Semi-supervised GraphNN for Pileup Noise Removal

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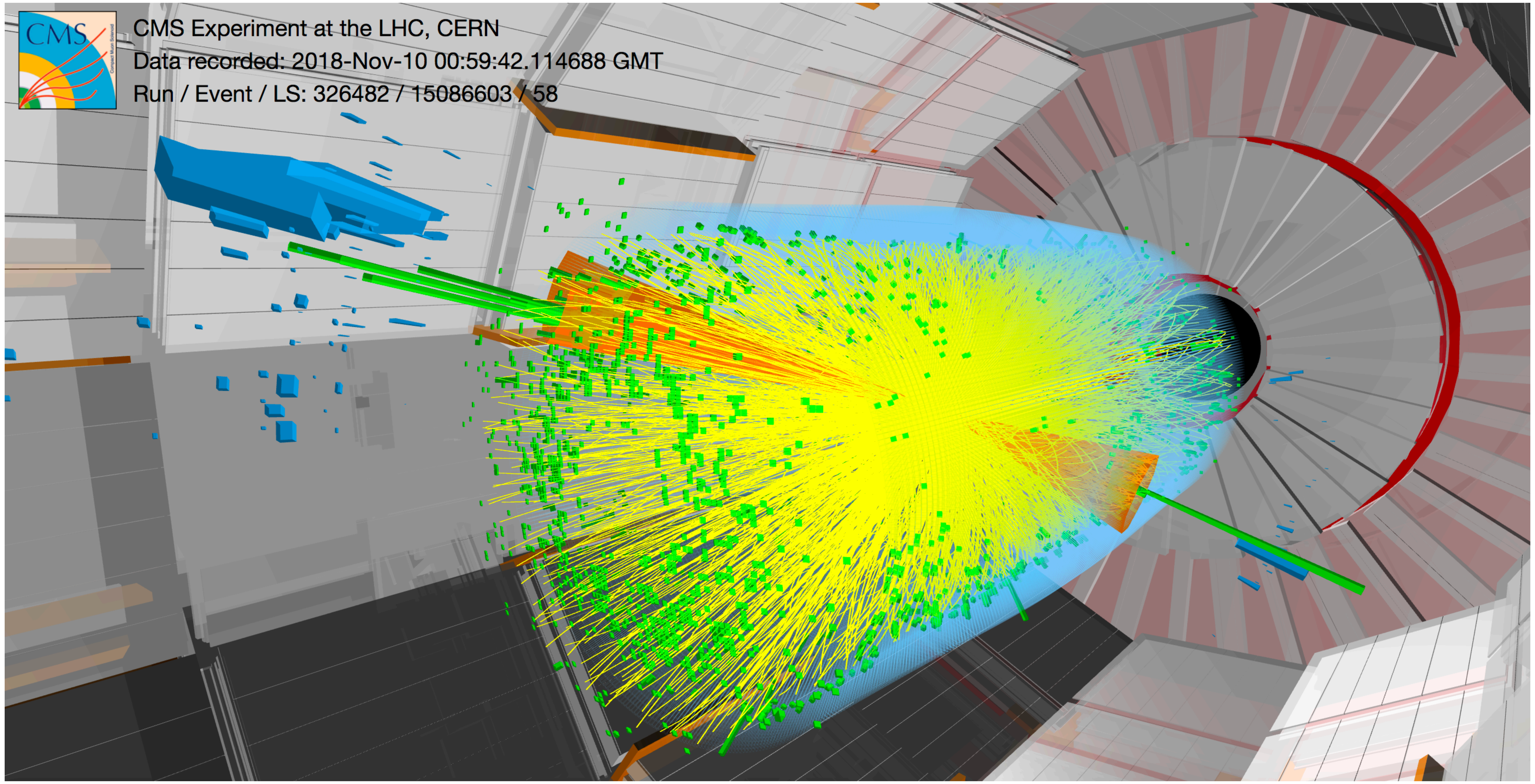
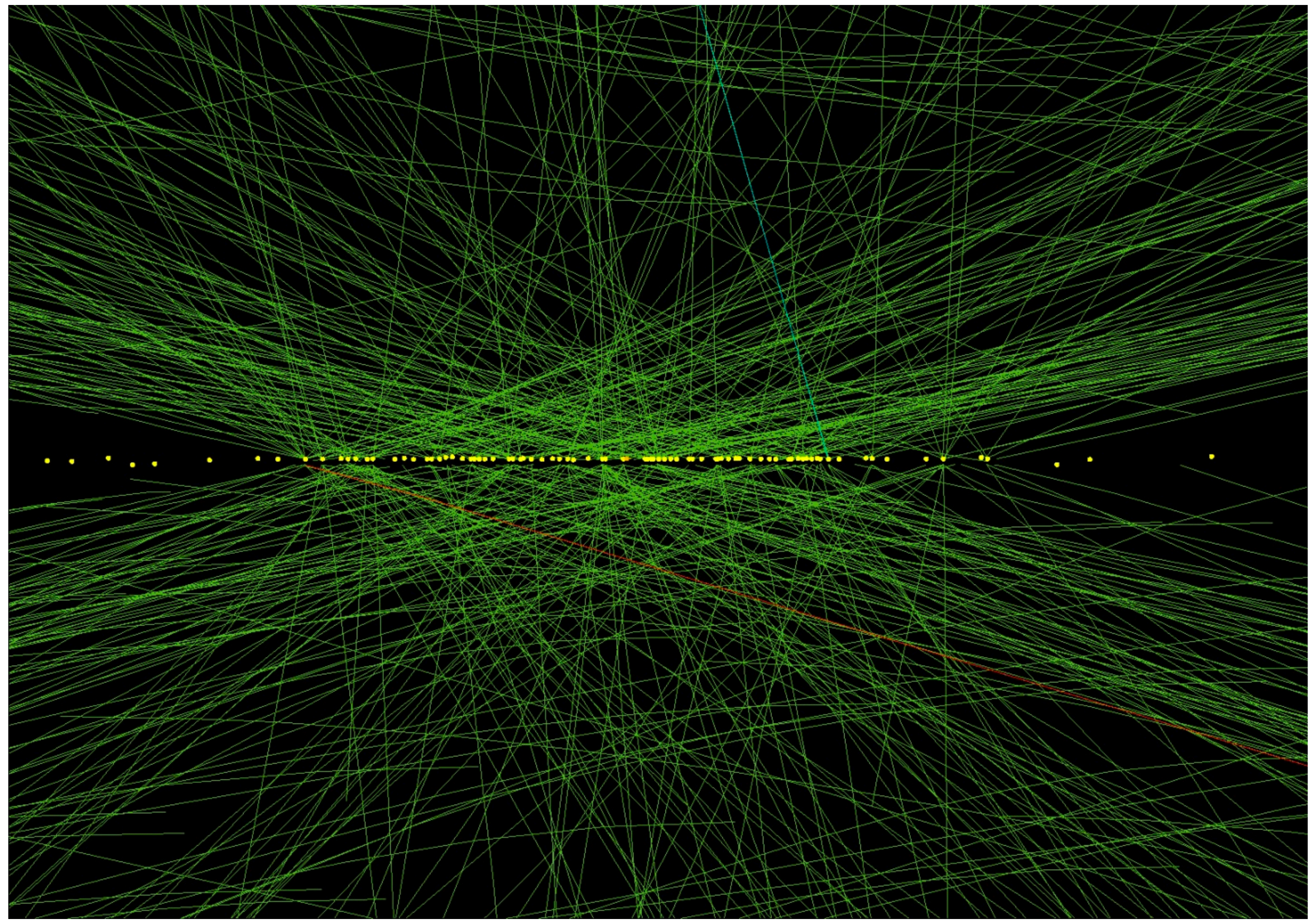
EPE Machine Learning

