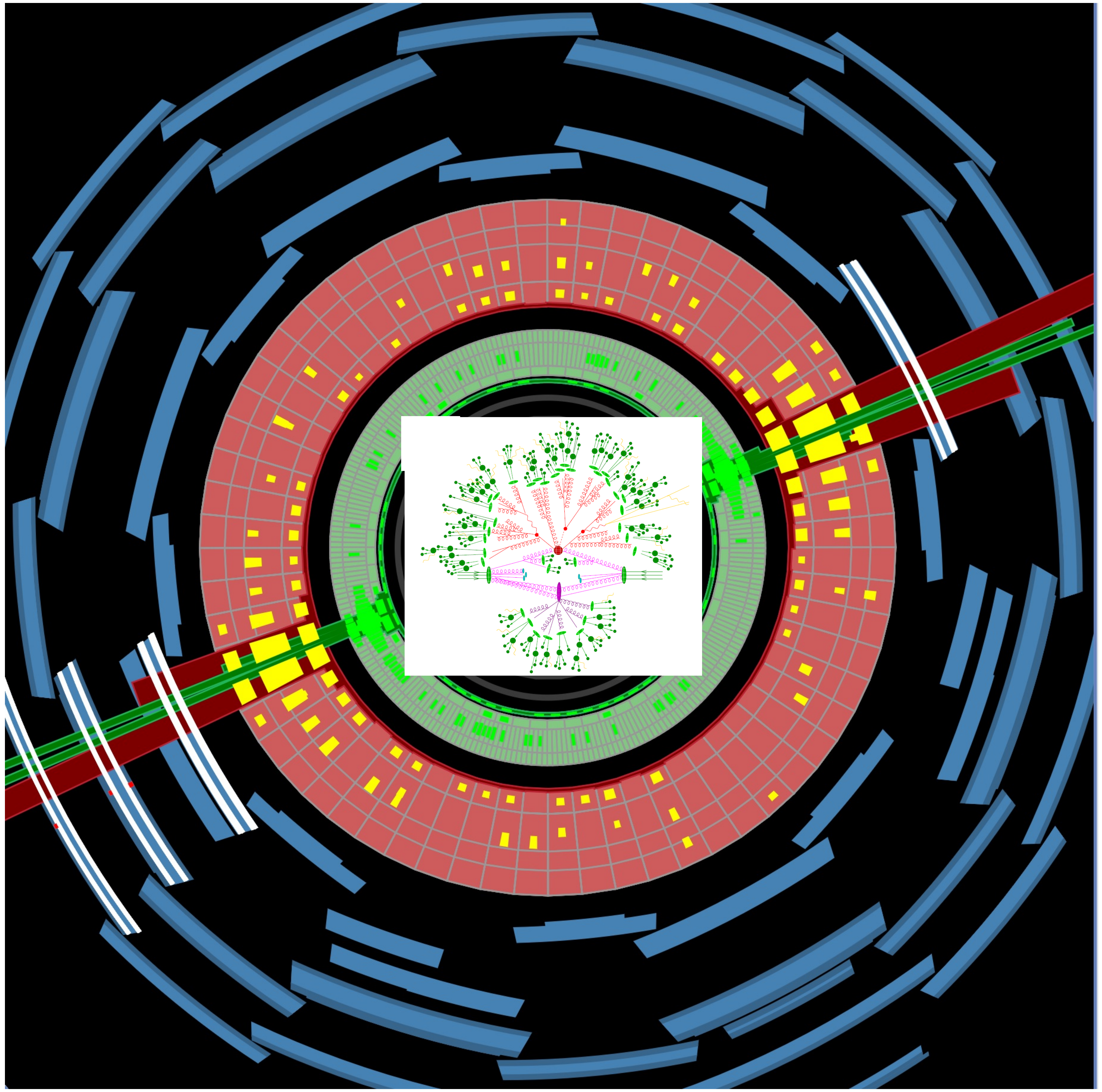
4. (Bonus) Enabling profiling with ML



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Unfolding as a Classification Task

Classifying the reco-level values into truth-level bins

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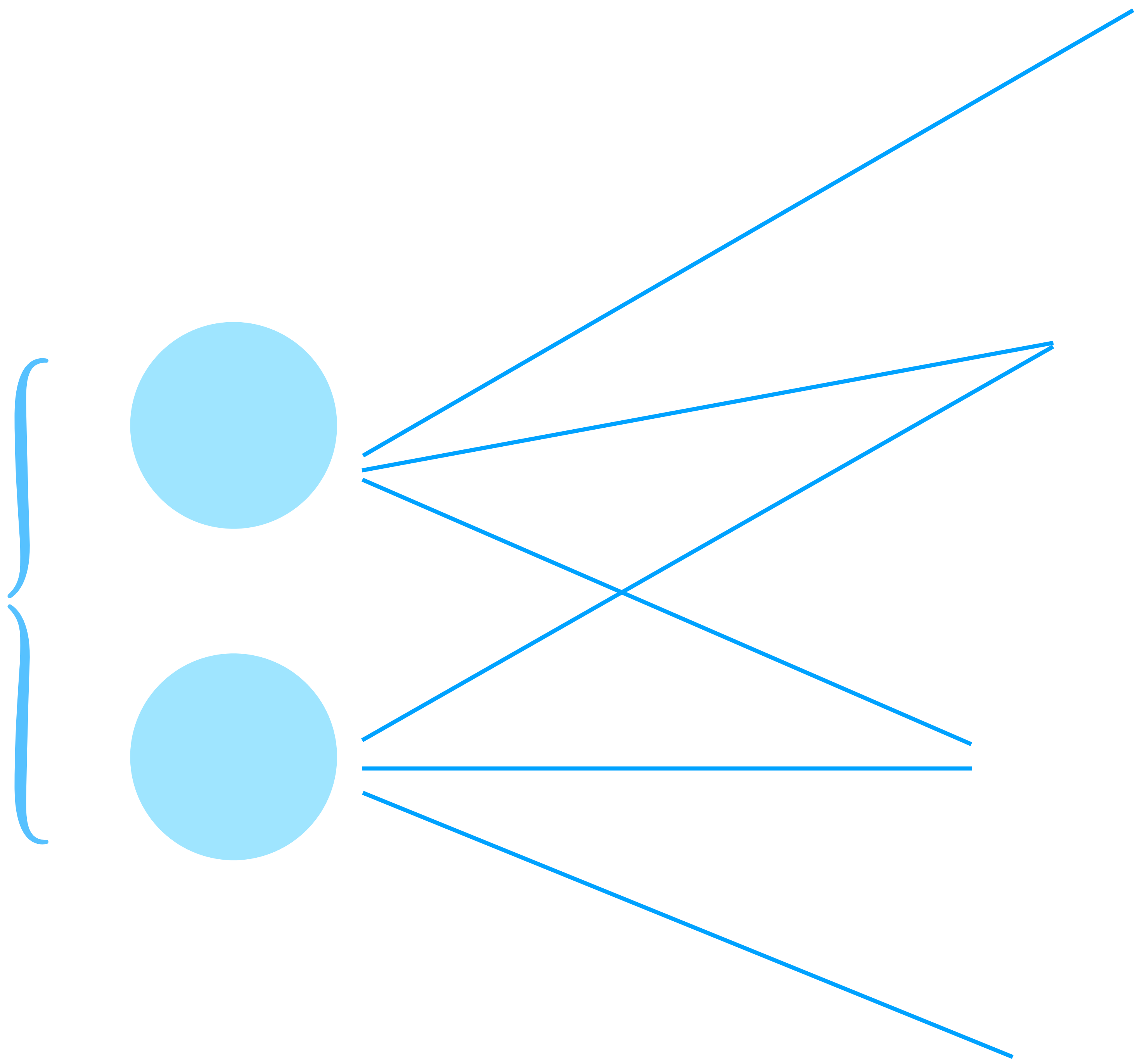
Number of the input variables (can readily adapt to high dim)



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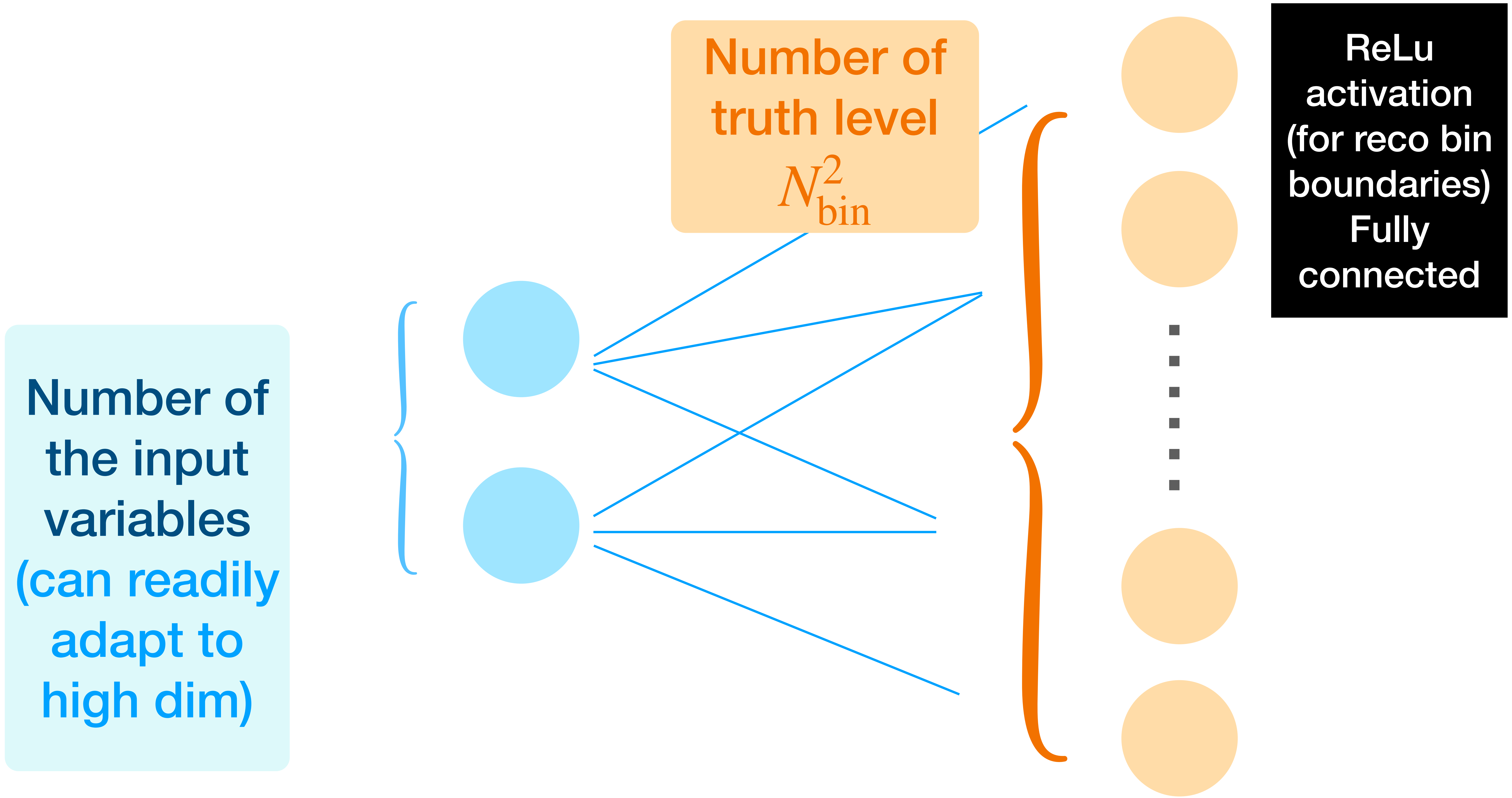

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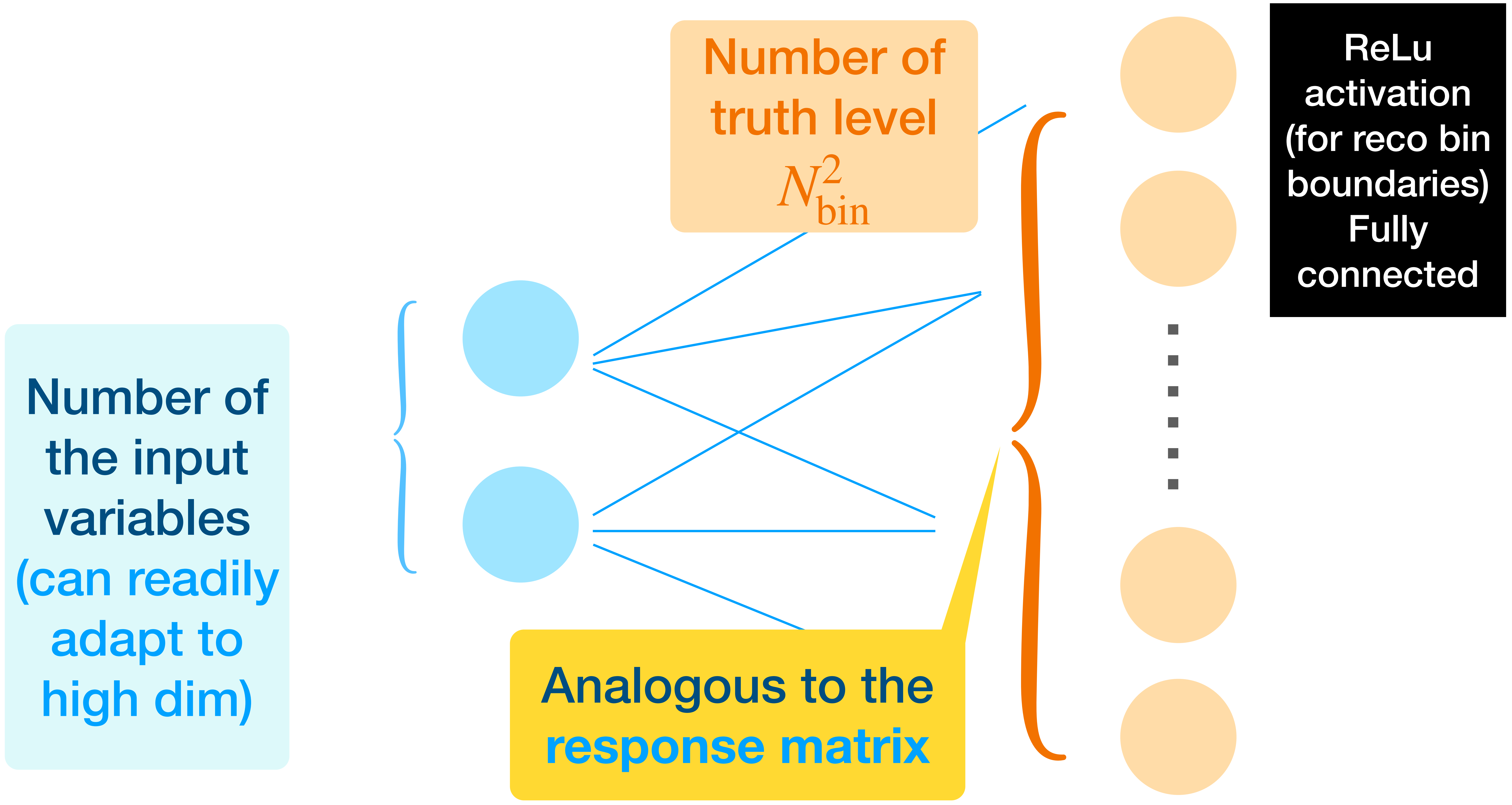

