



UNIVERSITÄT
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ZUKUNFT
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How to Unfold Top Decays

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Sofia Palacios Schweitzer¹, Tilman Plehn¹, Dennis Schwarz⁴*

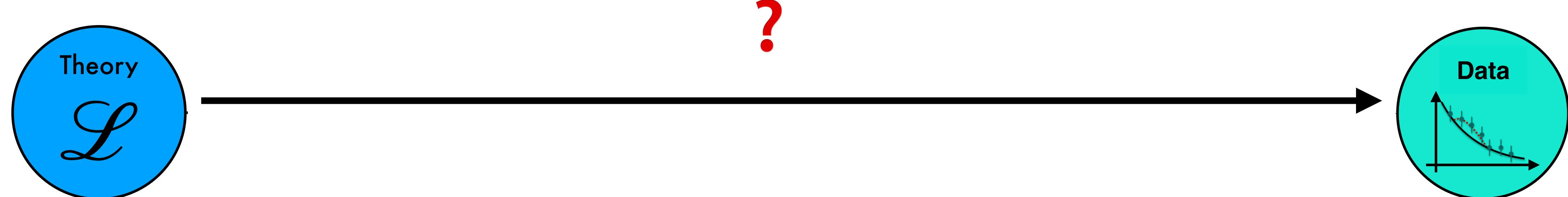
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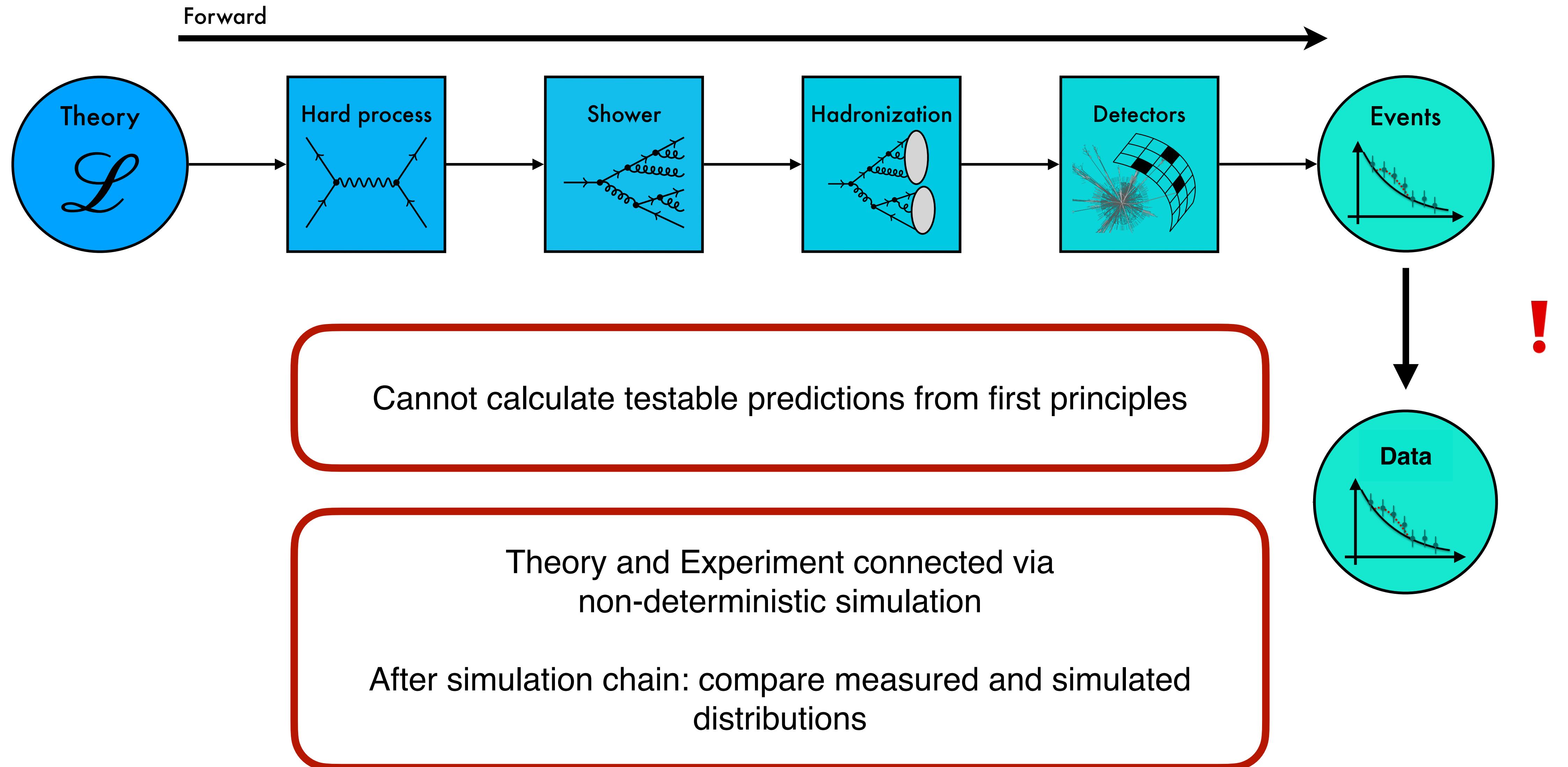
- 1 - Institut für theoretische Physik, Universität Heidelberg
- 2 - Deutsches Elektronen-Synchrotron DESY, Hamburg
- 3 - Institut für Experimentalphysik, Universität Hamburg
- 4 - Institut für Hochenergiephysik, Österreichische Akademie der Wissenschaften, Wien

Simulation Chain

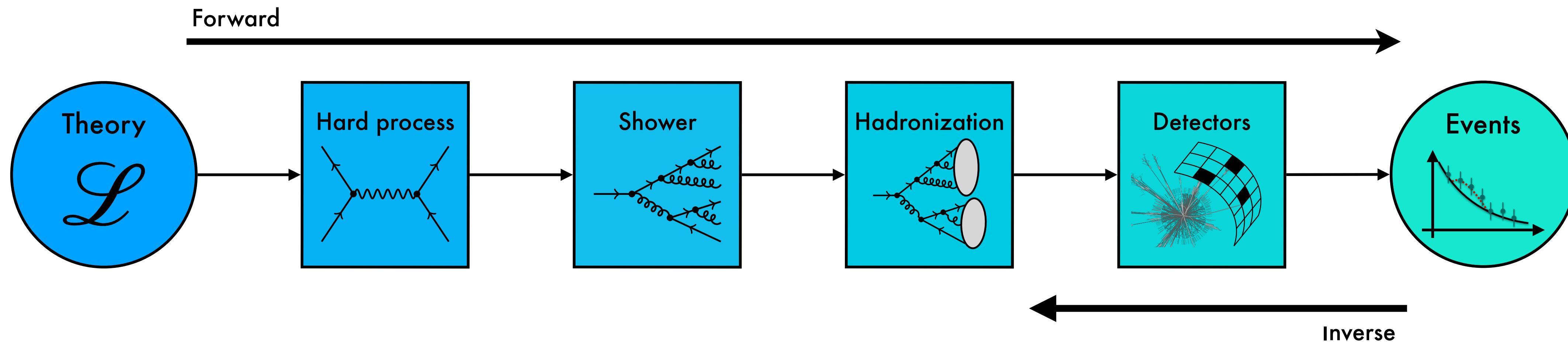


Cannot calculate testable predictions from first principles

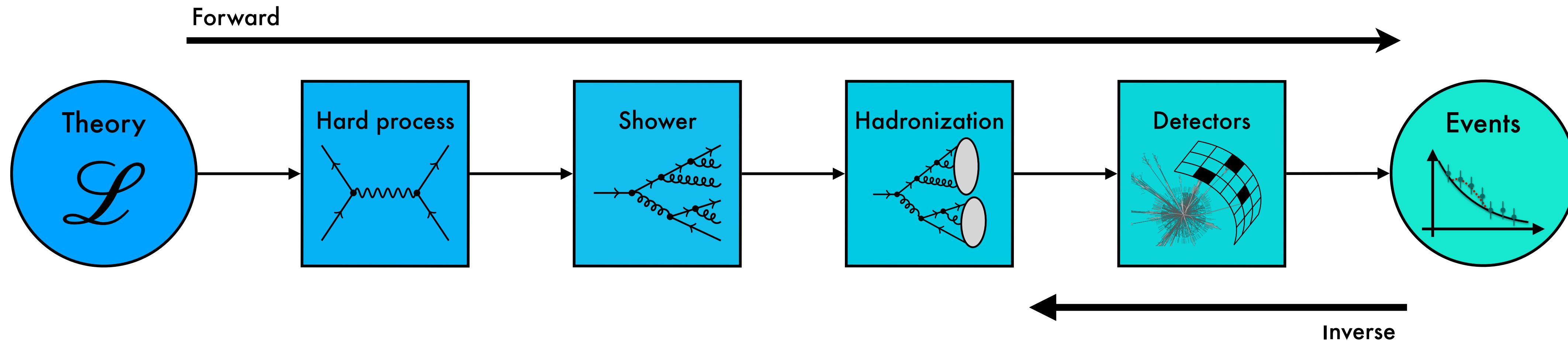
Simulation Chain



Simulation Chain – Inversion



Why unfolding?



Theory analyses don't care about detectors

Comparing data from different experiments (Global Analysis)

For some analysis direct access to theory parameters

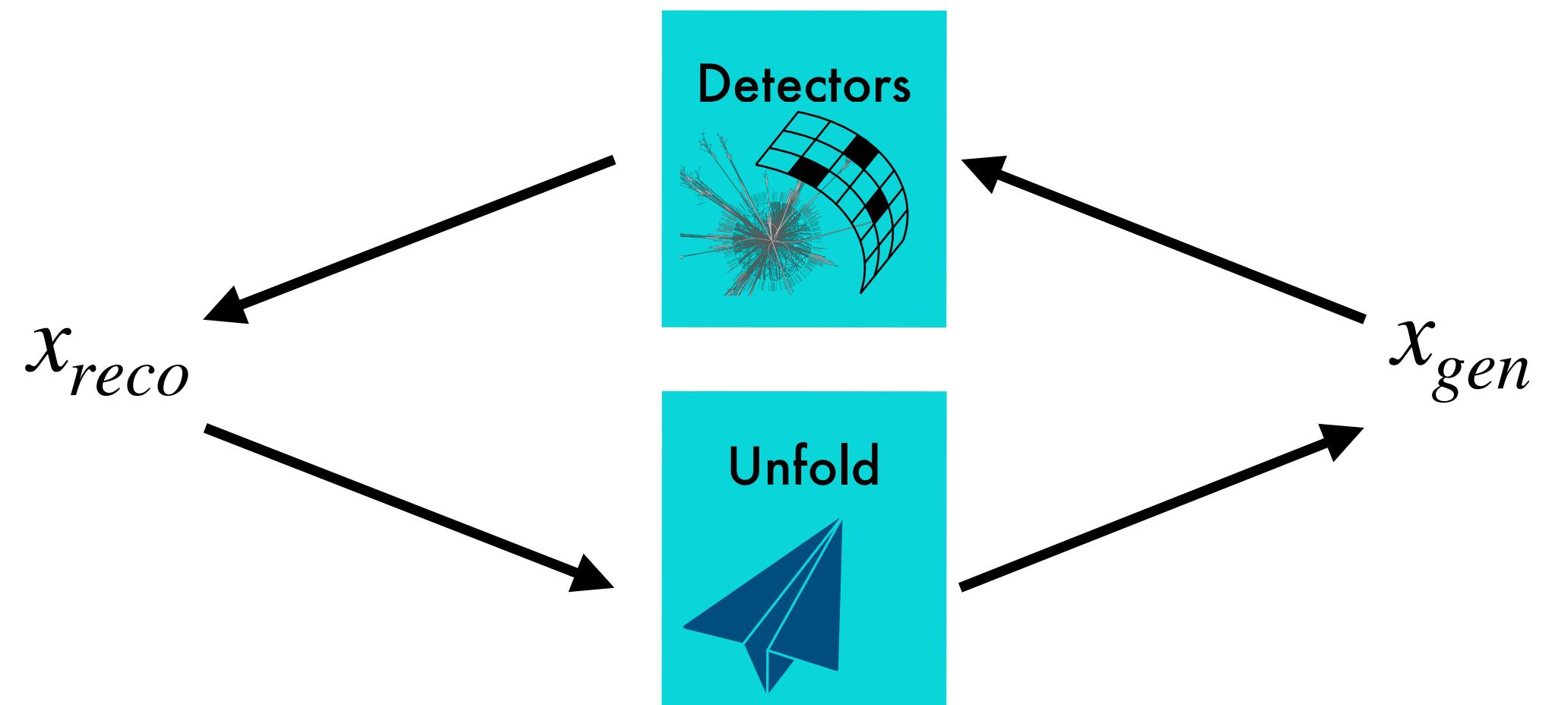
Resolution

Data preservation

Unfolding – unchained

$$p(x_{reco}) = \int p(x_{gen})R(x_{reco}, x_{gen}) dx_{gen}$$

$$p(x_{gen}) = \int p(x_{reco})p(x_{gen} | x_{reco}) dx_{reco}$$



Unfolding – unchained

$$p(x_{reco}) = \int p(x_{gen}) \underbrace{R(x_{reco}, x_{gen})}_{p(\mathbf{x}_{\text{reco}} | \mathbf{x}_{\text{gen}})} dx_{gen}$$

$$p(x_{gen}) = \int p(x_{reco}) p(x_{gen} | x_{reco}) dx_{reco}$$

Classical methods are restricted to binned, one-dimensional distributions

We would like to learn high-dimensional, unbinned unfolding probability

Unfolding – unchained

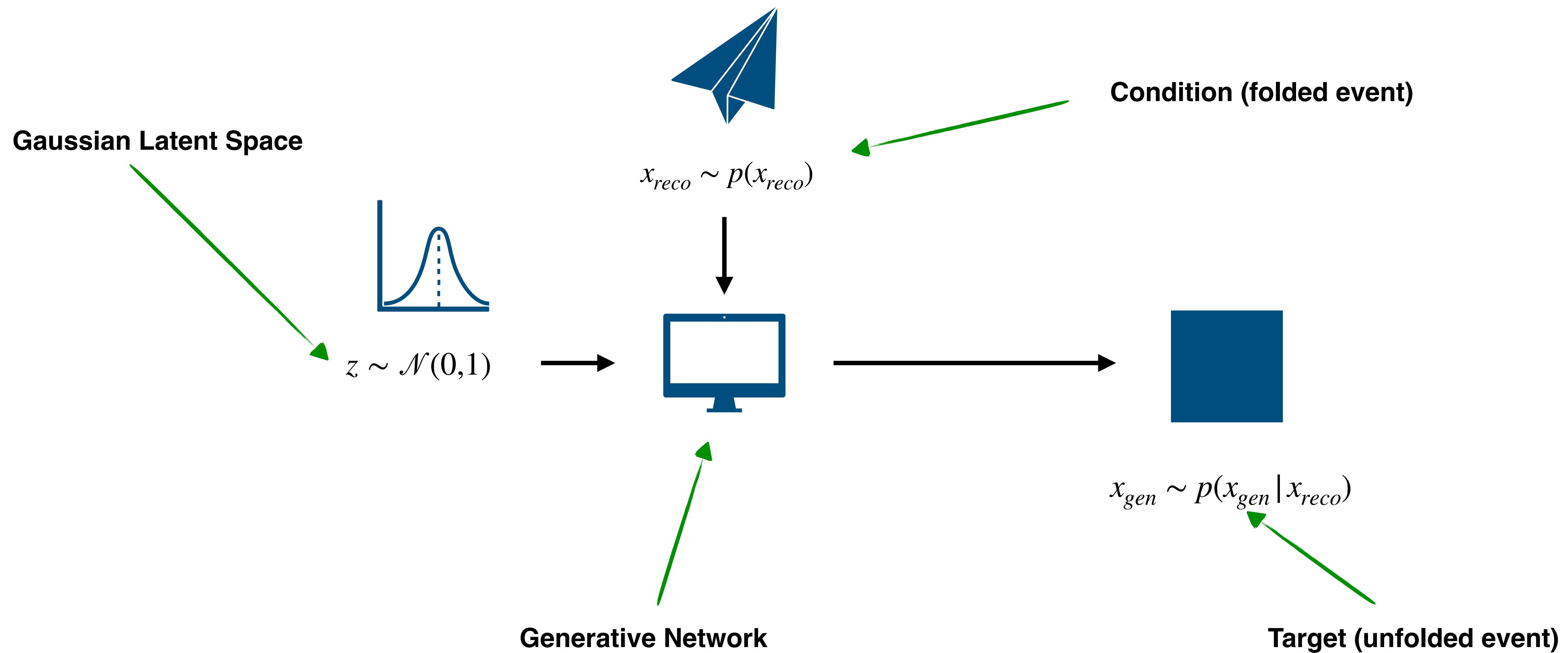
$$p(x_{reco}) = \int p(x_{gen}) \underbrace{R(x_{reco}, x_{gen})}_{p(\mathbf{x}_{\text{reco}} | \mathbf{x}_{\text{gen}})} dx_{gen}$$

$$p(x_{gen}) = \int p(x_{reco}) \underbrace{p(x_{gen} | x_{reco})}_{\text{target probability}} dx_{reco}$$

Classical methods are restricted to binned, one-dimensional distributions

We would like to learn high-dimensional, unbinned unfolding probability

Unfolding – generative methods

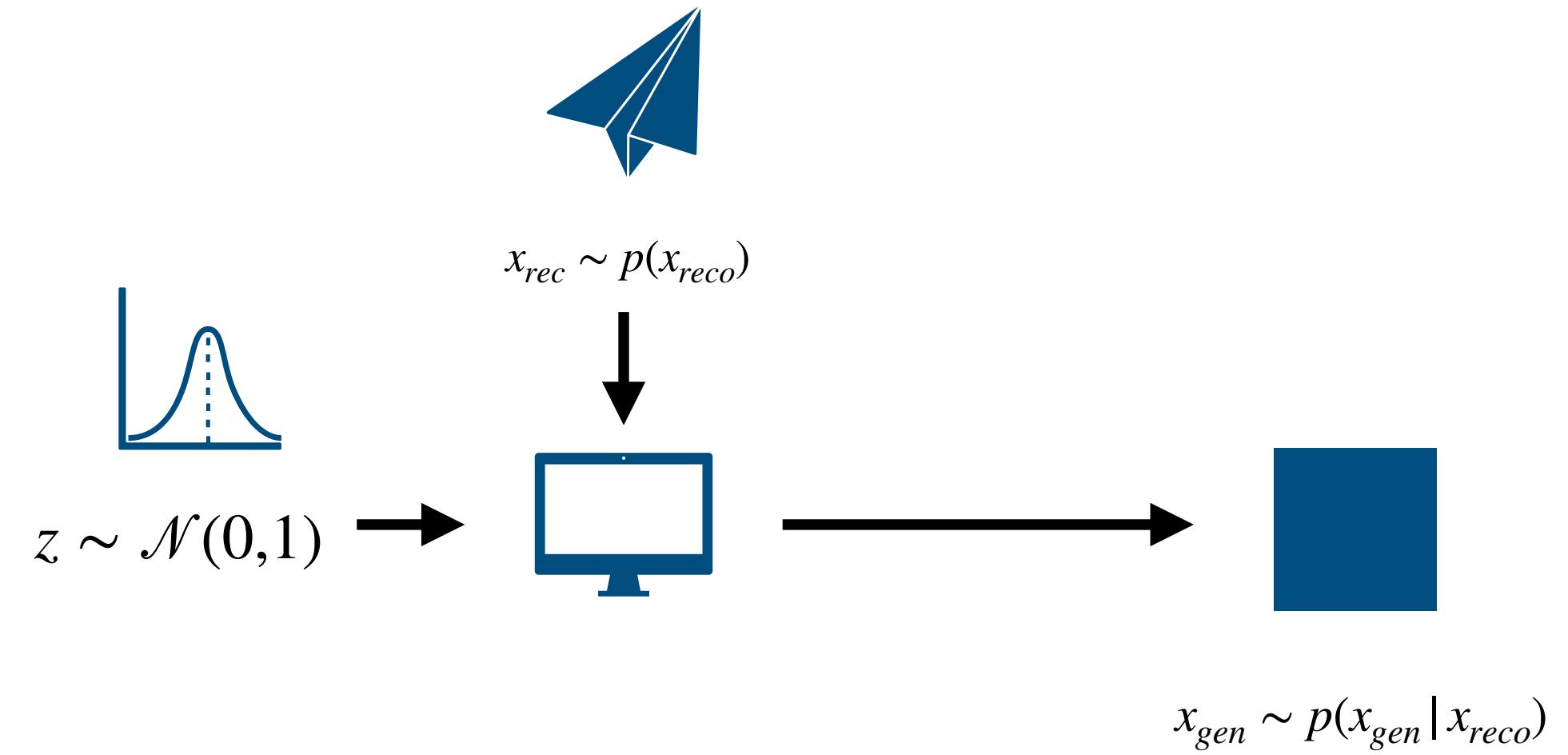


Unfolding – generative methods

Goal: learn transformation latent \rightarrow gen phase space conditioned on reco event

During training, use paired events of forward simulation

After training, repeated sampling from latent space with constant condition allows probabilistic single event unfolding

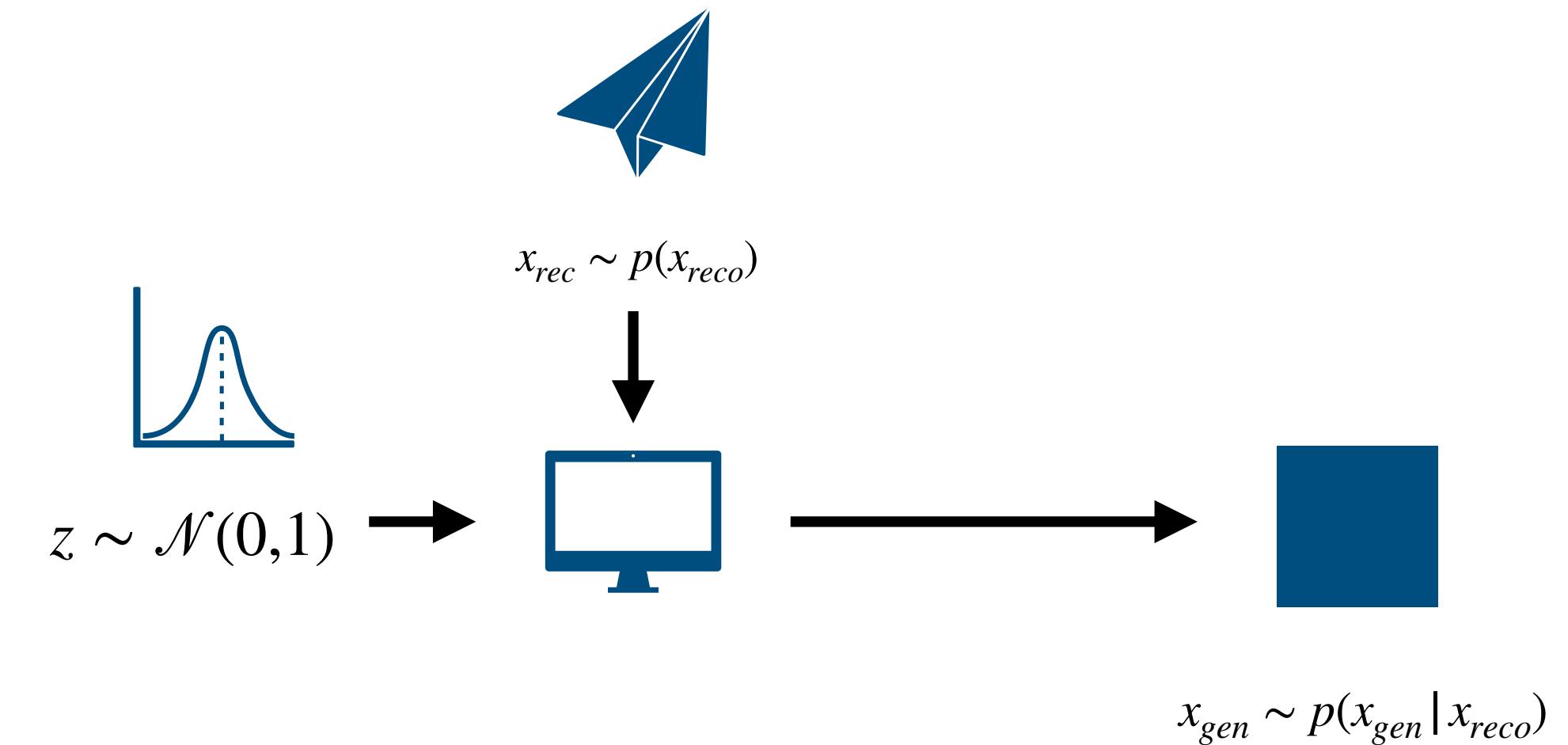


Unfolding – generative methods

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Bellagente et al. 1912.00477