May 3rd, 2022

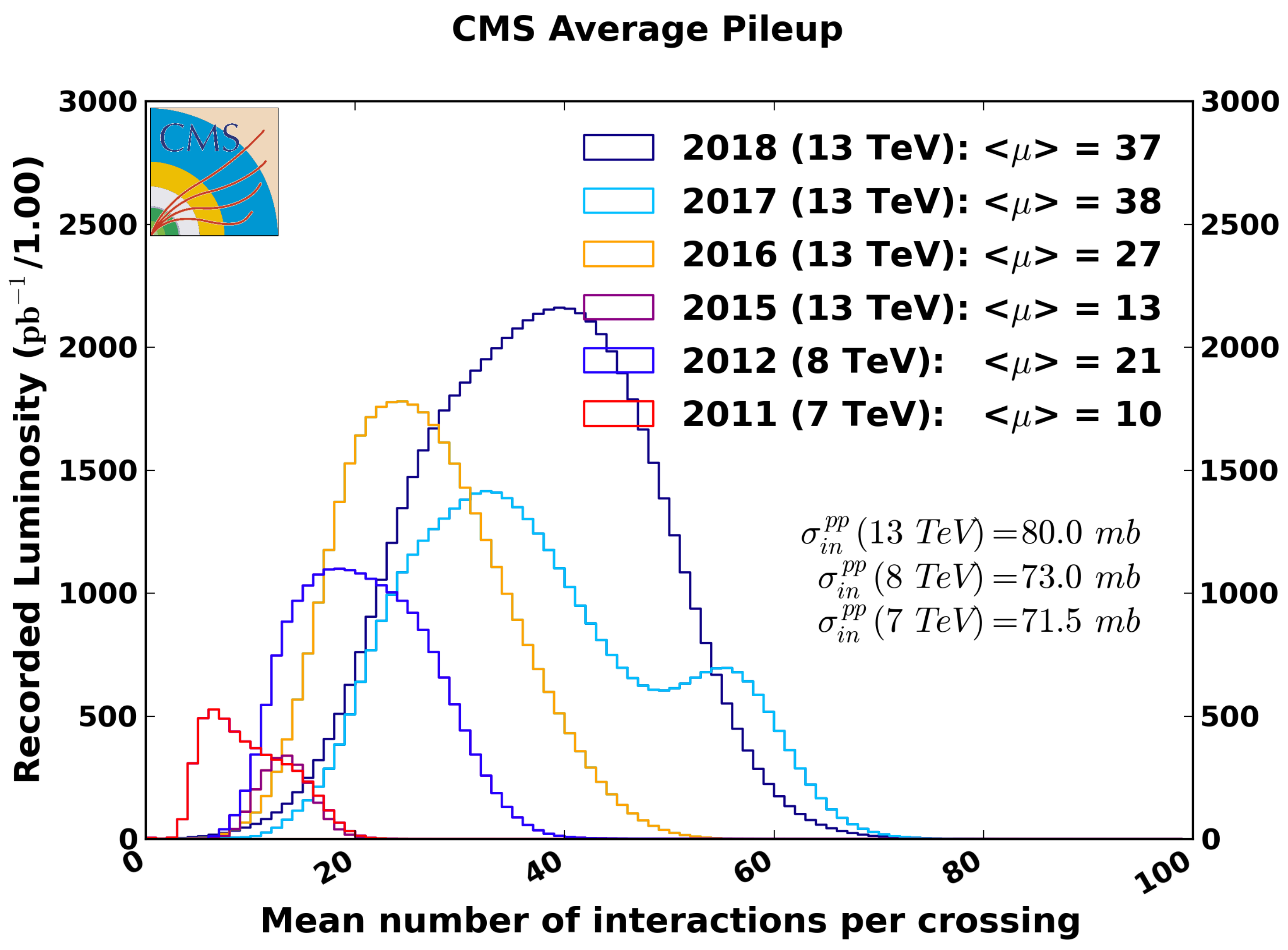
What is PileUp

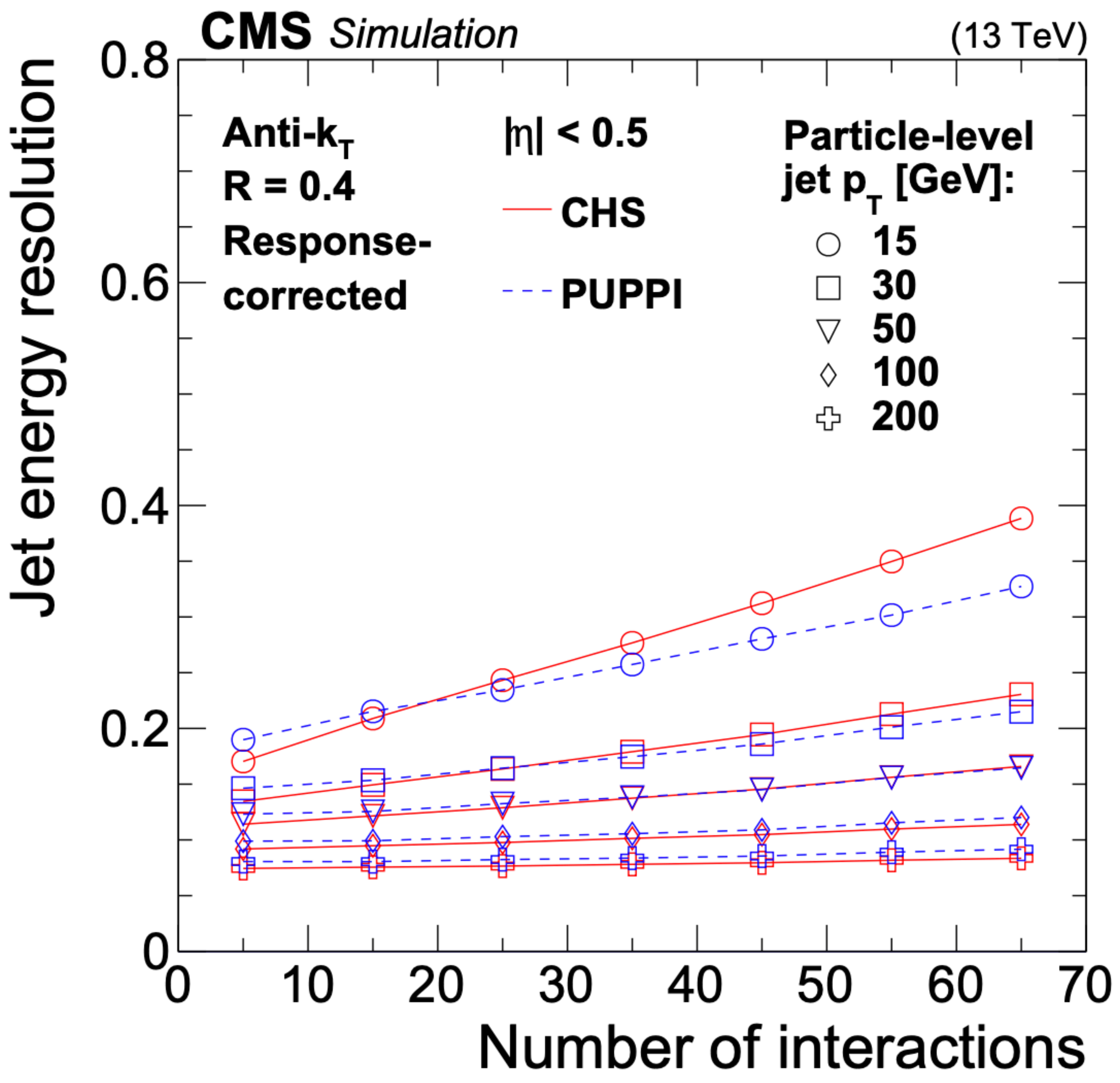


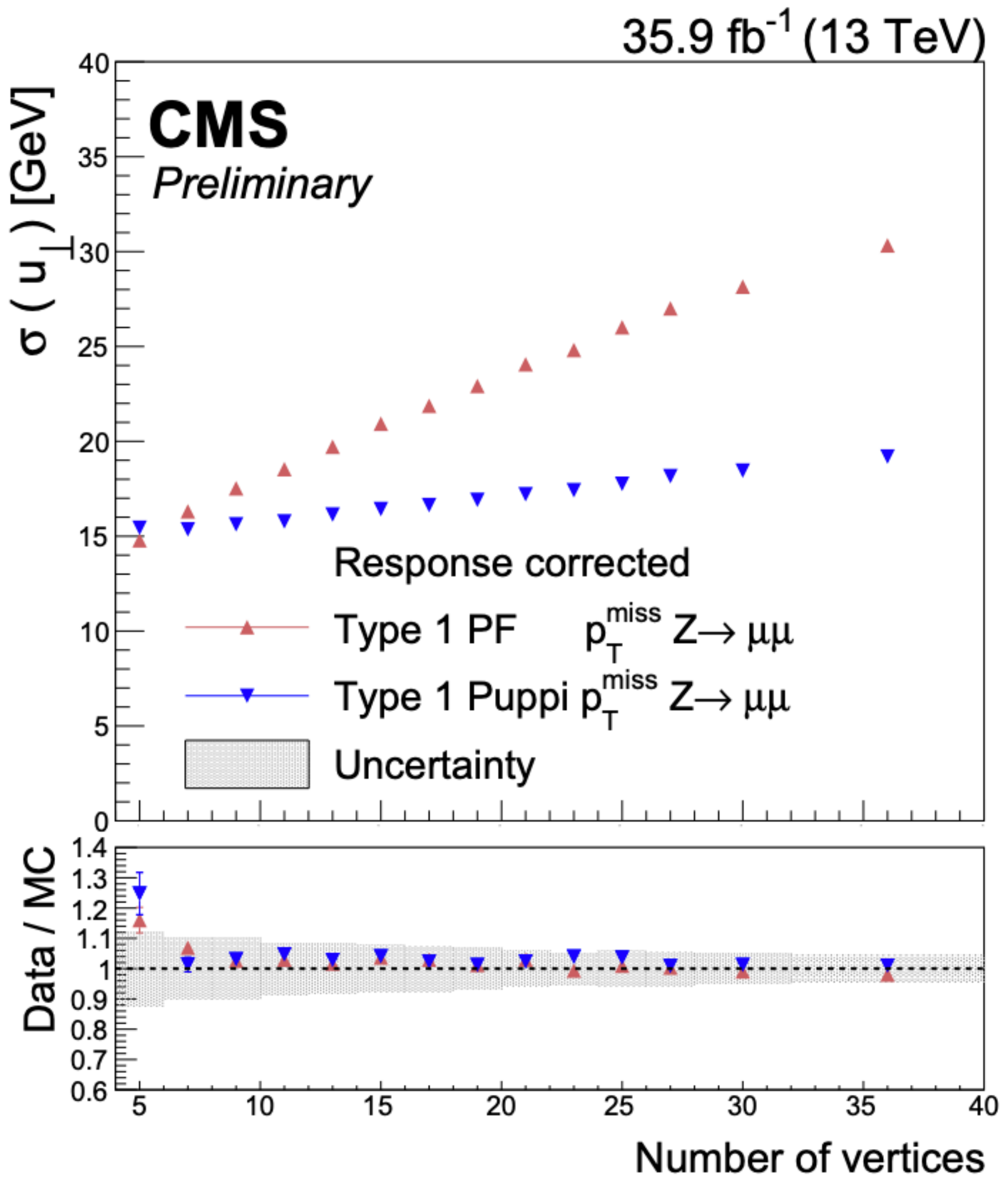


- Pileup (PU): additional proton-proton interactions in the same or nearby bunch crossings