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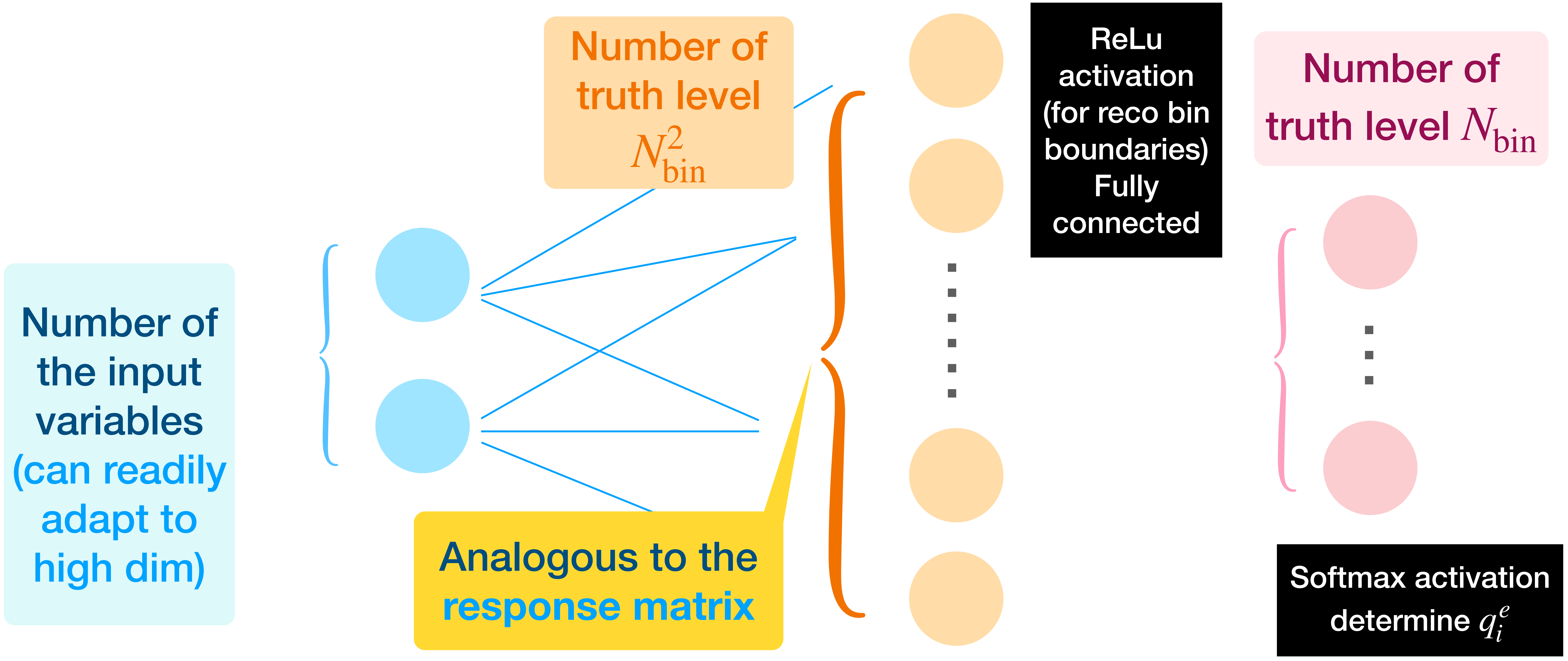

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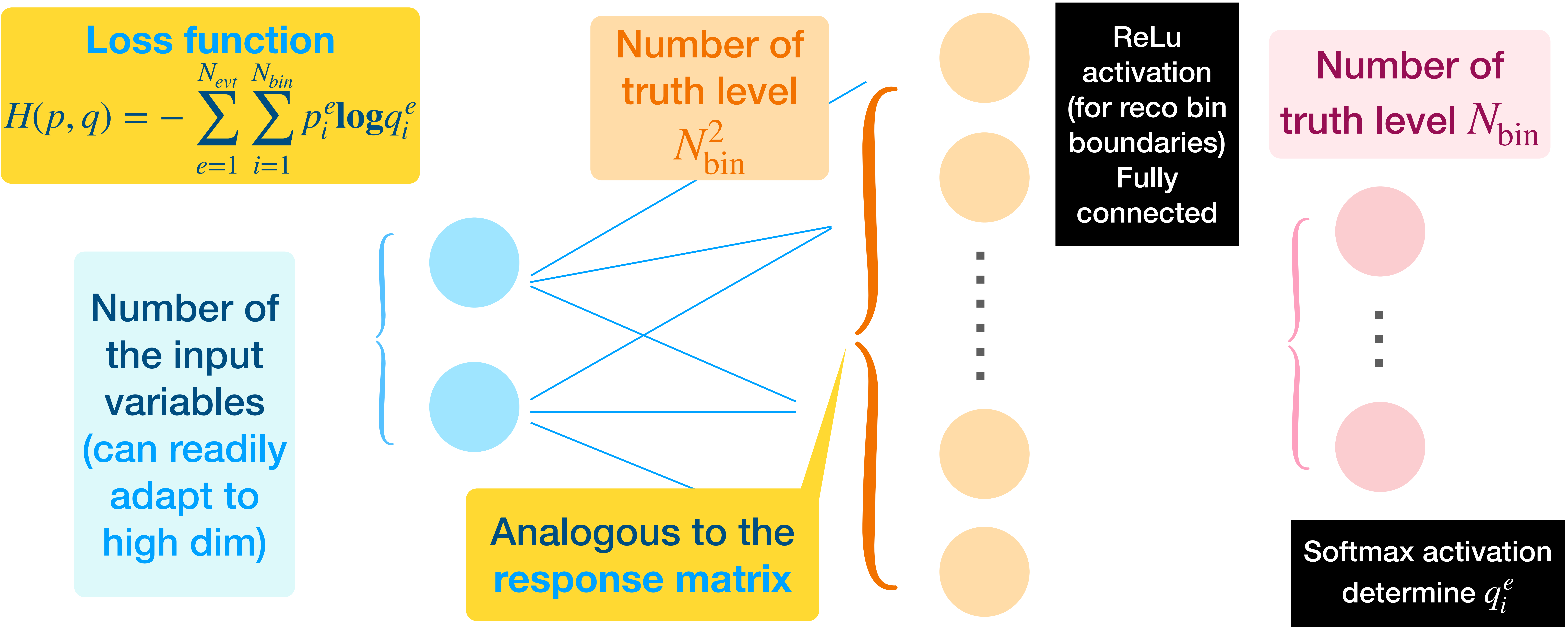

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Unfolding as a Classification Task

Classifying the reco-level values into truth-level bins

- Iterate to reduce prior dependence
  - Can start with flat prior $F(x_g) = const$.
  - Trained classifier applied to data $\rightarrow q_i^{e,\,\mathrm{data}}$ (predicted probability for truth bin i event e)
  - Update and obtain $F'_n(x) = \frac{1}{N_{evt,\,\mathrm{data}}} \sum_{e=1}^{N_{evt,\,\mathrm{data}}} q_i^{e,\,\mathrm{data}}$ for iteration n
  - Re-sample the MC & re-train the classifier
- (Ensembling to get the result)

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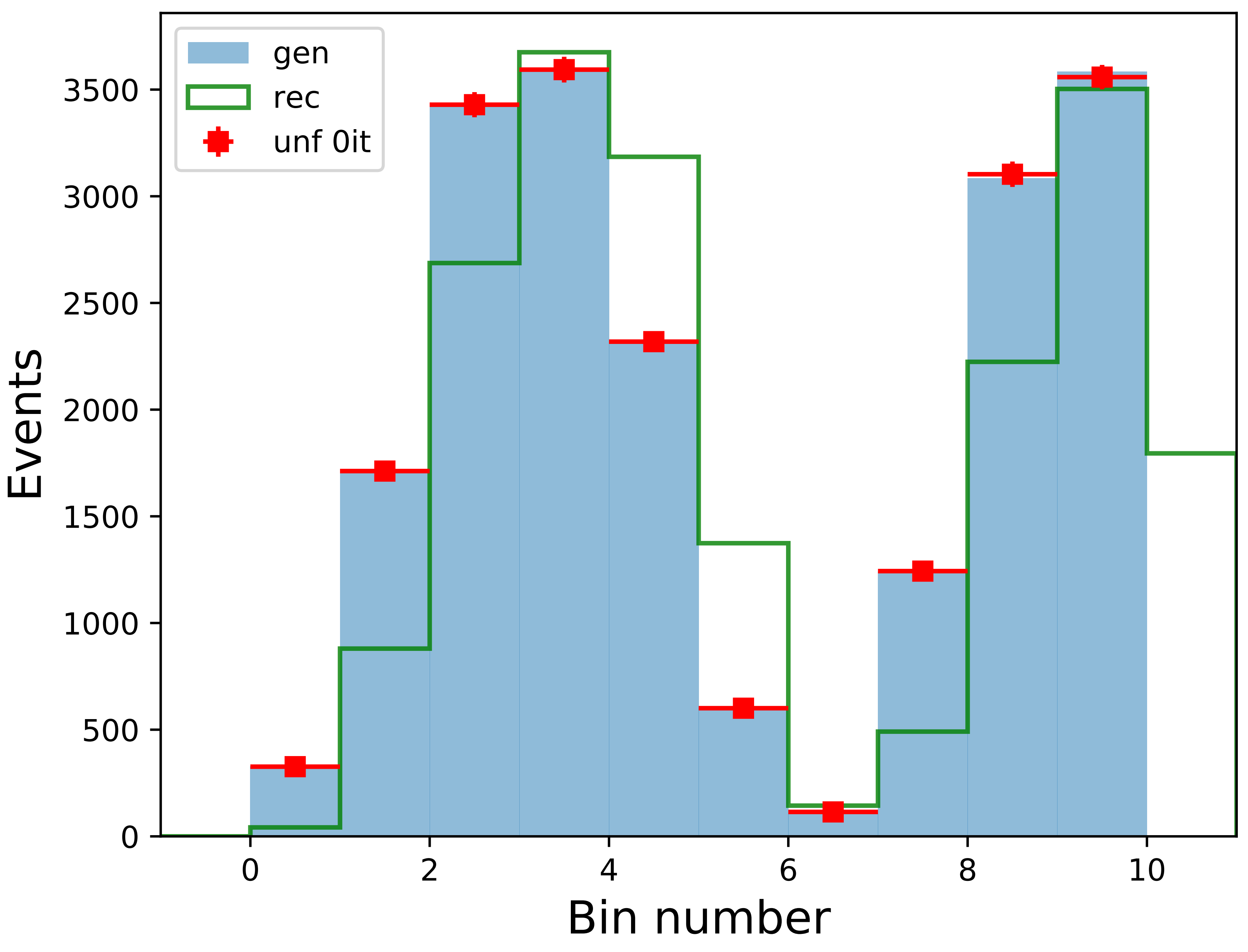