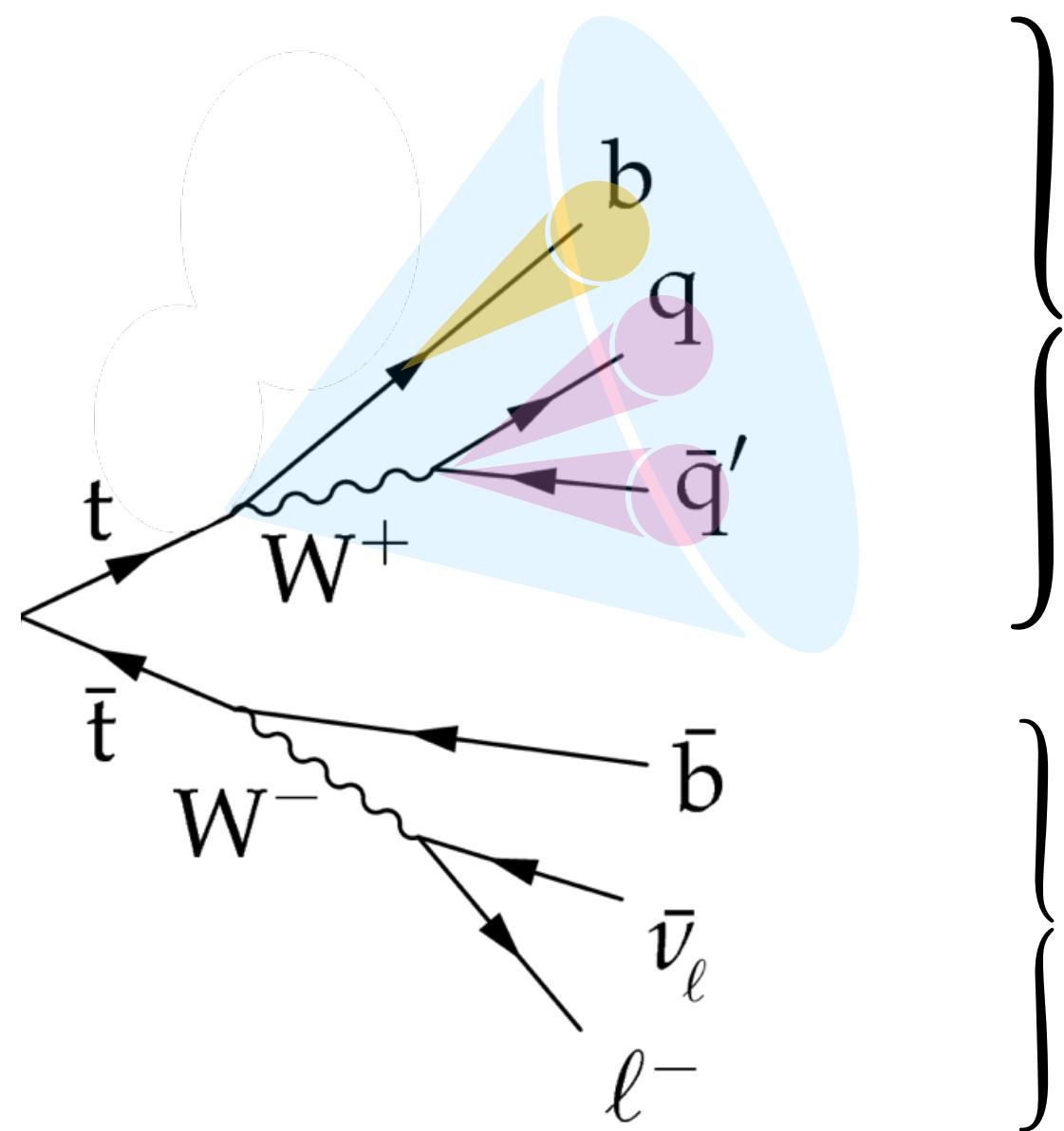
Bellagente et al. 2006.06685

Backes et al. 2212.08674

Huetsch et al. 2404.18807

BOOSTed top decays

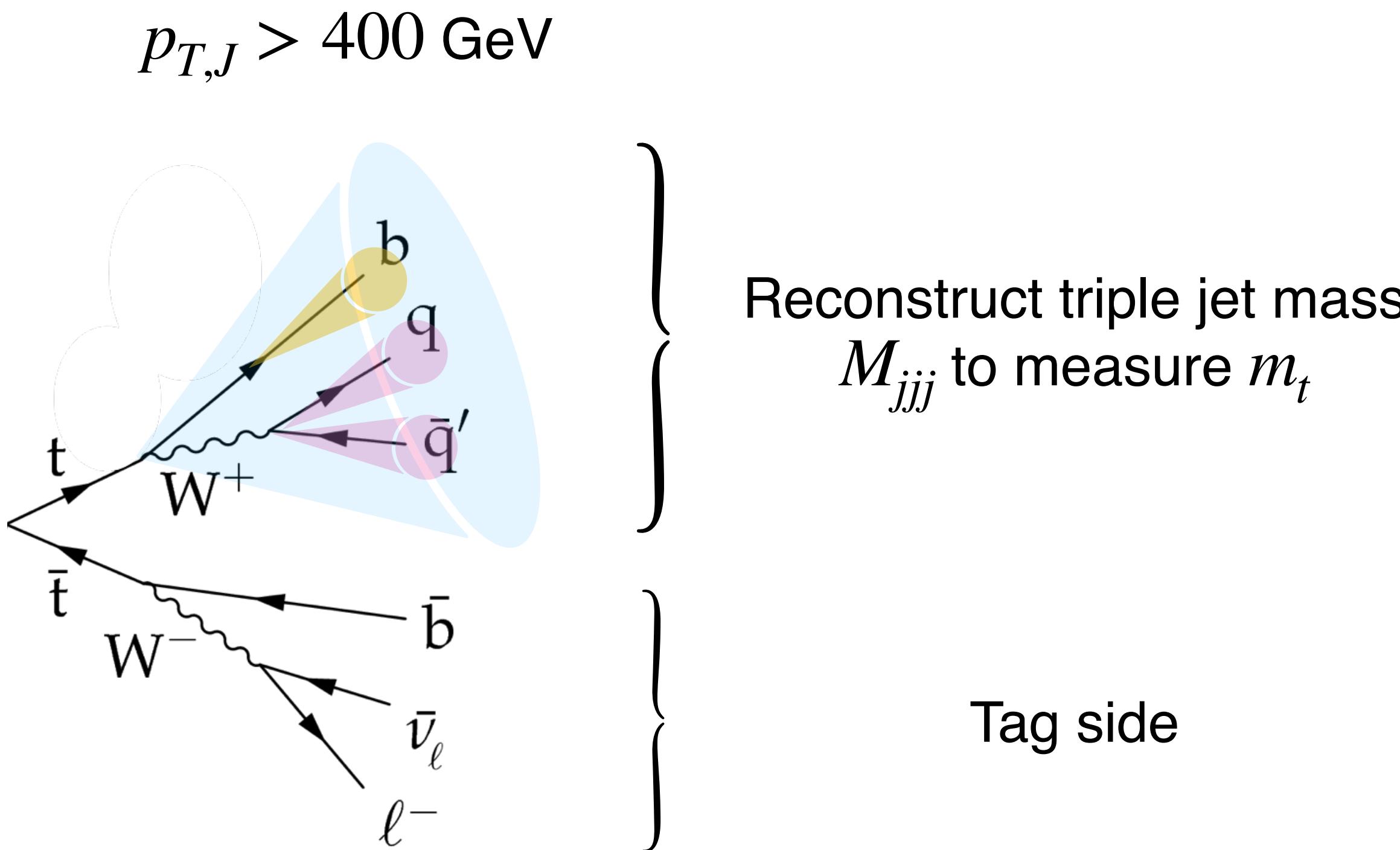
$p_{T,J} > 400 \text{ GeV}$



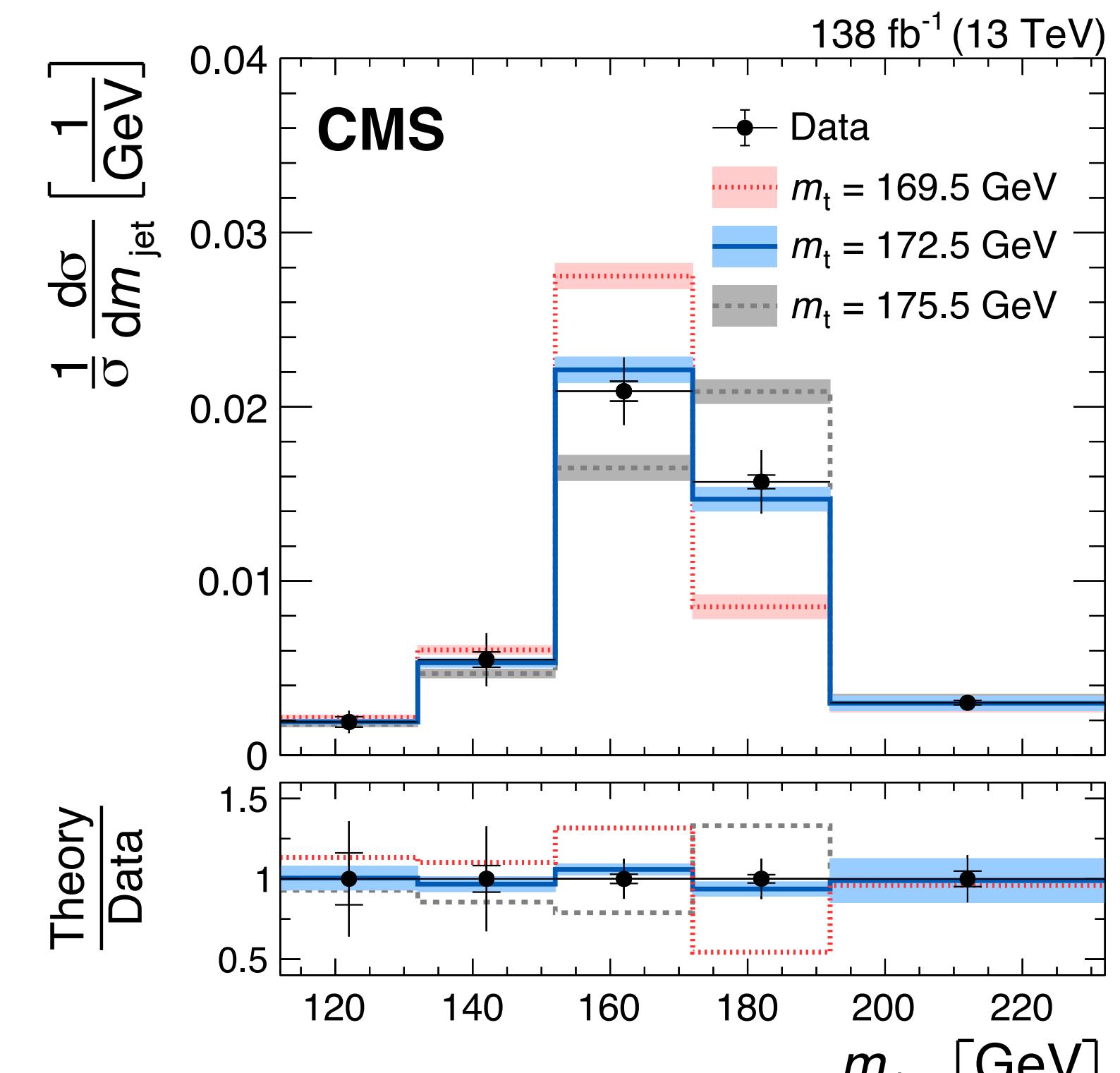
} Reconstruct triple jet mass
 M_{jjj} to measure m_t

} Tag side

BOOSTed top decays



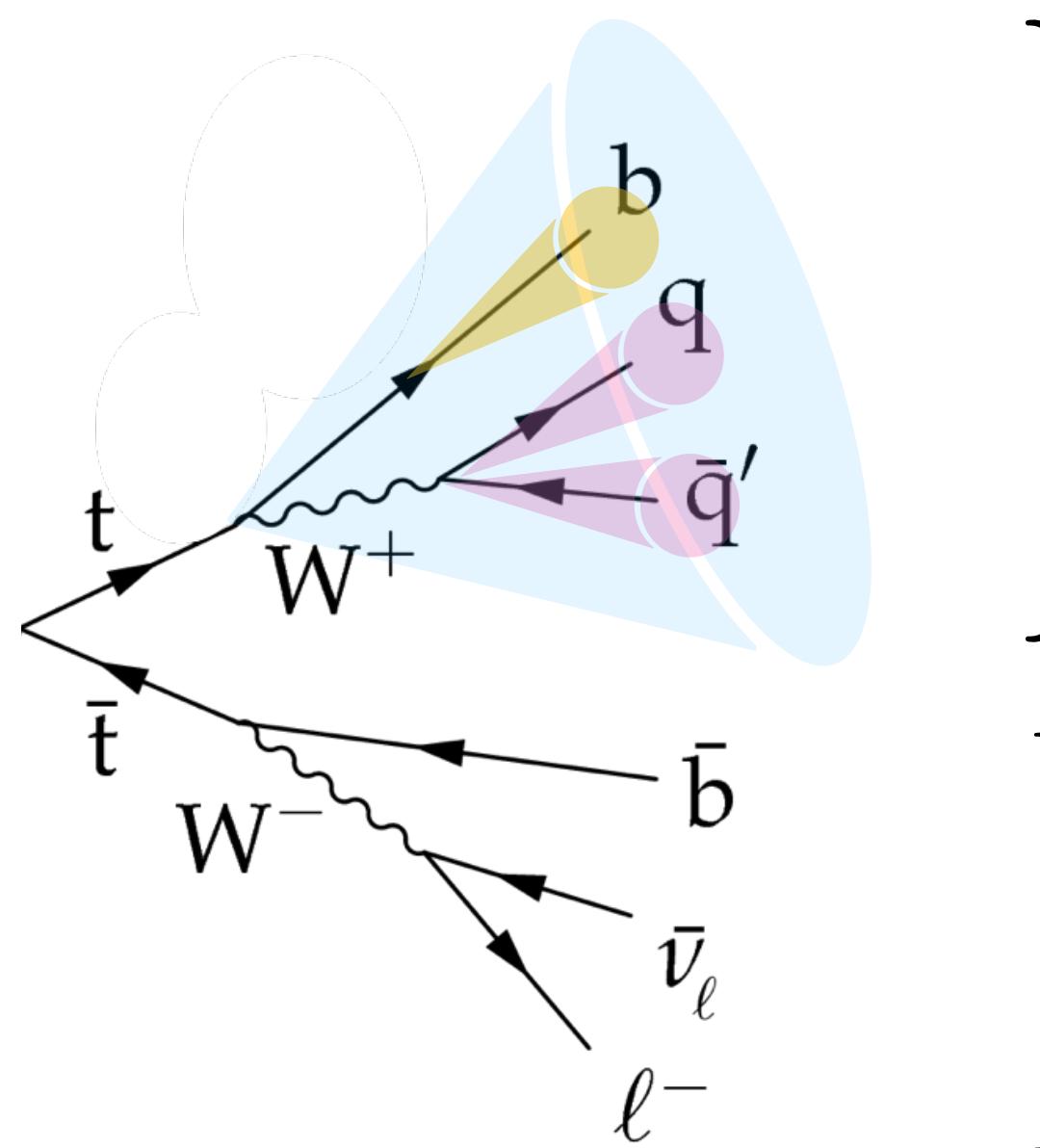
Previously done in CMS with TUnfold
(classical binned unfolding algorithm)



CMS 2211.01456

BOOSTed top decays

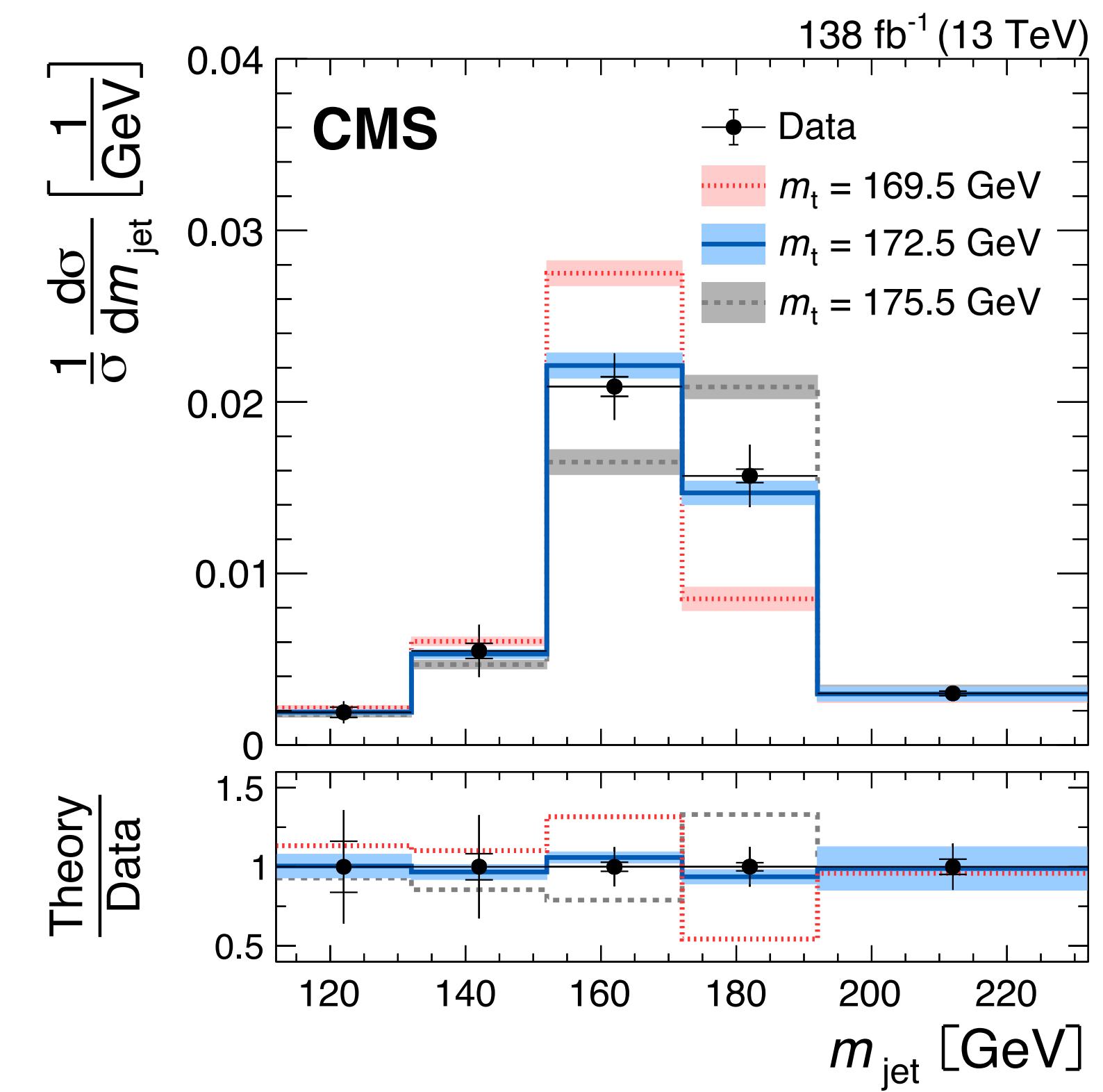
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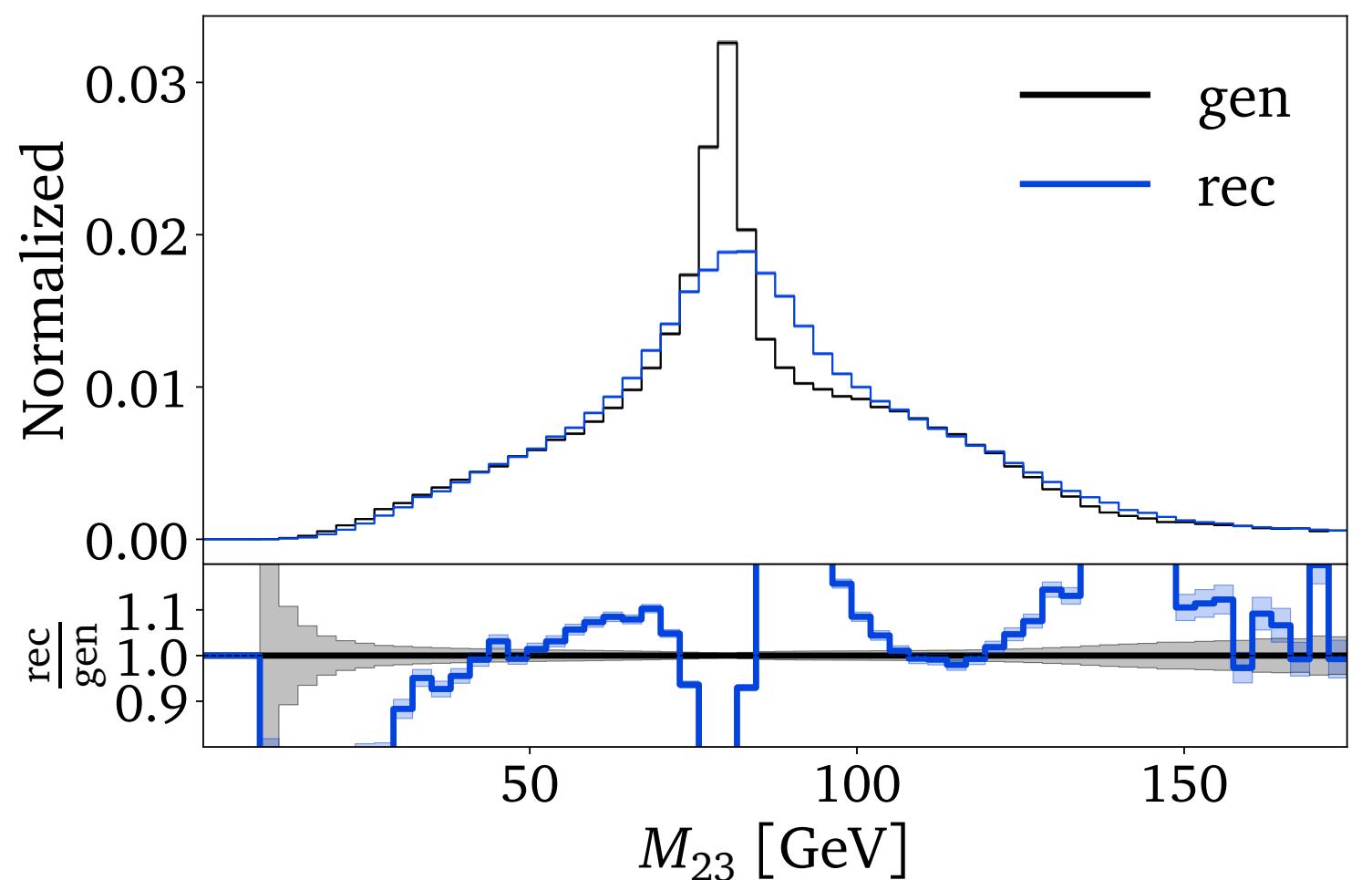
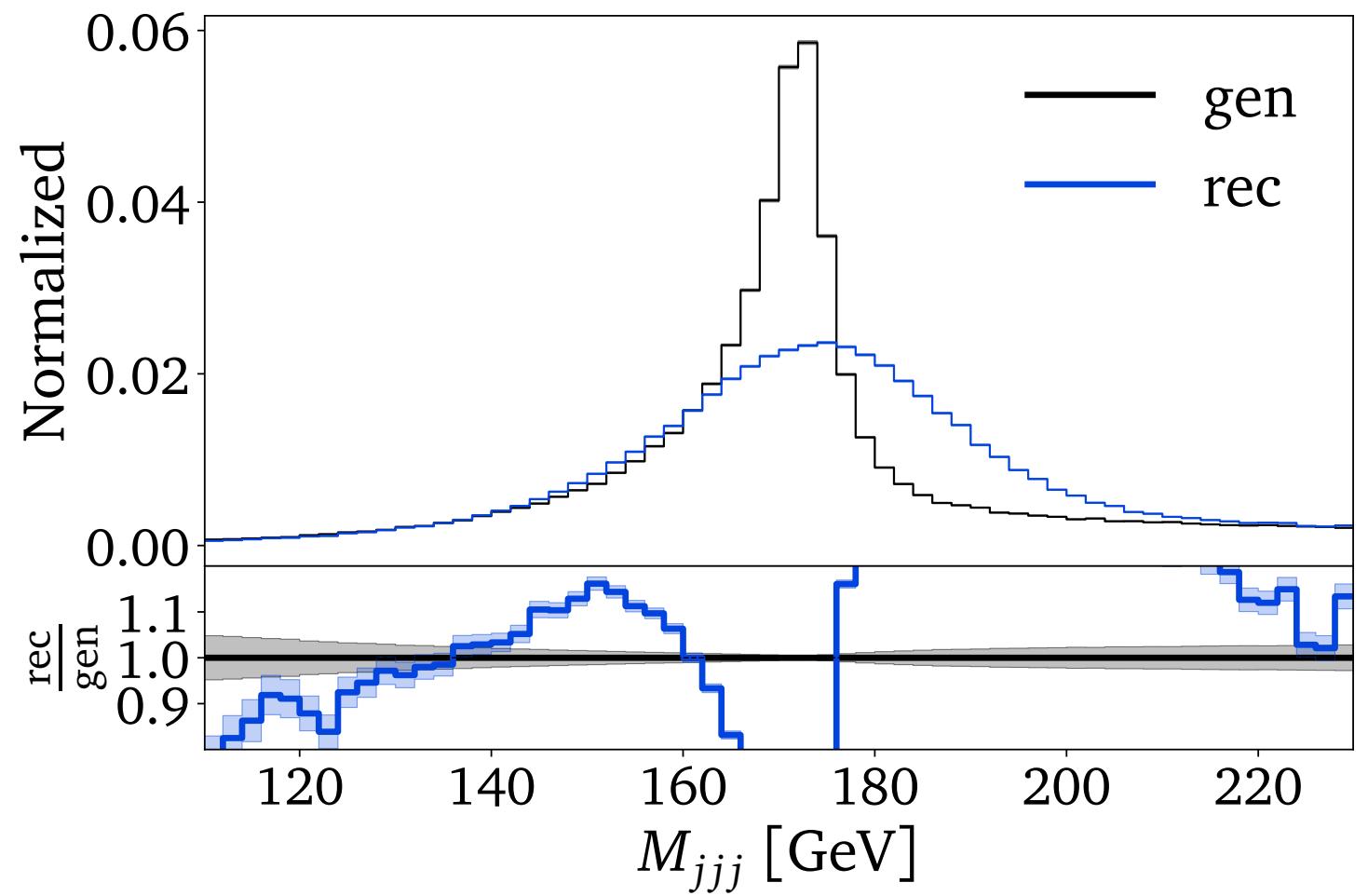


CMS 2211.01456

BUT leading uncertainty: choice of m_t in simulation + no access to full phase space
→ Could generative unfolding help?

