

# Generative Graph Neural Networks for Reconstructing Parton-Level Jets after Hadronization

Umar Sohail Qureshi (uqureshi@cern.ch)

Michael Taleb, Raghav (Rithya) Kunnawalkam Elayavalli

Department of Physics and Astronomy, Vanderbilt University, Nashville, TN, USA

Machine Learning for Jet Physics, LPNHE, Paris, France

November 6, 2024



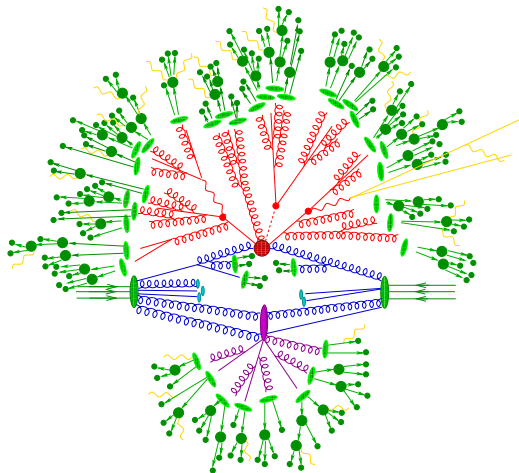
U.S. DEPARTMENT OF  
**ENERGY**

Office of  
Science



**VANDERBILT  
UNIVERSITY**

# The Anatomy of a Hadron-Hadron Collision



## Perturbative

- High  $Q^2$  scattering.
- Parton showering.

Possible because of factoring theorems!

## Non-Perturbative

- Hadronization.
- Multi-parton interactions.
- Underlying events.

Figure 1: Schematic of a hadron-hadron collision.

Image Credit: Stefan Hoche

# Hadronization Processes

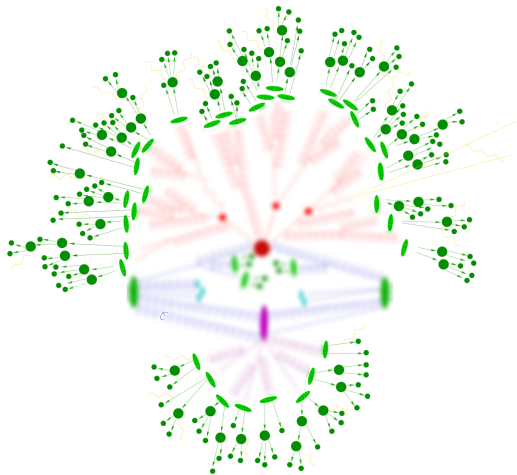


Figure 2: Schematic of a hadron-hadron collision.  
Image Credit: Stefan Hoche

## Hadronization

- Formation of hadrons from quarks and gluons.
- Incalculable using pQCD!

## Phenomenological Models

- Parameterized fits to data.
- Intractable to recover partonic event analytically.

# Probing the Intrinsic Parton Shower

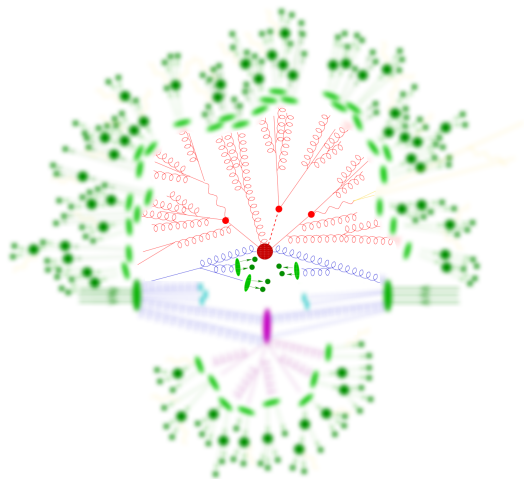


Figure 3: Schematic of a hadron-hadron collision.  
Image Credit: Stefan Hoche

## The Ultimate Goal

- Reconstruct the intrinsic (and immeasurable) parton shower from experimentally accessible quantities.