Why PileUp Mitigation



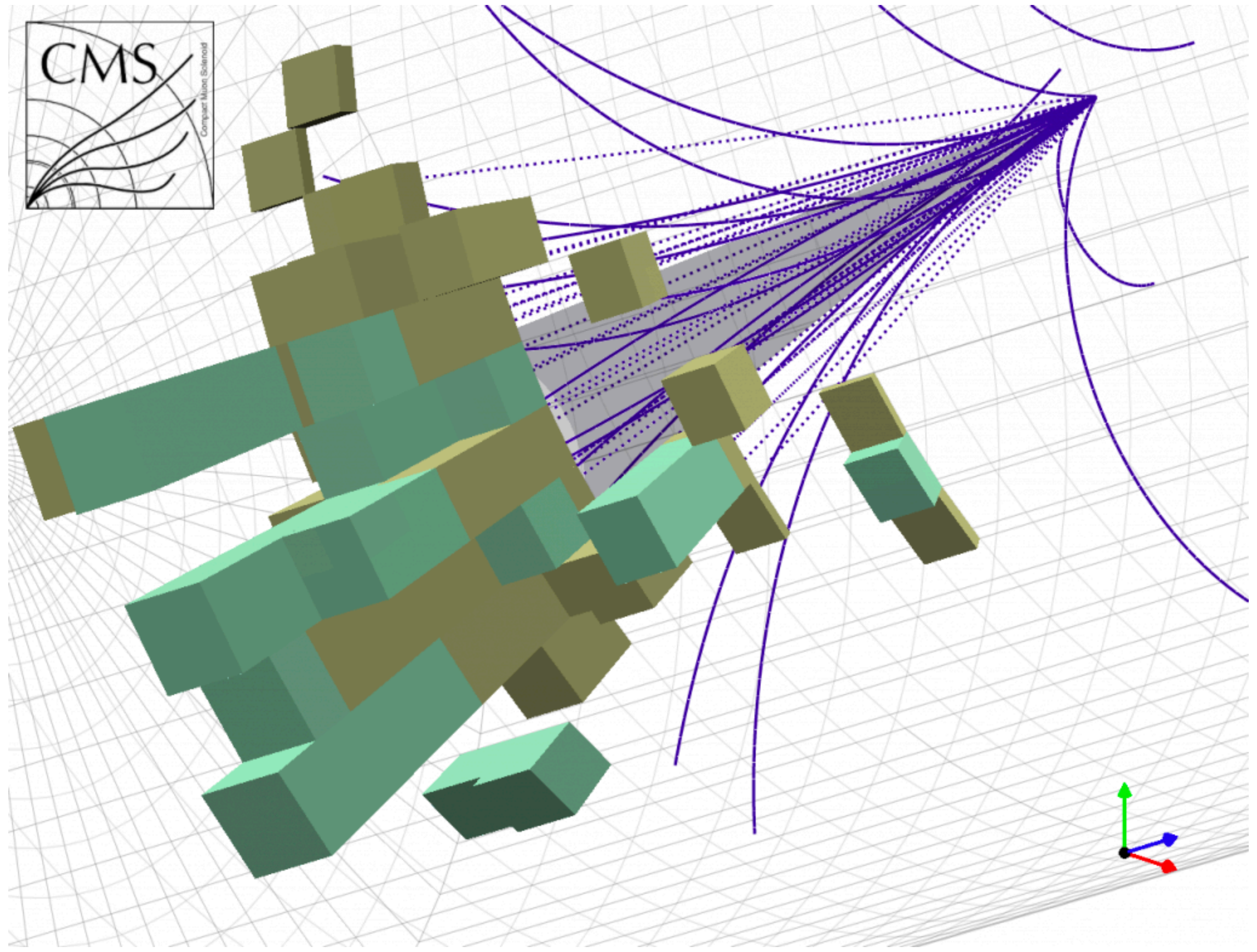


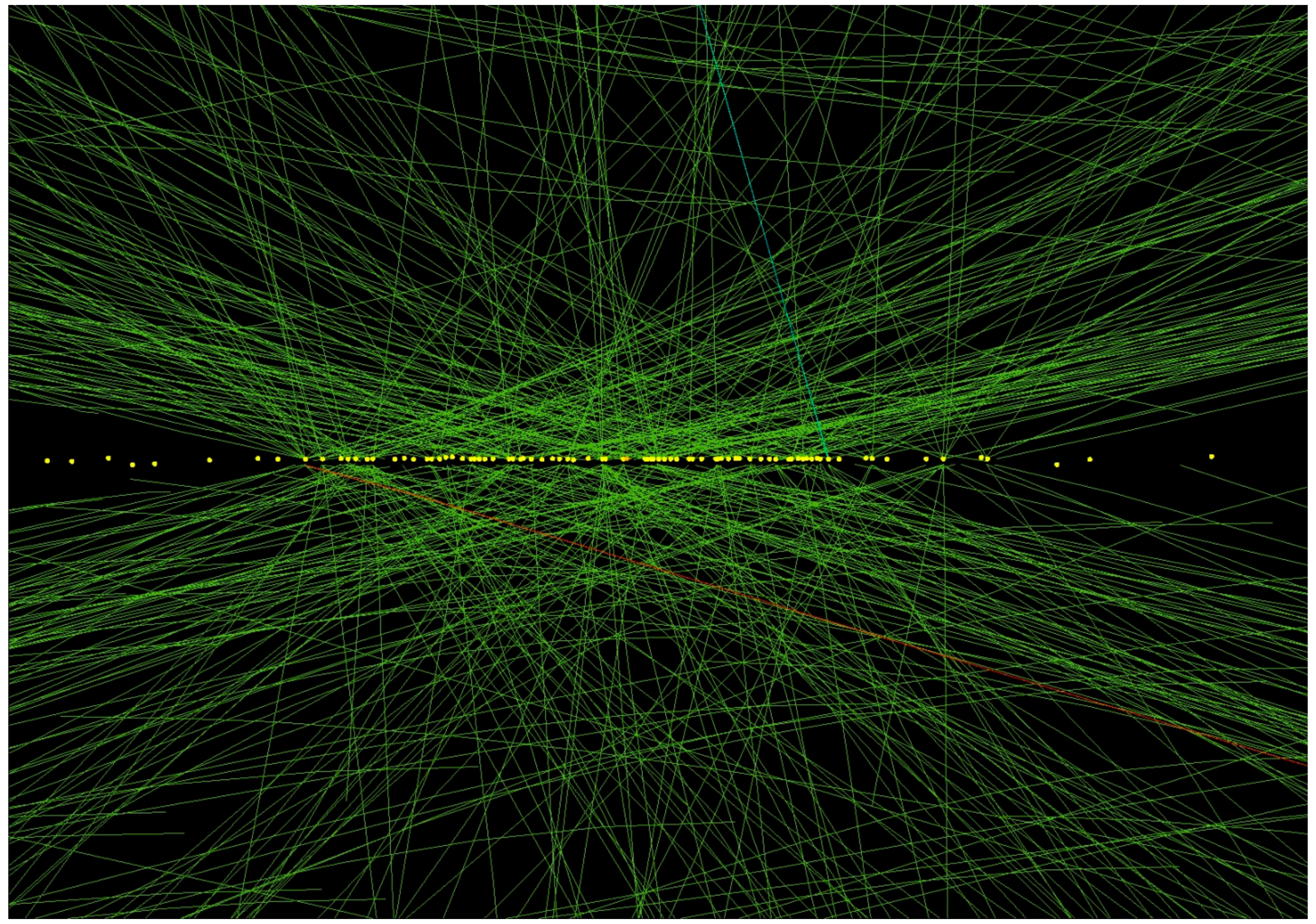


- PU at Run-II: ~30-40; expected to increase to 140-150 at HL-LHC
- PU can significantly affect the reconstruction and performance of many physics observables, such as jet mass, jet pT, and pTmiss
- PU mitigation is needed

PileUp Mitigation: How?

- Charged particles easy to deal with - Leading Vertex (LV) or Pileup (PU) charged particles can be easily identified because of excellent tracking and vertexing efficiency and

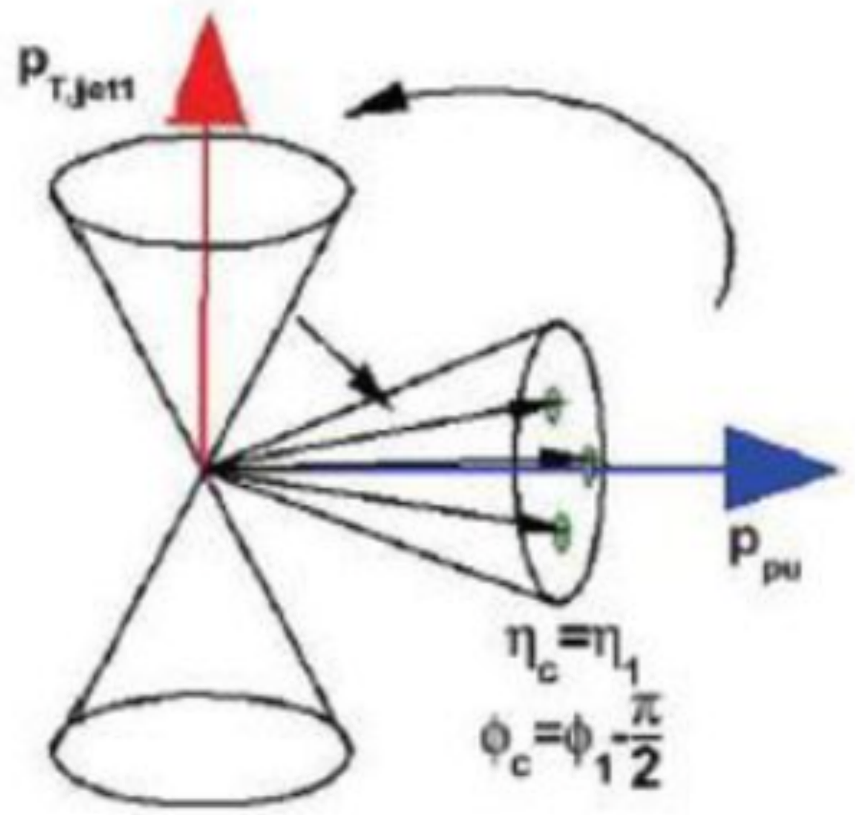




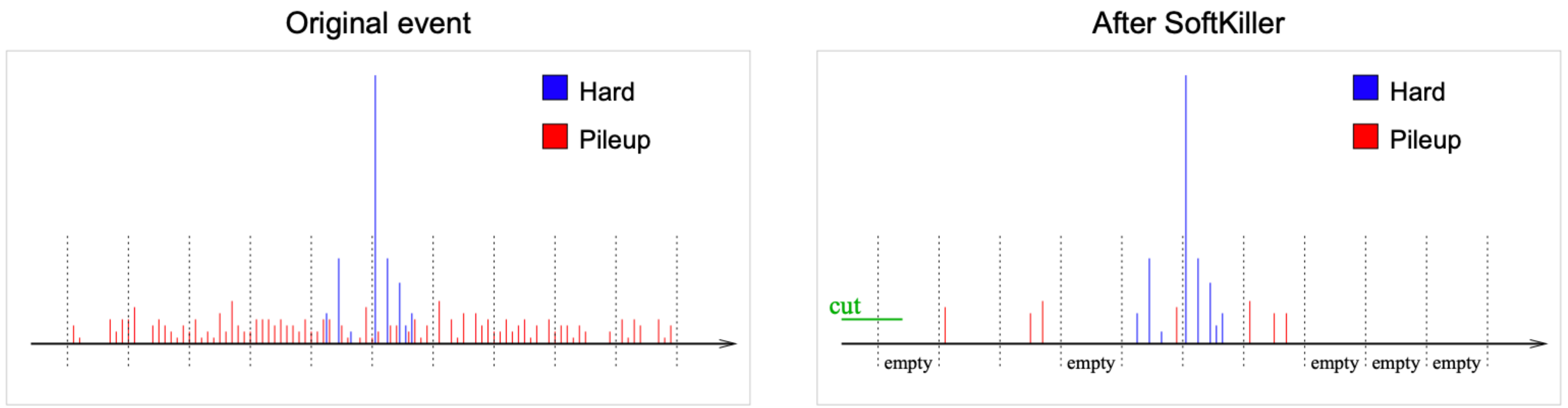
- Problem is how to identify pileup neutral particles and remove these

Classical PileUp Mitigation Techniques

- Run-I: Area-based pileup subtraction:
  - e.g., calculate the pileup energy density outside the jet cone; and use the average to correct jet energy



- Later on: Soft-Killer [Arxiv.1407.0408]
  - Pileup particles have lower pT; kill the pileup by removing "soft" particles
  - Calculate the median pT: $p_T^{\mathrm{cut}} = \mathrm{median}_{i \in \mathrm{patches}} p_{T,i}^{\max}$; cut on the median pT to remove pileup
  - pT is a particle's "self feature"; no strong connection with the other particles in the same event