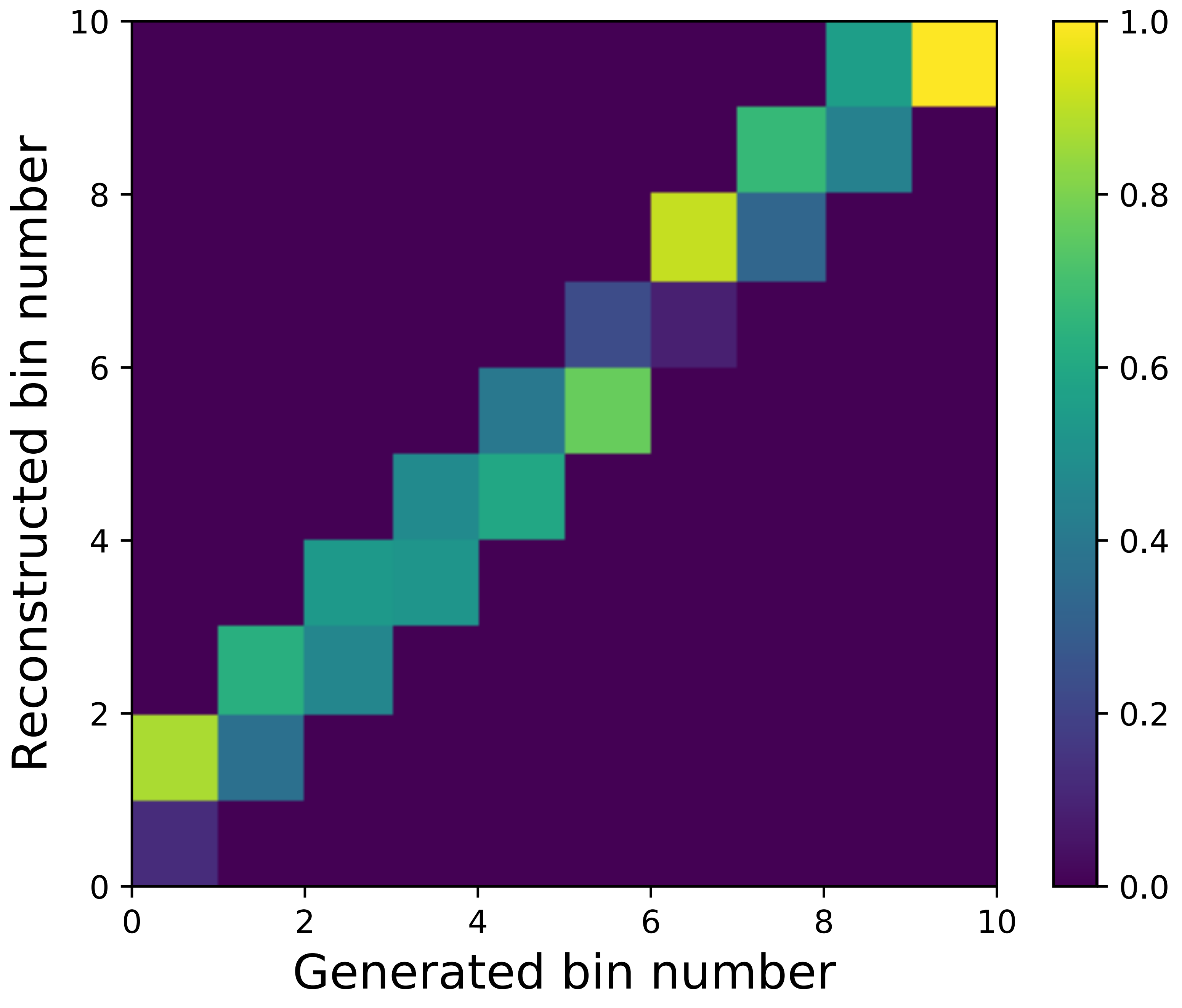

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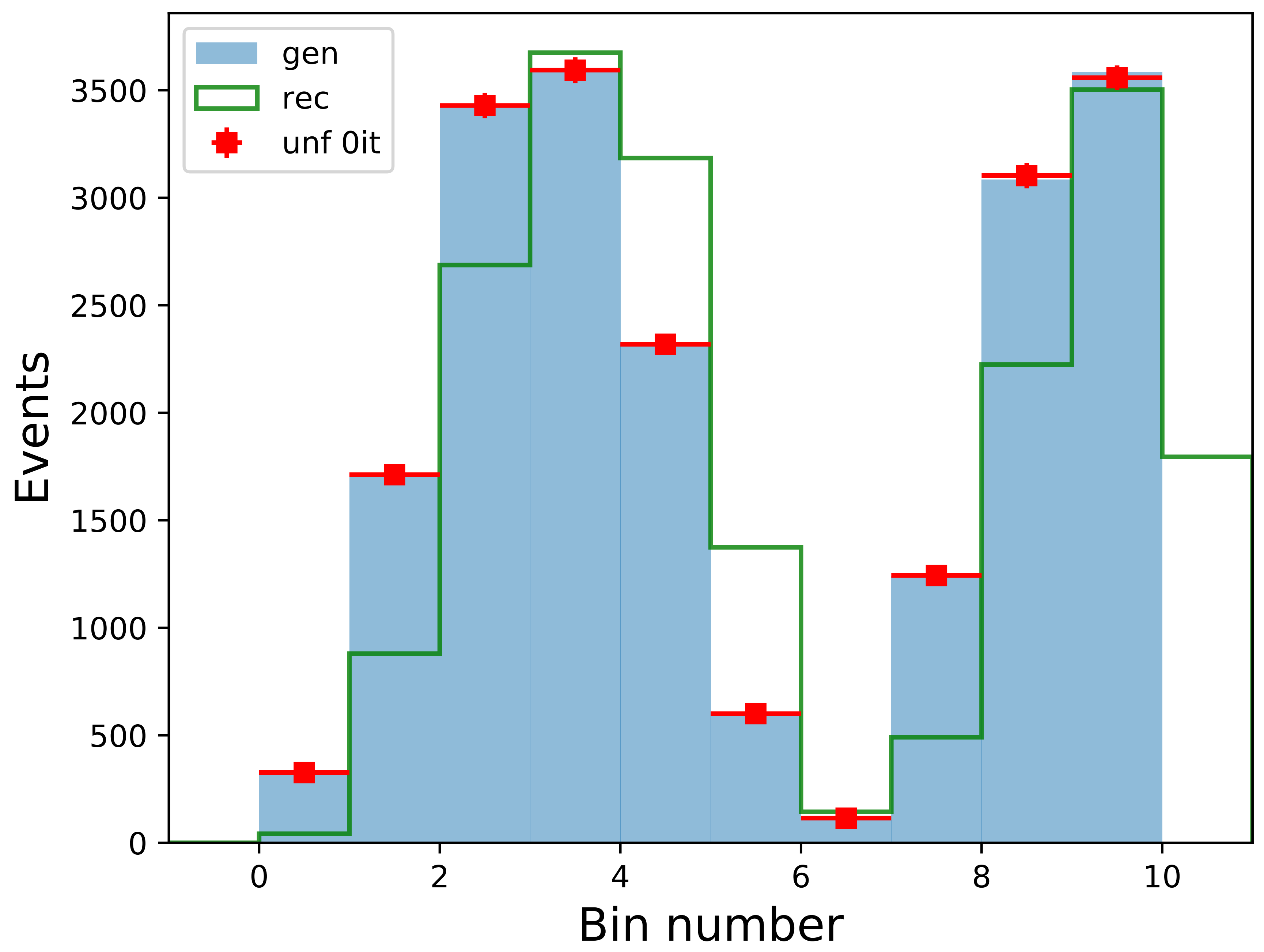

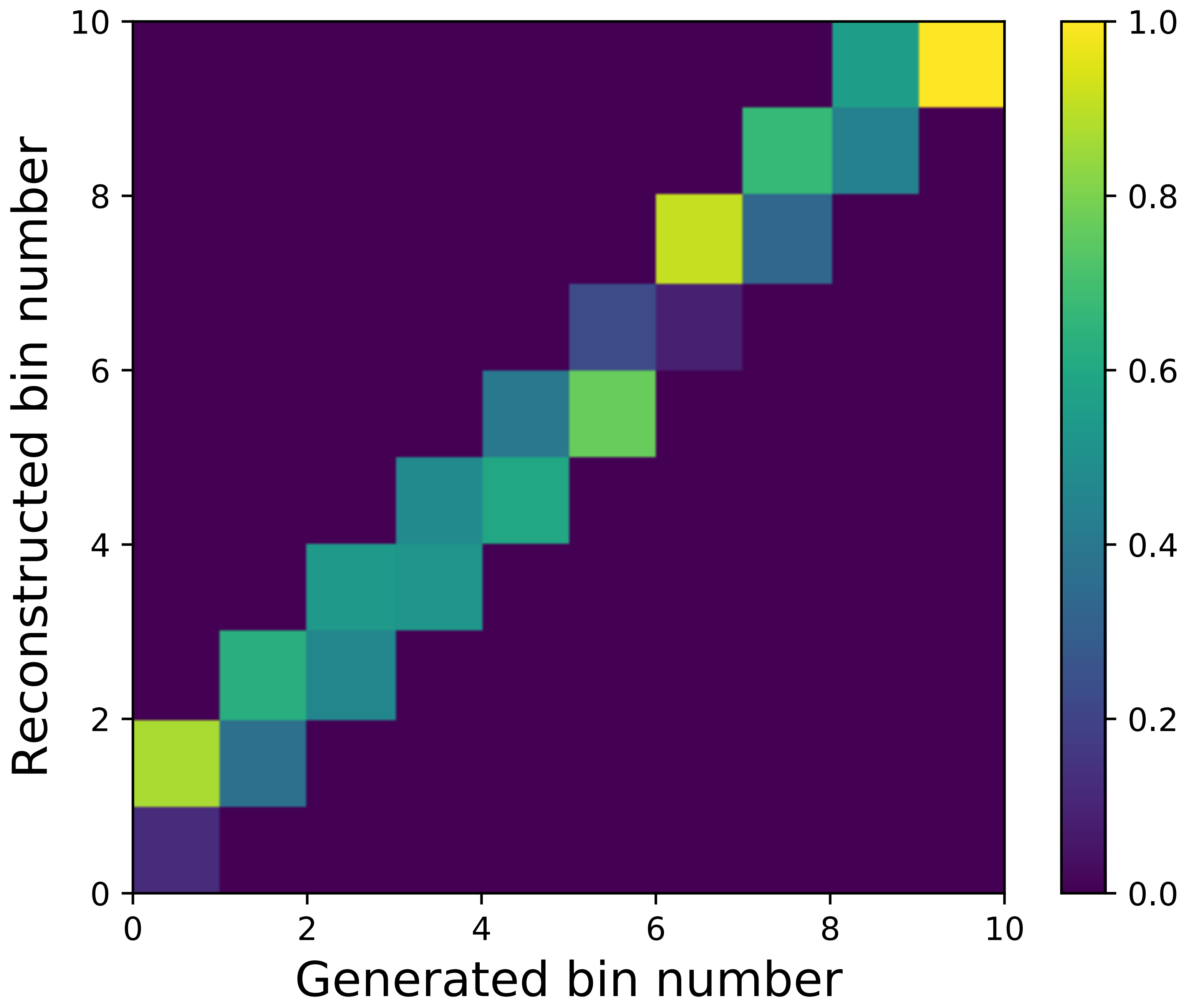

Performs very well even for huge off-diagonal response elements from a shift ($x_r \to x_g + 0.05$)!

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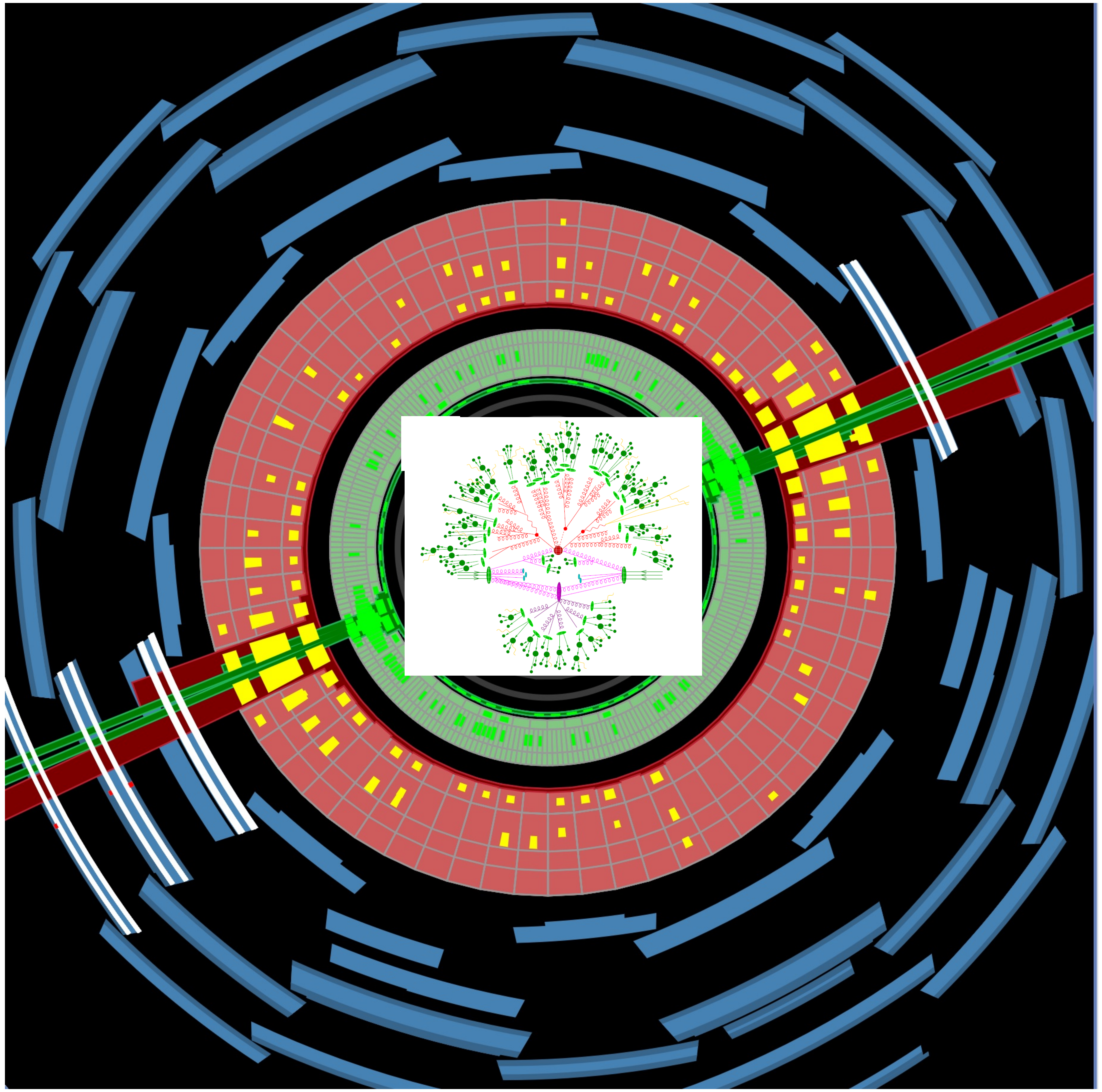
3. Fast regularized neural posterior estimation with flows

4. (Bonus) Enabling profiling with ML



Optimizing reco Observable ($\mathcal{O}_d$) with ML

2203.16722

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- Step 0: What is the observable?
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What to unfold?

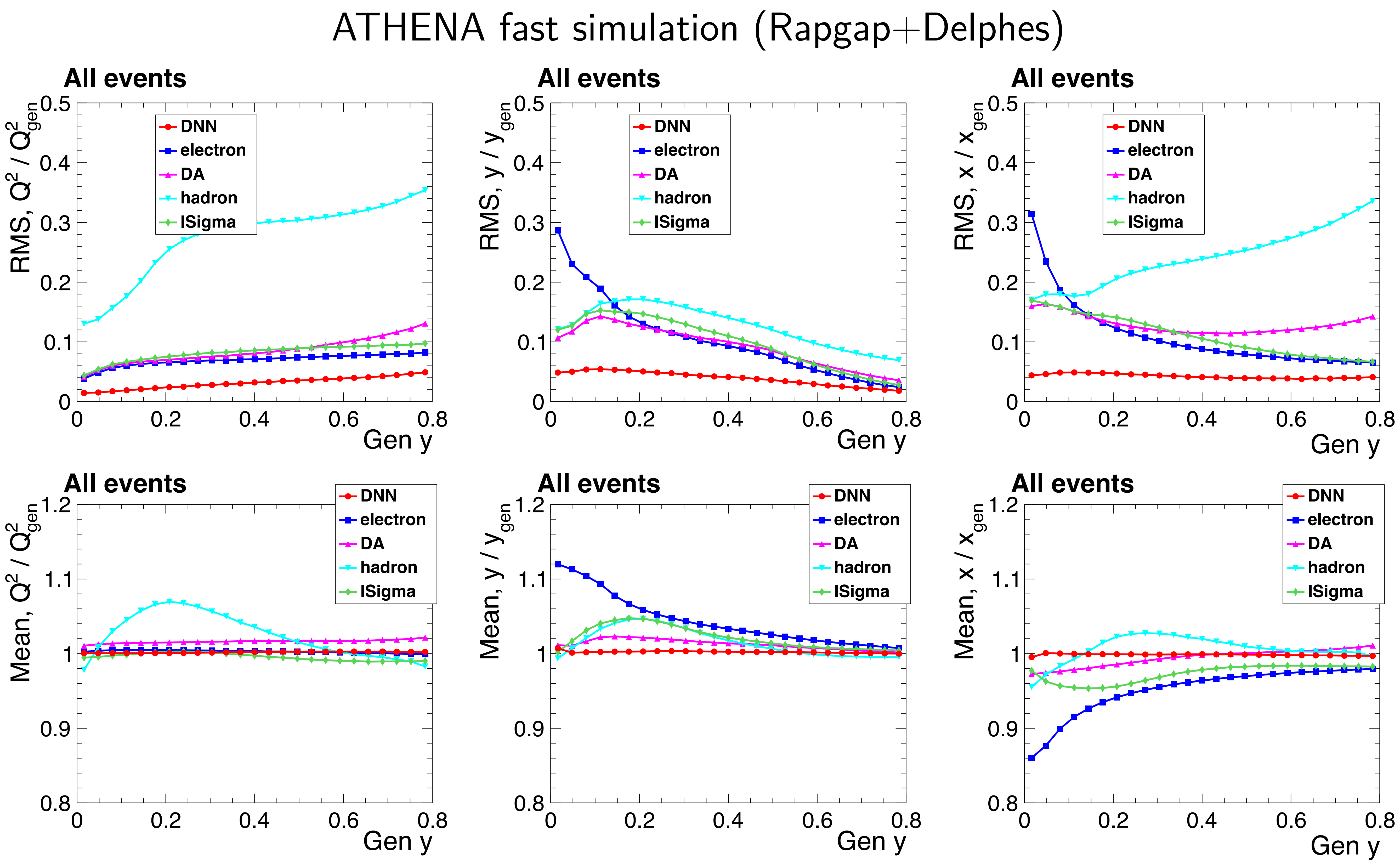
- Usually we discuss the art of matrix inversion (i.e. How)
- Step 0:   What is the observable?
  - Can we do better than simply adding variables / going to higher dimension?
  - YES!
  - Particle-level: from a list of 4-vectors, must be linked to theory for comparison
  - Detector-level: from energy flow objects

Optimizing reco Observable ($\mathcal{O}_d$) with ML

2203.16722

2110.05505

What to unfold?