## Predicting Parton-Level Jets

- We find the expected parton-level jet for a given hadron-level jet.
- Learn a mapping  $f : \mathcal{H} \rightarrow \mathcal{P}$ .

## Event Generation (PYTHIA 8.312)

- $pp$  beams with  $\sqrt{s} = 14$  TeV.
- Photon-tagged events  $qg \rightarrow q\gamma$ .
- $\hat{p}_T > 1000$  GeV.
- Anti- $k_t$   $R = 0.8$  parton-level and hadron-level jets.
- Visible final-state particles.
- $800 < \text{Jet } p_\perp < 2000$  GeV.
- 100K events to ensure sufficient statistics.



[pythia.org/latest-manual/welcome.html](http://pythia.org/latest-manual/welcome.html)

## Graph Representation of Pythia Quark Jets

Jets represented as graphs, connected by  $\Delta R$ :

$$\text{Vertices : } \mathcal{J} = \left\{ (p_\perp^i, \eta^i, \phi^i)_{i=1}^n \right\}$$

$$\text{Edges : } E = \left\{ \Delta R(i, j)_{i, j=1}^n, i \neq j \right\}$$

Fully connected graphs, no self-loops.

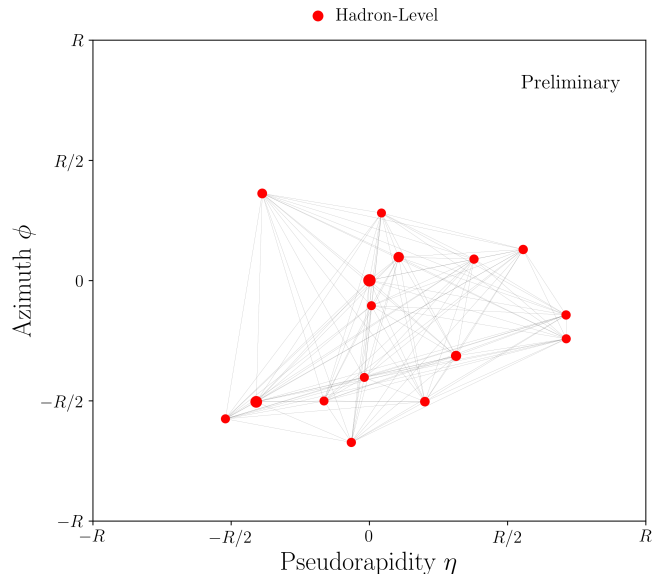
# Preprocessing: Centering the Jets

- The  $(\eta, \phi)$  coordinates of jet constituents are centered based on the jet  $(\eta, \phi)$  using the  $E$ -scheme jet axis:

$$\bar{\eta} = \frac{\sum_{i \in \text{jet}} \eta_i p_{T,i}}{\sum_{i \in \text{jet}} p_{T,i}}, \quad \bar{\phi} = \frac{\sum_{i \in \text{jet}} \phi_i p_{T,i}}{\sum_{i \in \text{jet}} p_{T,i}}$$

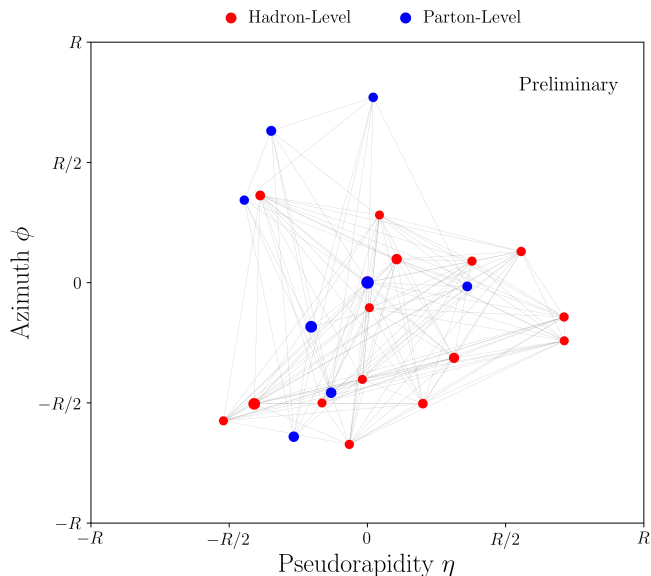
$$\eta_i \rightarrow \eta_i - \bar{\eta}, \quad \phi \rightarrow \phi_i - \bar{\phi}$$