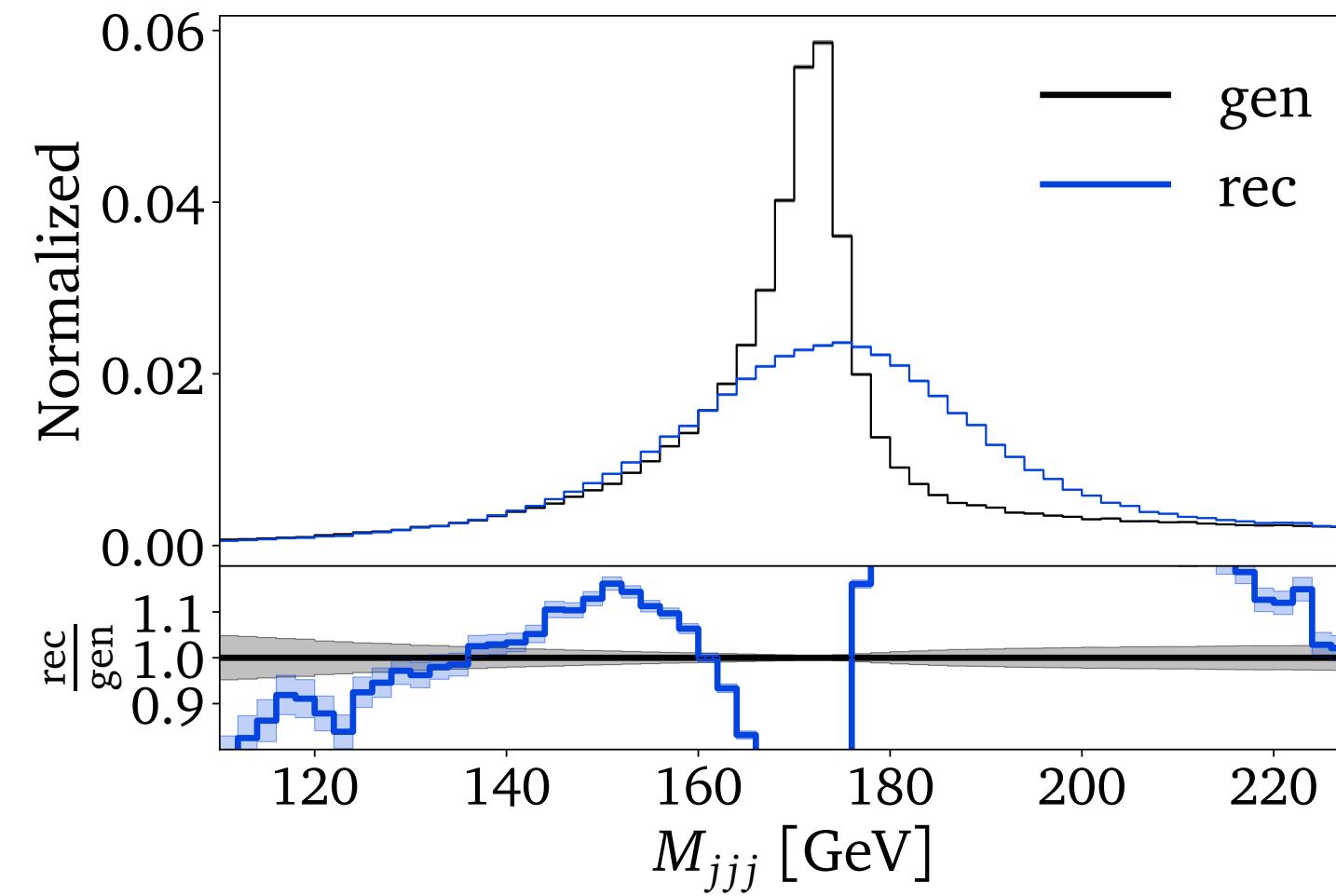
Challenging aspects of top - unfolding

1. Multiresonant phase space

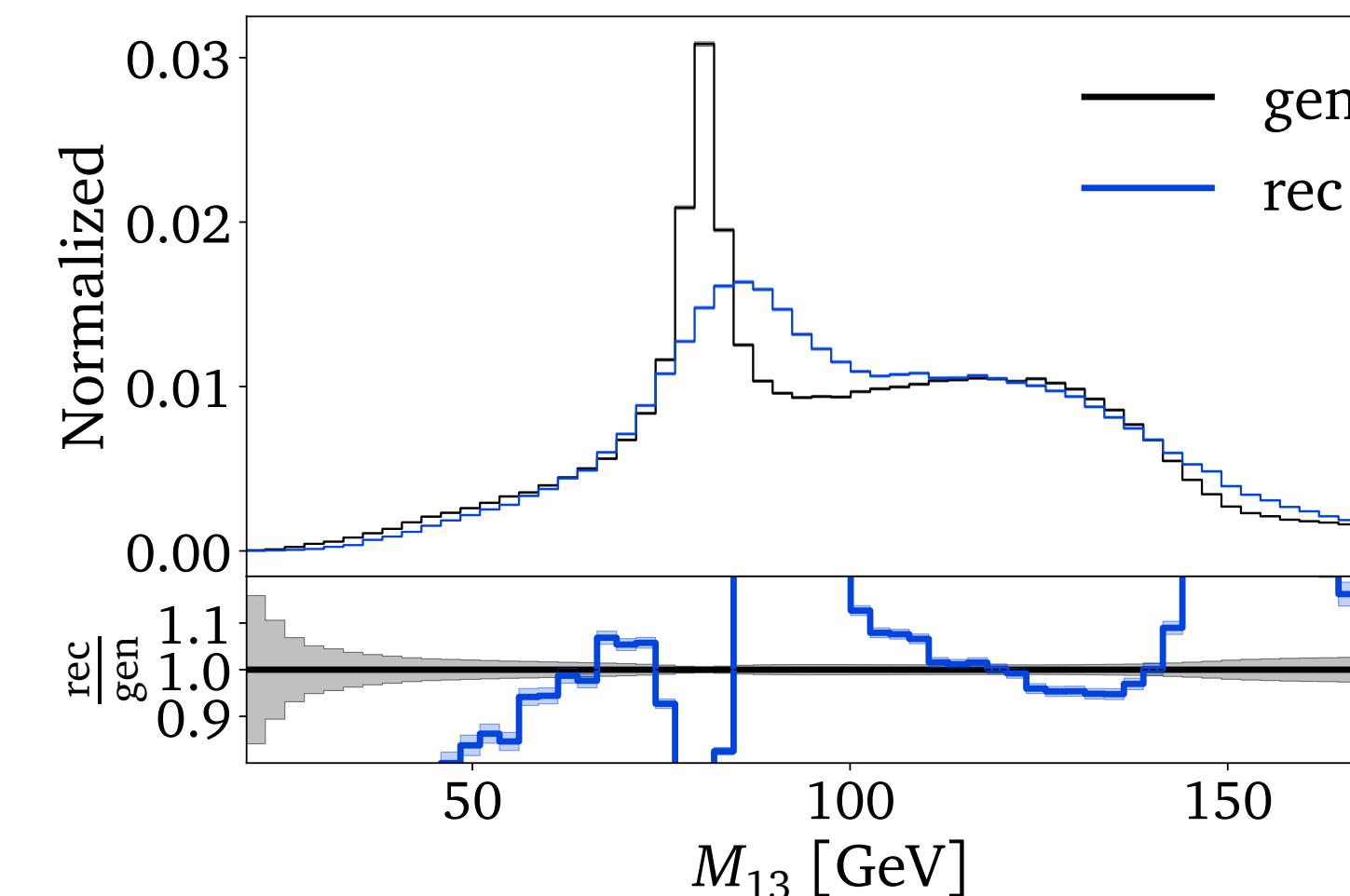
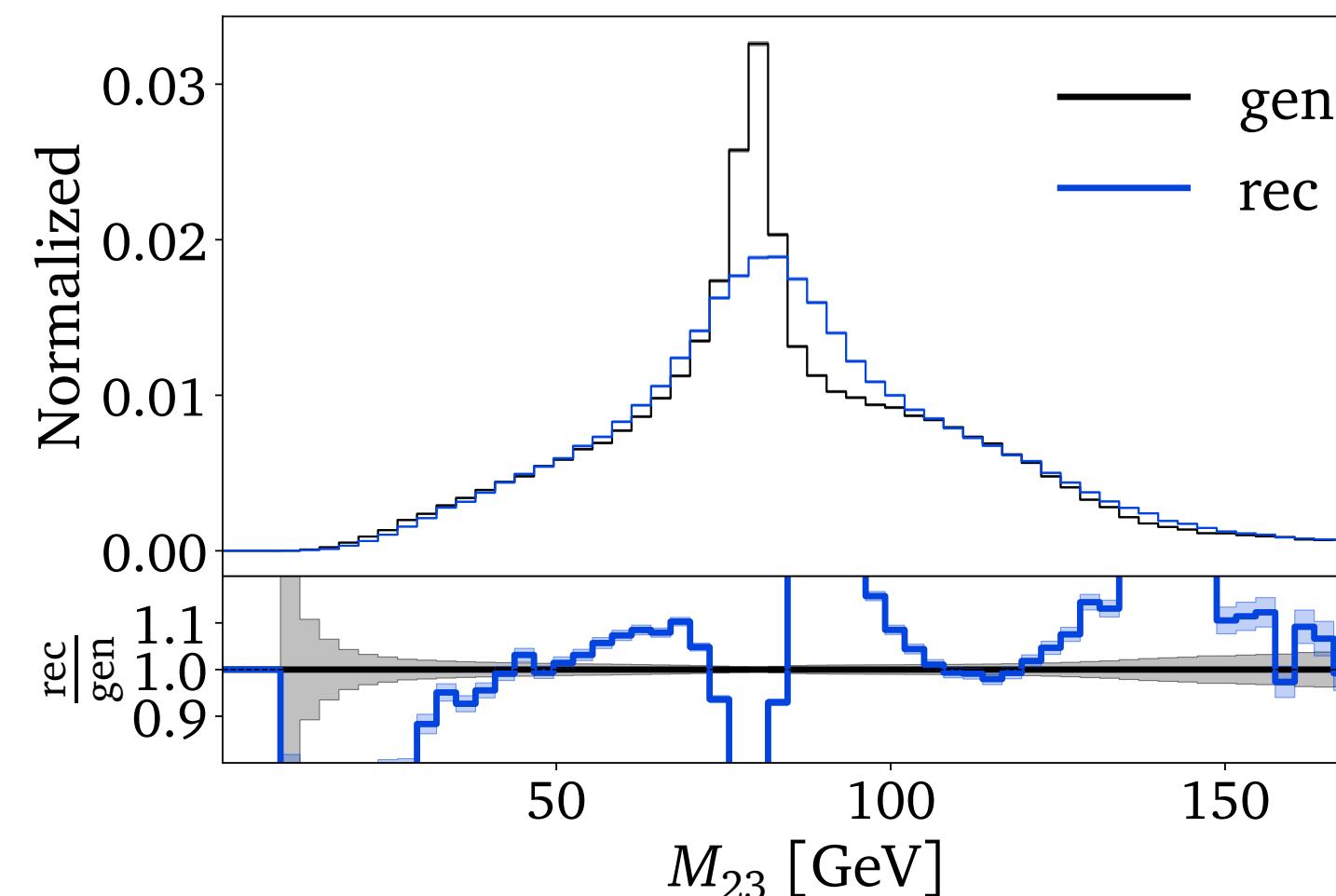
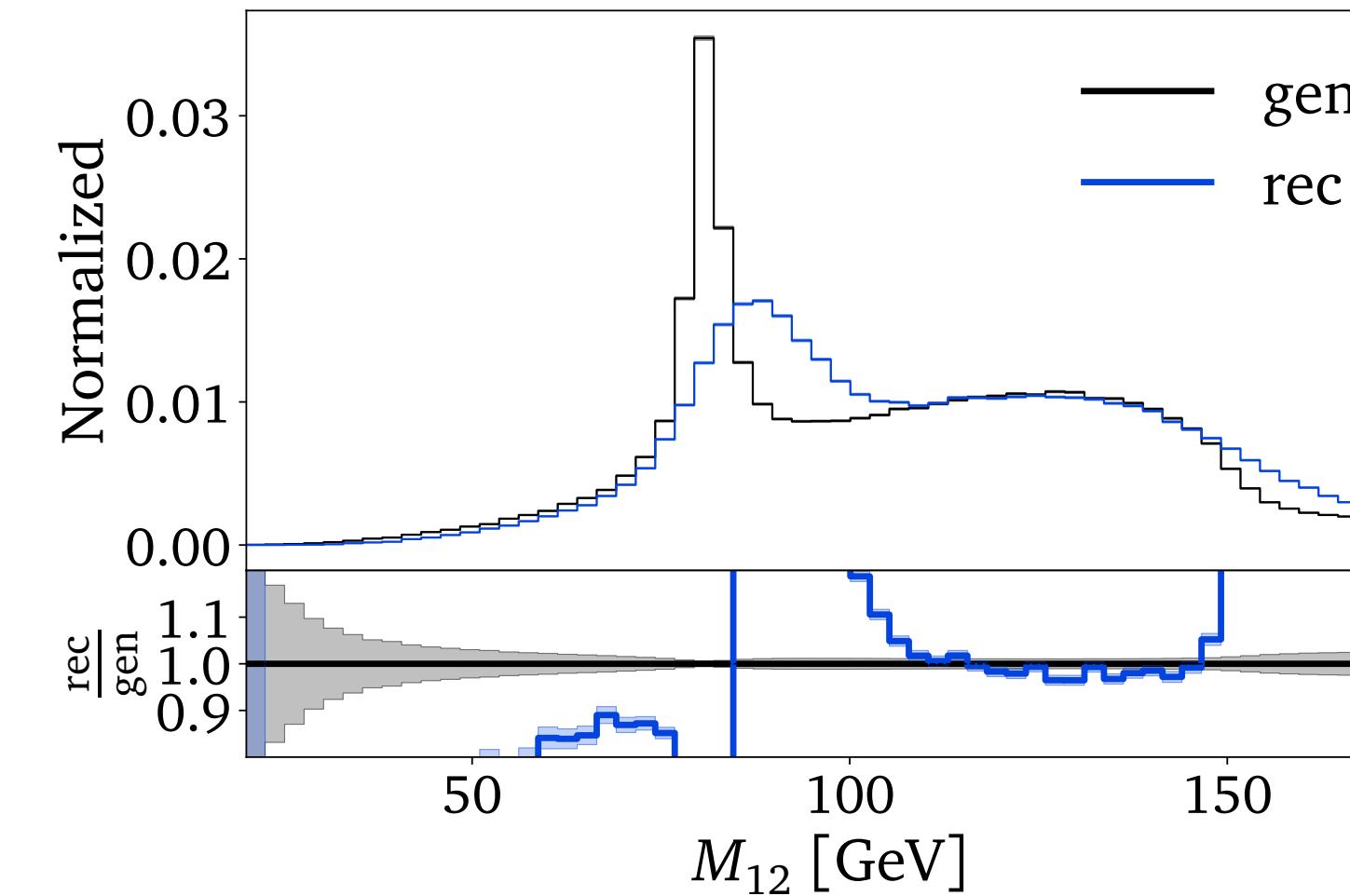


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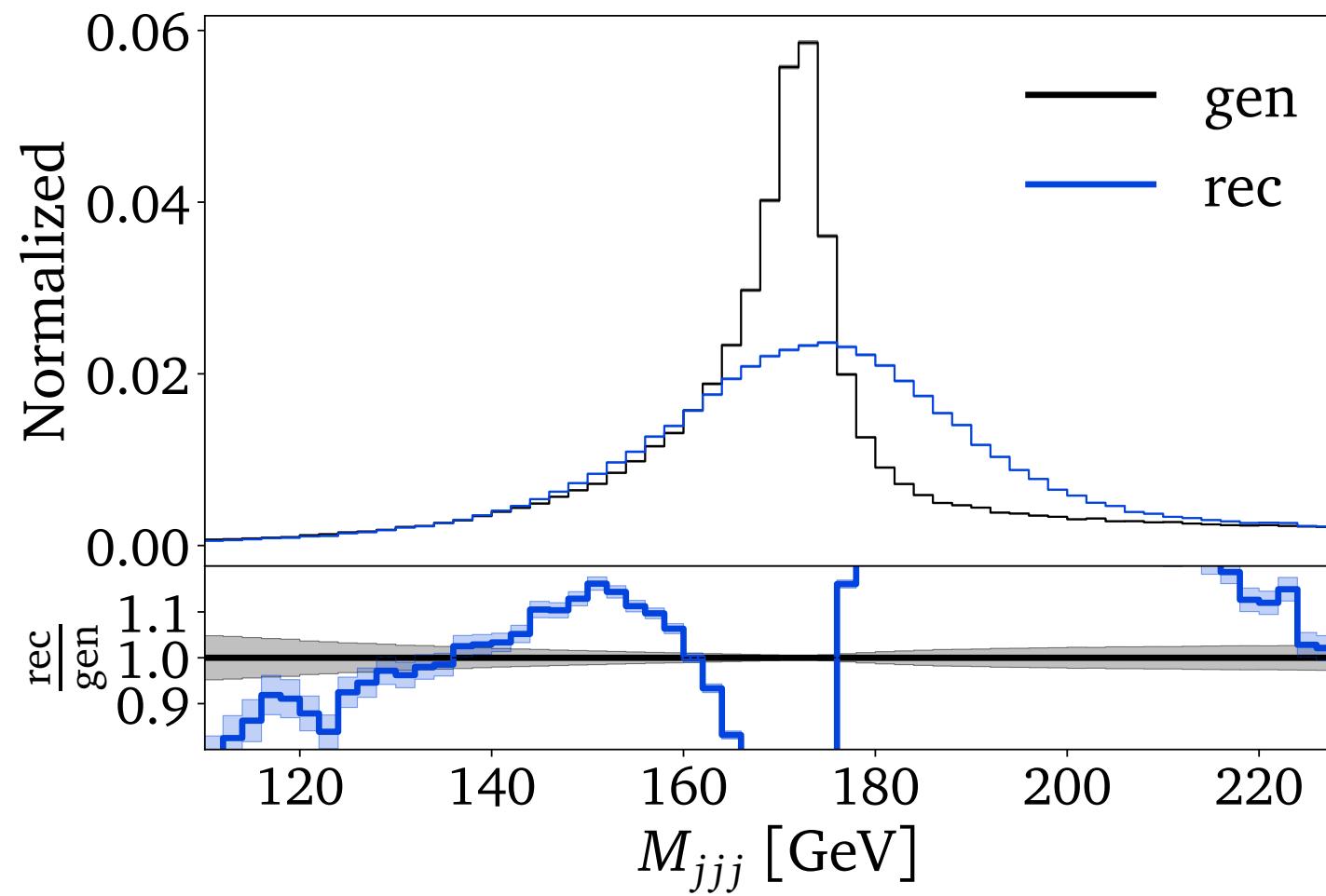