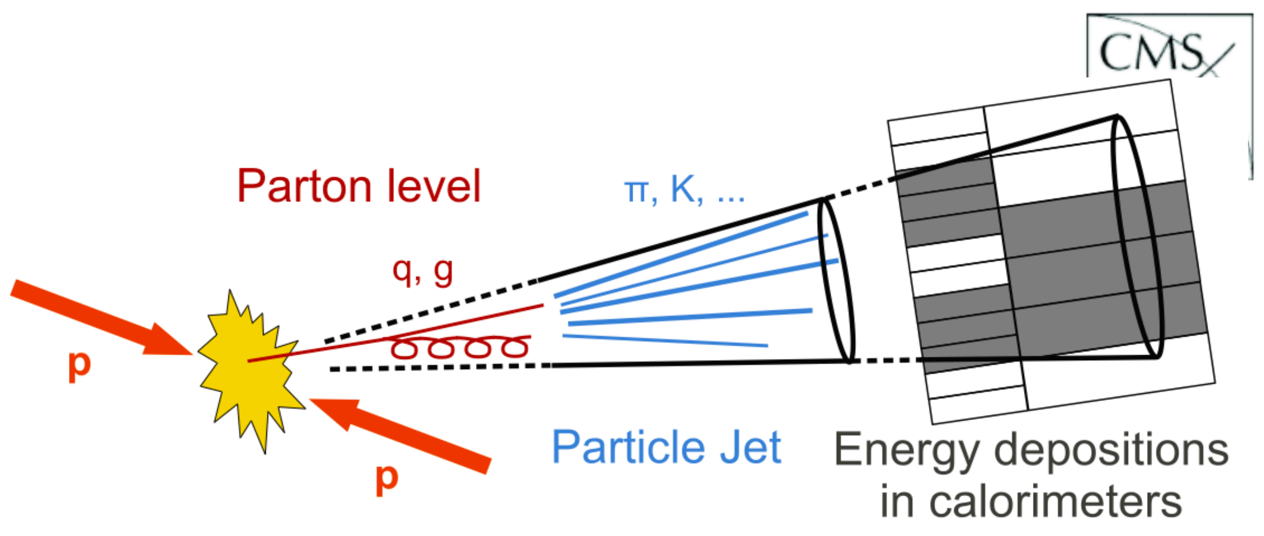
Classical PileUp Mitigation Techniques

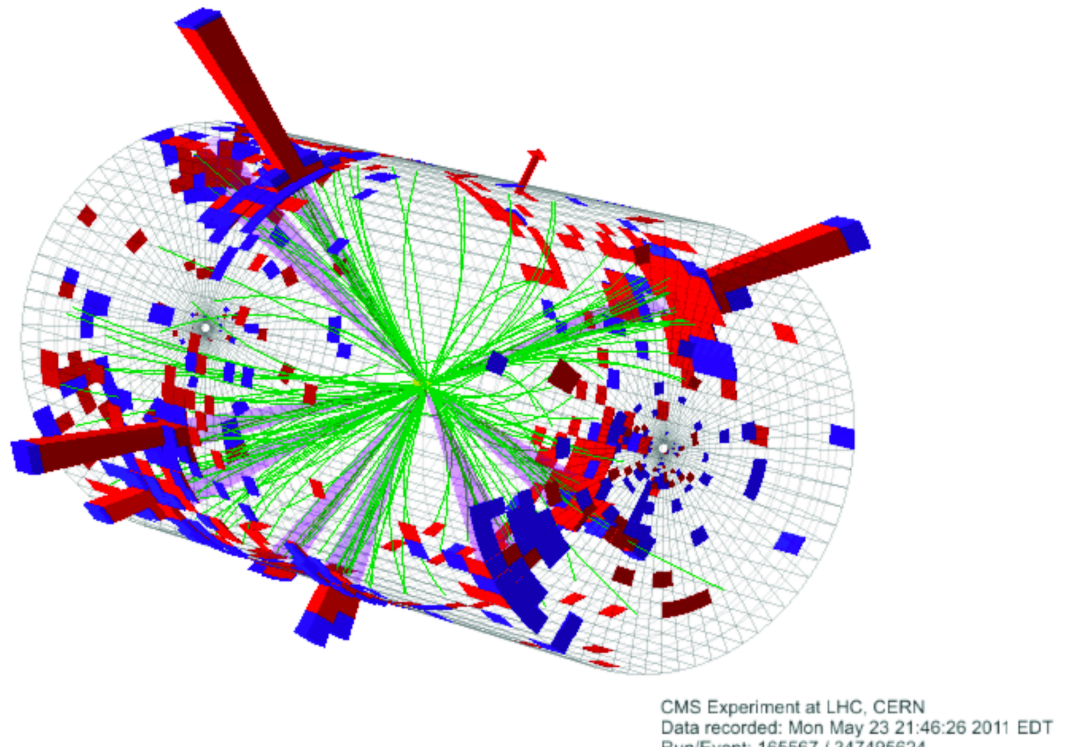
- PUPPI: [Arxiv:1407.6013]
  - Makes use of the neighboring particle features: LV particles are usually surrounded by LV particles; PU particles are more isotropic
  - Calculate a local shape variable alpha:

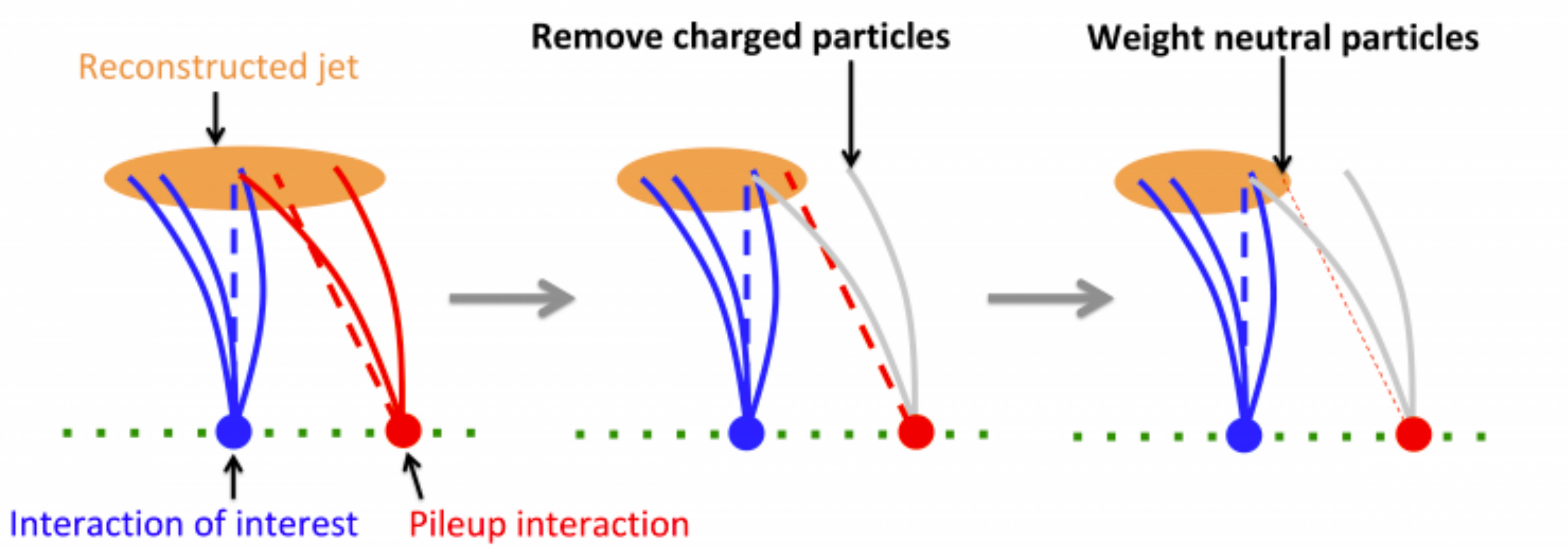
$$\alpha_i = \log \sum_{j \in \text{event}} \xi_{ij} \times \Theta(R_{\min} \leq \Delta R_{ij} \leq R_0),$$

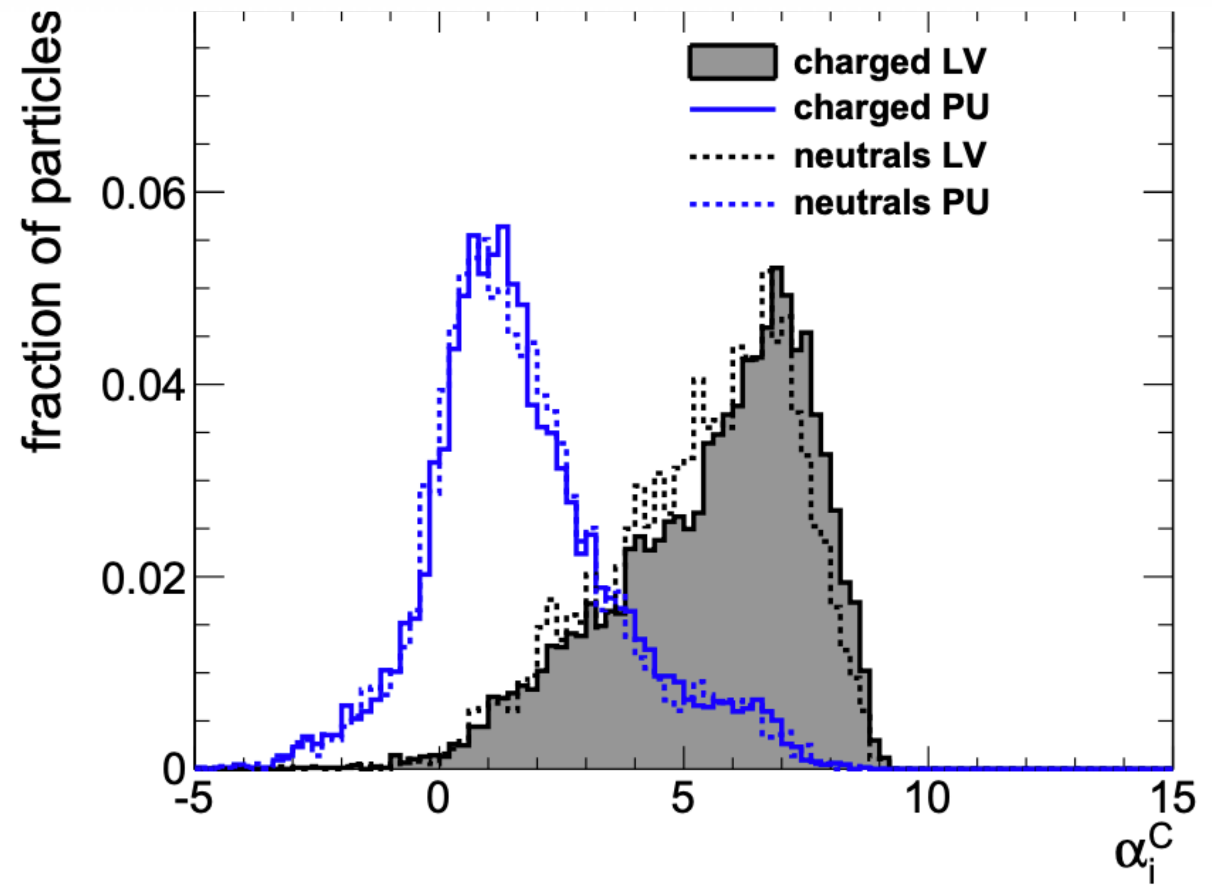
$$\text{where } \xi_{ij} = \frac{p_{Tj}}{\Delta R_{ij}}.$$

  - Alpha is aggregating information from the neighboring particles. e.g., aggregating ξ_{ij} only from the neighboring charged LV particles
  - Per-particle weight (PUPPI weight, in the range of 0-1) is calculated based on alpha; particle 4-momenta are rescaled based on the PUPPI weight