# Graph Representations of Quark Jets



- Pythia 8.312,  $pp \sqrt{s} = 14$  TeV.
- Anti- $k_T$ ,  $R = 0.8$
- $800 < p_T < 2000$  GeV.

# Graph Representations of Quark Jets



- Pythia 8.312,  $pp \sqrt{s} = 14$  TeV.
- Anti- $k_T$ ,  $R = 0.8$ .
- $800 < p_T < 2000$  GeV.



# Machine Learning Model

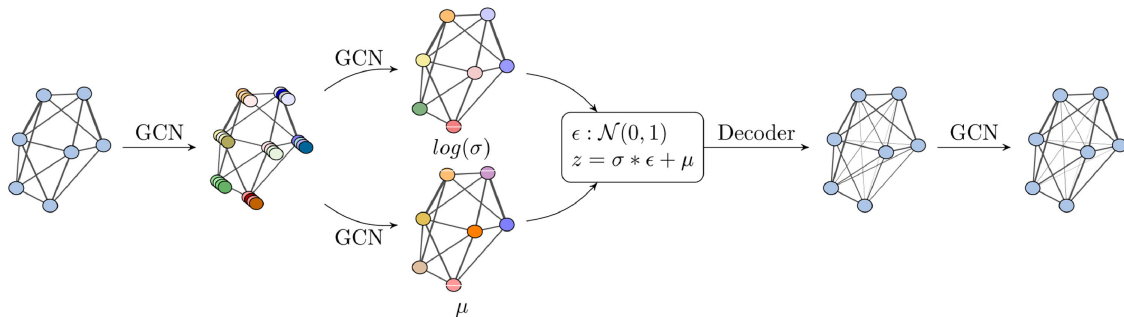


Image Credit: Tina Behrouzi et. al.

## Variational Graph Autoencoder (VGAE)

- Input hadron-level jets  $\mathcal{H}$ .
- Output parton-level jets  $\mathcal{P}$ .

- Encoder: learns an embedding  $(z, \mu)$  for  $\mathcal{H}$  in latent space.
- Decoder: learns reconstructing parton-level jets  $\mathcal{P}$  from embedding.

## Model Training

- Implemented using PyTorch-geometric.
- Trained using on an Nvidia A100.
- Train-validation split of 90%-10%.
- Adam optimizer, 3000 epochs.

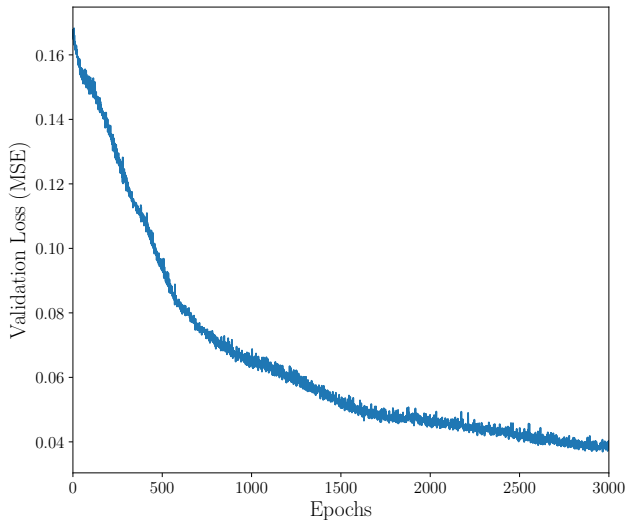


Figure 4: Validation loss over time.