2. Combinatorics

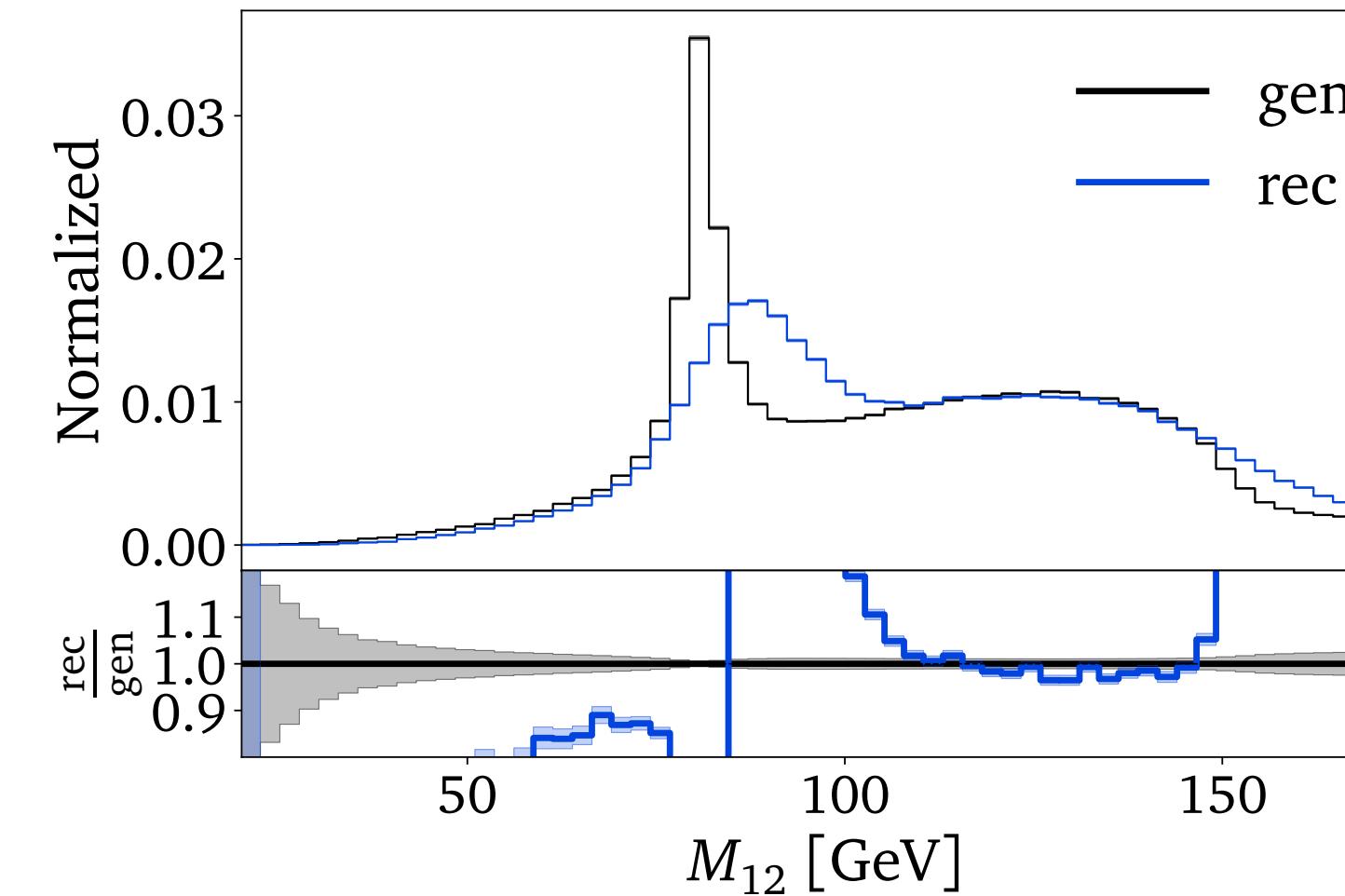


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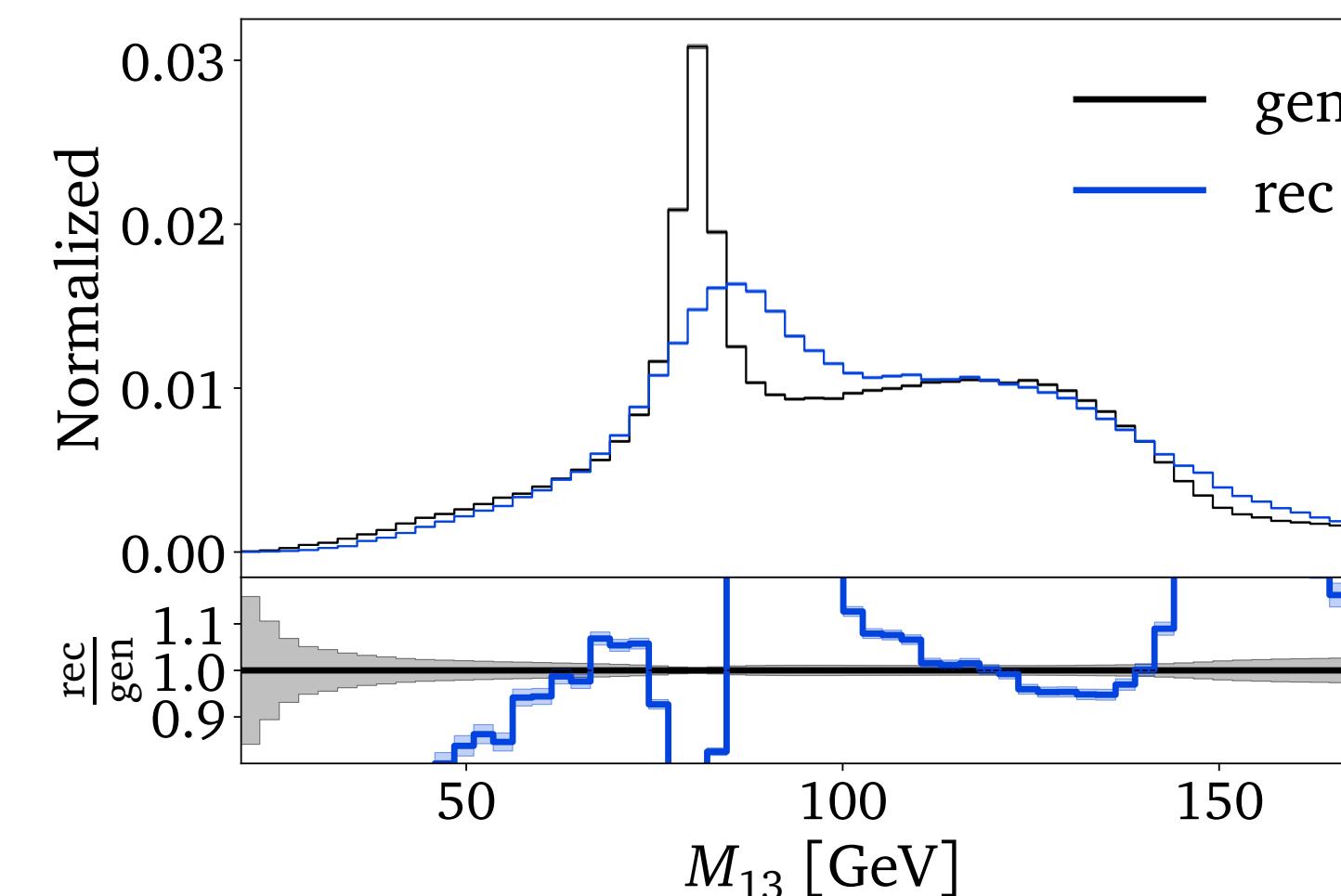
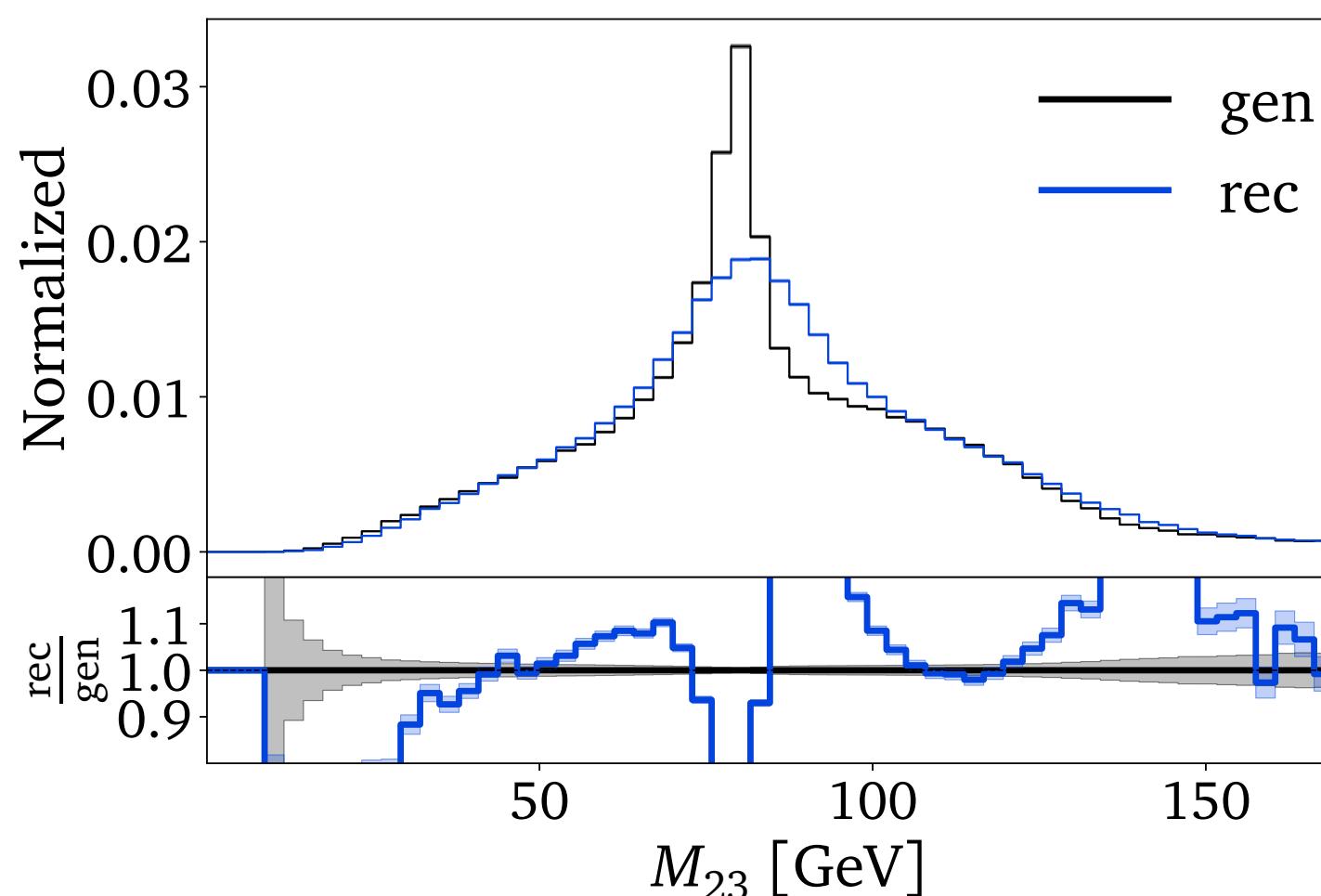
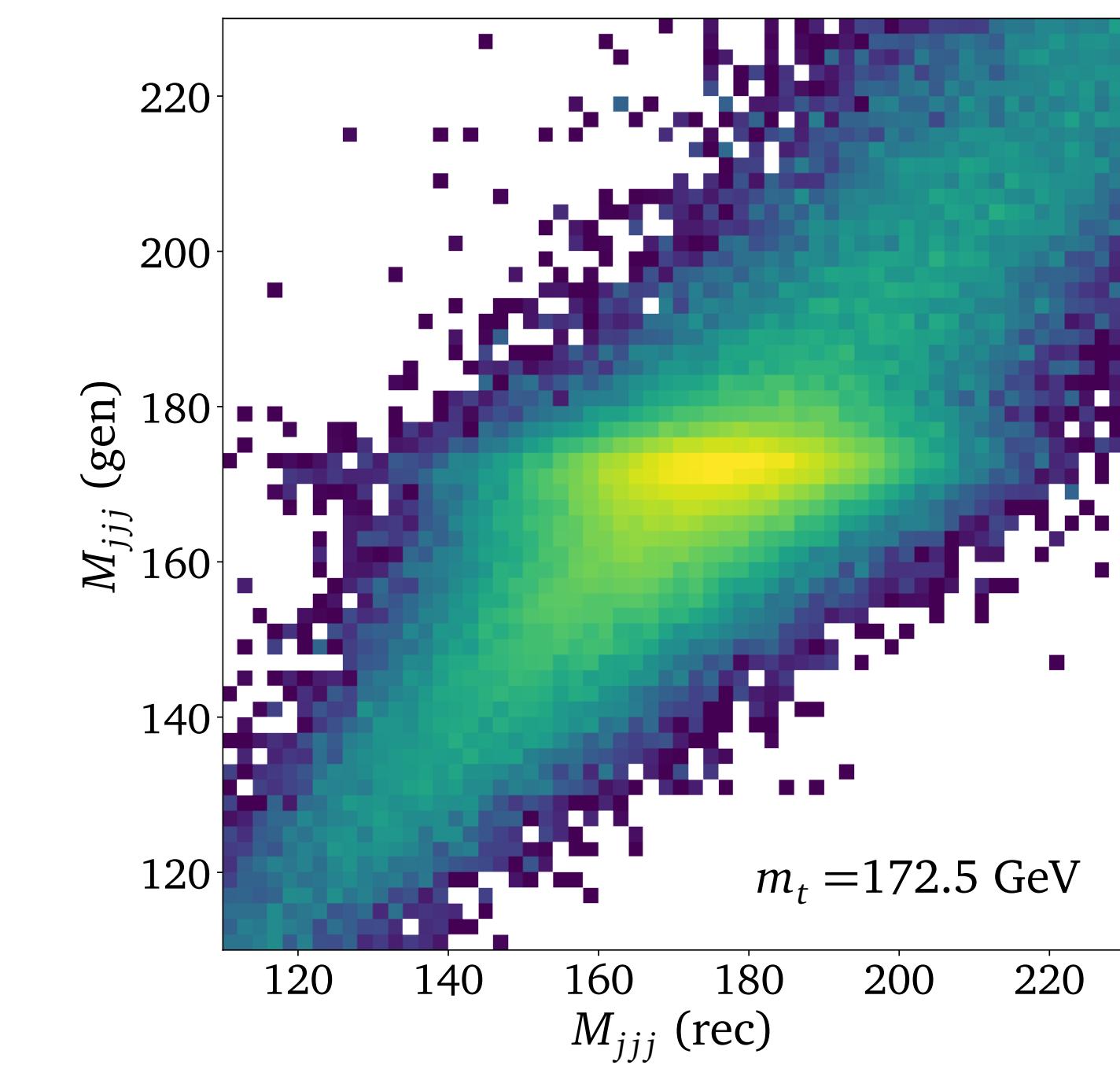
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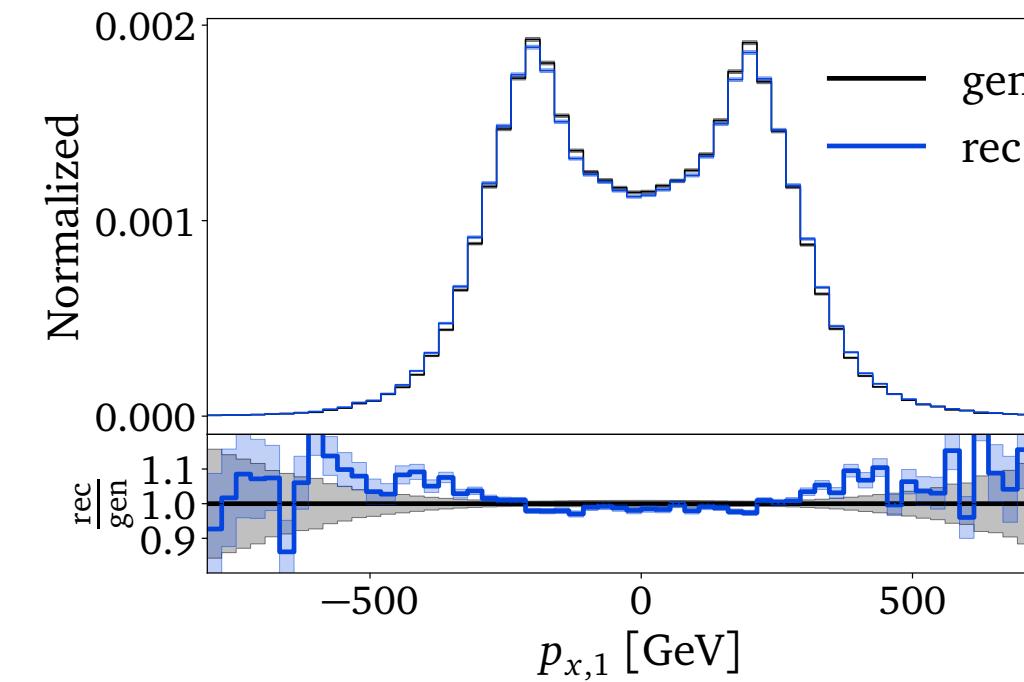
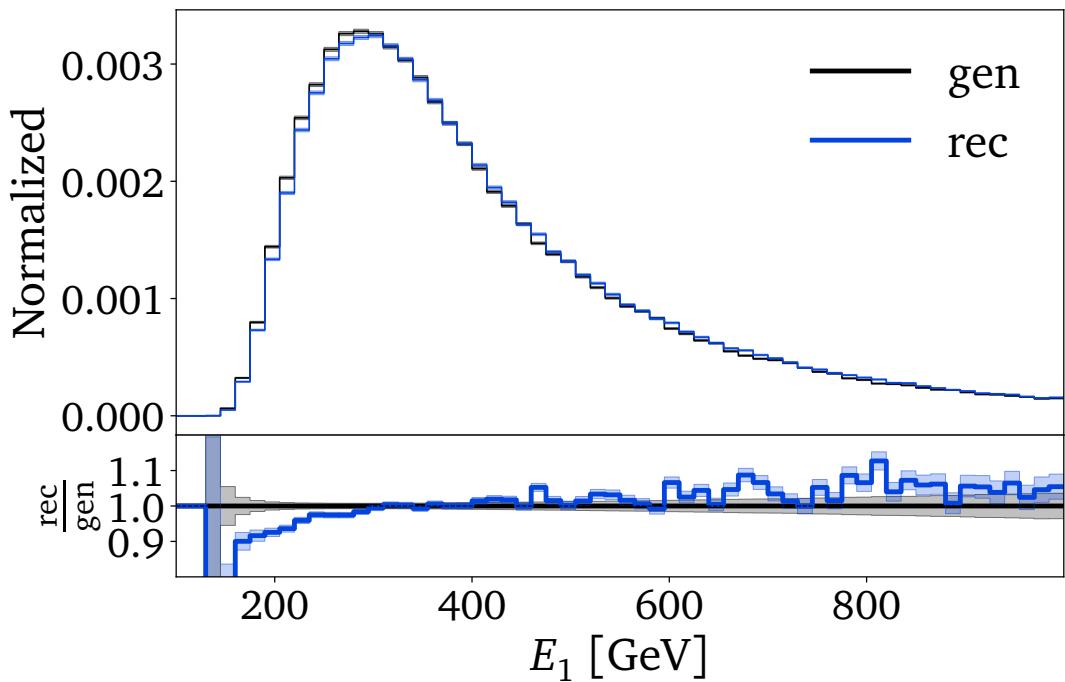


3. Detector Smearing



Choosing the right parametrization

Reco and gen level difference not significantly visible, only in correlations



1. The naive

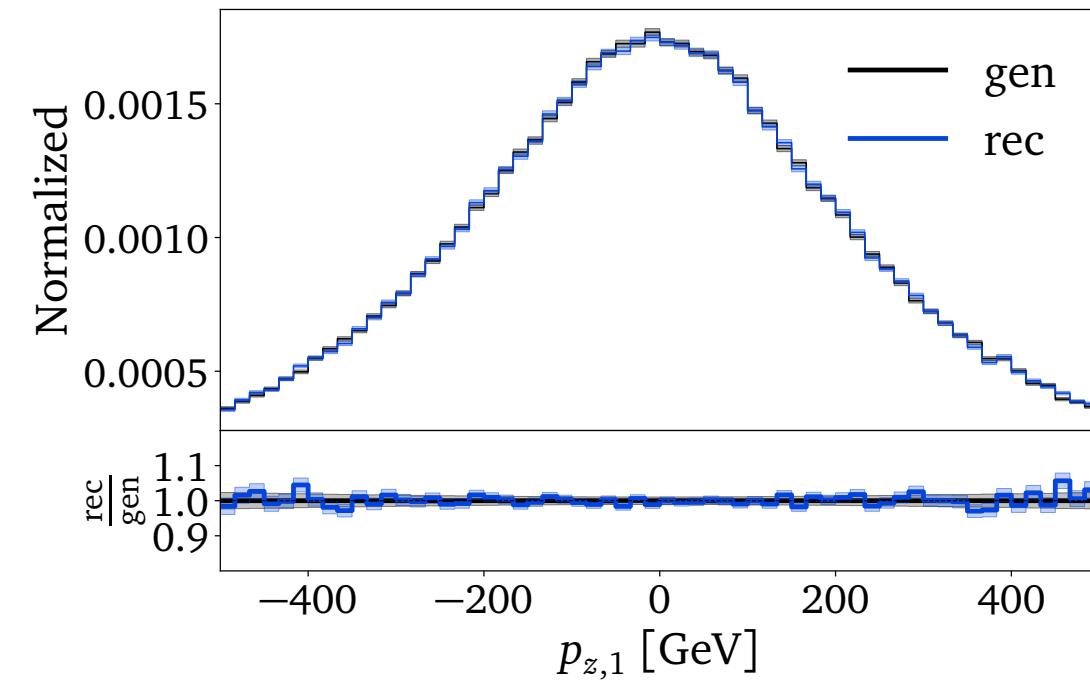
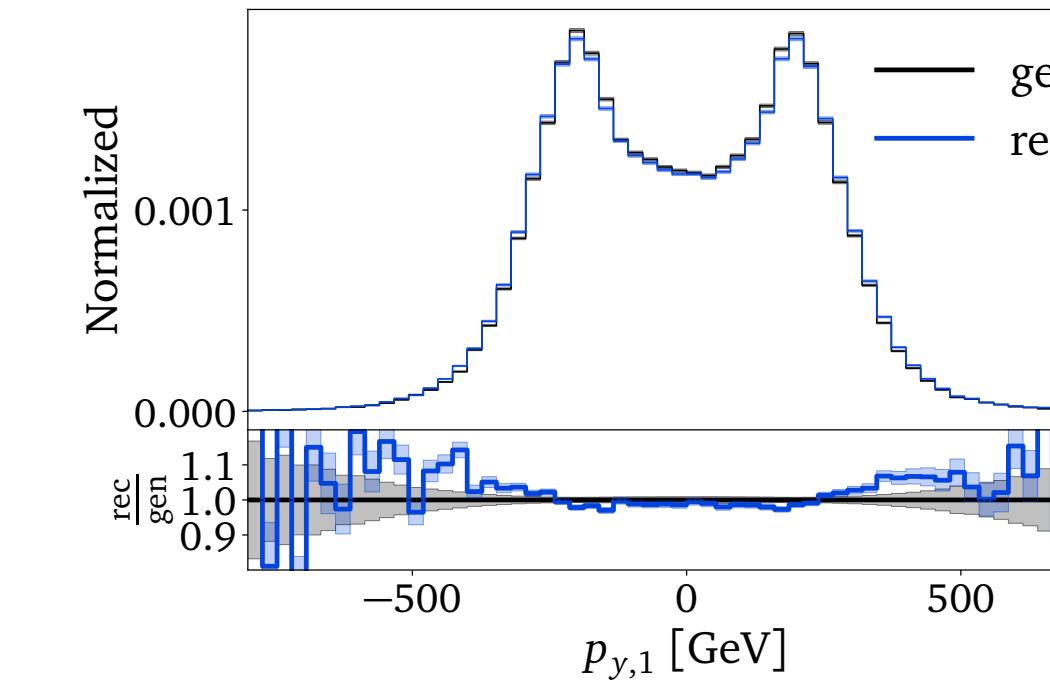
$$\left. \begin{array}{l} p_1 = (E_1, \vec{p}_1) \\ p_2 = (E_2, \vec{p}_2) \\ p_3 = (E_3, \vec{p}_3) \end{array} \right\}$$

$$M_{jjj}(p_1, p_2, p_3)$$

$$M_{ij}(p_i, p_j)$$

12 dimensional correlation

8 dimensional correlation + combinatorics difficult



Choosing the right parametrization

2. The less naive

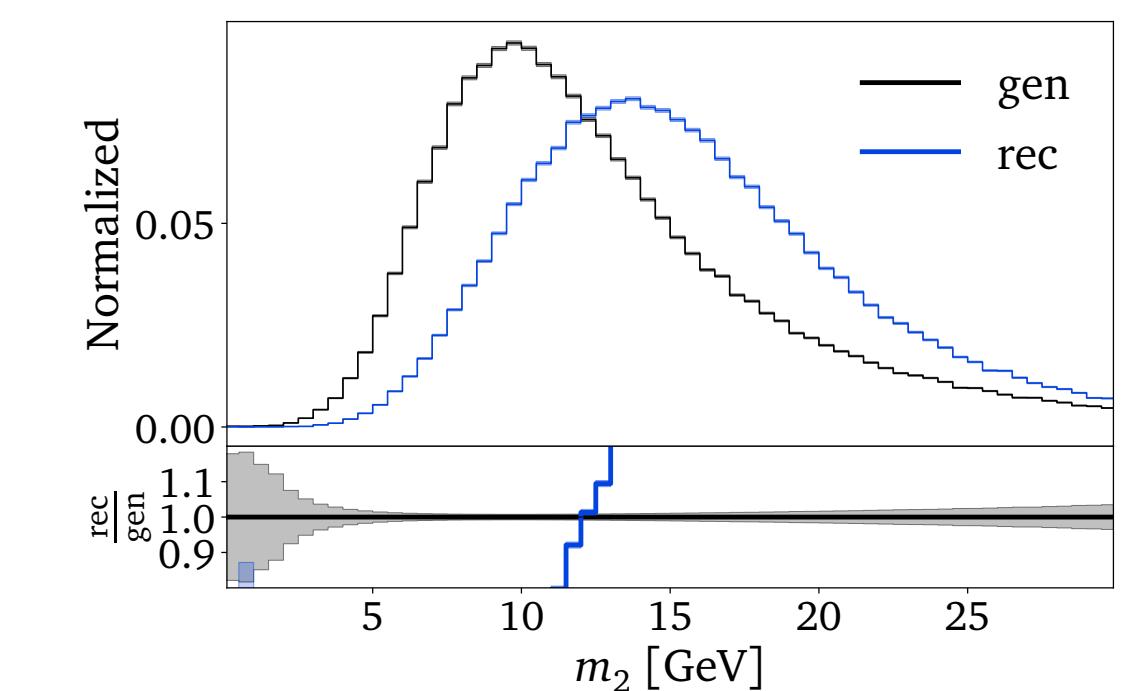
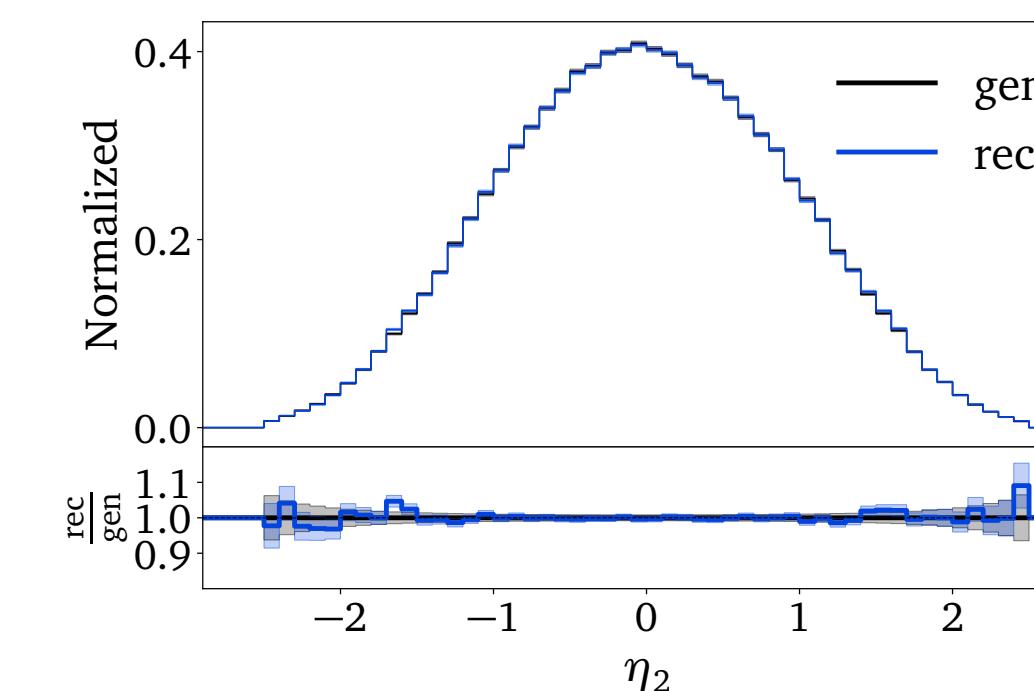
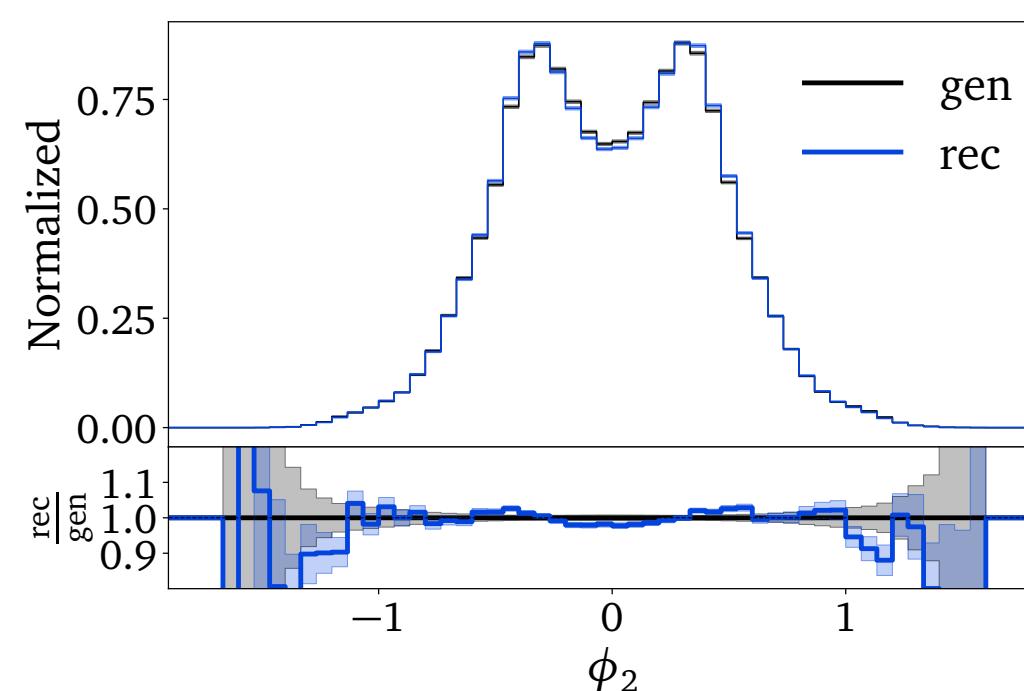
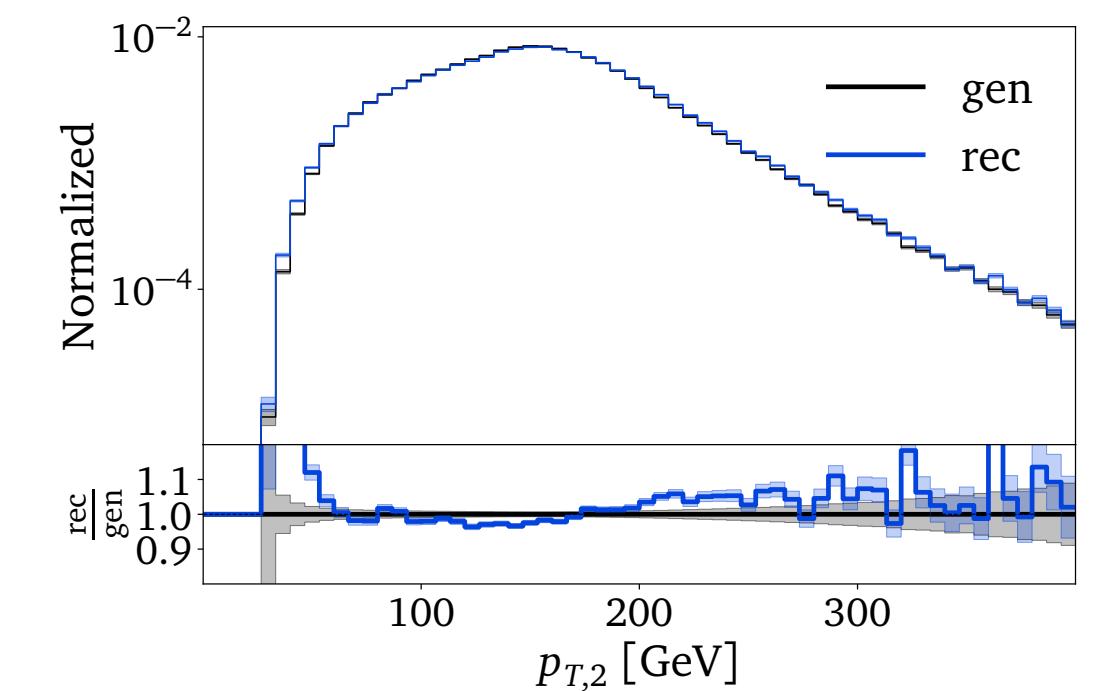
$$\left. \begin{array}{l} p_1 = (p_{T,1}, \phi_1, \eta_1, m_1) \\ p_2 = (p_{T,2}, \phi_2, \eta_2, m_2) \\ p_3 = (p_{T,3}, \phi_3, \eta_3, m_3) \end{array} \right\}$$

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Reco and gen level difference visible