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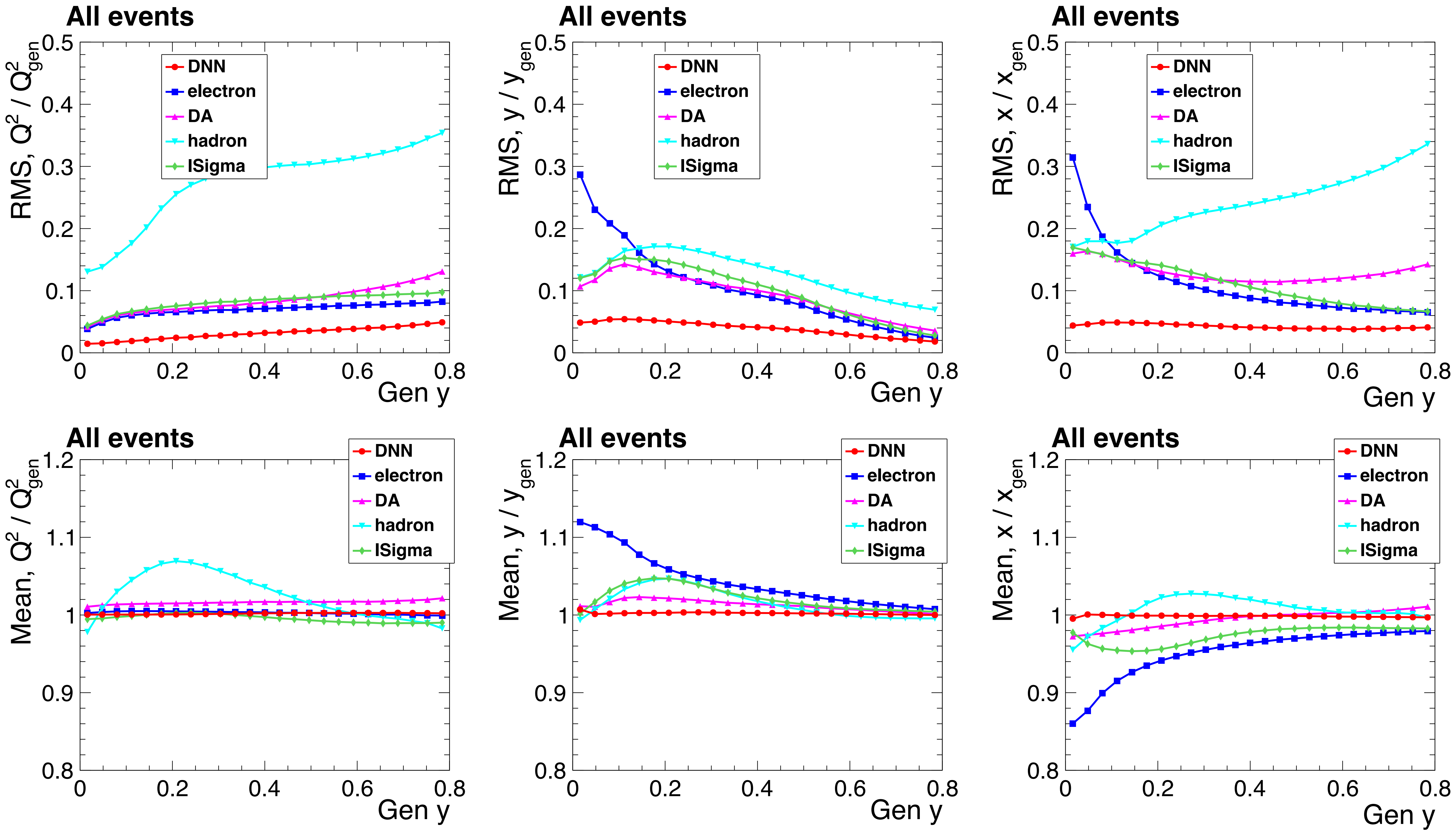
What to unfold?

- ML-assisted reconstruction goals
  - Reduce bias
  - Improve resolution

ATHENA fast simulation (Rapgap+Delphes)



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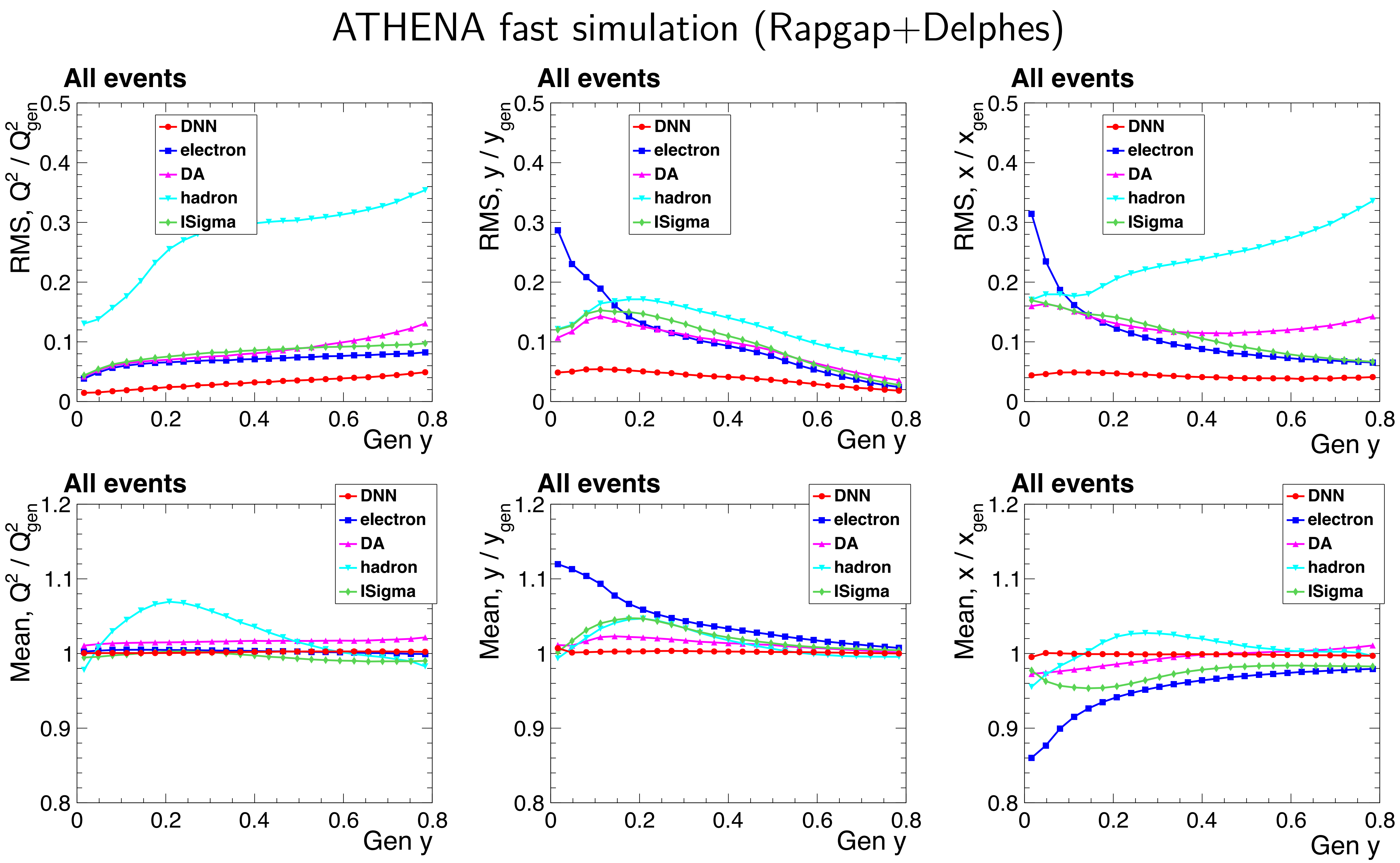
- QED-regression DNN for a Deep Inelastic Scattering (DIS) example: learns Q^2, x, y from distorted inputs



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QED-regression DNN gives the finest resolution & corrects for acceptance effects

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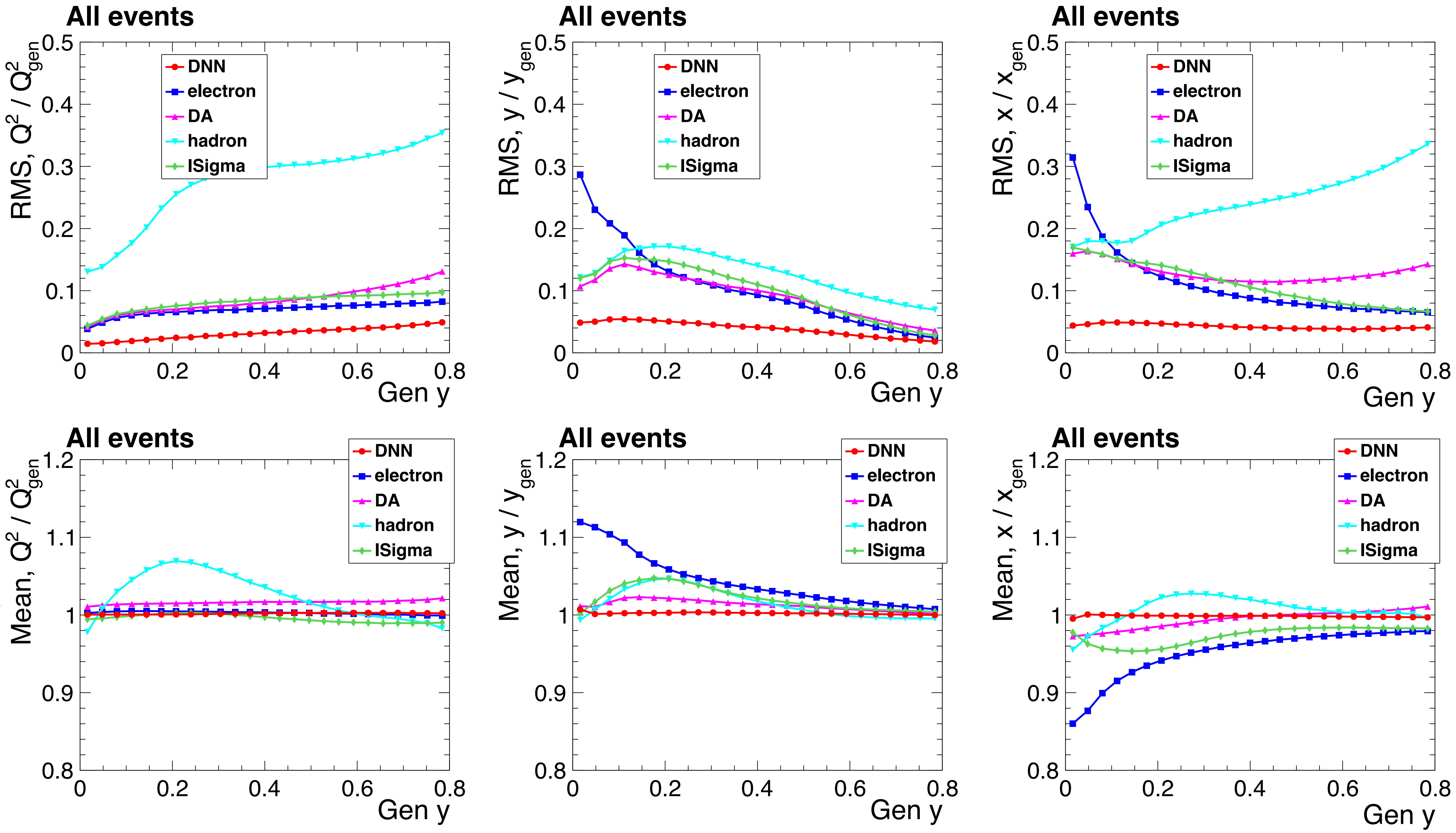

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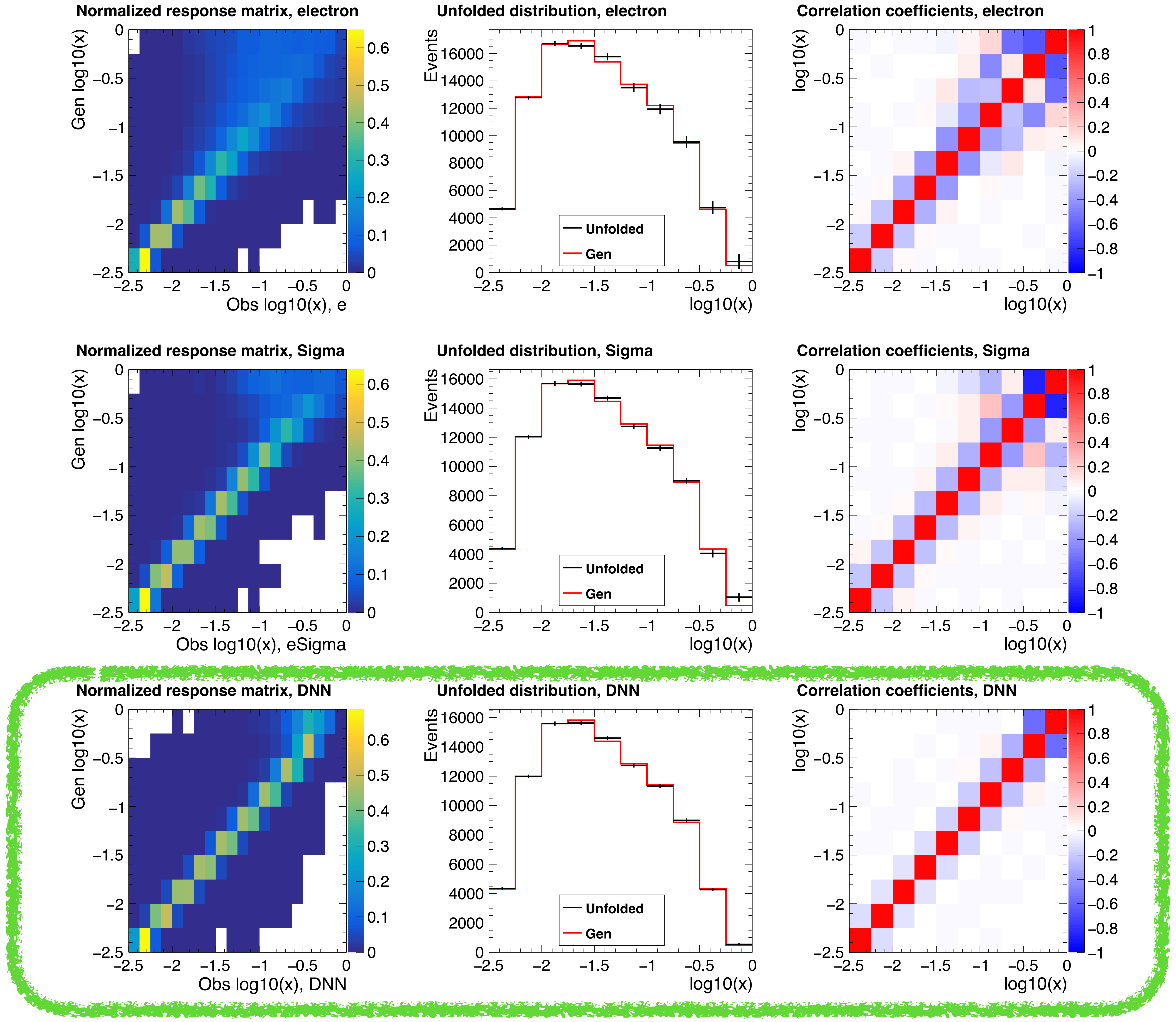