# Comparing Jets: The Energy Mover's Distance Metric

## EMD Metric (PhysRevLett.123.041801)

- Quantifies the distance between two jets.
- The minimum “energy” required to rearrange a jet  $\mathcal{G}$  to  $\mathcal{G}'$ .

$$\mathcal{E}(\mathcal{G}, \mathcal{G}') = \min_{\{f_{ij} \geq 0\}} \sum_{i=1}^M \sum_{j=1}^{M'} f_{ij} \left( \frac{\Delta R_{ij}}{R} \right) + \left| \sum_{i=1}^M E_i - \sum_{j=1}^{M'} E'_j \right|,$$

$$\sum_{j=1}^{M'} f_{ij} \leq E_i, \quad \sum_{i=1}^M f_{ij} \leq E'_j, \quad \sum_{i=1}^M \sum_{j=1}^{M'} f_{ij} = E_{\min},$$

$\mathcal{E}(\hat{\mathcal{P}}, \mathcal{P})$  gives a discrepancy measure between reconstructed graphs  $\hat{\mathcal{P}}$  and the ground truth  $\mathcal{P}$ .

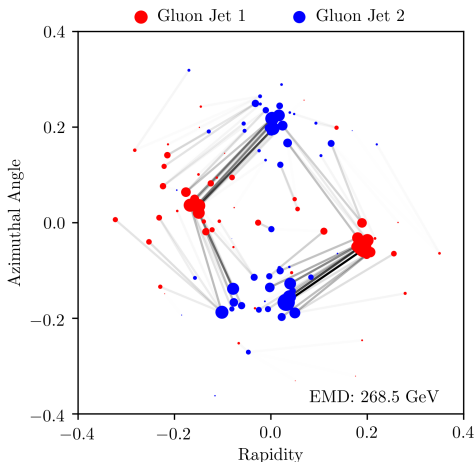
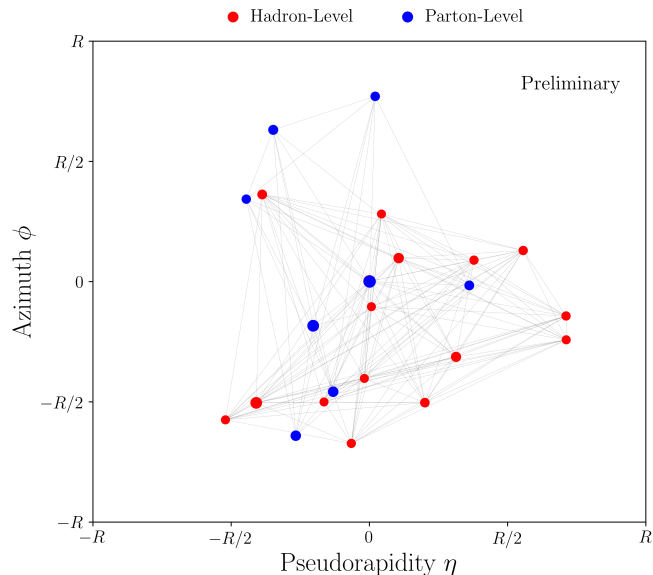