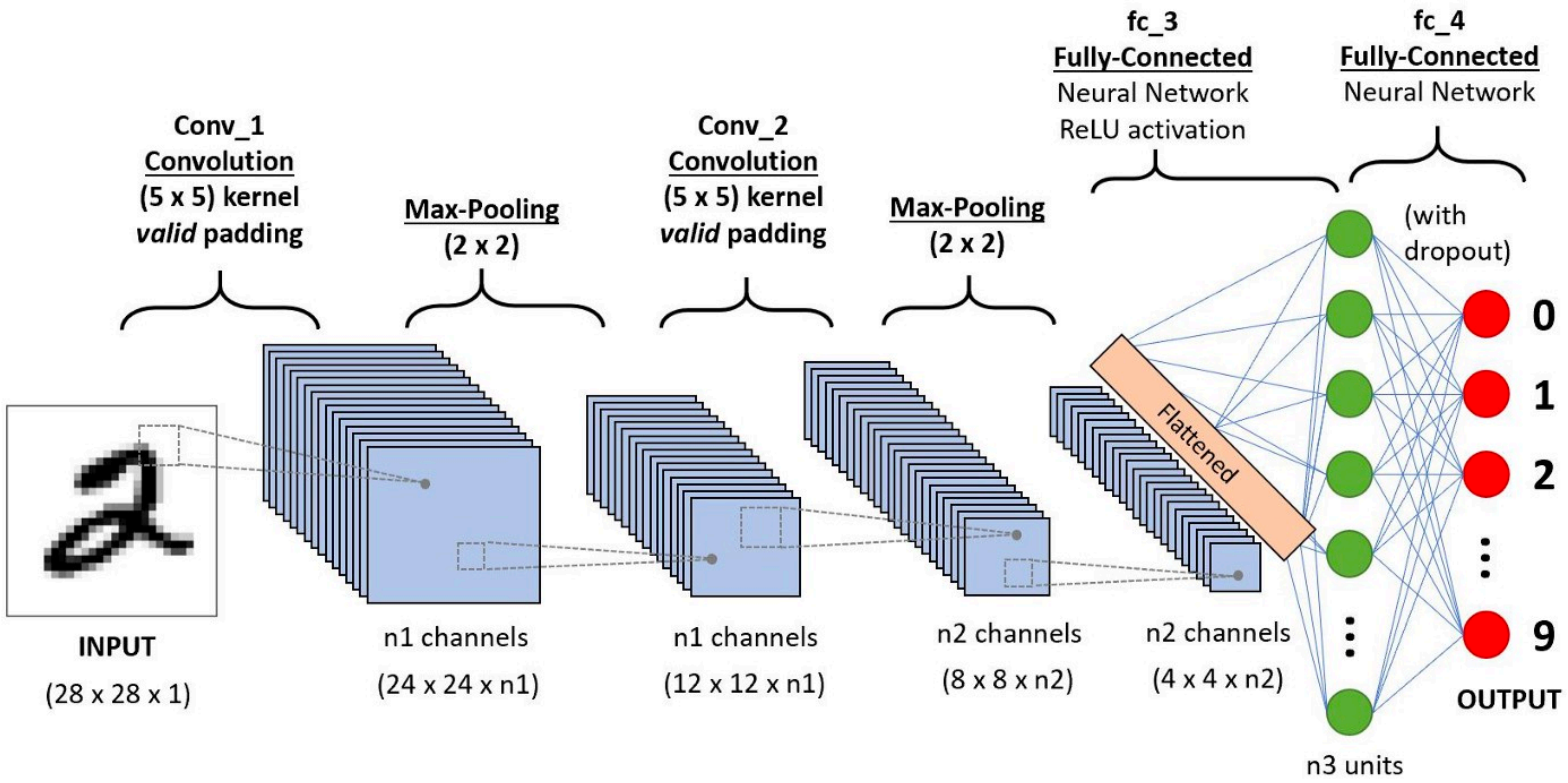
Learned From Classical Techniques

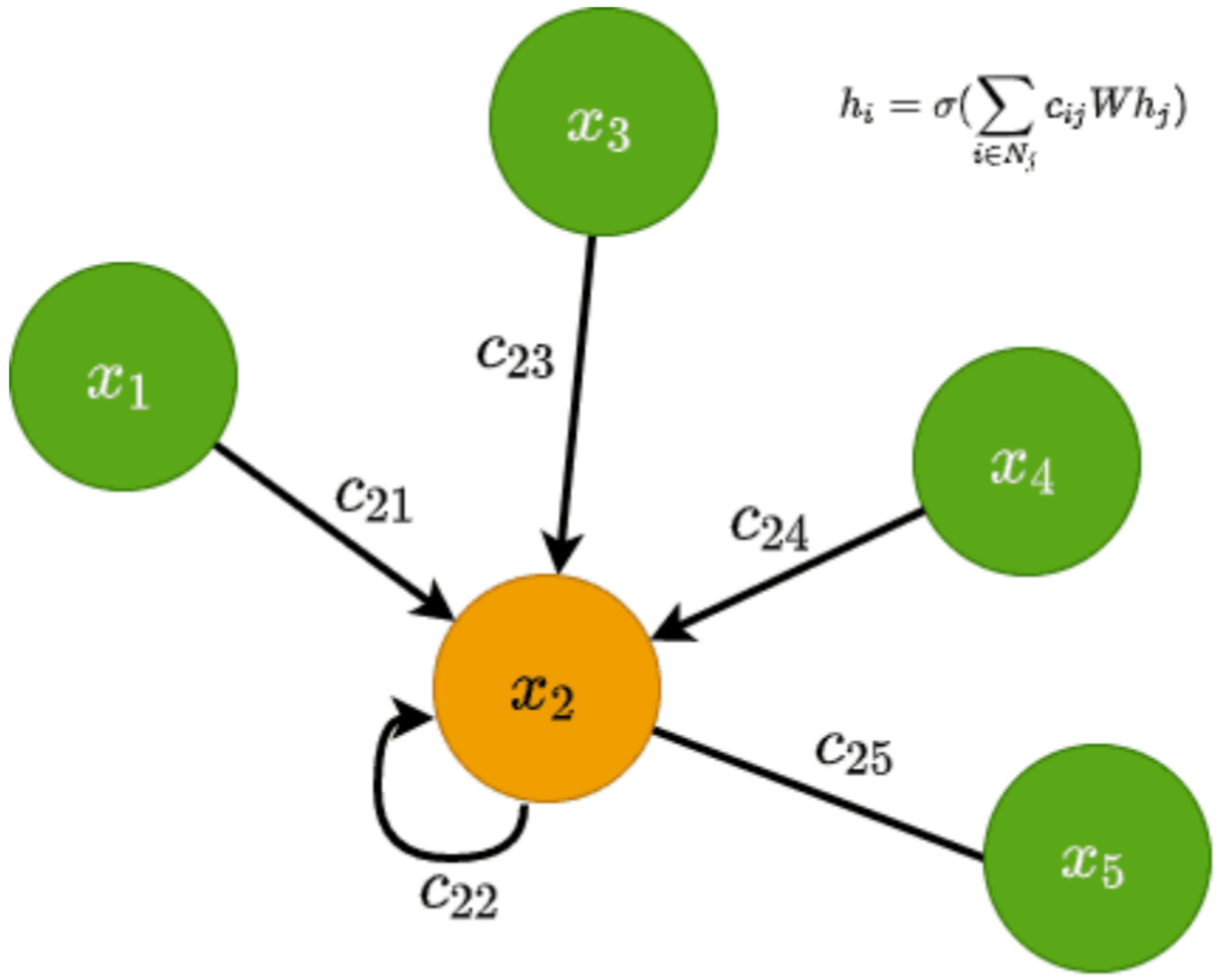
- Information we can use for pileup mitigation
  - Per-particle individual features: PU particles low pT; LV particles high pT; PU particles more in the forward region; LV particles more in the central region
  - Particle neighboring features: PU particle neighbors are more likely to be PU; LV particle neighbors are more likely to be LV

- To put together make use all such information together:
  - Combining particle individual features and neighboring features;
  - Avoid preselections, cut tunings, matrix selectetc

- GraphNN is an efficient and effective way to do this.

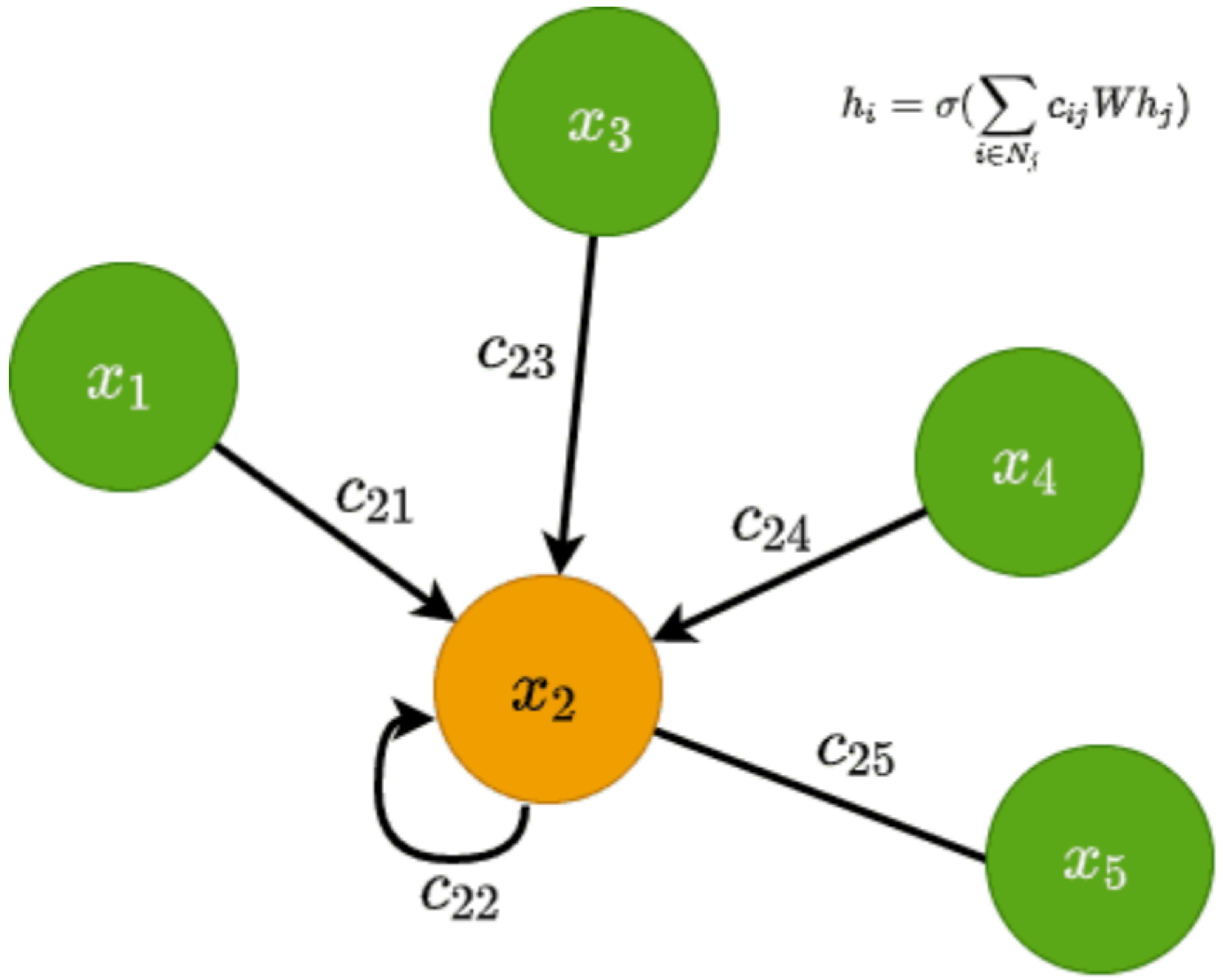
CNN -> GNN





- Convolutional Neural Networks work on Euclidean space and can aggregate information from the "real" neighbors adjacent to each target.
- Moving to Non-Euclidean space; do the similar type of "convolutions" to extract and aggregate information from neighboring particles -> Graph Neural Network (More general and more powerful)

Graph Neural Networks



- One Graph (G) has nodes (V) and edges (E): G = (V,E)
- For one node x_i, represented with h_i. the available information includes:
  - Target node itself: h_i
  - Neighboring nodes: $\{h_j\}$
  - Neighboring edges: $\{e_{ij}\}$
- "message passing". The node representation upgrade in the k-th iteration, is a function of $(h_i, \{h_j\}, \{e_{ij}\})$
  - $h_i^{k+1} = f(h_i^k, h_j, e_{ij})$
- Can aggregate information from both target node, neighboring node, and the edges
- Information upgrades have a lot of degrees of freedom;
  - Can include different types of symmetries in the expression; works very well on point-cloud data (HEP data is mostly point-cloud)