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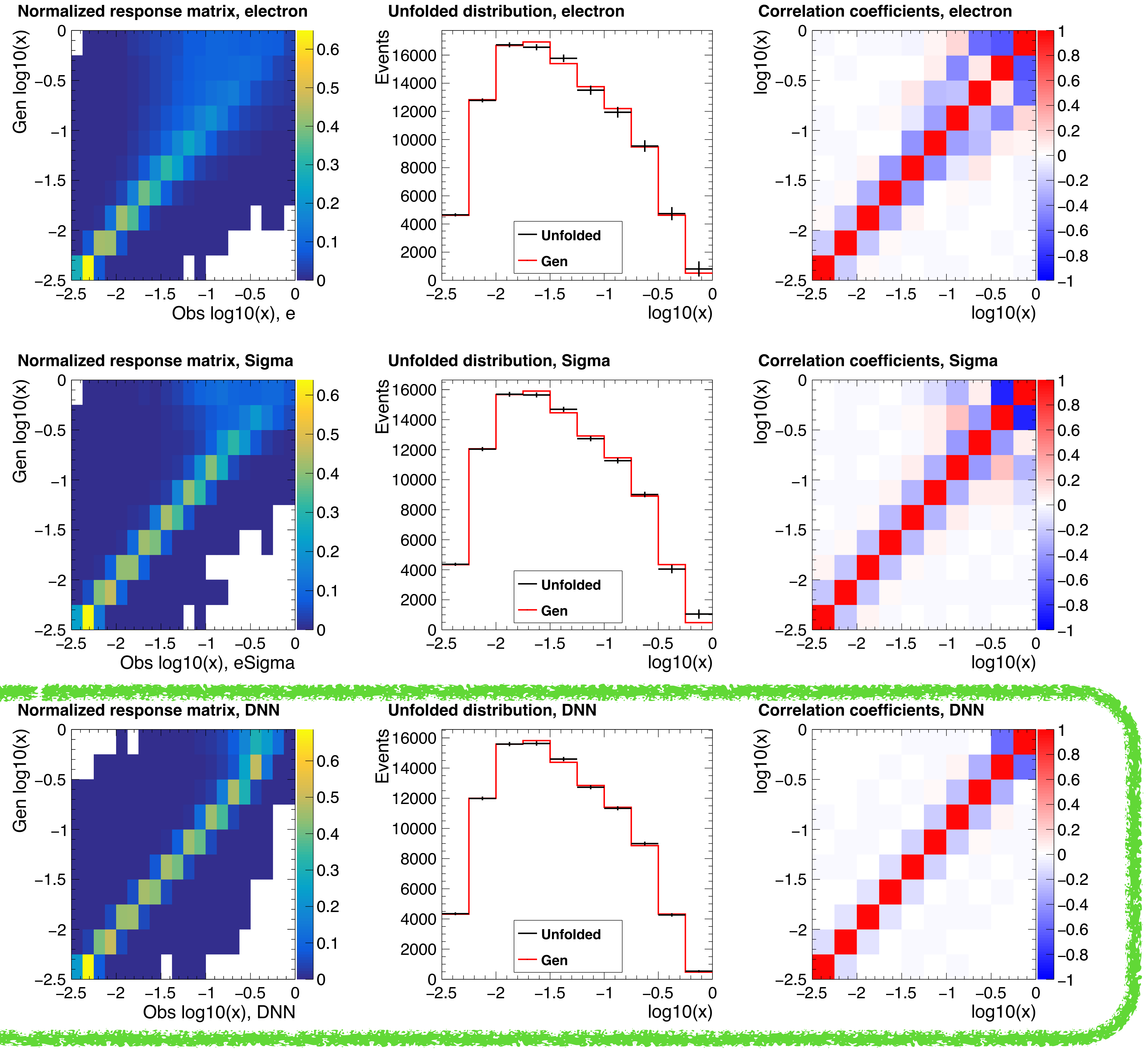
What to unfold?

- ML-assisted reconstruction reco-level observables has the most diagonal fractions throughout phase space

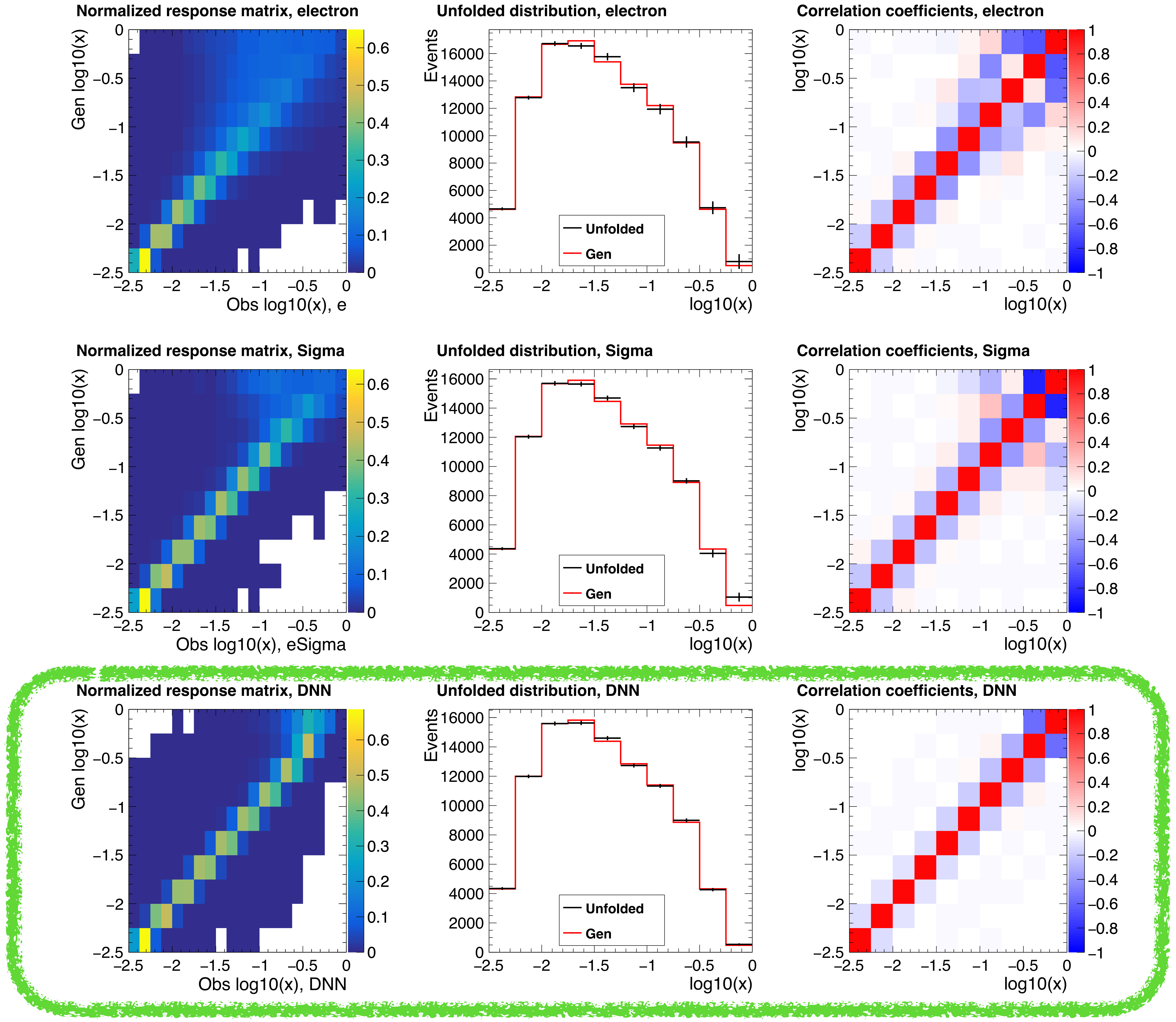


Optimizing reco Observable ($\mathcal{O}_d$) with ML

2203.16722

What to unfold?

- ML-assisted reconstruction reco-level observables has the most diagonal fractions throughout phase space
- Loss function = (particle-level target) + (particle-level - detector-level)^2



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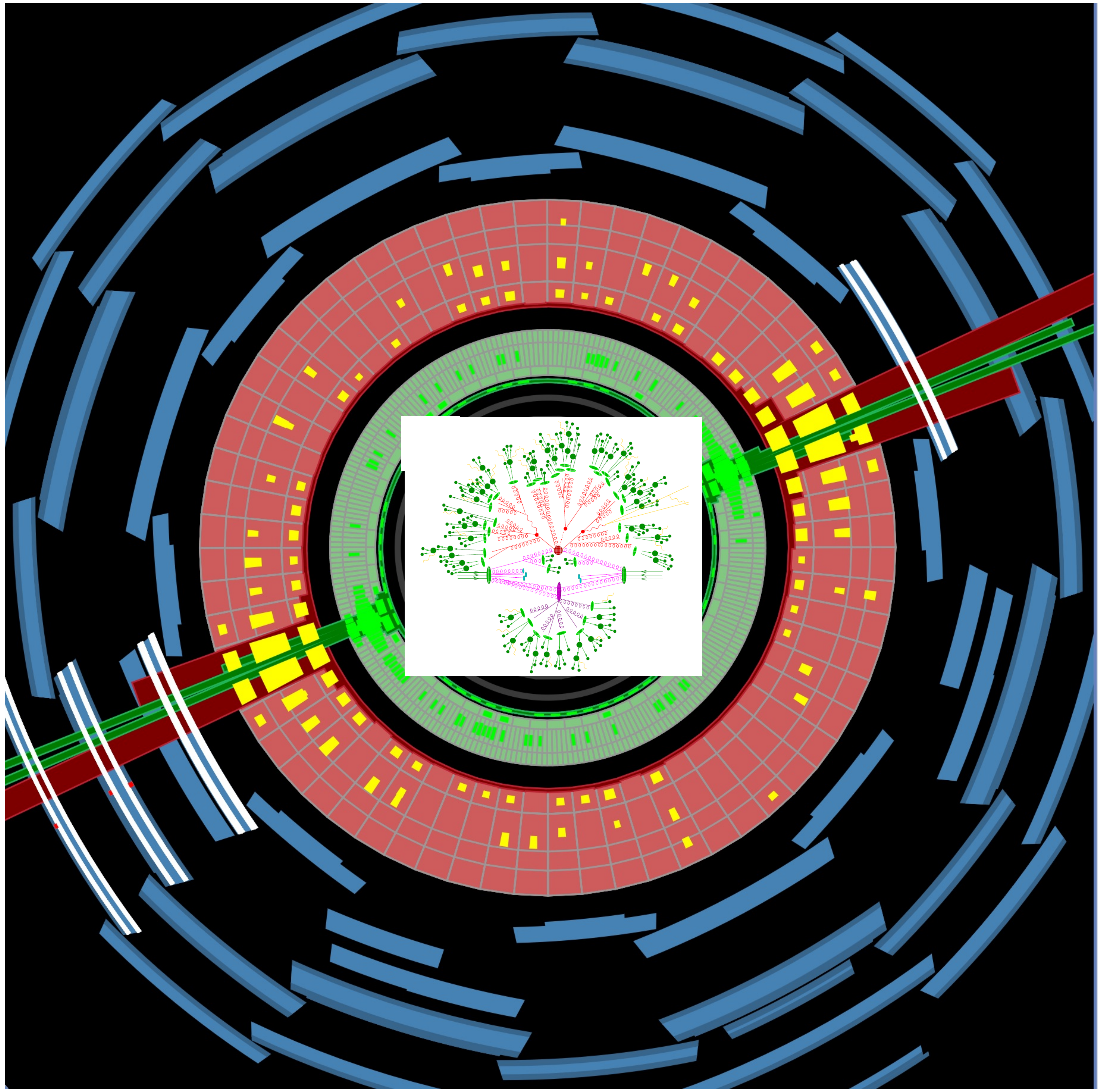

Fully Bayesian Unfolding:

1201.4612

2406.xxxxx

Neural Posterior Unfolding

Fast regularized neural posterior estimation with NFs

- Motivations
  - Bayesian: access to full posterior
  - Circumvent MCMC for sampling to fit parameters via amortized ML: directly learn $\Pr(t_j \mid m_i)$ from prior pairs that are passed through R
  - Normalizing Flows (NFs) as the density estimator is inherently regularized through model selection (i.e. the validation loss)
  - Still sensible in phase space poorly constrained by data (i.e. response matrix with degeneracy)

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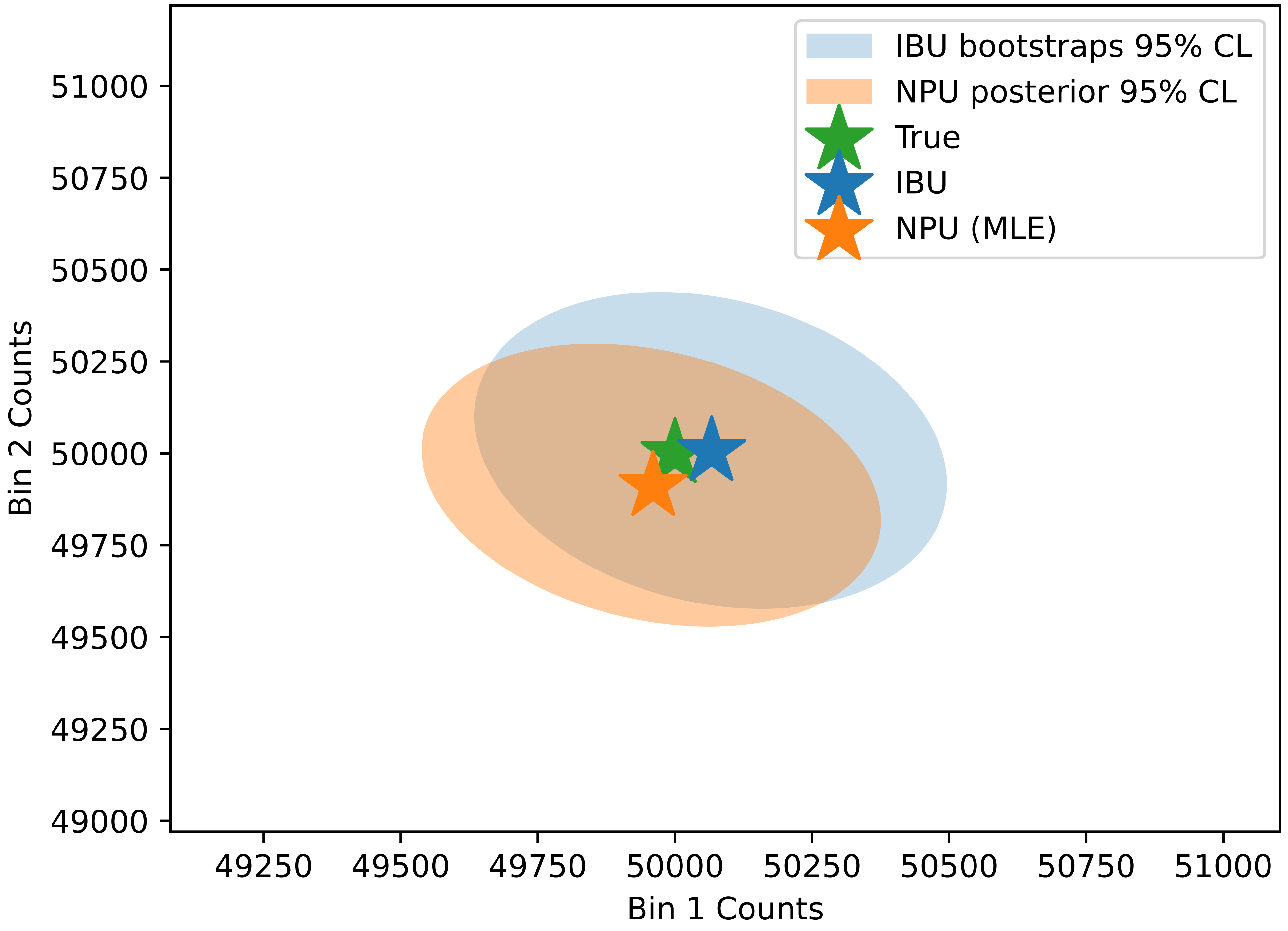