Choosing the right parametrization

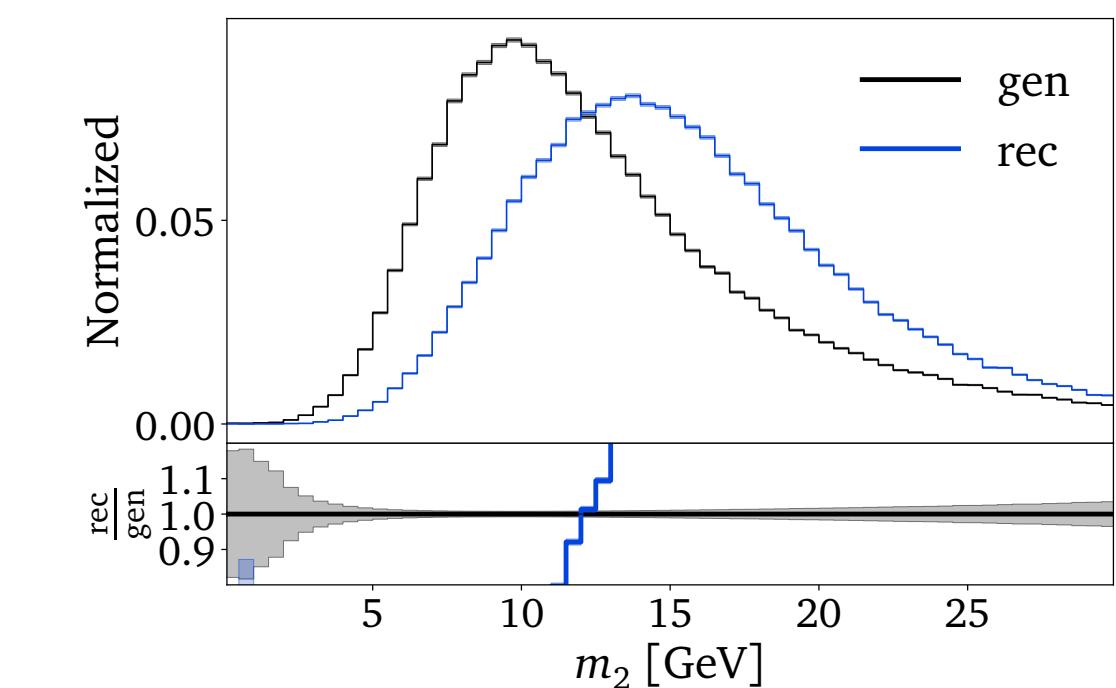
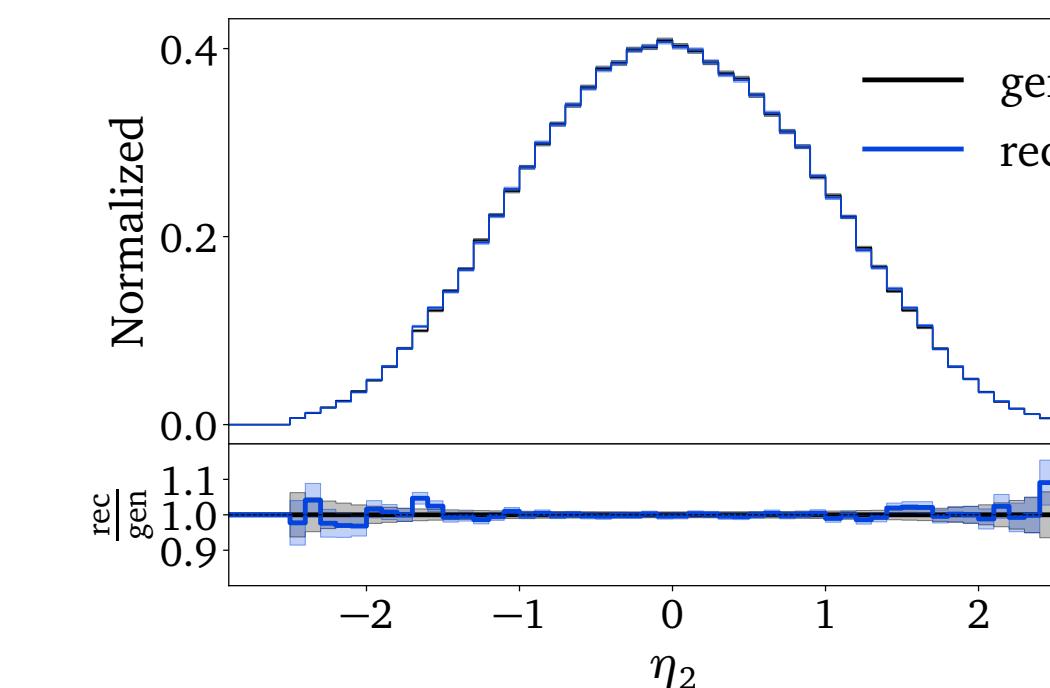
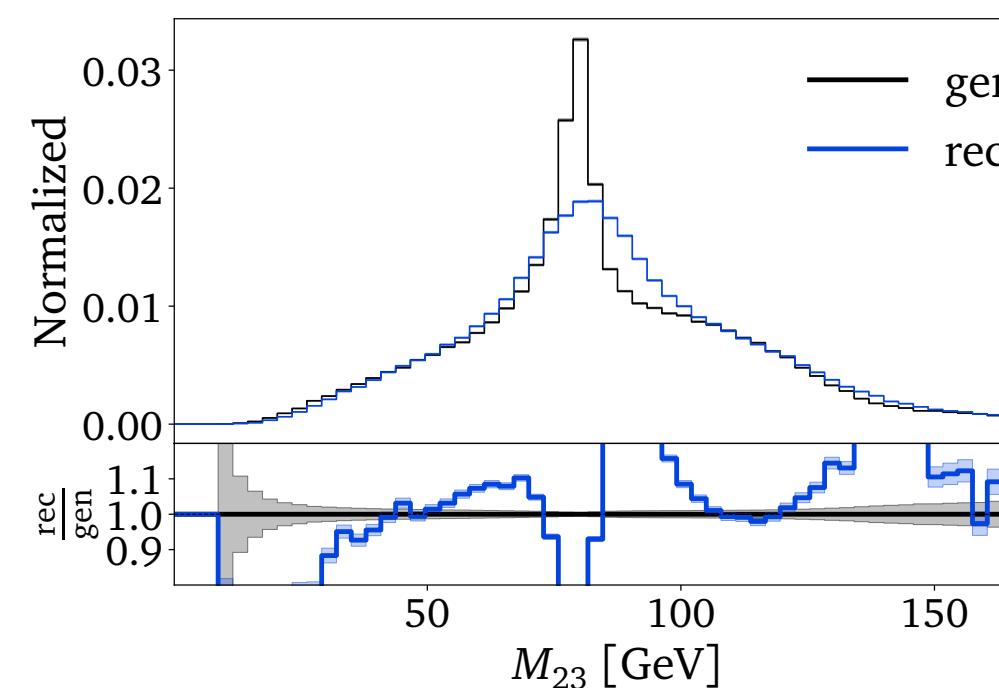
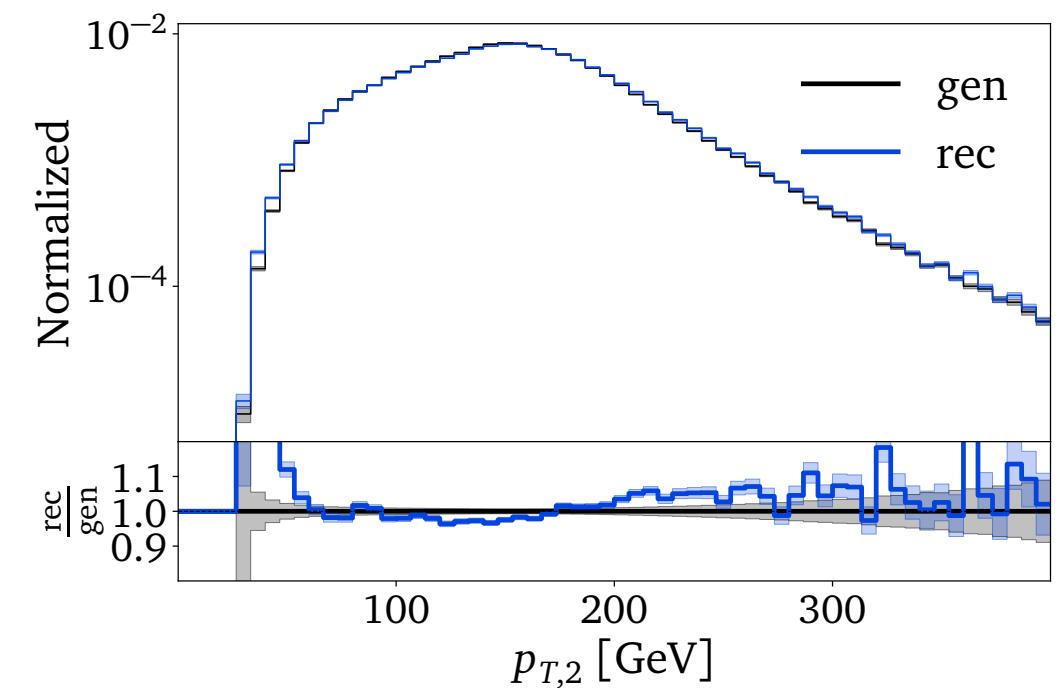
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$$M_{jjj}^2 = \sum_{ij, i>j} M_{ij}^2 - \sum_i m_i^2$$

6 dimensional correlation

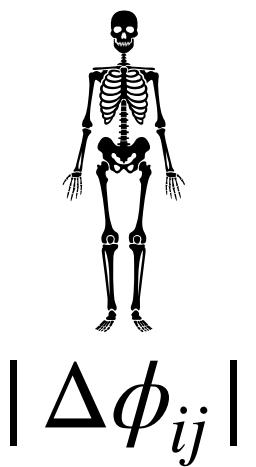
Direct input +
combinatorics simple



Reco and gen level difference
visible

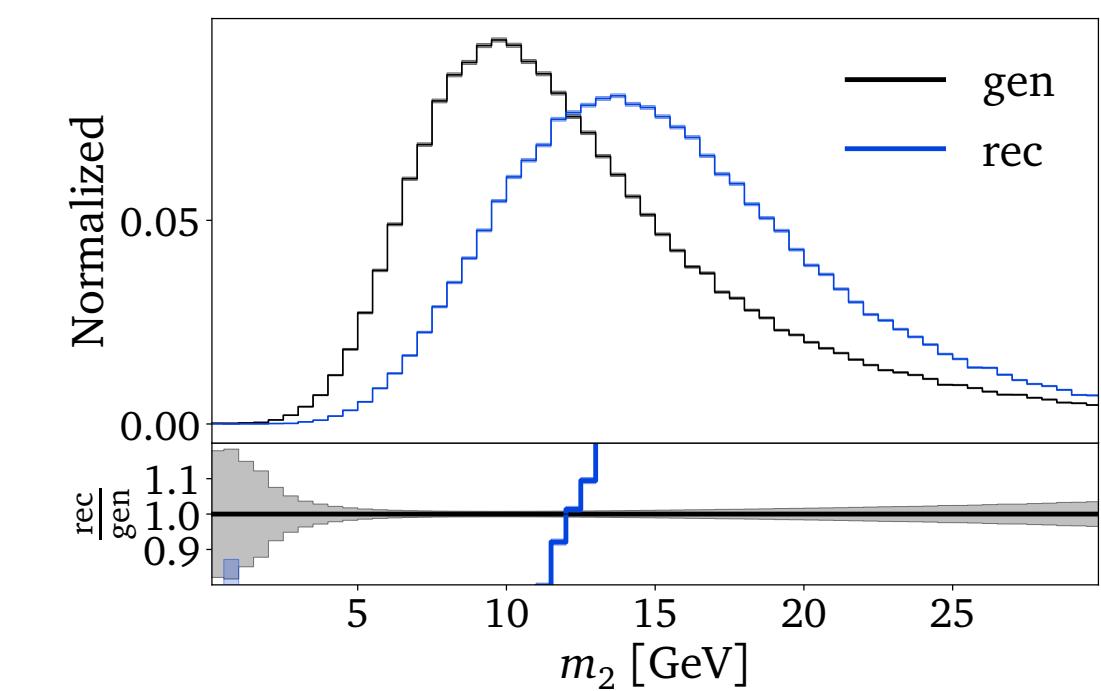
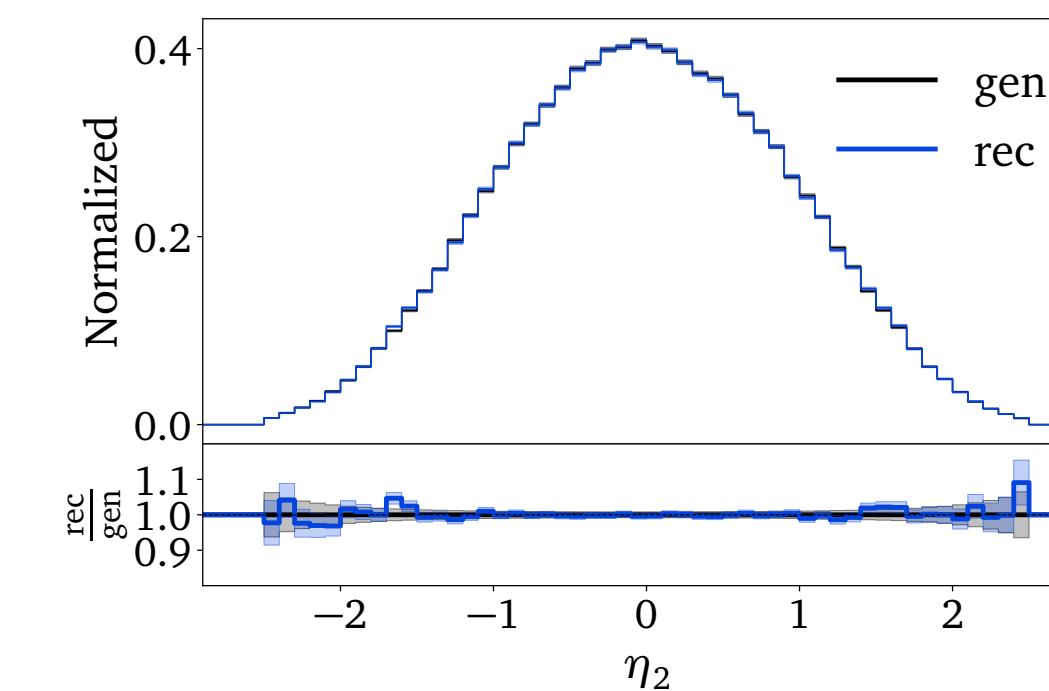
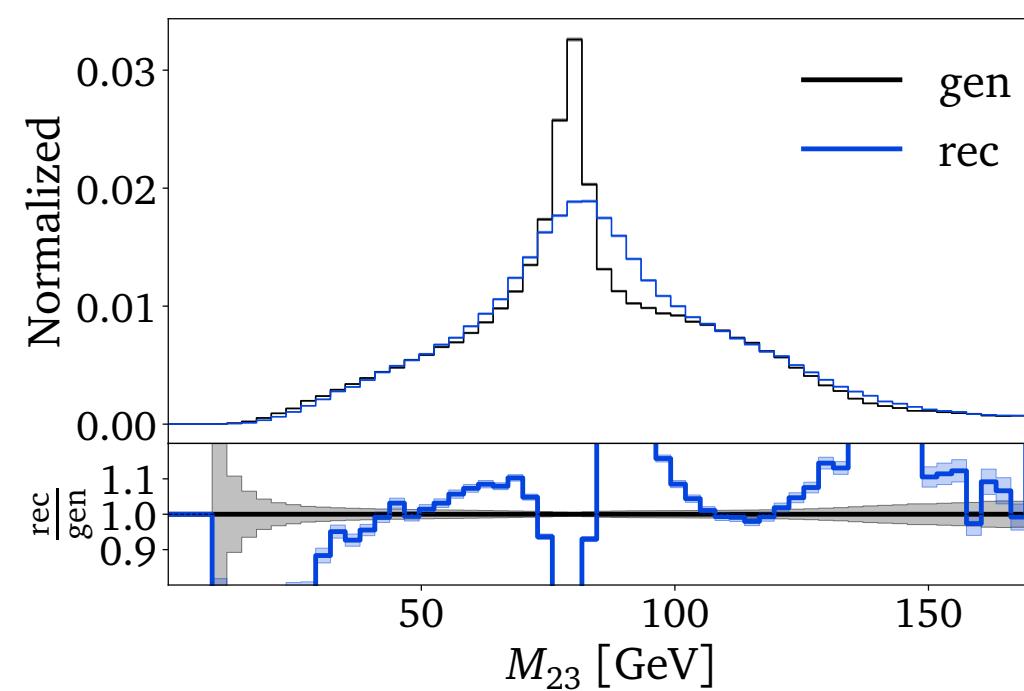
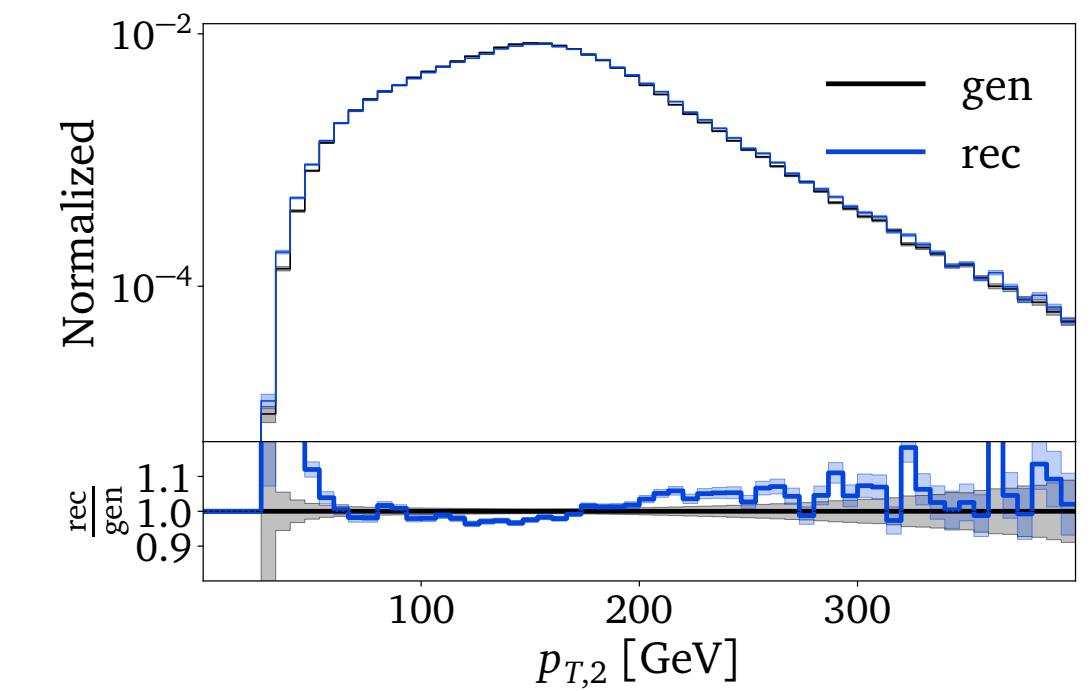
Choosing the right parametrization

3. The least naive



$|\Delta\phi_{ij}|$

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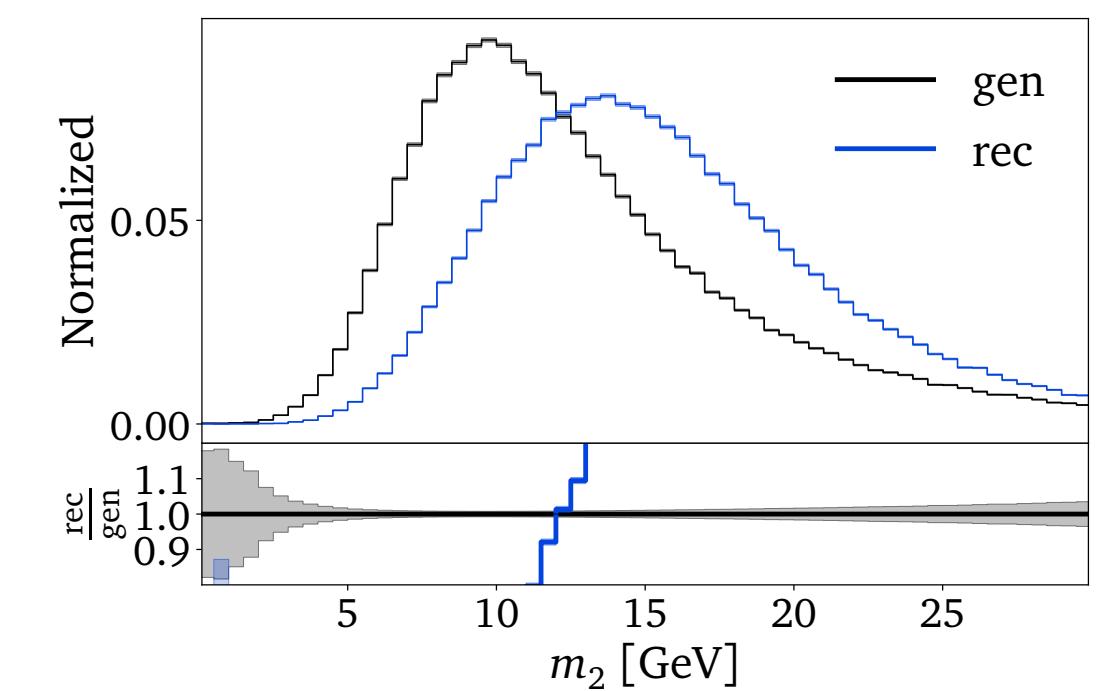
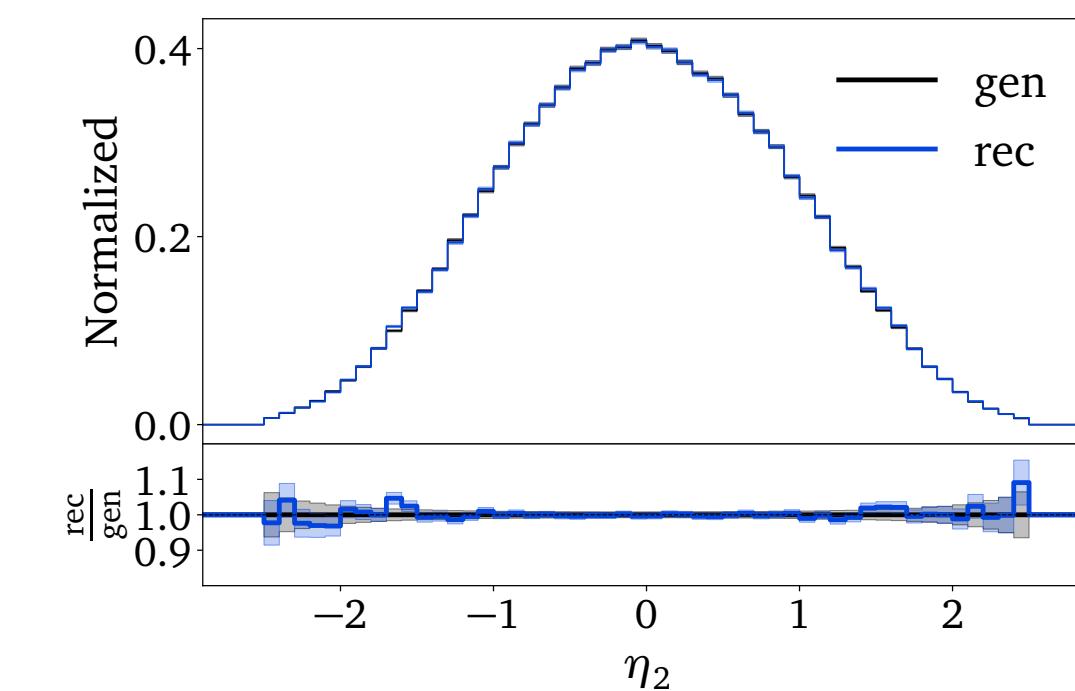
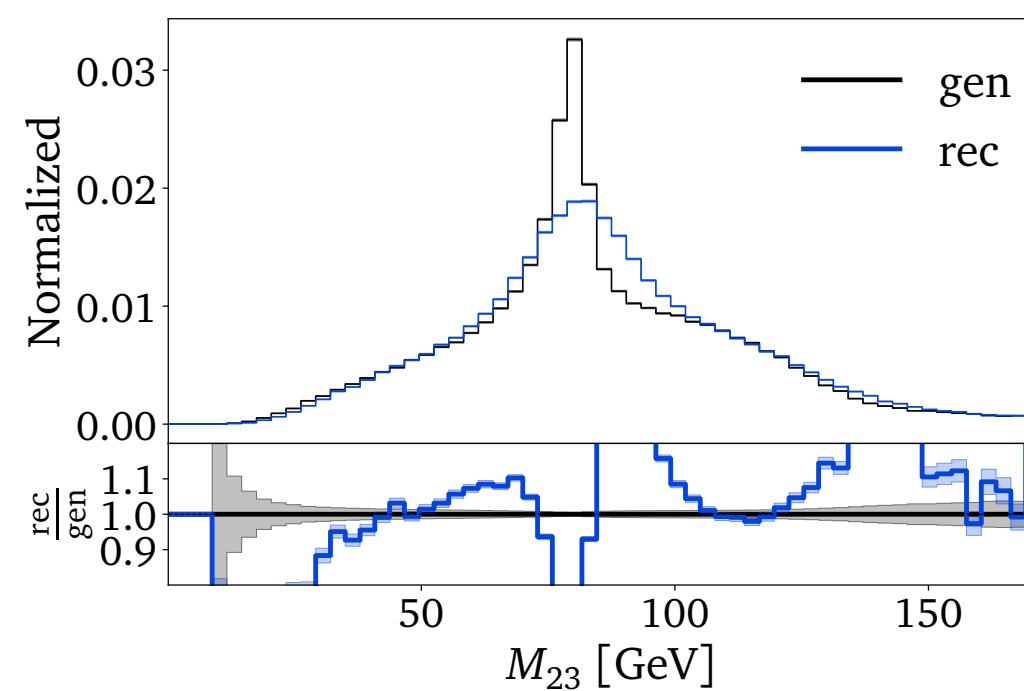
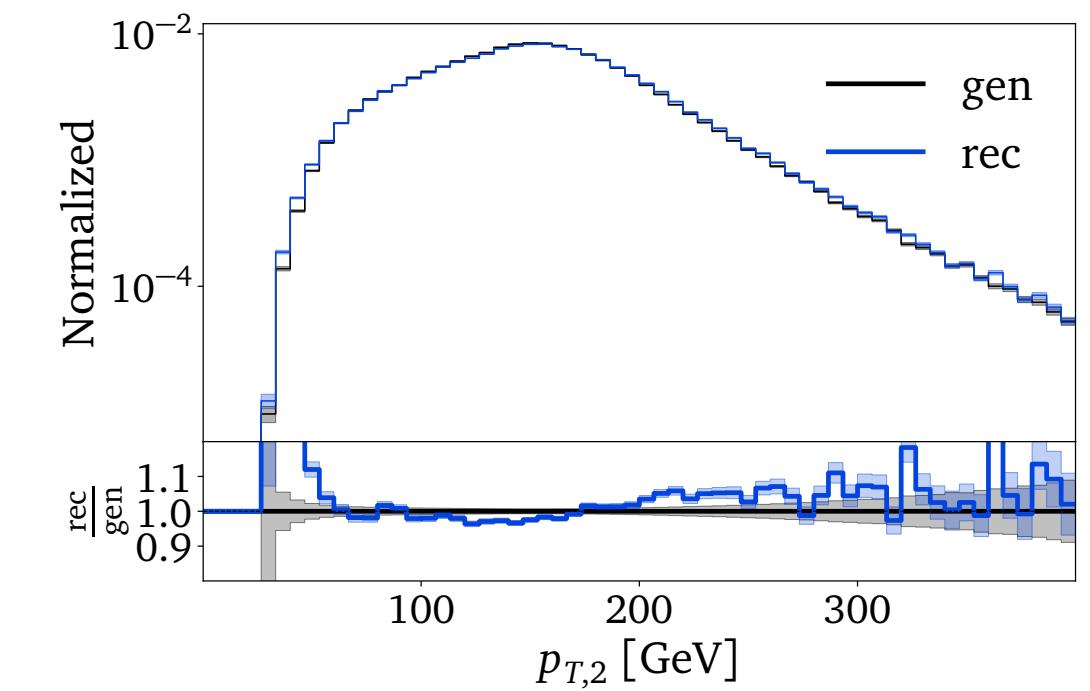