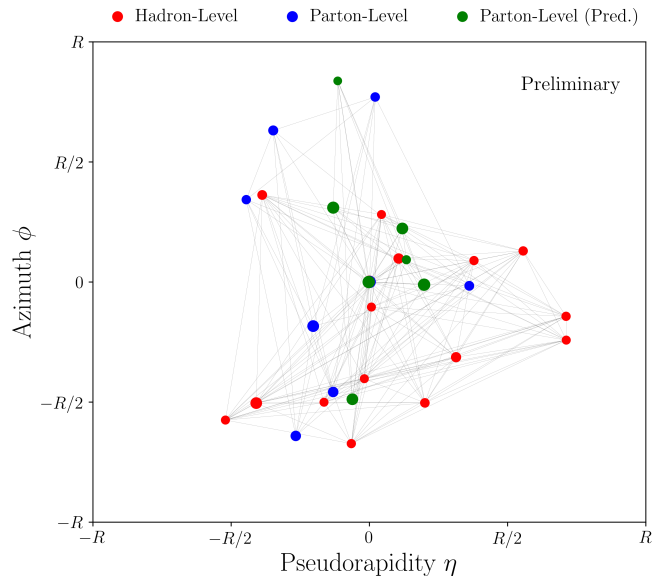
Figure 5: EMD between two gluon jets.

# Results: Predictions on Unseen Data



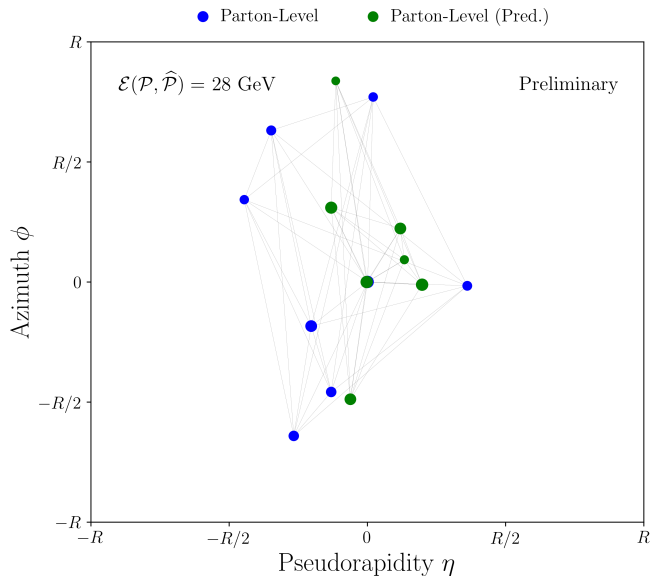
- Pythia 8.312,  $pp \sqrt{s} = 14$  TeV.
- Anti- $k_T$ ,  $R = 0.8$ .
- $800 < p_T < 2000$  GeV.

# Results: Predictions on Unseen Data



- Pythia 8.312,  $pp \sqrt{s} = 14$  TeV.
- Anti- $k_T$ ,  $R = 0.8$ .
- $800 < p_T < 2000$  GeV.

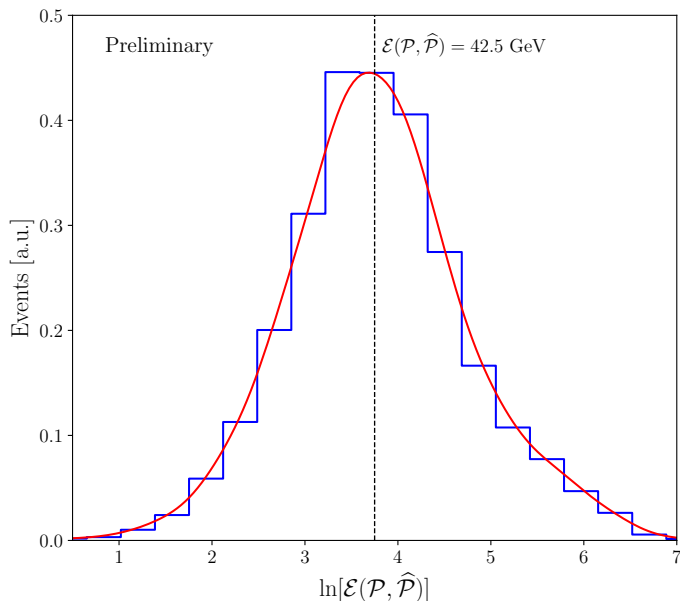
# Results: Predictions on Unseen Data



Can compare predictions  $\hat{\mathcal{P}}$  with ground truth  $\mathcal{P}$  using EMD!