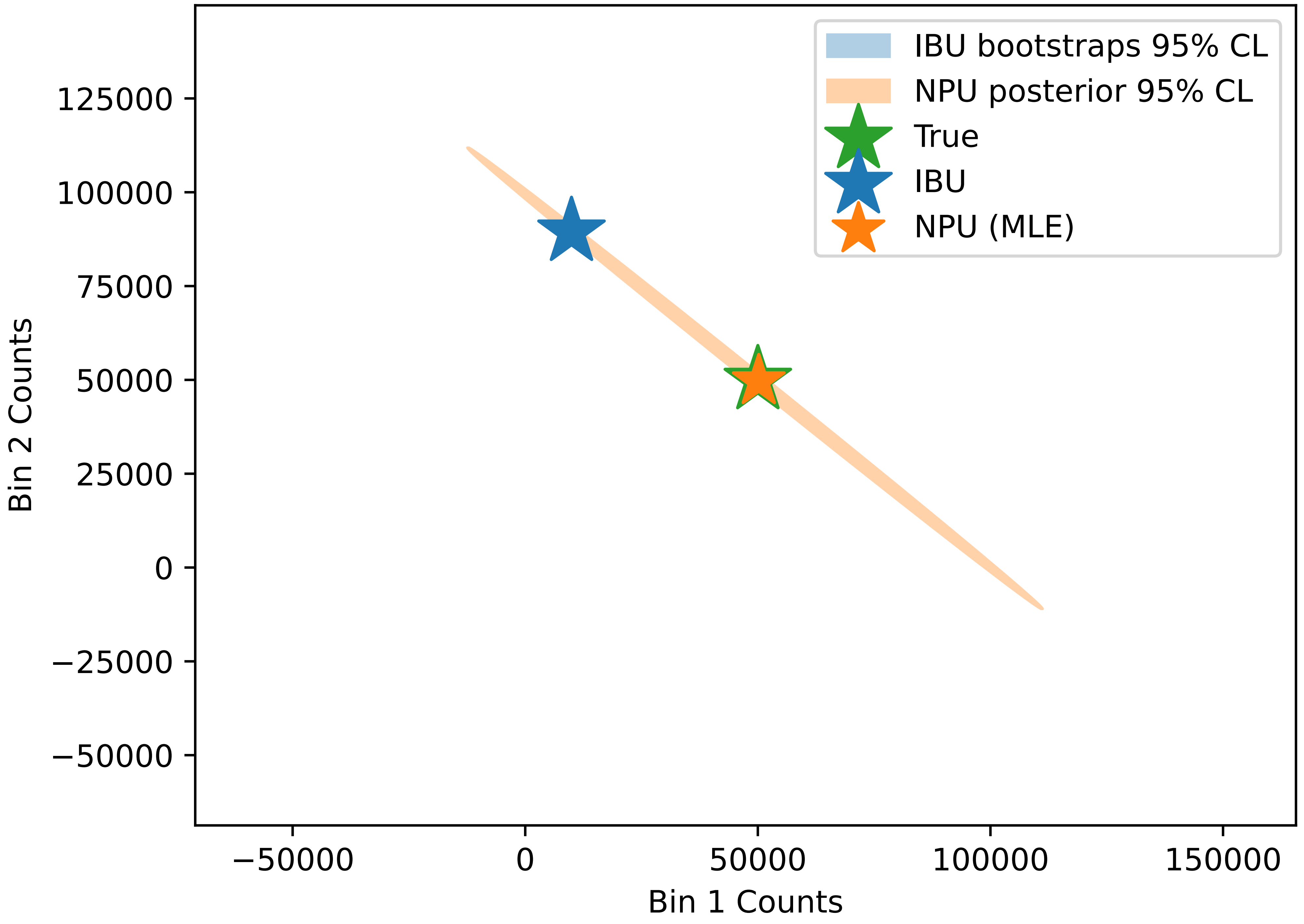

Correlation coefficient = 1
Small migration

Correlation coefficient = 0
Response degenerate

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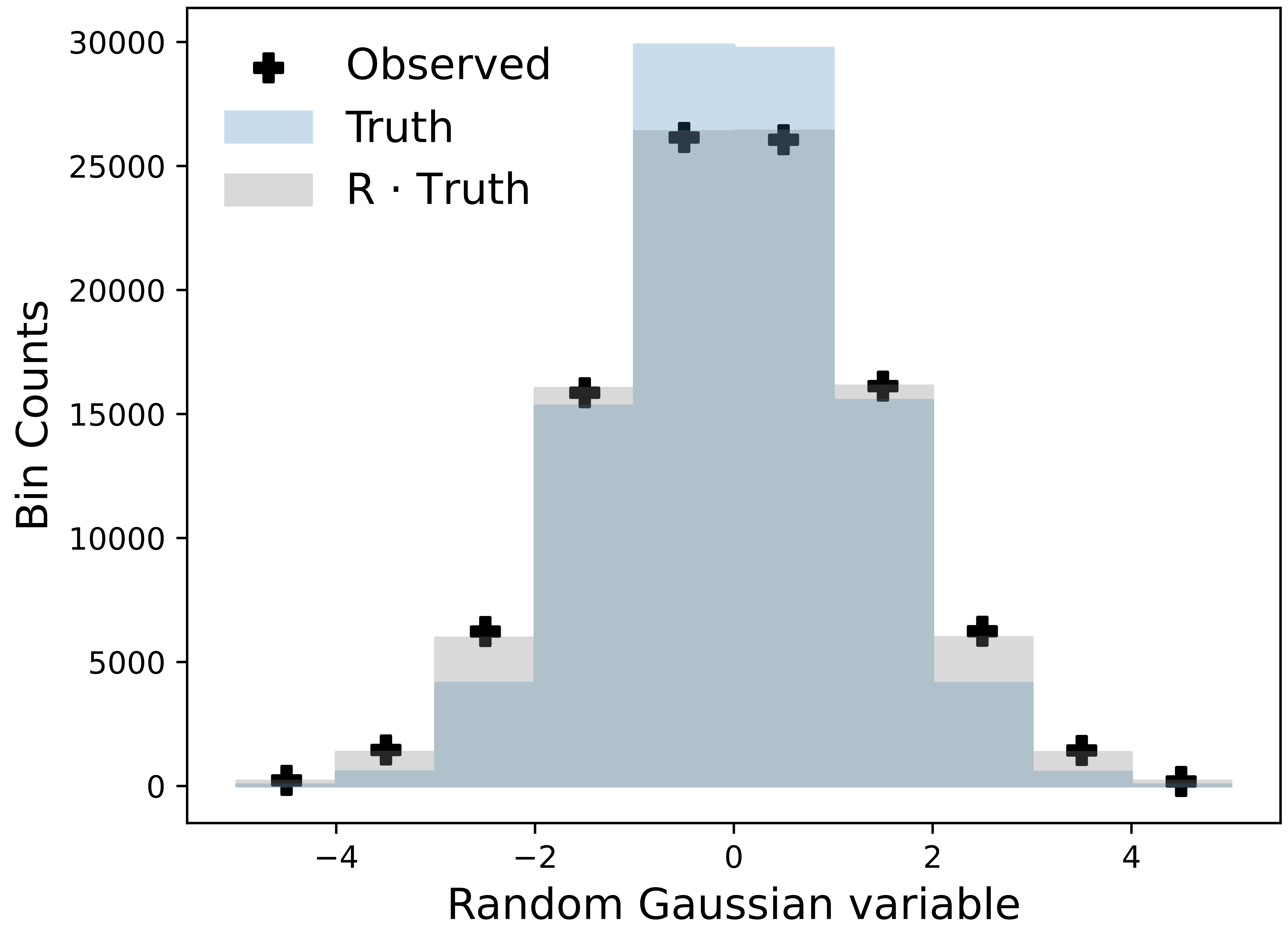

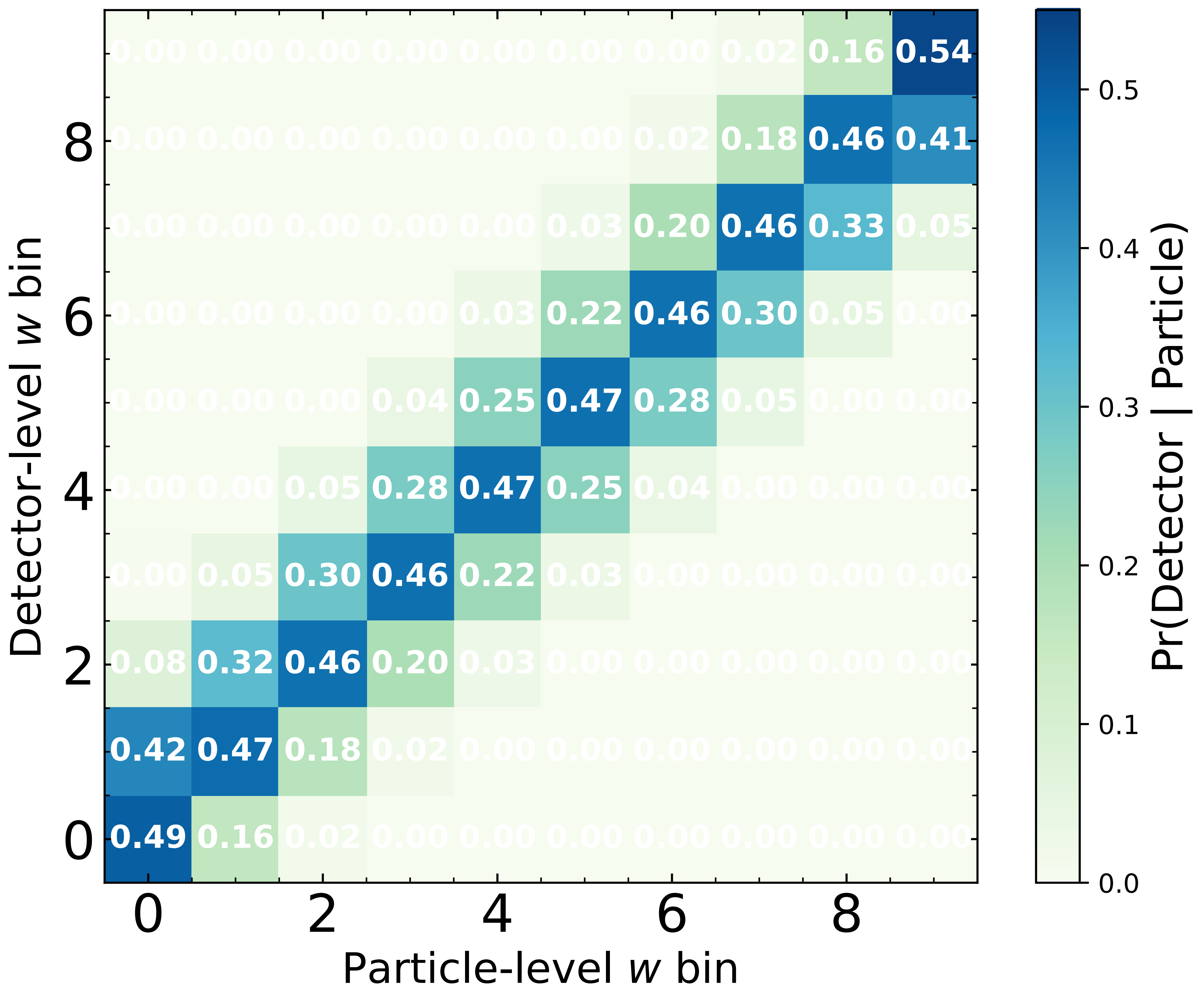

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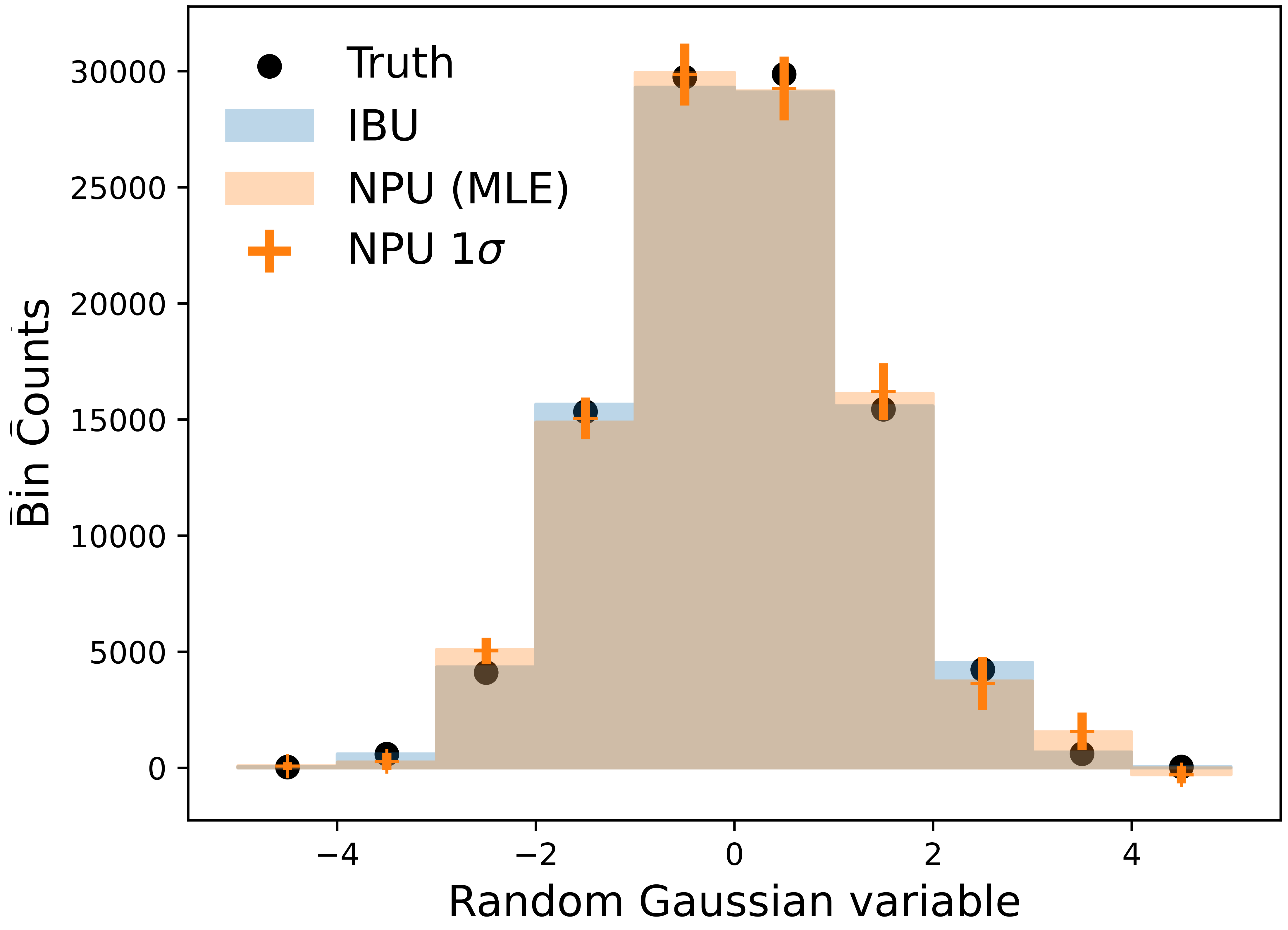