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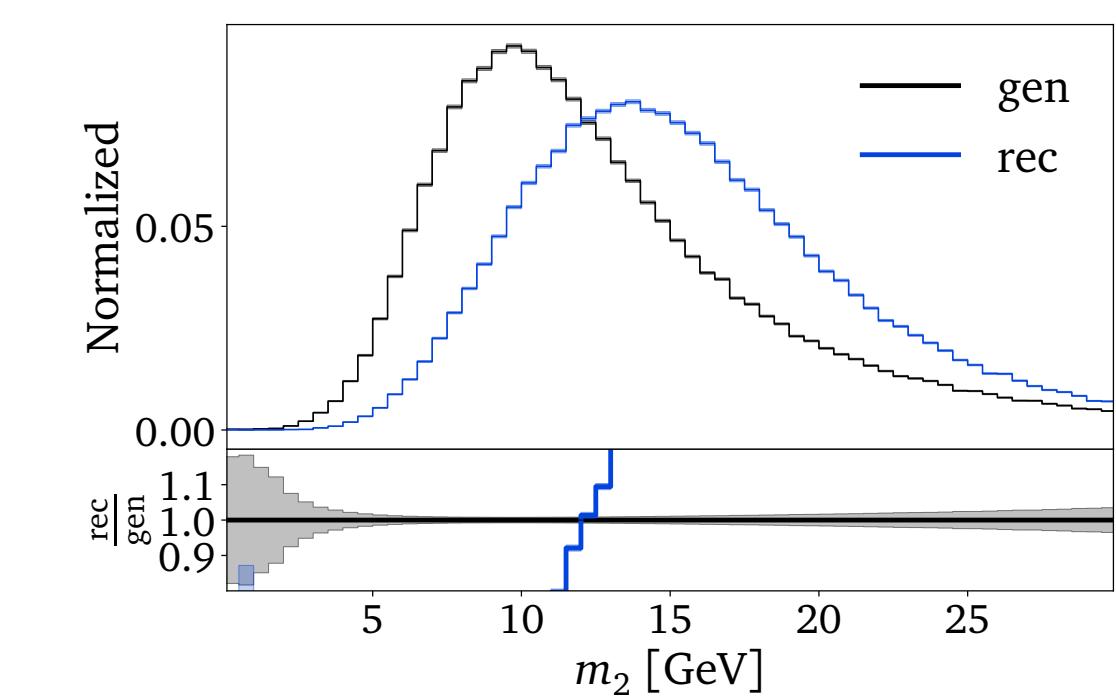
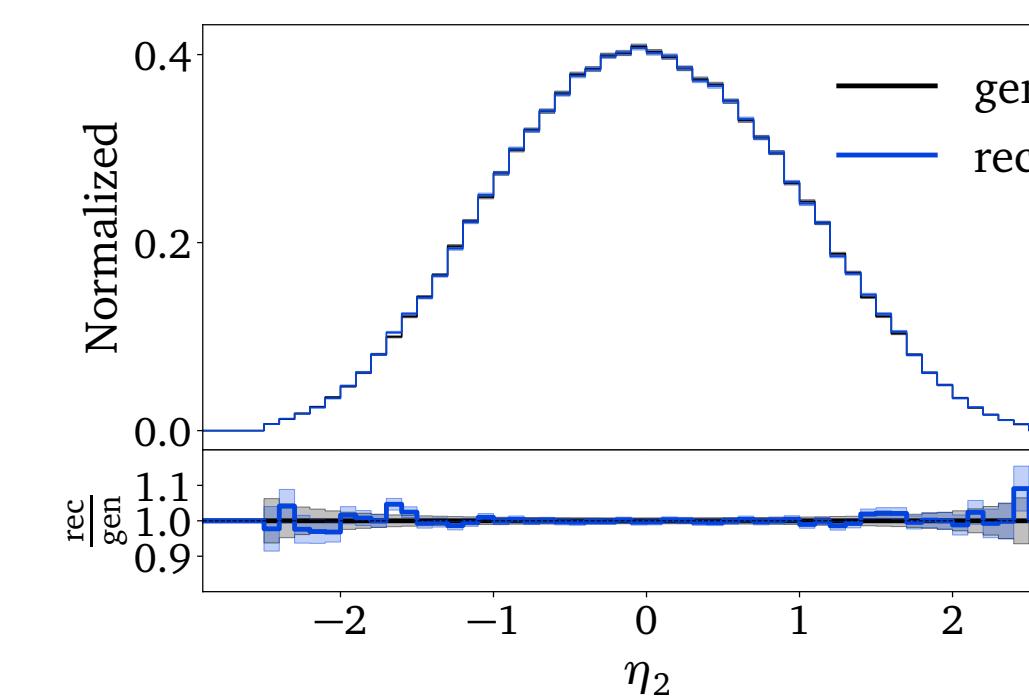
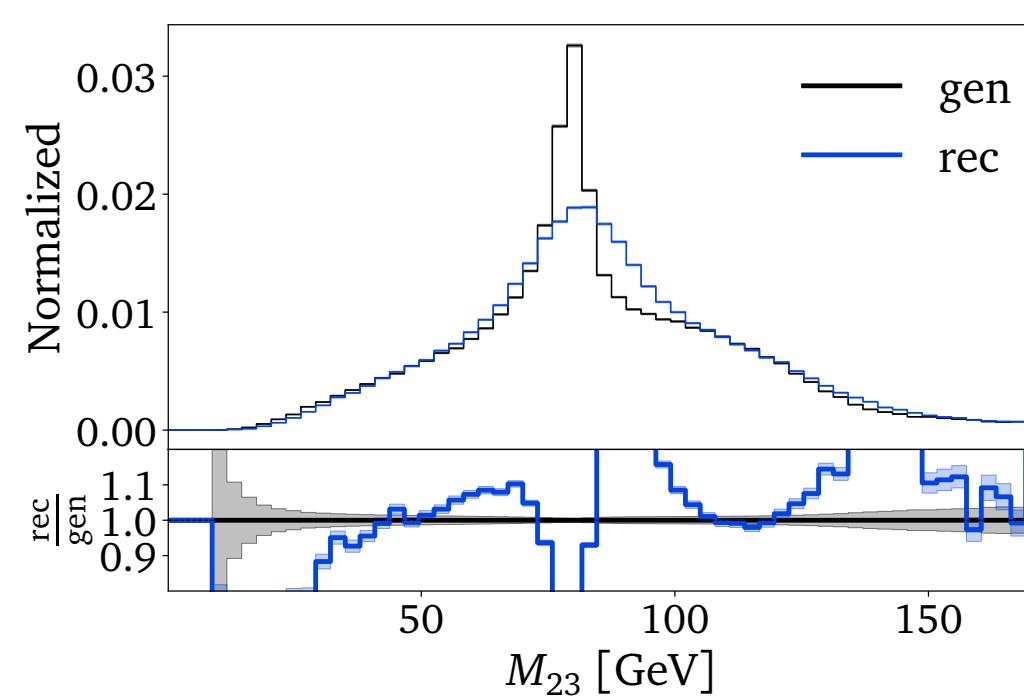
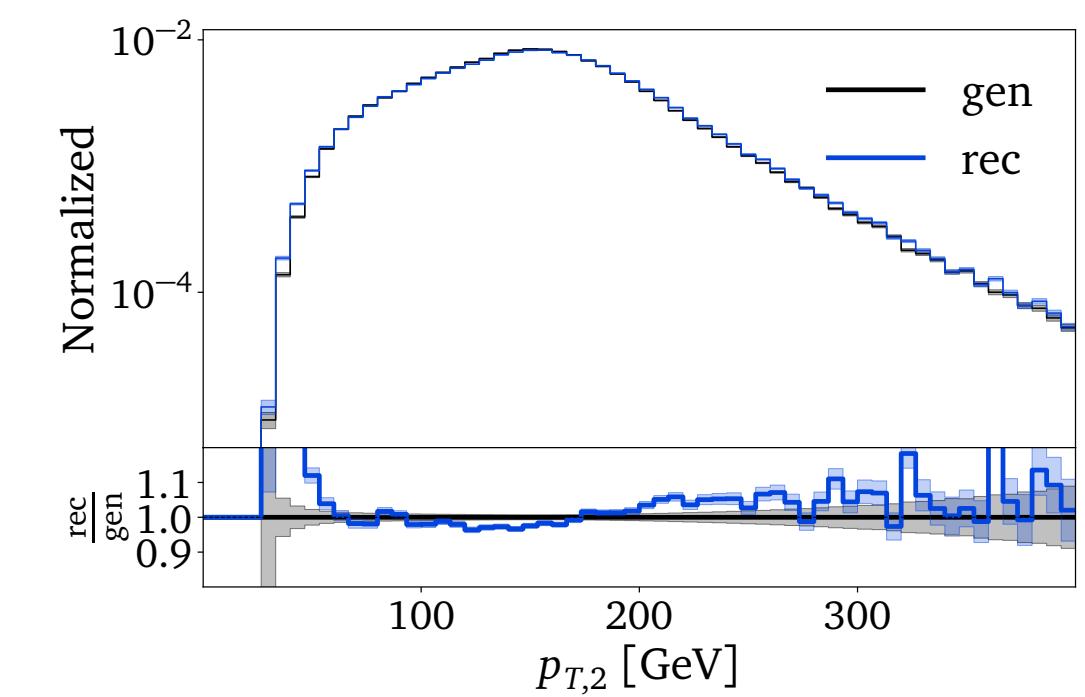
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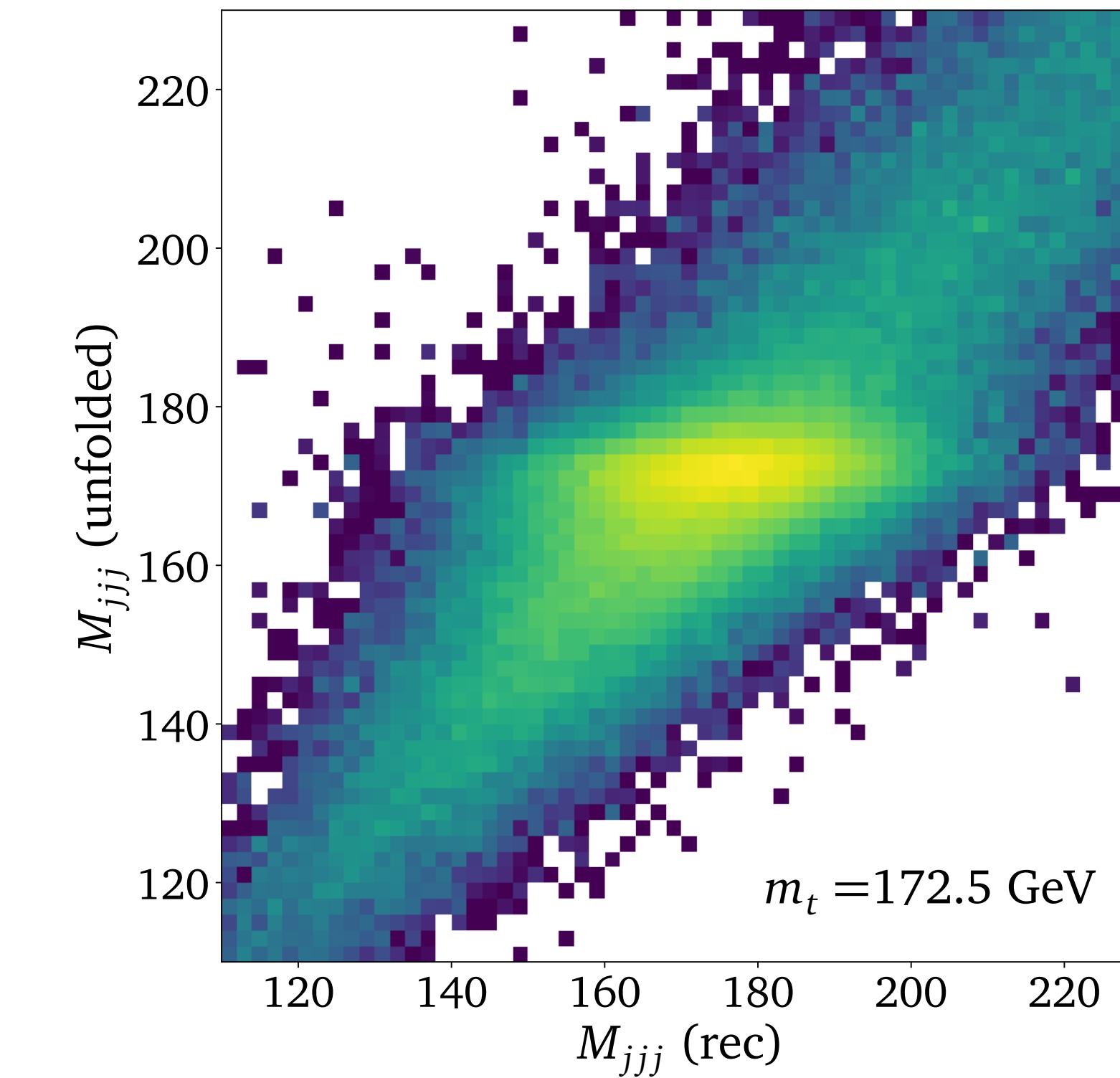
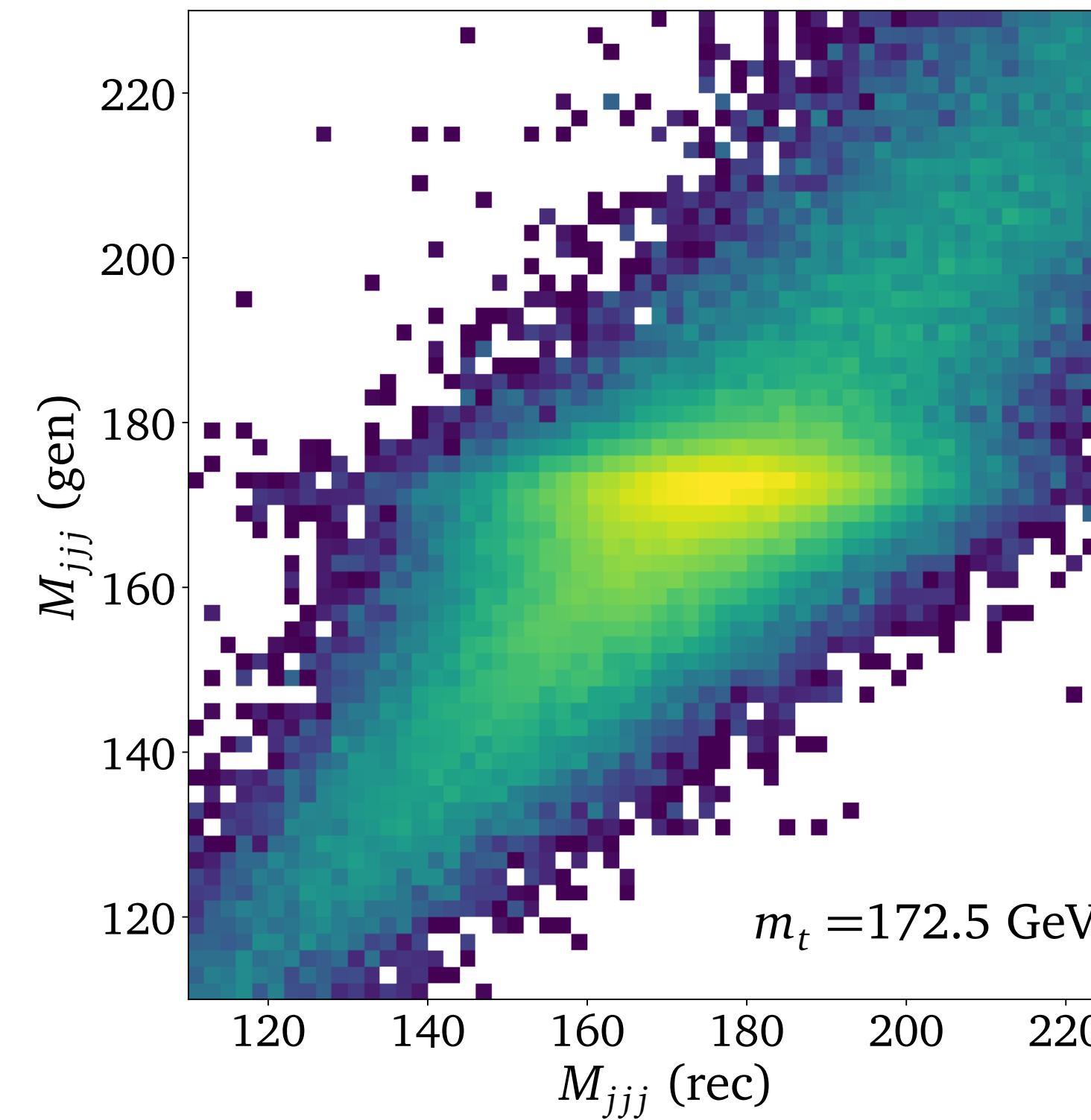
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$$M_{jjj}^2 = \sum_{ij, i>j} M_{ij}^2 - \sum_i m_i^2$$

For mass measurement, we only use 6 dimensional subset of phase space to increase network performance



Model-Dependence



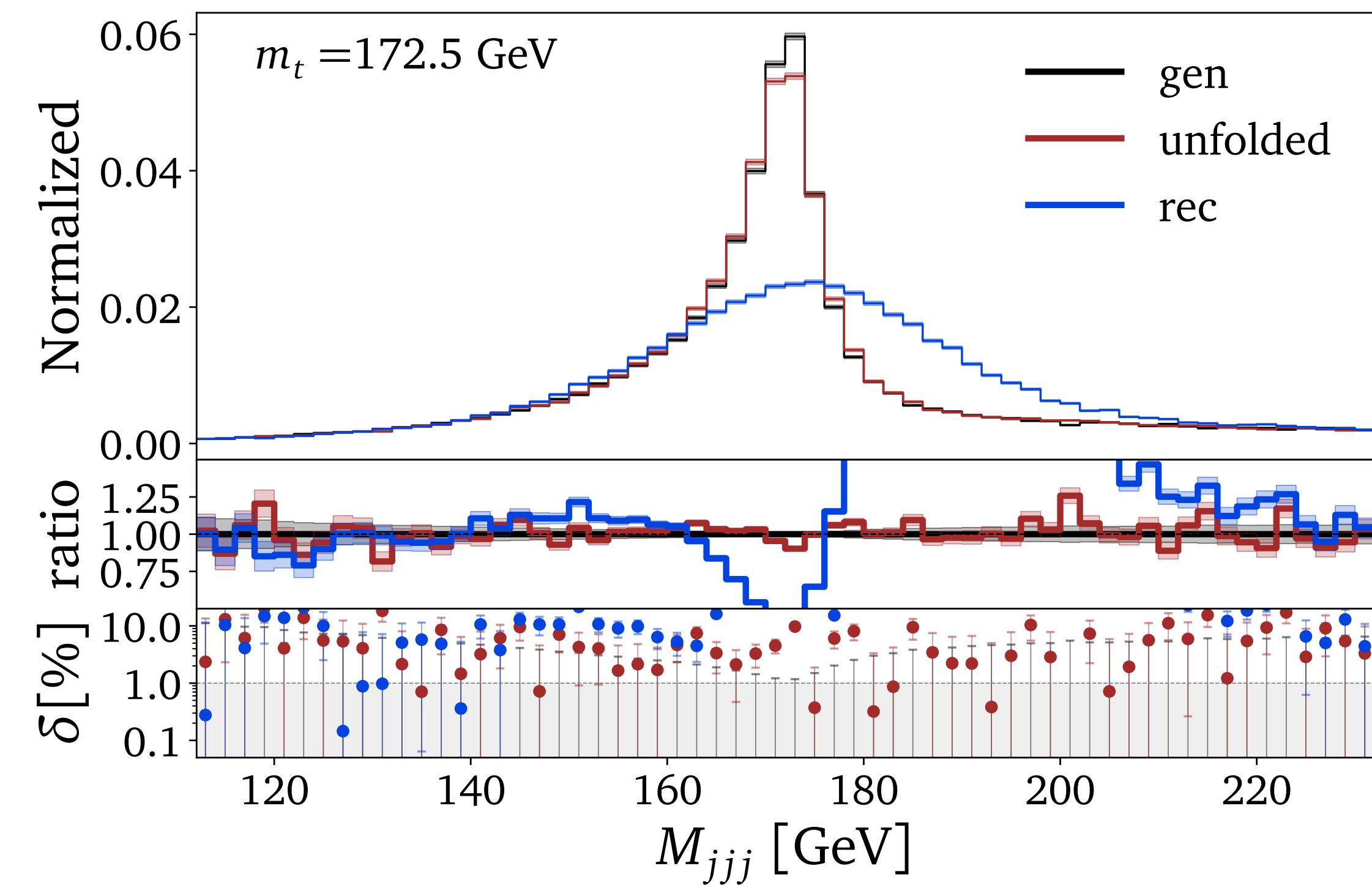
Correct migration learned?

Model-Dependence?

Train with full CMS simulation with
 $m_t = 172.5 \text{ GeV}$

Unfolded distribution of triple jet mass within
 $\mathcal{O}(1\%)$ of truth gen level

BUT: Test data also simulation with
 $m_t = 172.5 \text{ GeV}$



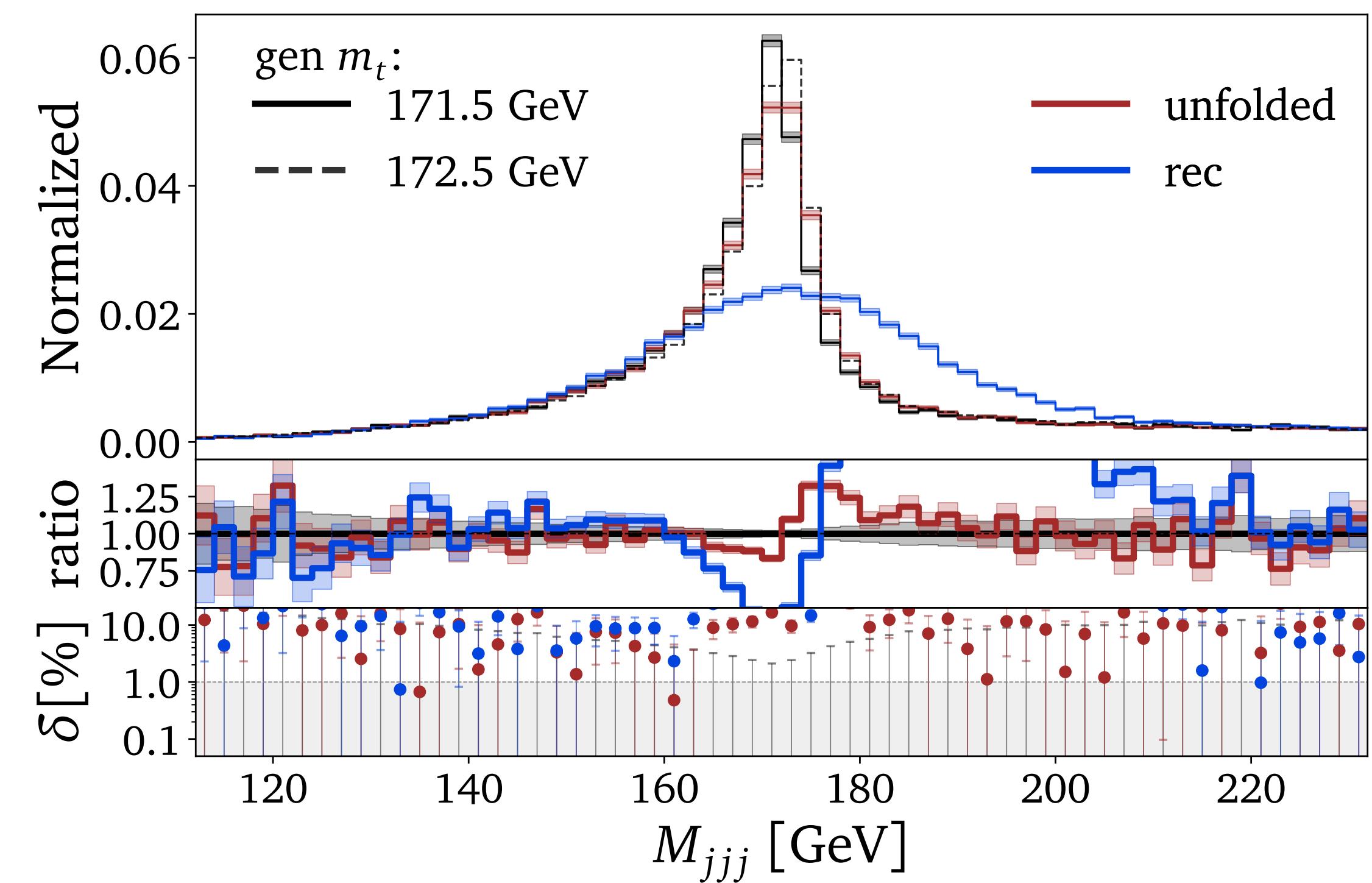
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For pseudo-data with different top masses :
Algorithm falls back to prior ($m_t = 172.5$ GeV)