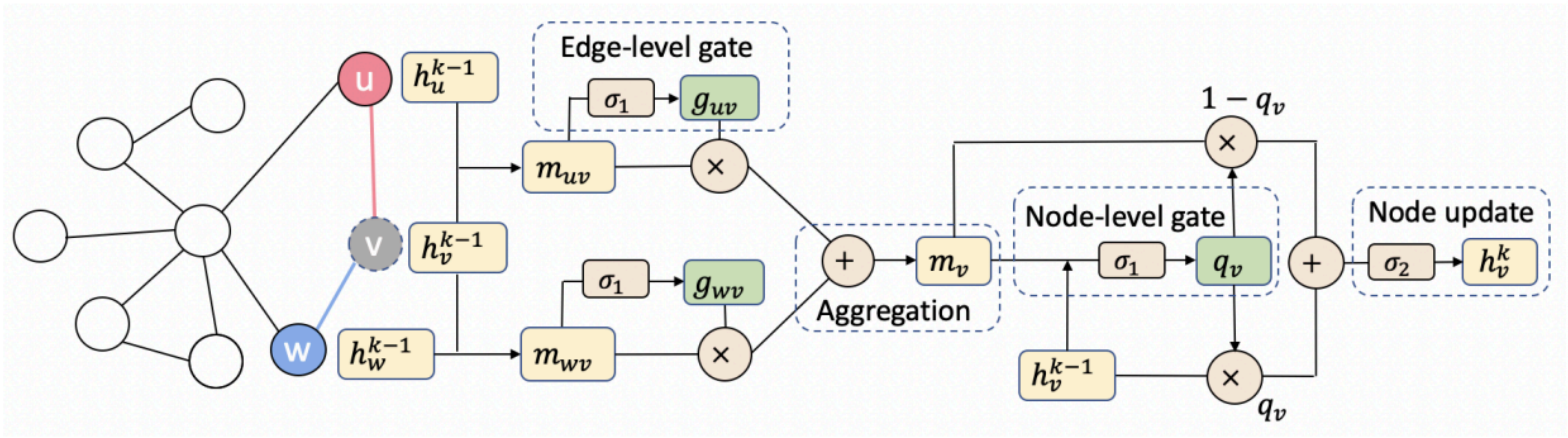
Typical Graph Neural Networks

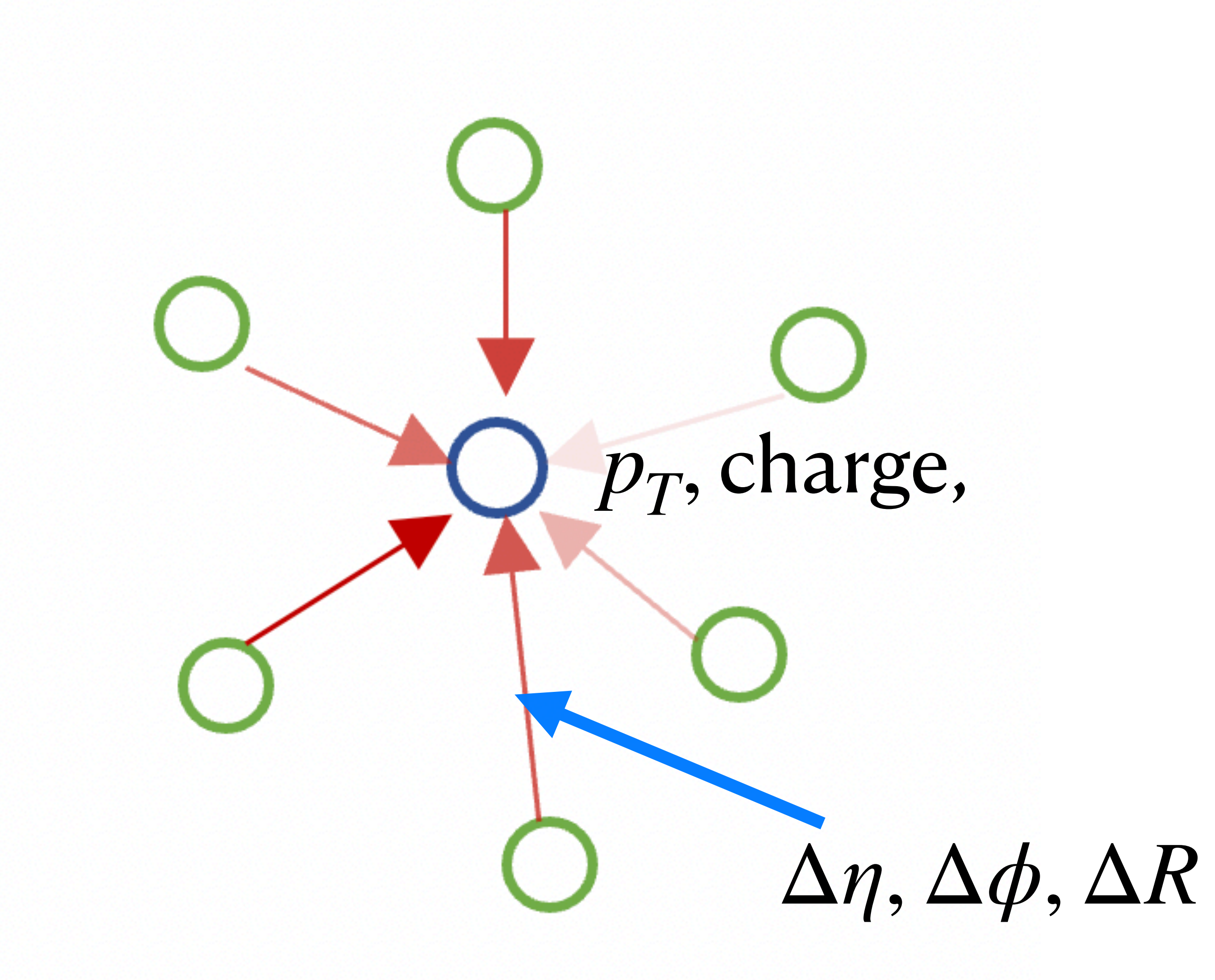
- GraphSage:
  - Poor the neighboring information together, combine with the target node information
  - $h_u^{k+1} = f(h_u^k, \{h_{v_j}^k\}, \{e_{u,v_j}^k\}) = \sigma(h_u^k w_1^k + \sum_{v_j} h_{v_j}^k w_2^k)$

- Gate models:
  - Add one gate G_u^k to control the message passing ("importance"):
  - $\bar{h}_u^{k+1} = f(h_u^k, \{h_{v_j}^k\}, \{e_{u,v_j}^k\})$
  - $h_u^{k+1} = G_u^k \bar{h}_u^k + (1 - G_u^k) h_{v_j}^k$, where $G_u^k = Sigmoid(\bar{h}_u^k, h_u^k)$ is in the range of 0-1

- Attention models:
  - "Attention" to different nodes and edges
  - $\sum_{v_i} h_{v_i}^k \rightarrow \sum_{v_i} \mathrm{Att}_{u,v_j}^k h_{v_j}^k$, where $\sum_{v_i \in N} \mathrm{Att}_{uv_j}^k = 1$ for normalization

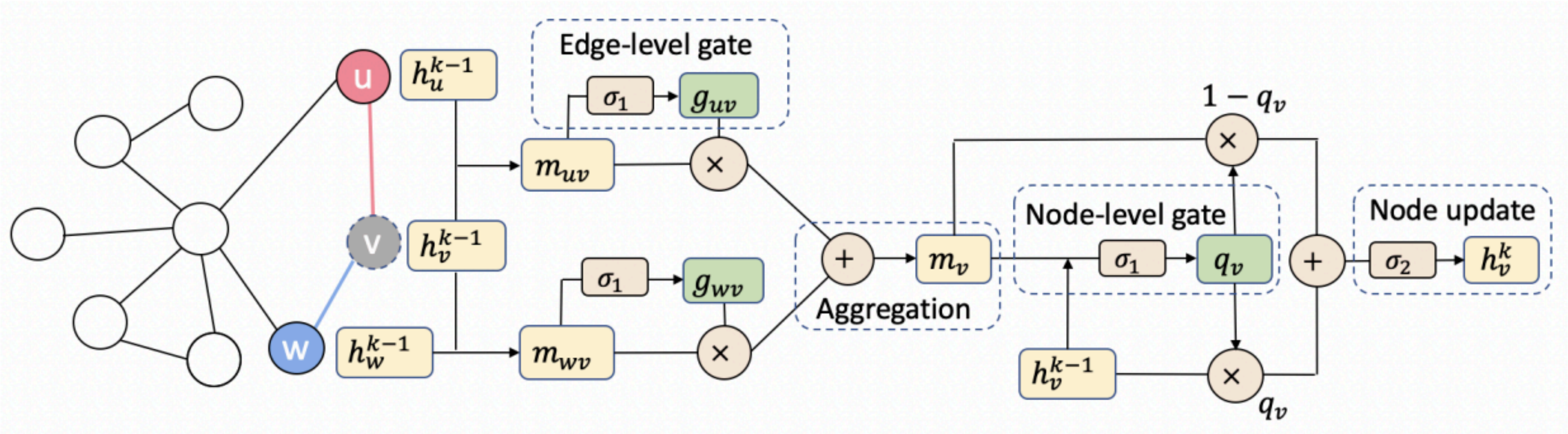
Our Model Architecture

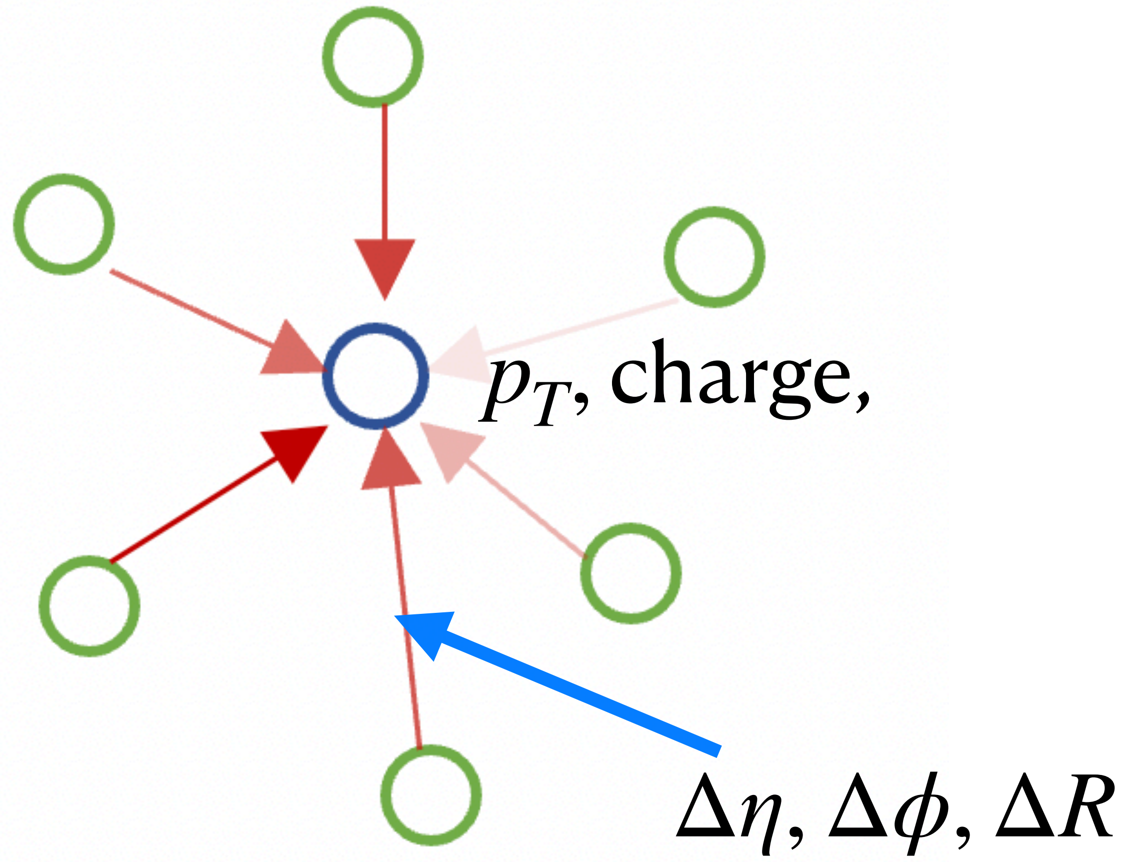




- Build graph in $\eta - \phi$ space. Connect the particles in the $\Delta R = 0.4/0.8$ cone.Input features:
  - Node features: p_T , charge
  - Edge features: $\Delta\eta$, $\Delta\phi$, and ΔR between particles
- Outputs are a weight between 0 and 1, representing the probability that the particle is produced from the LV
- Model architecture: gated model

Our Model Architecture





Message formulation: $m_{uv} = \left[h_u^{k-1}, h_v^{k-1}, \Delta\eta_{uv}, \Delta\phi_{uv}, \Delta R_{uv}, h_g^{k-1}\right]$,

Aggregation: $m_v = \sum_{u \in N(v)} g_{uv} m_{uv}$, where $g_{uv} = \mathrm{Sigmoid}(W_1 m_{uv} + b_1)$