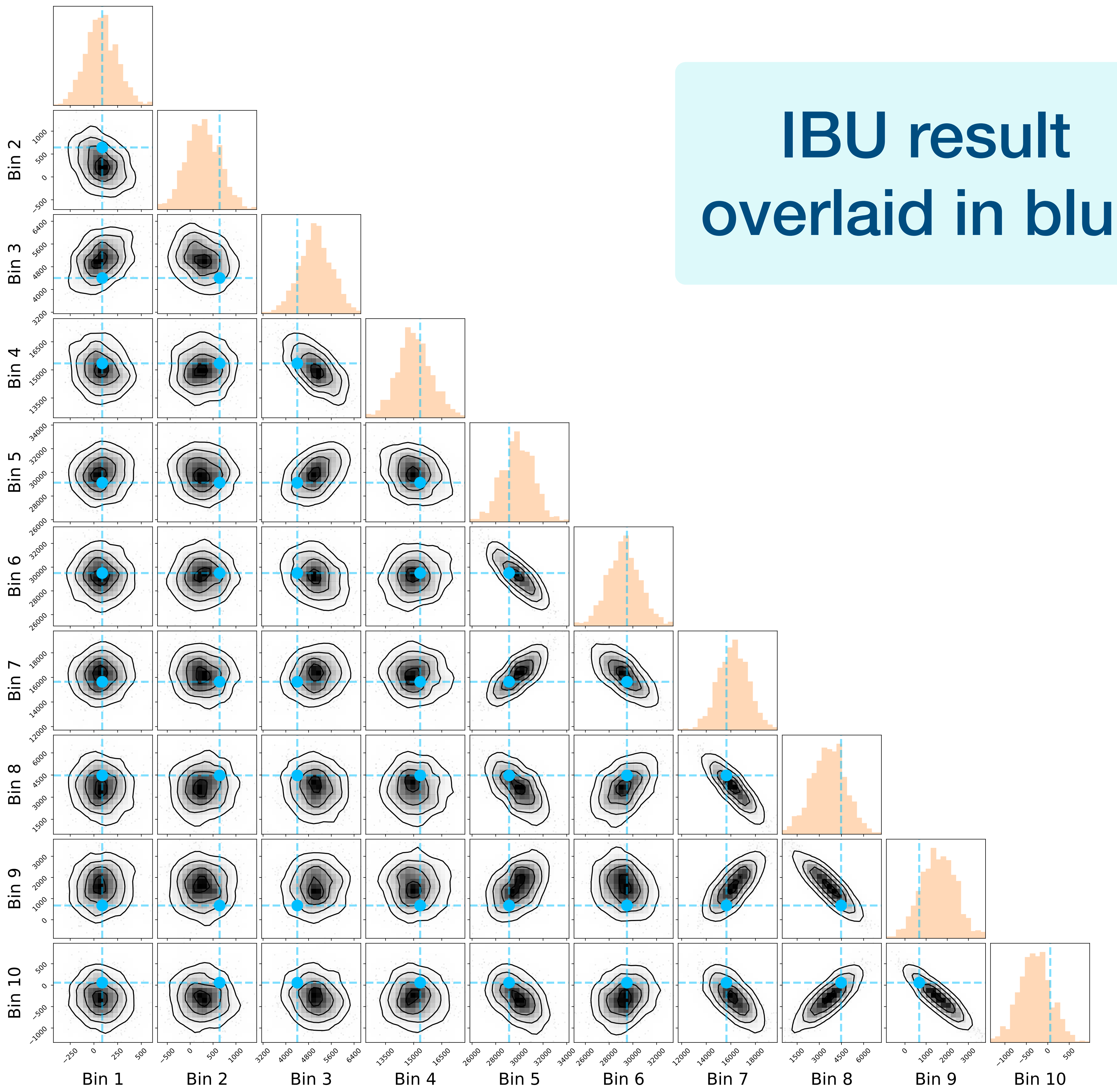

IBU result overlaid in blue

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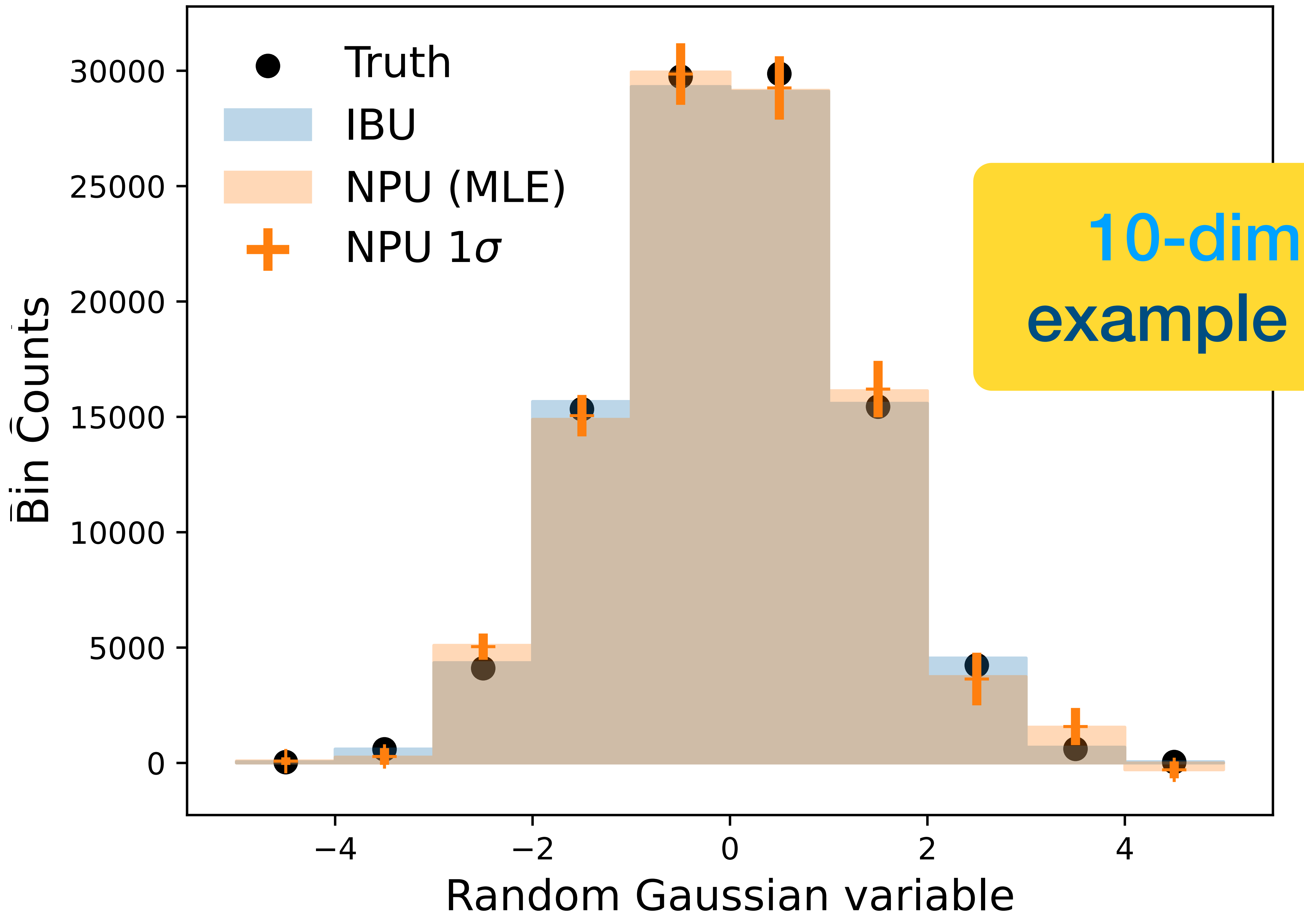
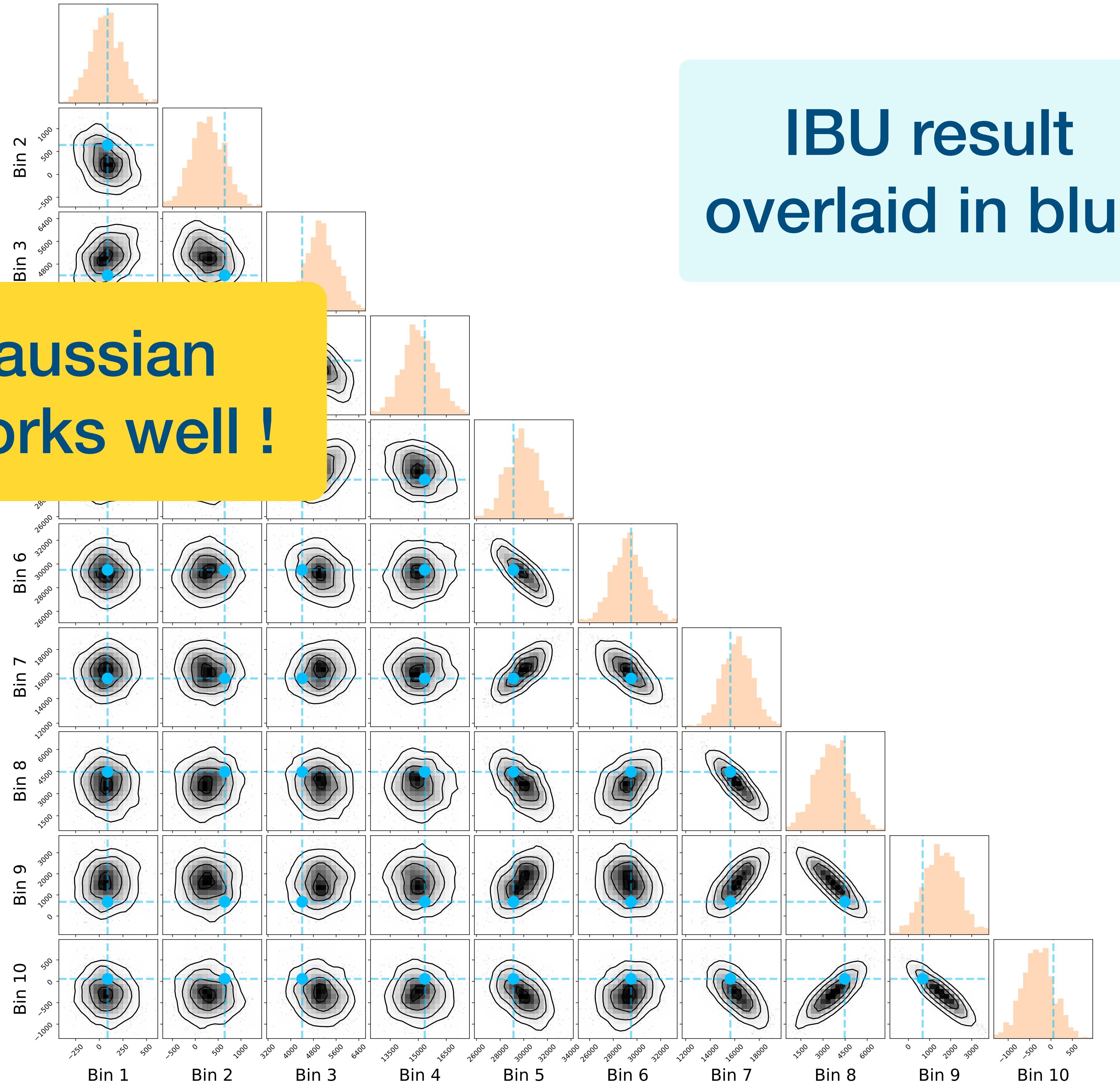


10-dim Gaussian example works well !



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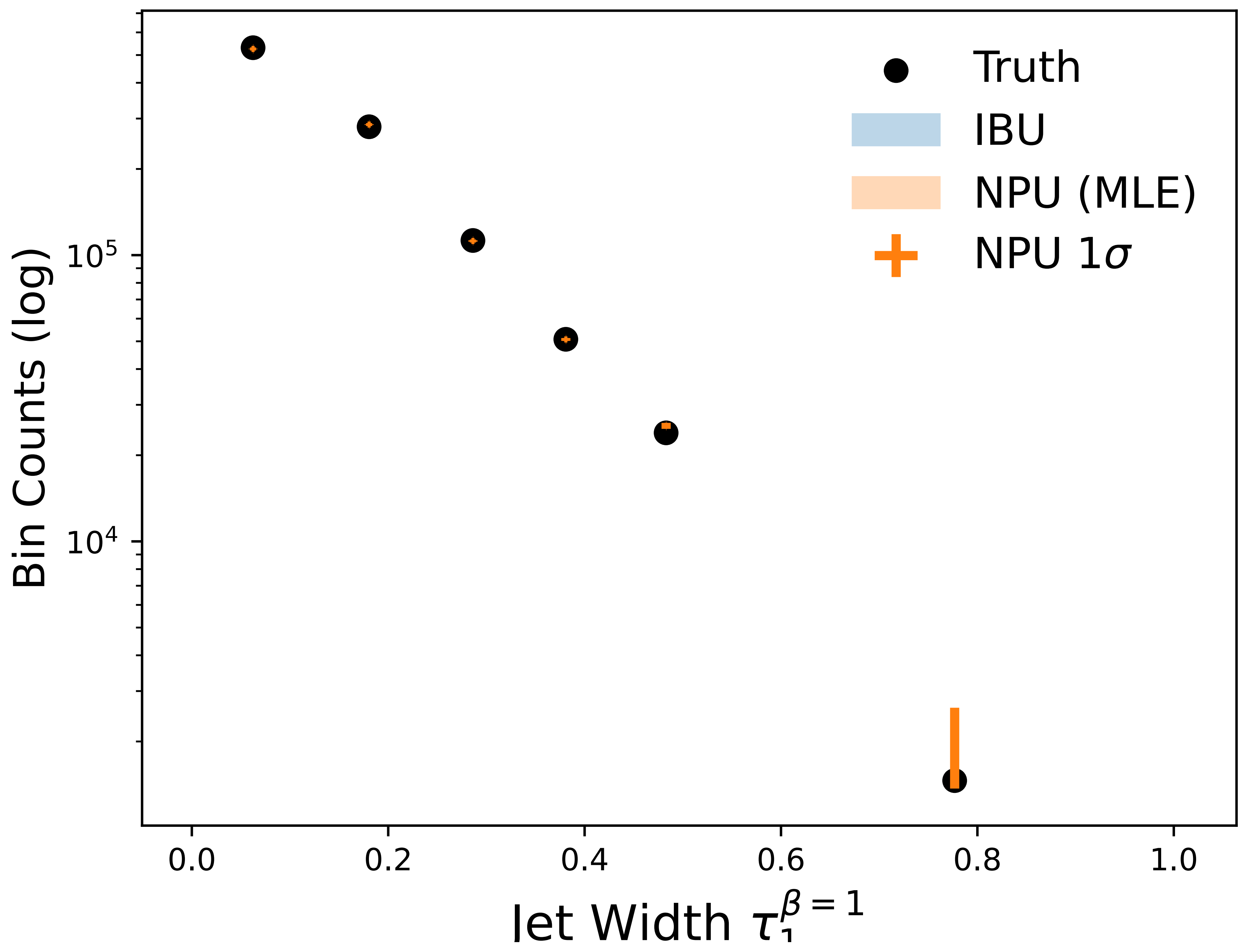