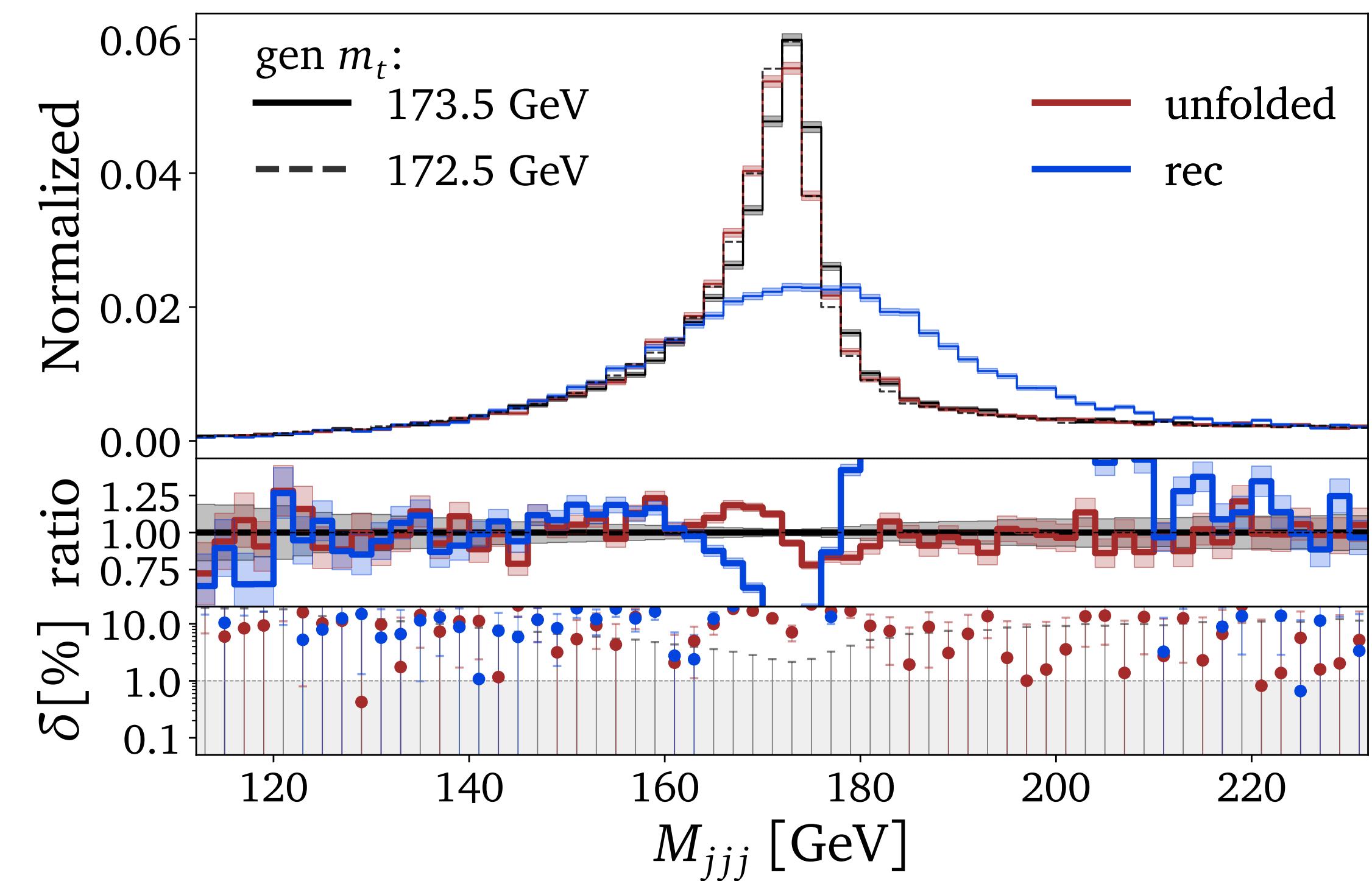
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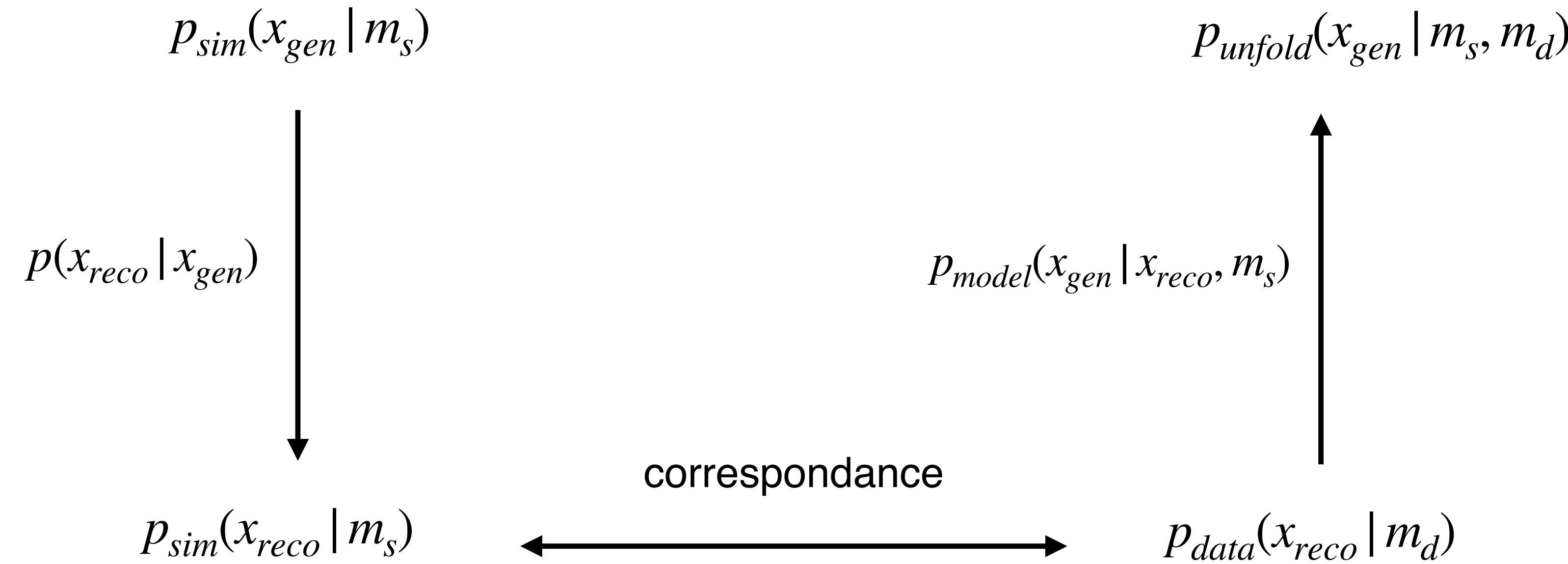
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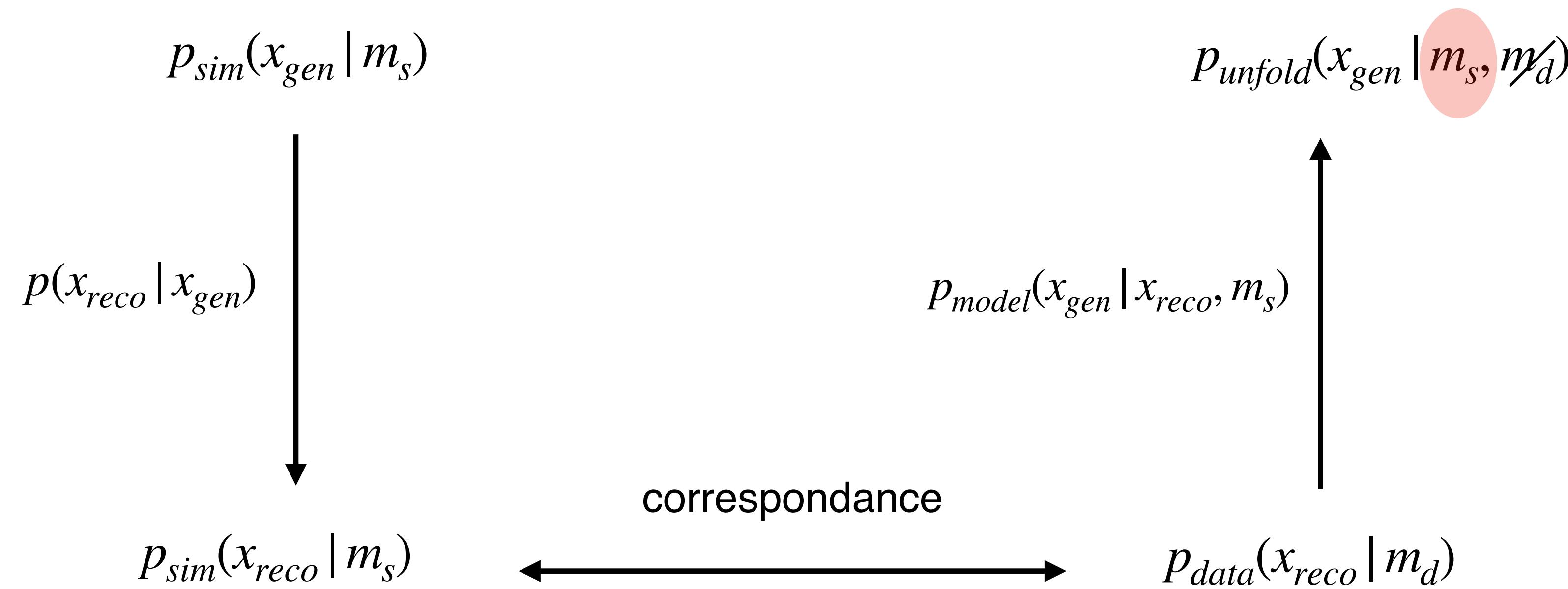
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Removing Model-Dependence

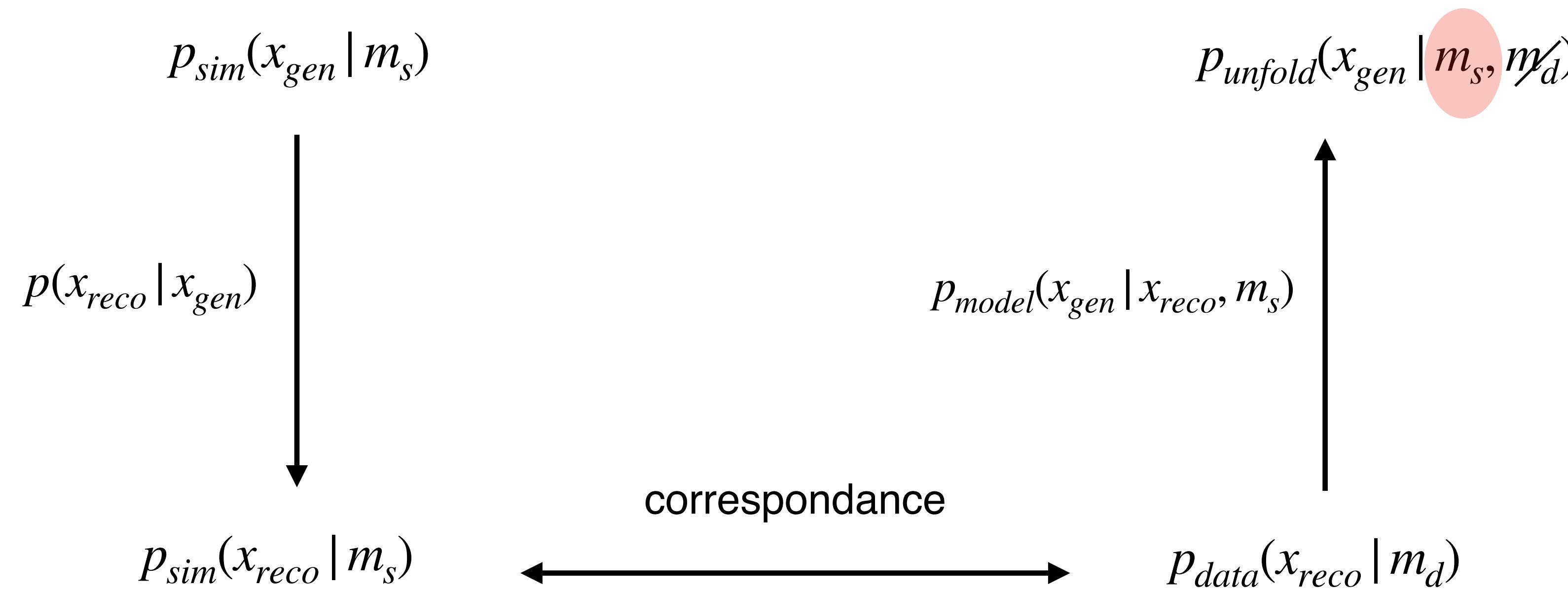


Removing Model-Dependence



→ **Solution: Strengthen m_d dependence, but how?**

Removing Model-Dependence



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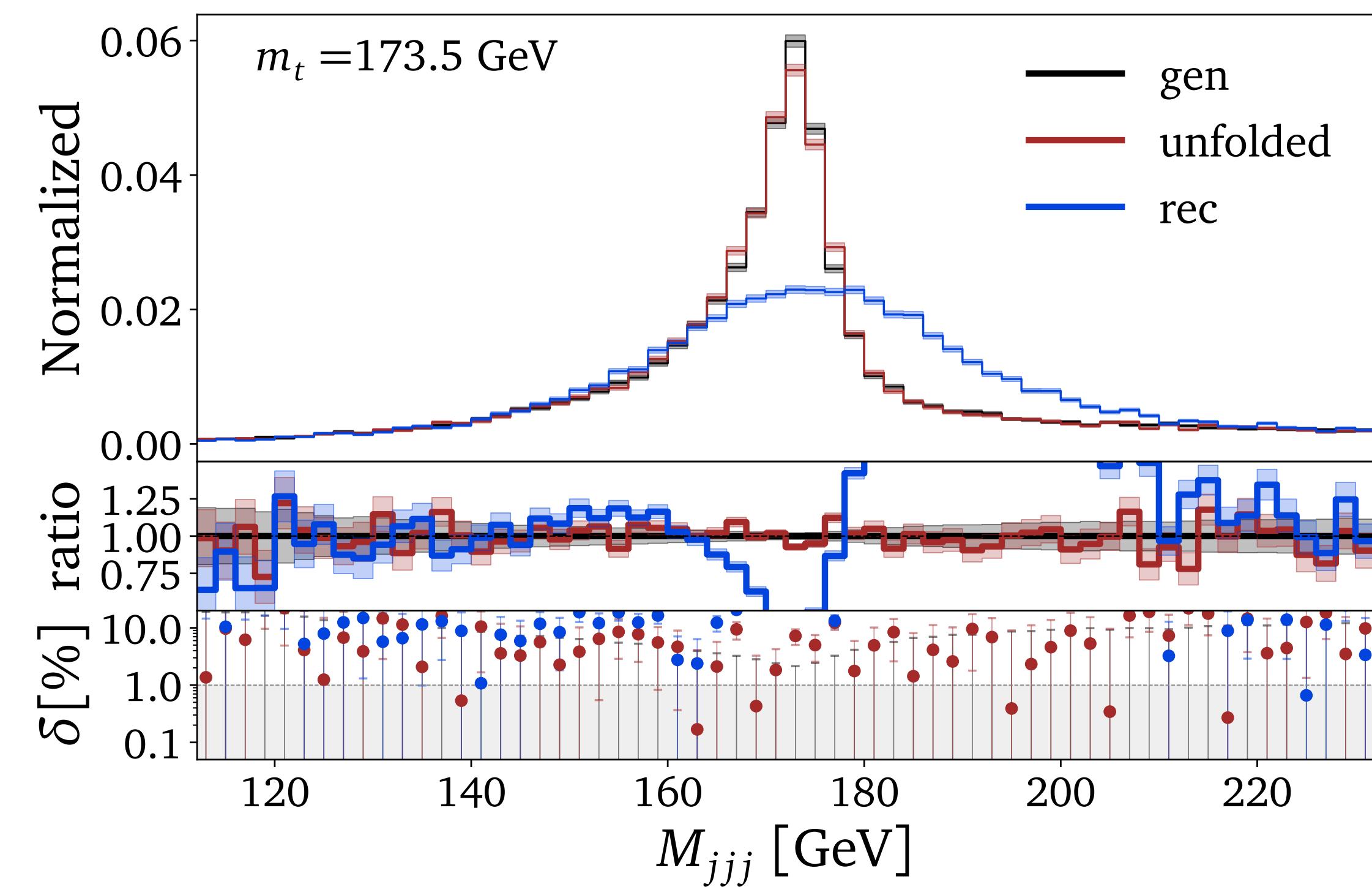
1. Augment training data with simulation from different top masses
2. Estimate batch-wise $m_d \approx \text{weighted-median}(M_{jjj}^{batch})$ on reco level

Removing Model-Dependence!

Train with full CMS simulation with
 $m_t = [172.5 \text{ GeV}, 169.5 \text{ GeV}, 175.5 \text{ GeV}]$

Test by unfolding simulation with
 $m_t = 171.5 \text{ GeV} \& 173.5 \text{ GeV}$

Unfolded distribution of triple jet mass within
 $\mathcal{O}(1\%)$ of truth gen level **without bias**



Removing Model-Dependence!

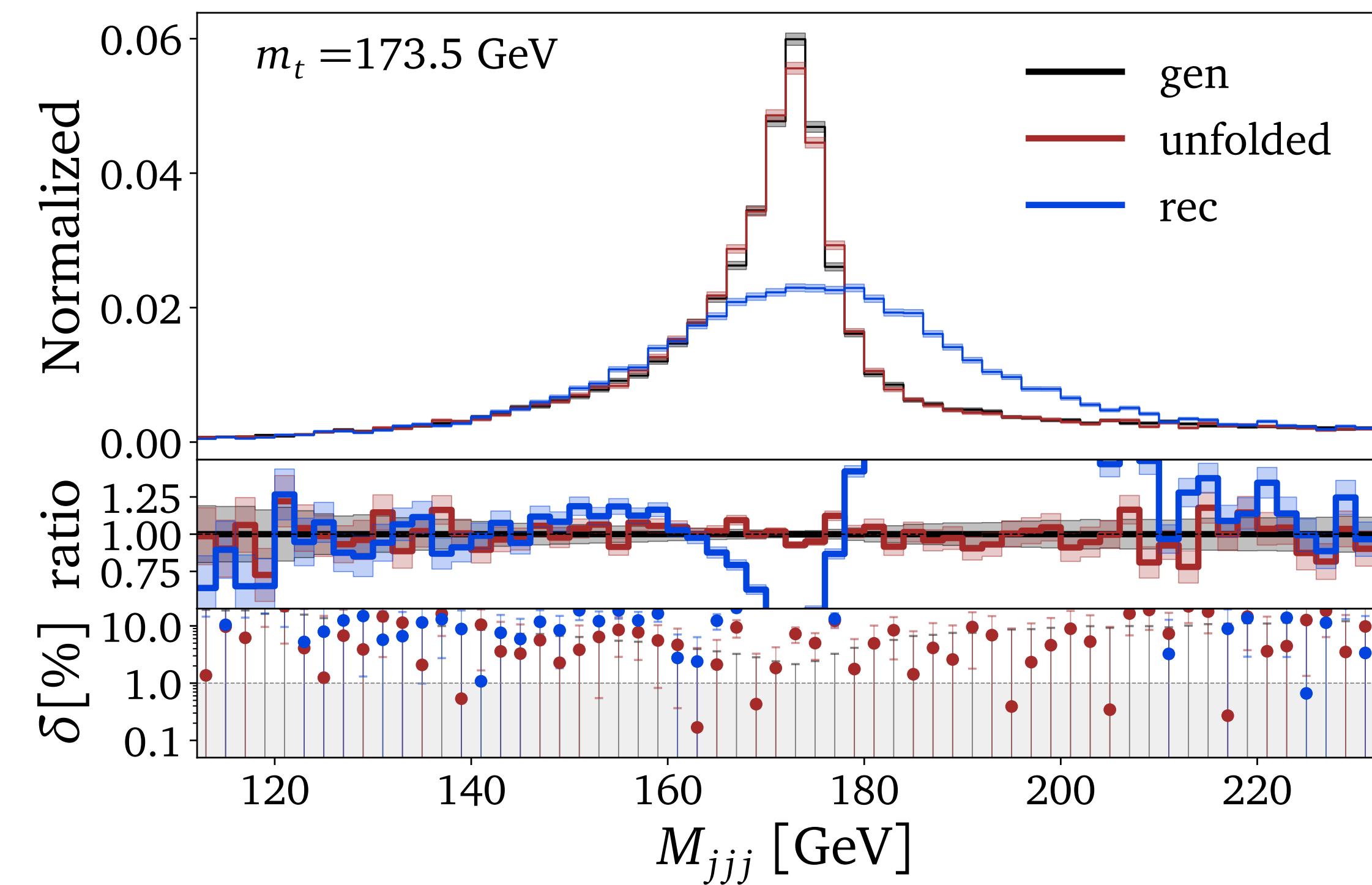
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Unfolded distribution of triple jet mass within
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ML task becomes much harder



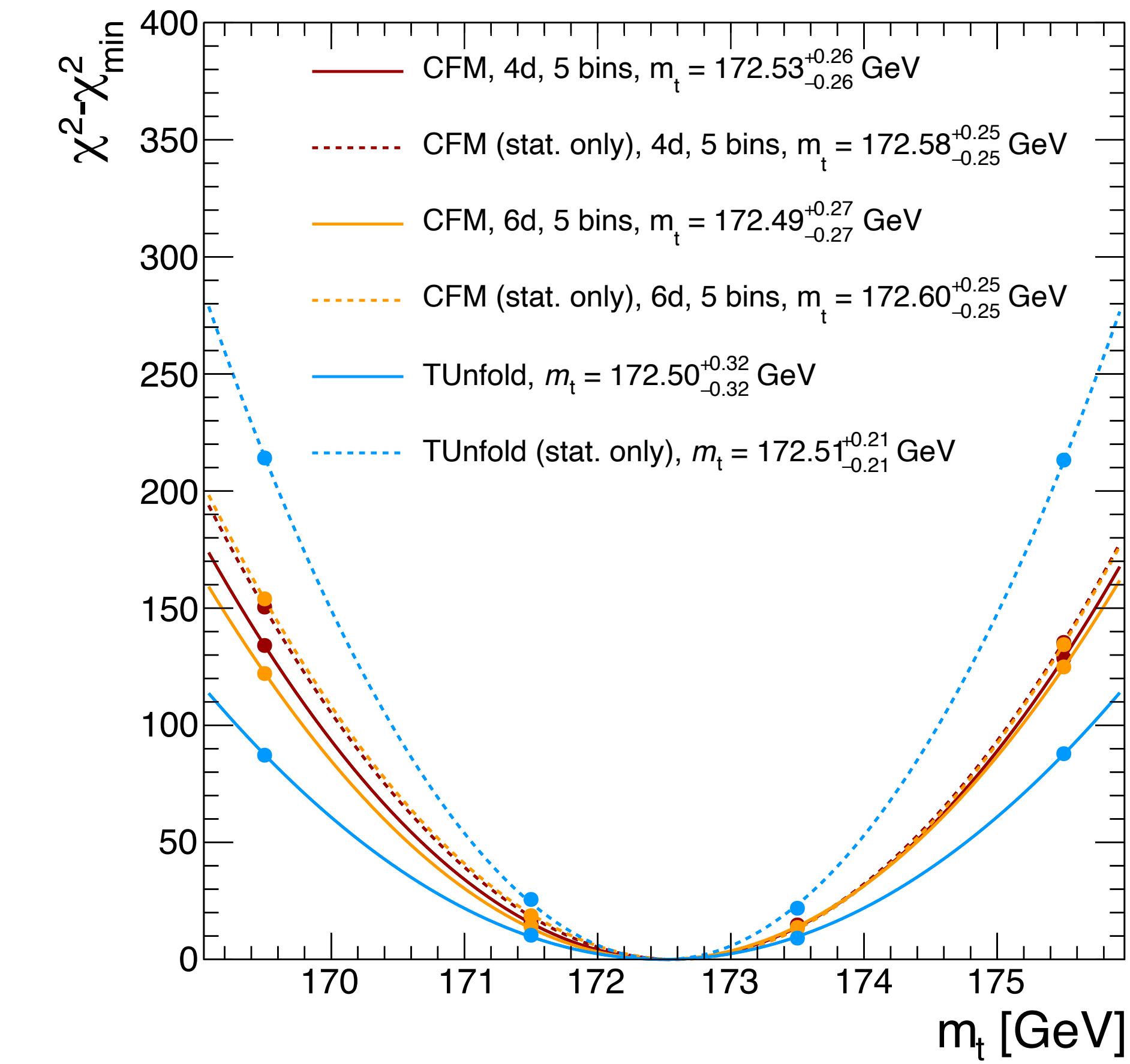
Mass Measurement

For a fixed top mass:

Choose subset of test data of 41000 reco level events

Unfolded 1000 bootstrapped replicas

Estimate covariance matrix and mean by 1000 different unfolded distributions



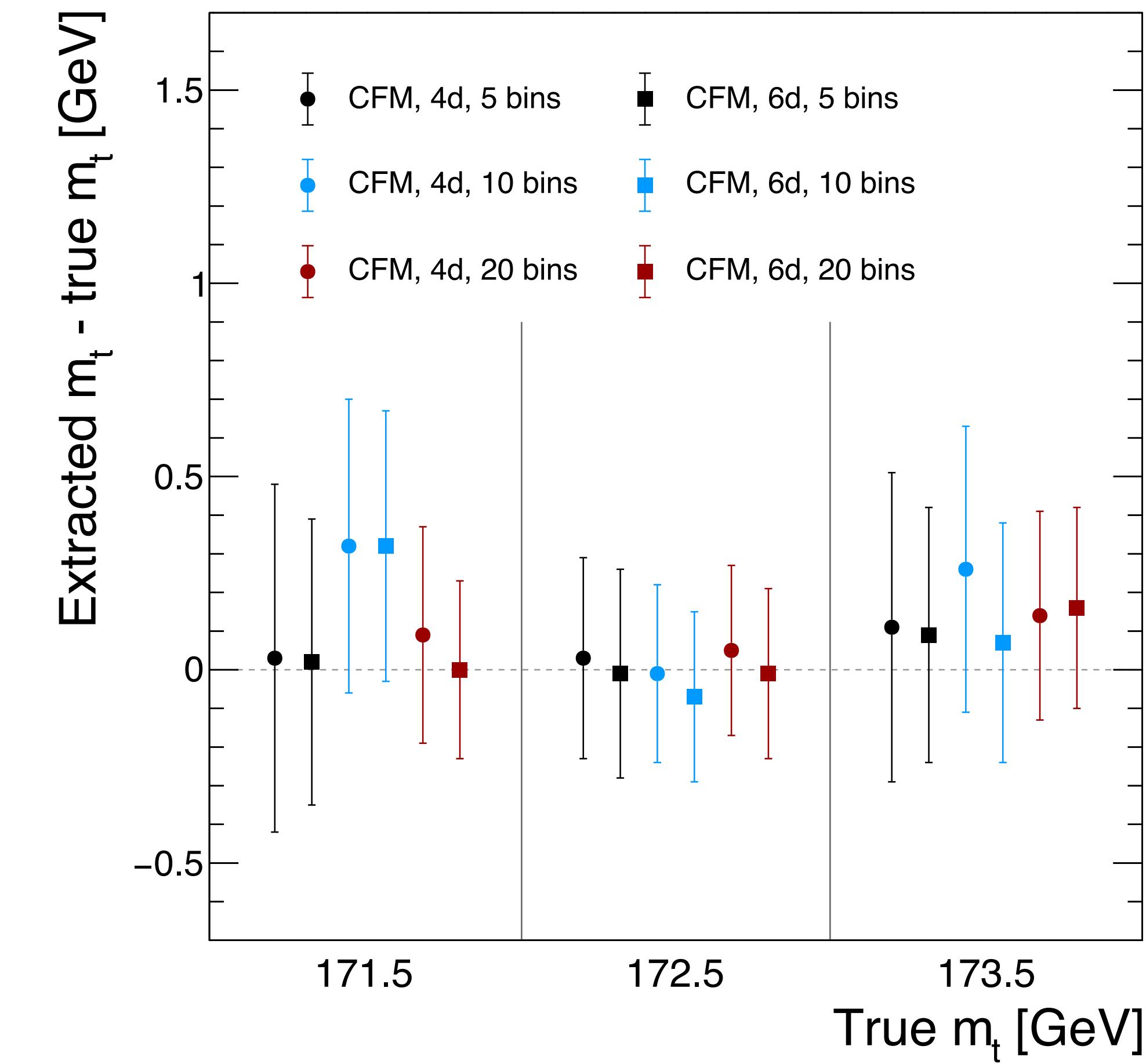
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→ Reliably unfold triple jet mass without bias