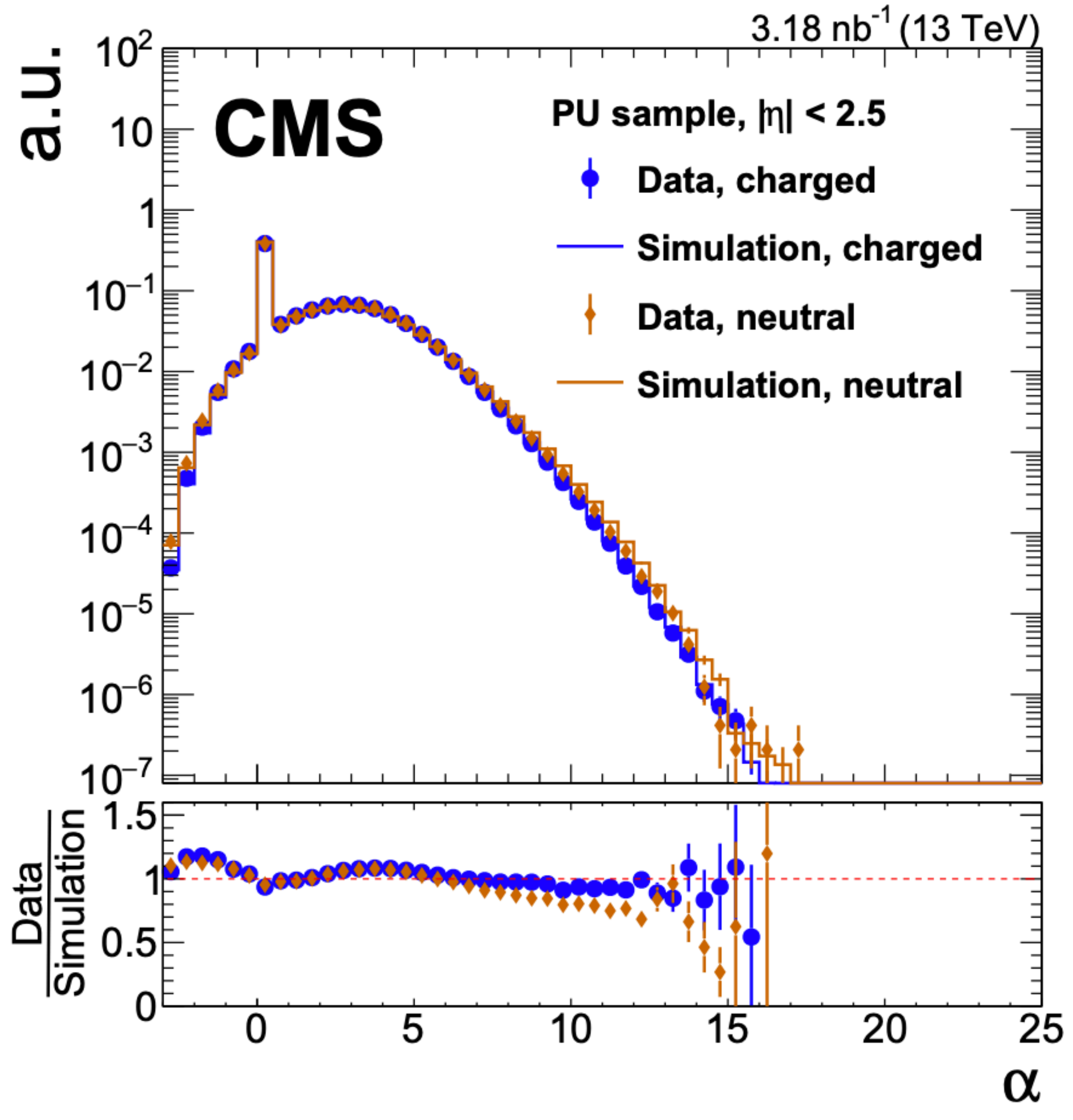
Node-level gate: $q_v = \mathrm{Sigmoid}(W_2[h_v^{k-1}, m_v] + b_2)$

Node update: $h_v^k = \mathrm{ReLU}(q_v(W_3 h_v^{k-1} + b_3)) + (1 - q_v)(W_4 m_v + b_4))$,

Semi-Supervised Learning

- To operate at particle level, the current ML models would require the prior knowledge of whether the particle is produced from PU or LV, as the ground truth information
  - For charged particles, it is easy to retrieve, even in the real data
  - For neutral particles, currently very hard to recover truth information, sometimes mixed LV/PU; no truth information in the real data

- How about we train the model using the charged particles, and then do inference on neutral particles?
  - This semi-supervised ML method would allow us to train directly on real data/ full simulation, without worrying about the labels for the ground truth information
  - This semi-supervised training strategy would work on different ML models and architectures



Masking & Training Details

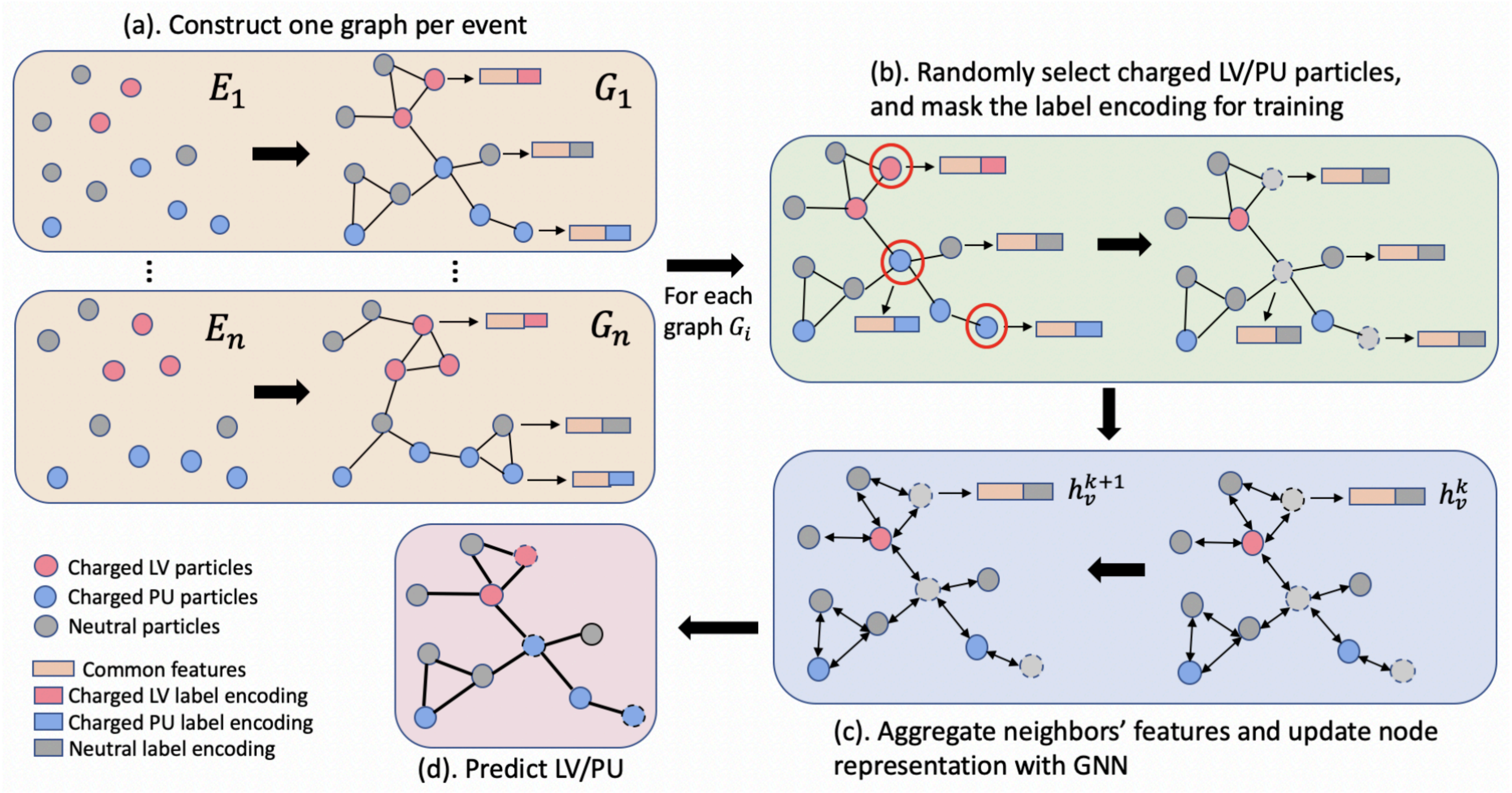


Figure 1: A diagram illustrating the SSL model training flow

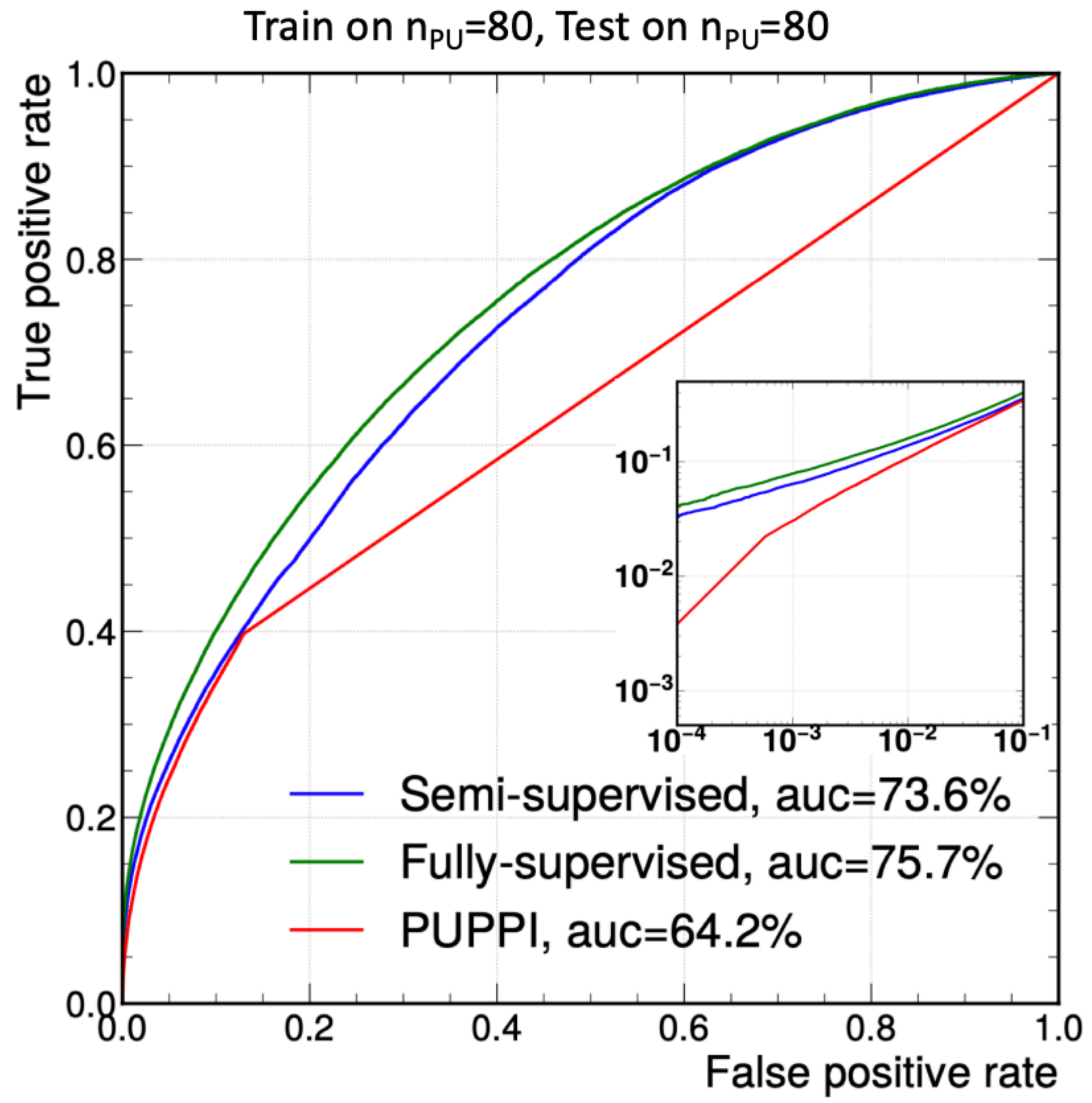
- Build graph in $\eta - \phi$ space
- Randomly select and mask a subset of charged particles
- Train on these charged particles
- Move to the next event and repeat