- Pythia 8.312,  $pp \sqrt{s} = 14 \text{ TeV}$ .
- Anti- $k_T$ ,  $R = 0.8$ .
- $800 < p_T < 2000 \text{ GeV}$ .

# Results: EMD Metric Distribution

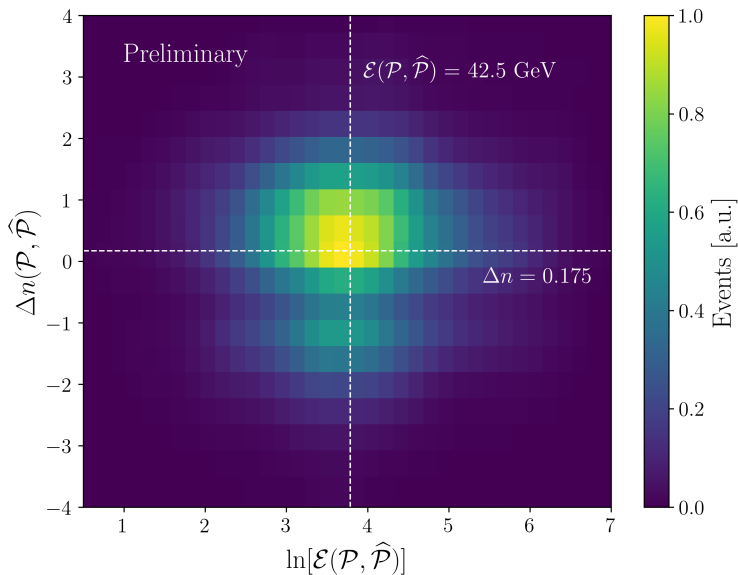


Predicted jets close to ground truth (Pythia)!

Benchmark EMDs:

- Good:  $\ln \mathcal{E} \leq 4$ 
  - Jets are similar.
- Fair:  $4 \leq \ln \mathcal{E} \leq 5.5$ 
  - Jets are fairly similar.
- **Bad:  $\ln \mathcal{E} \geq 5.5$** 
  - Jets are disparate.

# Results: Predictions for Parton Multiplicities

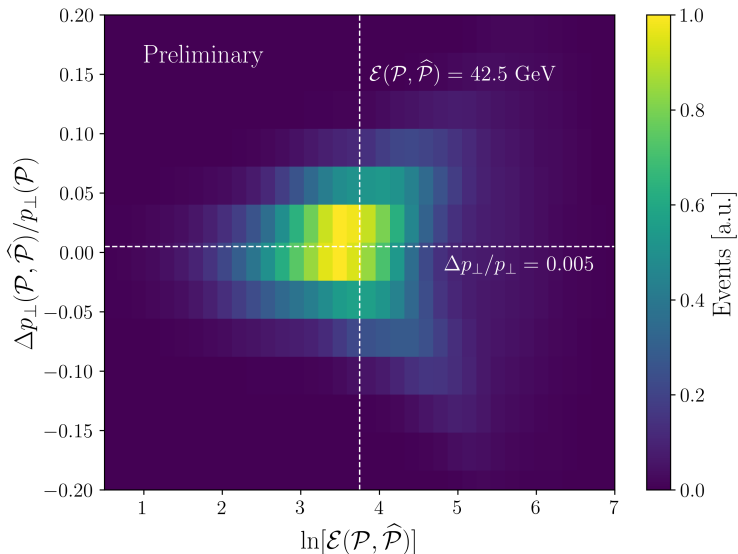


Correlation of EMD and the difference in prediction and ground truth parton multiplicities.

- Accurate prediction of multiplicities.
- Average particle multiplicity is  $\sim 22$ .
- Peak at  $\Delta n = 0$ .
- Almost all data:  $|\Delta n| < 2$ .