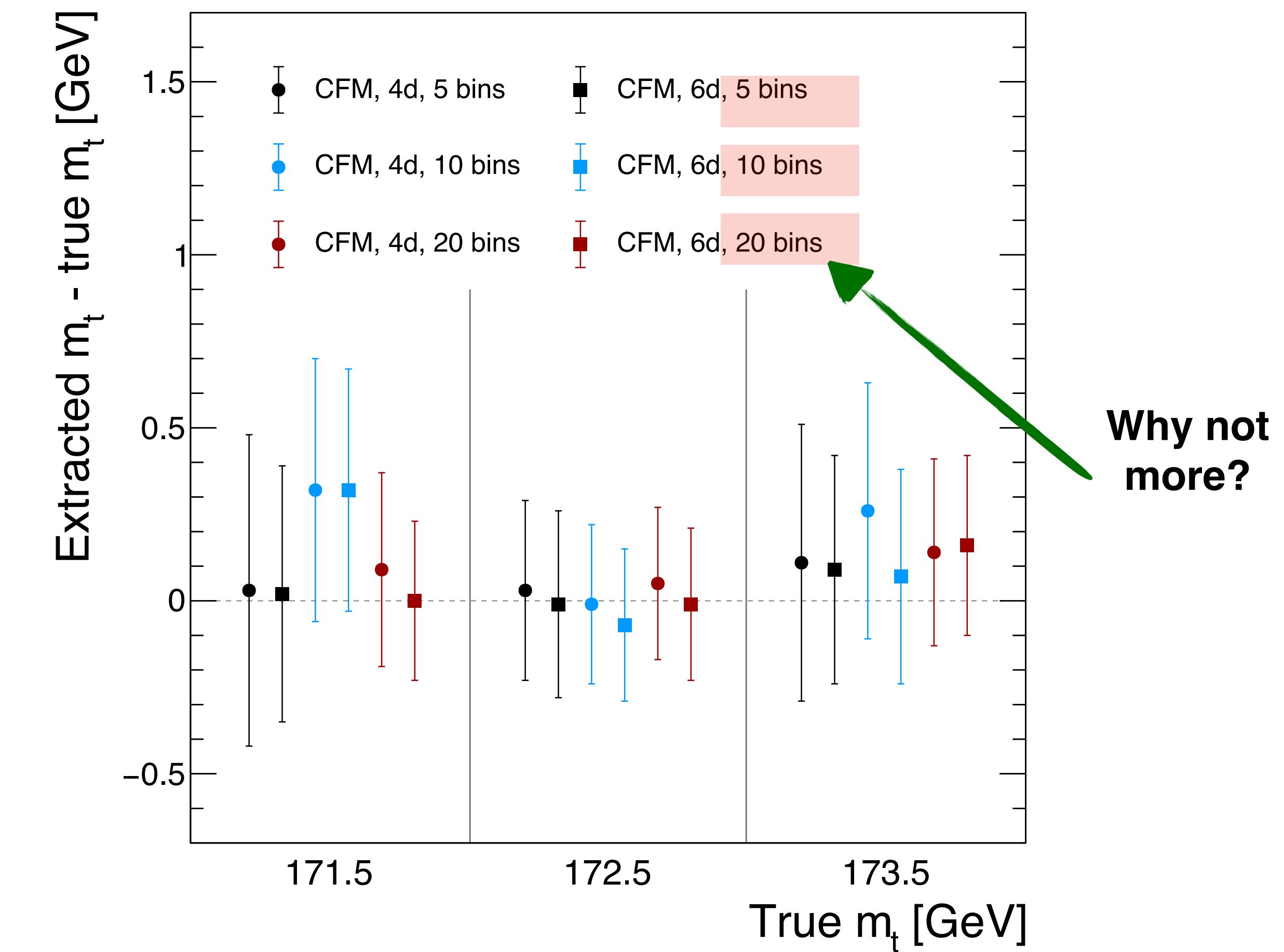
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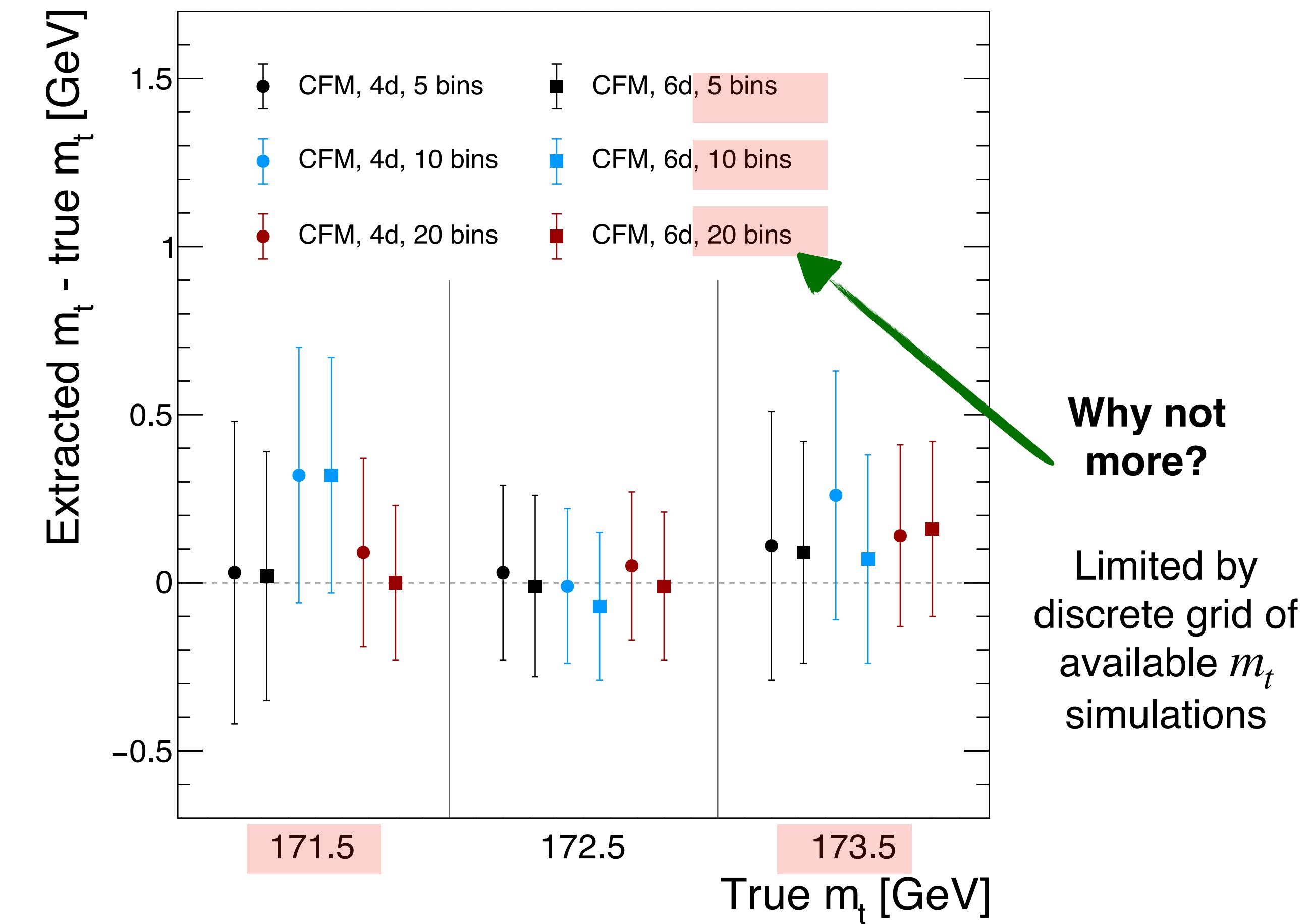
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Unfolded 1000 bootstrapped replicas

Estimate covariance matrix and mean by 1000 different unfolded distributions

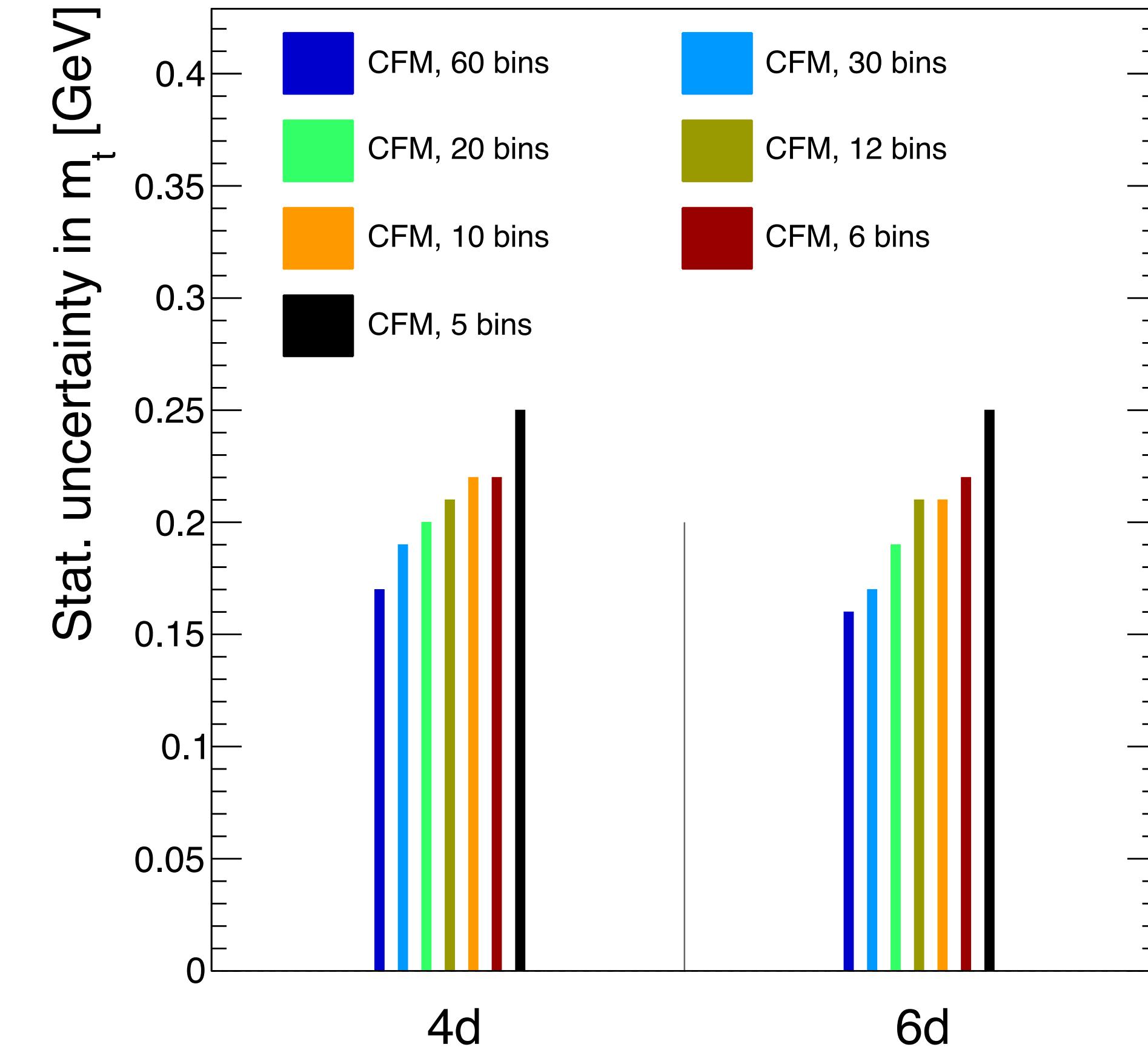


→ Reliably unfold triple jet mass without bias

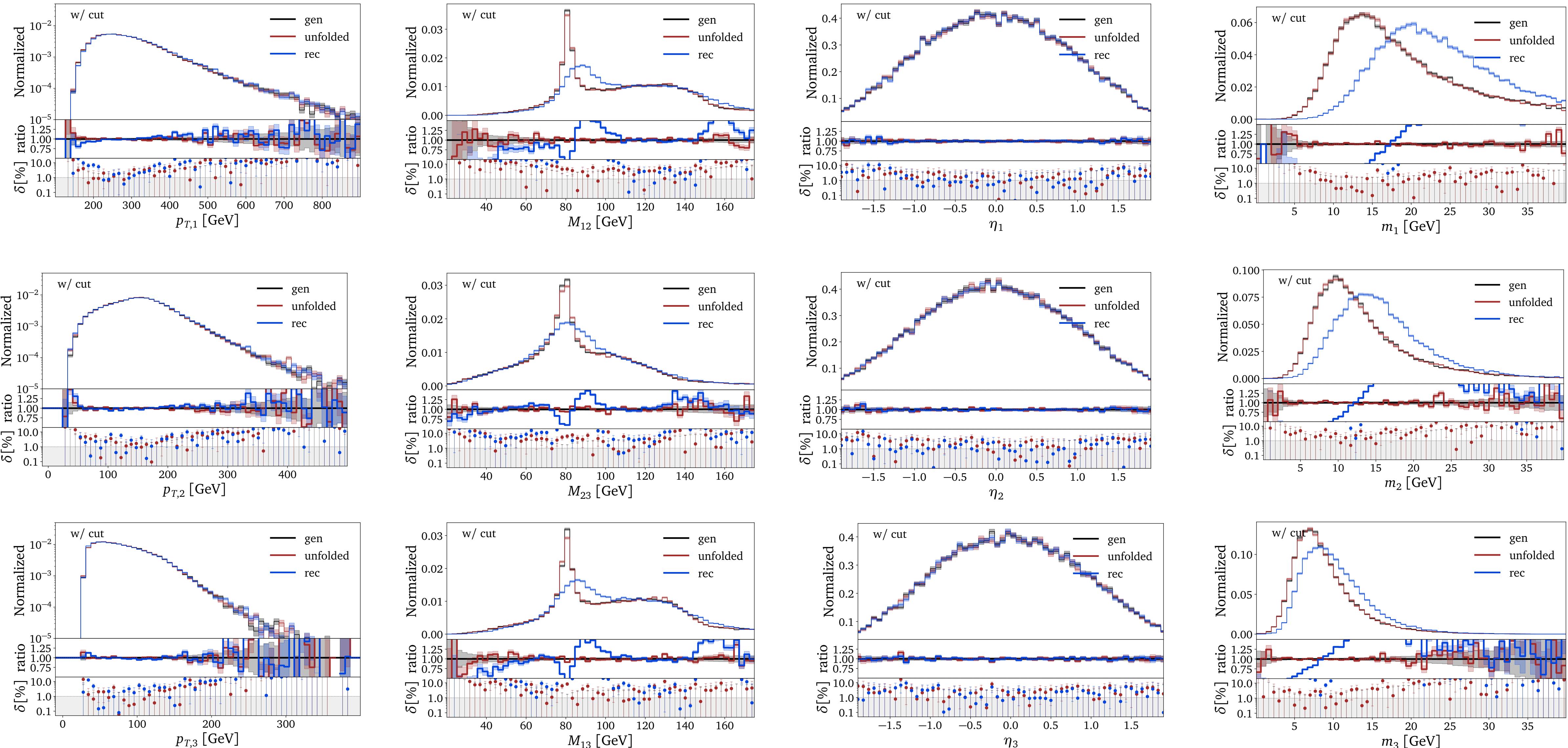
Mass Measurement

For $m_t = 172.5$ GeV, we have a close grid of available simulations (± 1 GeV)

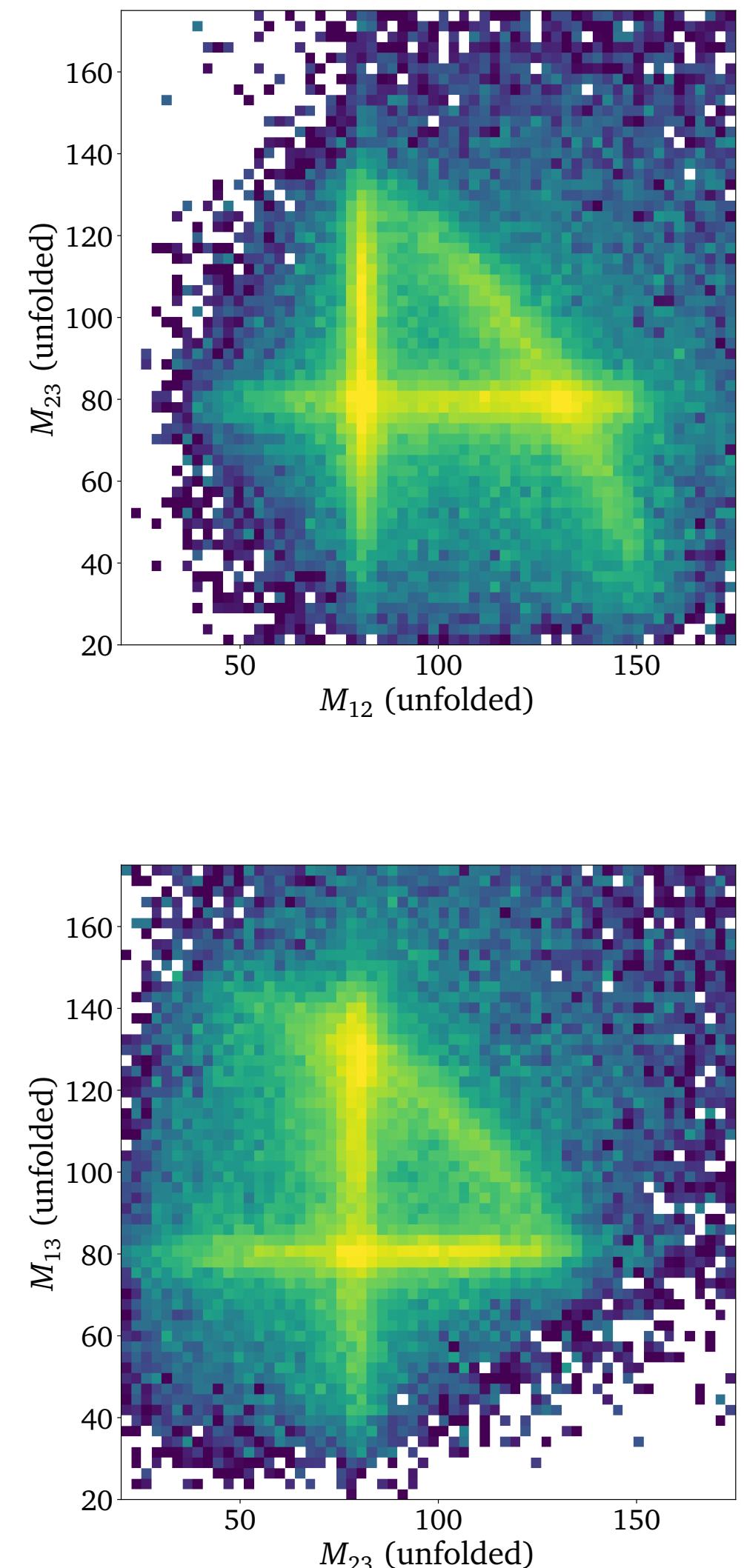
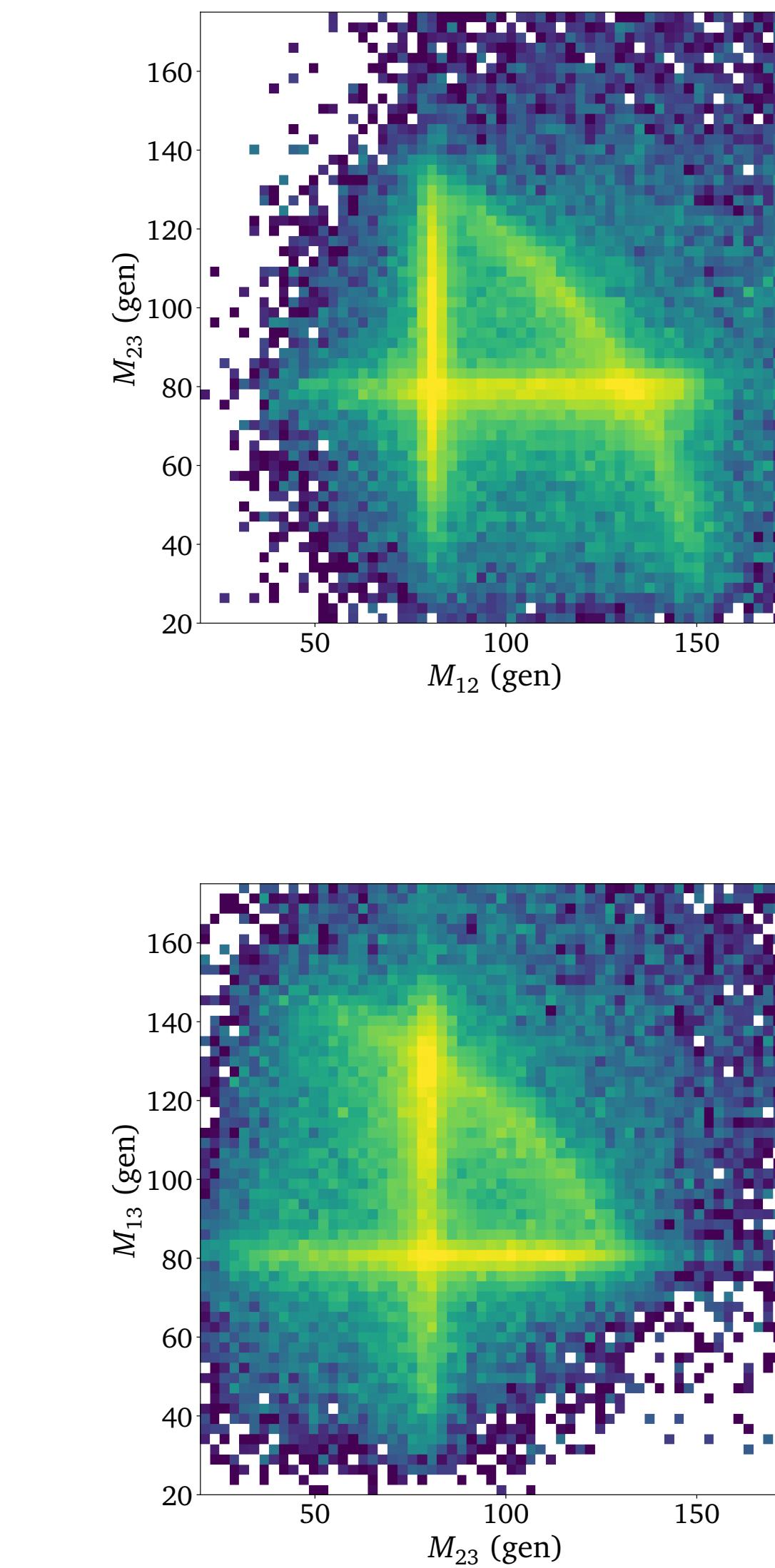
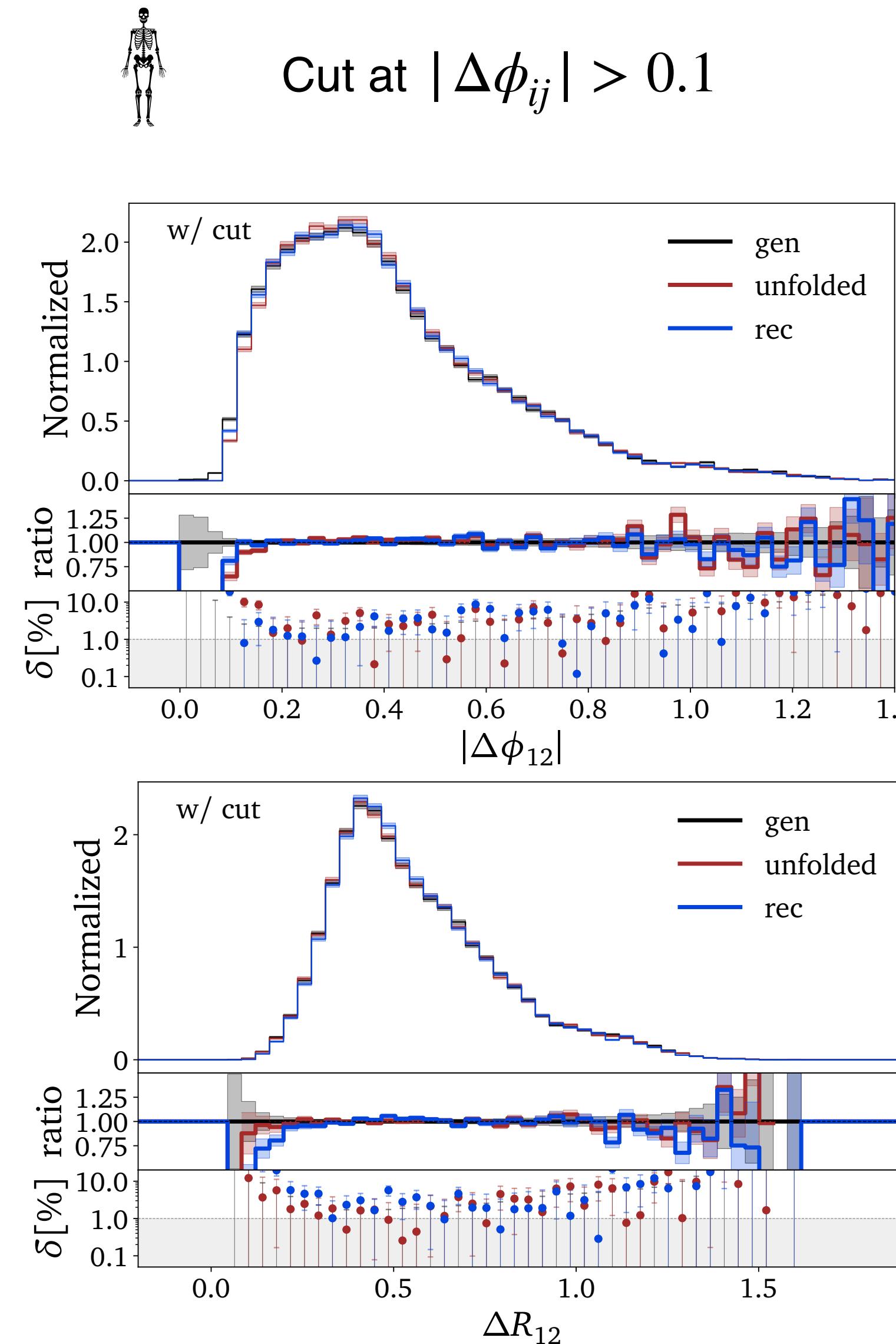
Statistical uncertainty for 60 bins decreases by 36%



Full Phase Space Unfolding (12d)



Full Phase Space Unfolding (12d) - Correlations



And now what?

Generative machine learning allows for unbinned,
high dimensional unfolding

Unbiased networks can enhance precision in e.g.
top mass measurement

Crucial step to build generative unfolding into
existing LHC analysis

Proposal of analysis pipeline:

1. Event Selection
2. Unfold subset
3. Jet calibration
4. Measure top mass
5. Resimulate
6. Unfold full phasespace

And now what?

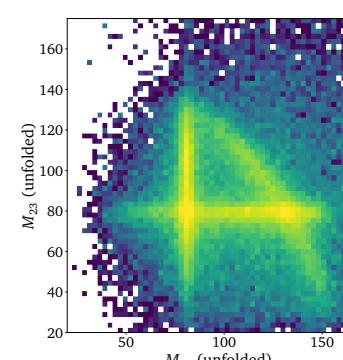
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Are there any questions?