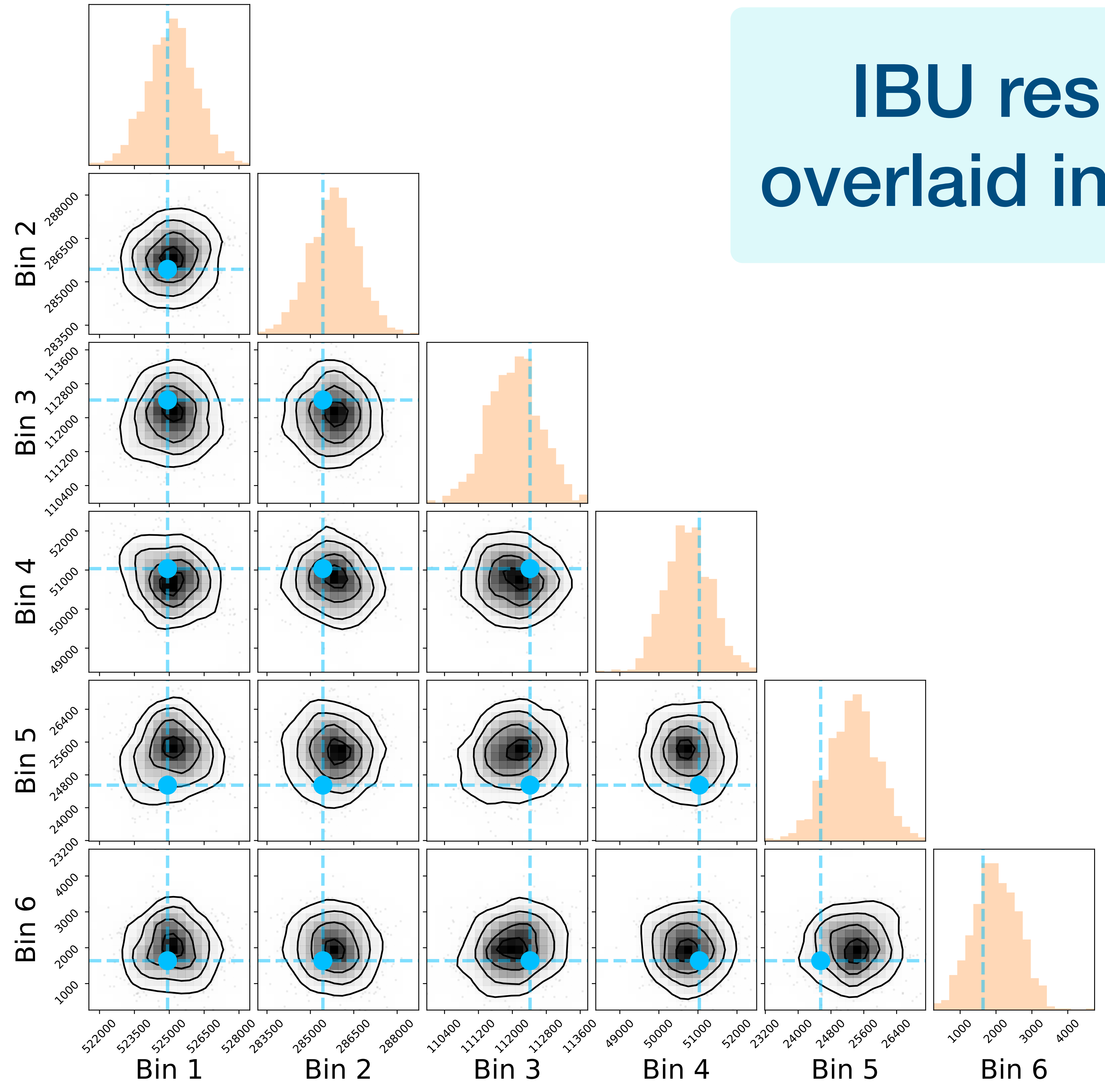

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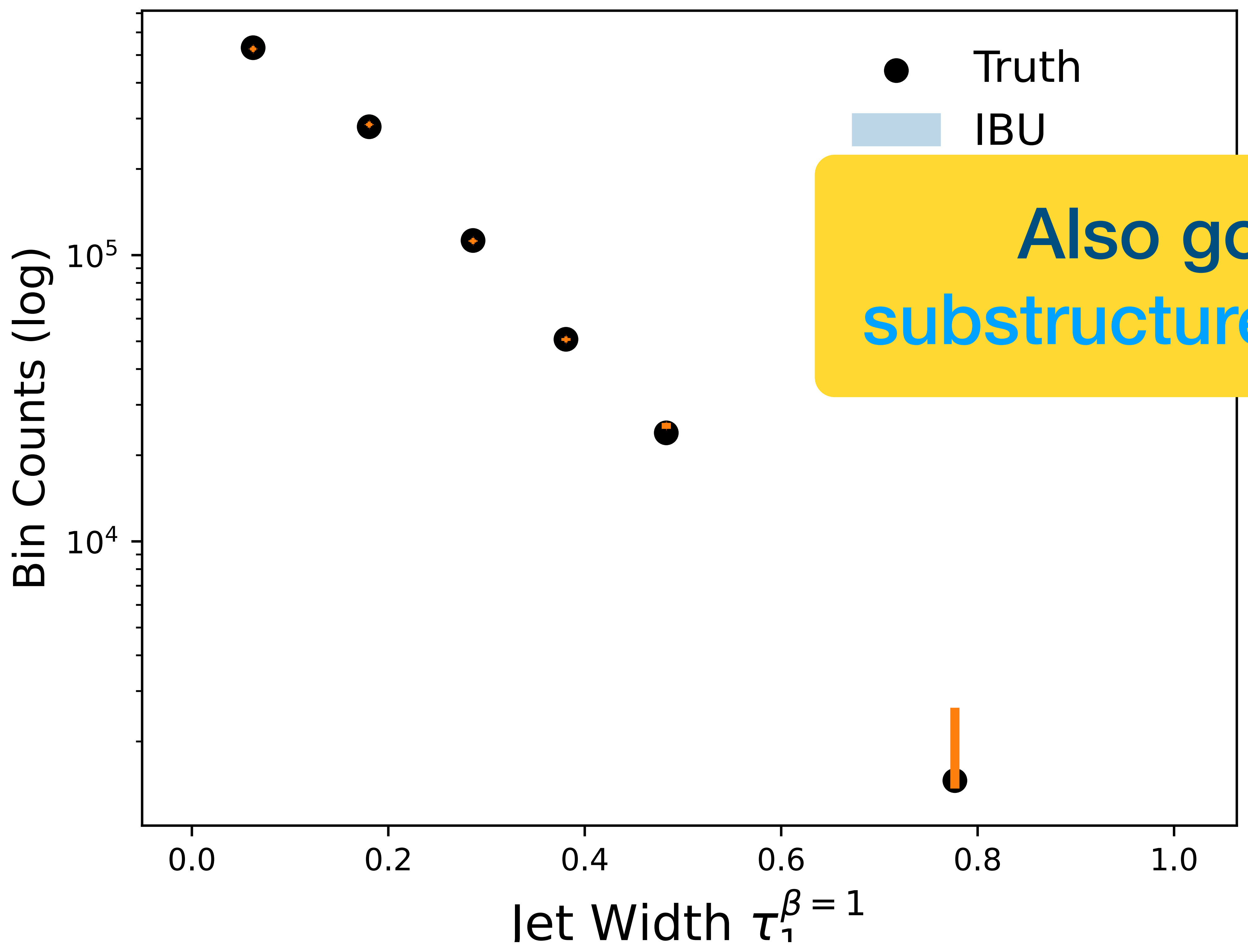

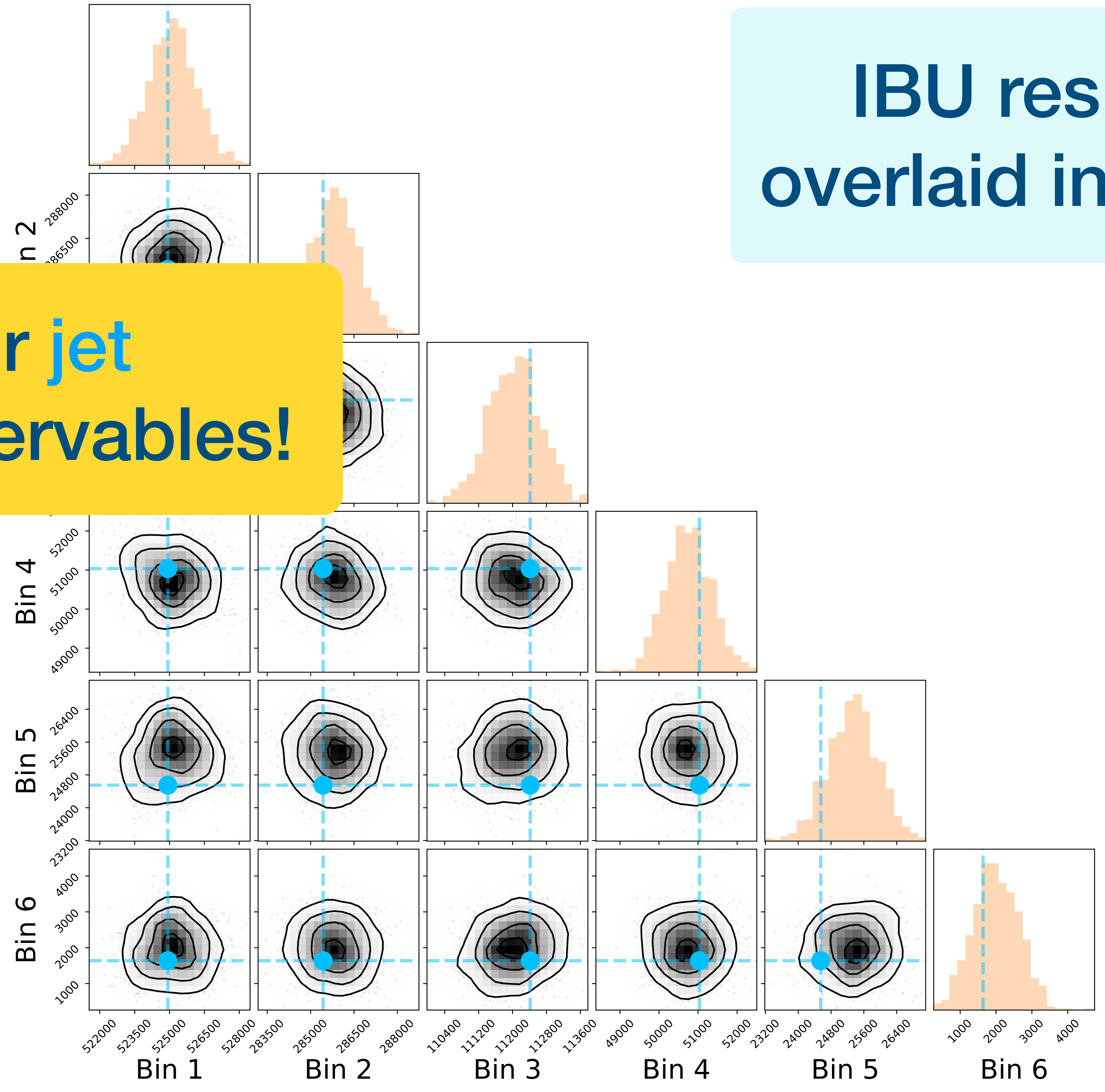

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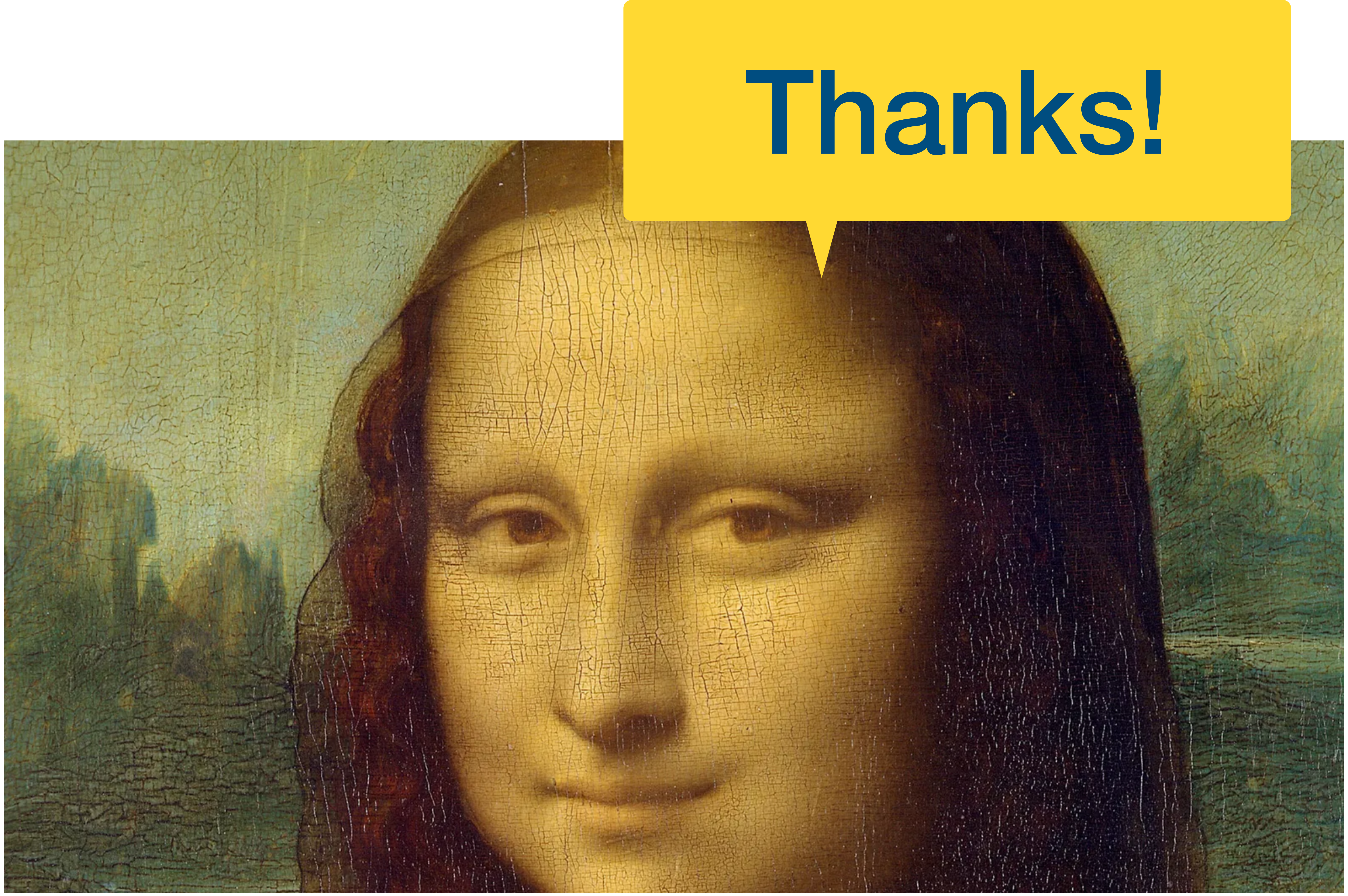
Also good for jet substructure observables!


Thanks!

Backup