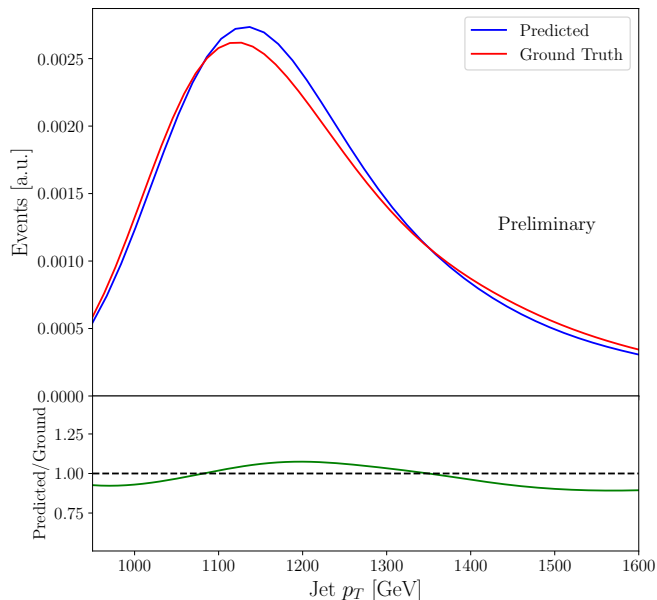
# Results: Predictions for Parton Jet $p_T$



Correlation of EMD and the fractional difference in jet  $p_T$ .

- Accurate prediction of  $p_T$ .
- Peak at  $\Delta p_T/p_T \approx 0$ .
- Almost all data:  $|\Delta p_T/p_T| < 0.1$ .

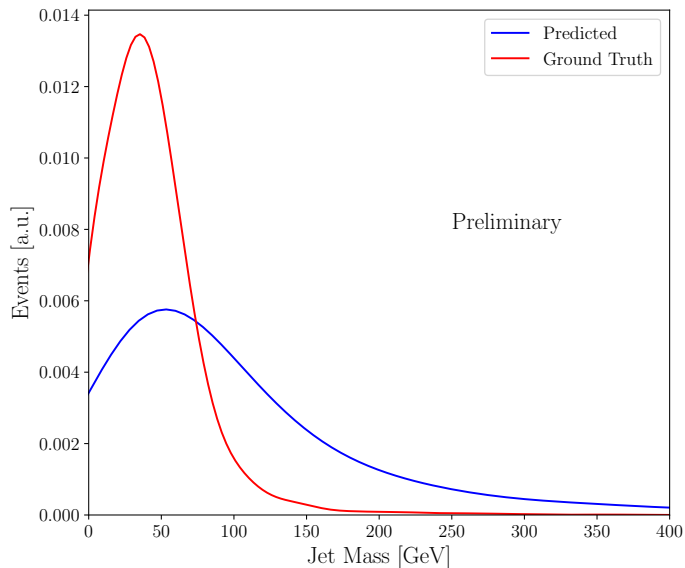
# Results: Parton Jet $p_T$ Spectra



Comparison of predicted and ground jet  $p_T$  spectra.

- Accurate prediction of  $p_T$ .
- Almost all data  $\varepsilon < 0.1$ .

# Results: Parton Jet Mass Spectra



Comparison of predicted and ground jet mass spectra.

- Poor prediction of jet mass.
- Distribution is shifted and significantly more spread out.

## Summary

- We present a first look at using generative neural networks to reconstruct parton-level jets after hadronization.
- Our method captures the entire parton-level jet.
- Jury is still out on substructure observables.

## Future Work

- Investigate the predictions for more jet substructure observables.
- Better ML models? Loss functions?
- Study the inclusion of detector effects, underlying events, and pileup.

# Acknowledgements

- I thank Professor Rithya Kunnawalkam Elayavalli for their invaluable support and guidance.
- This work is supported in part by DOE Office of Science Award DE-SC0024660 and a Vanderbilt Immersion Grant.

Thank you! Questions?