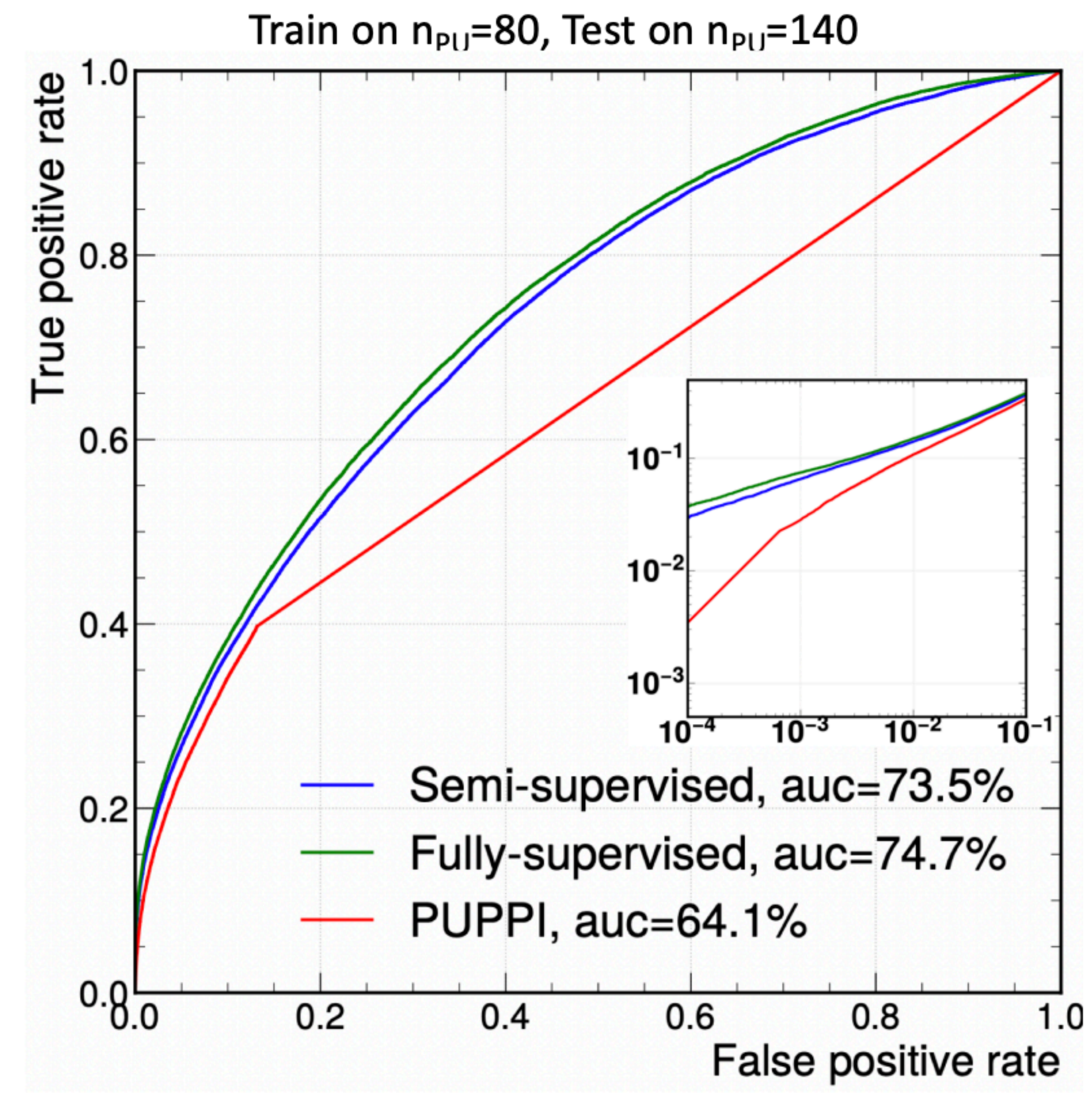
Training Datasets

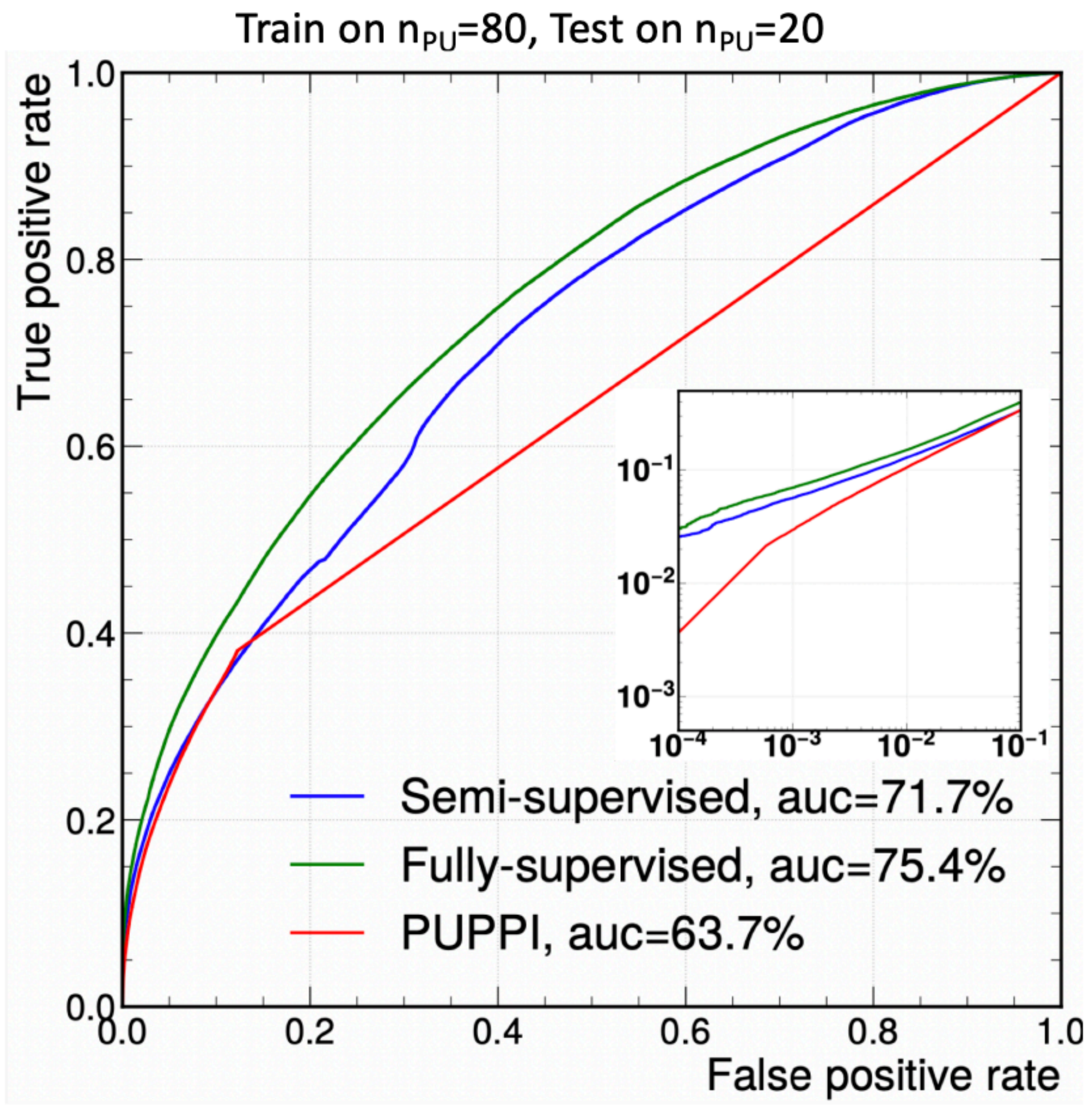
- Using similar setup as the PUPPIML
  - Pythia 8.223 + Delphes 3.3.2 for simulation
  - $Z(\nu\nu)$+jets signal processes
  - Pythia-generated QCD events as pileup; Poisson distribution sampled with the average pileup of 80 and 140
  - Charged particle flag for the LV and PU is set to be perfect
- Number of different particles per event at PU=80 (with pT>0.5GeV cut)

# Particles	Charged	Neutral
LV	85	50
PileUp	1600	800

Per-Particle Performances

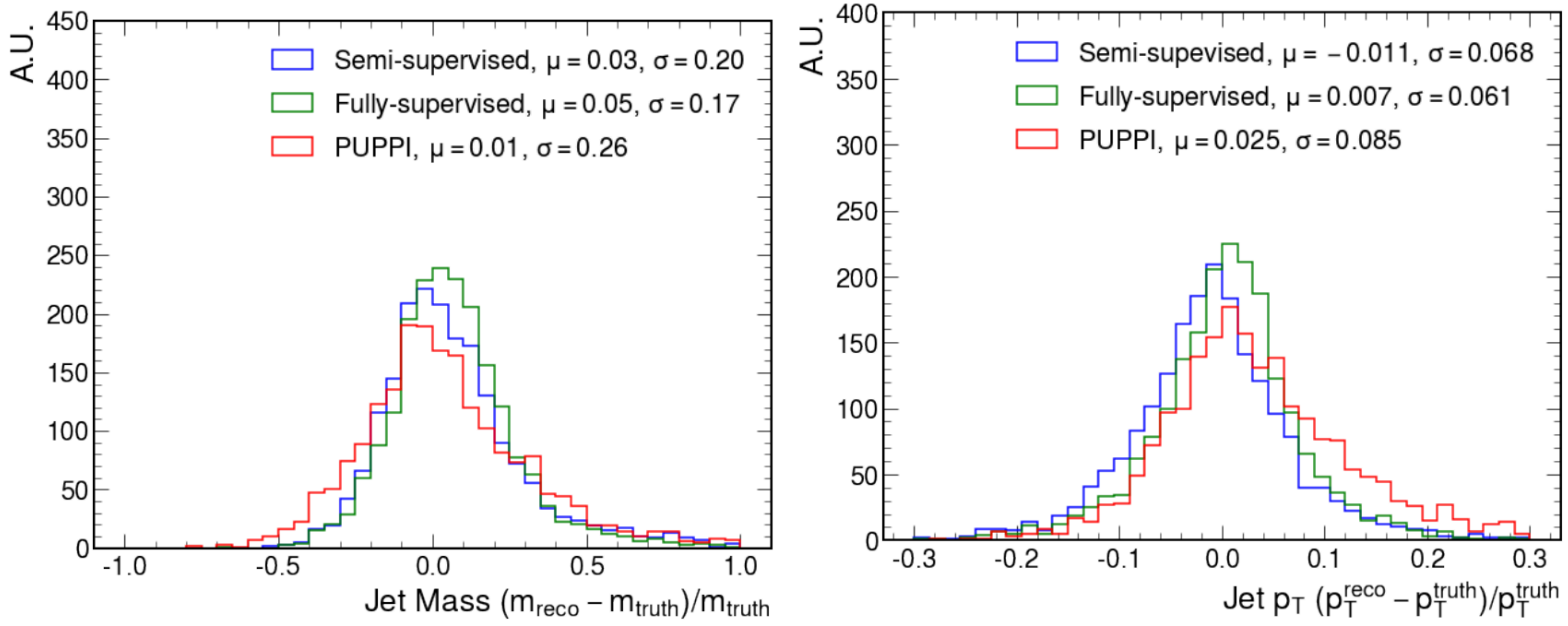






- Train on nPU=80; test on nPU=80; both supervised and semi-supervised outperforms PUPPI; supervised and semi-supervised results are close
- Train on nPU=80, still performs well on nPU=149 and nPU=20

Performance on Jet Mass, pT (PU80)



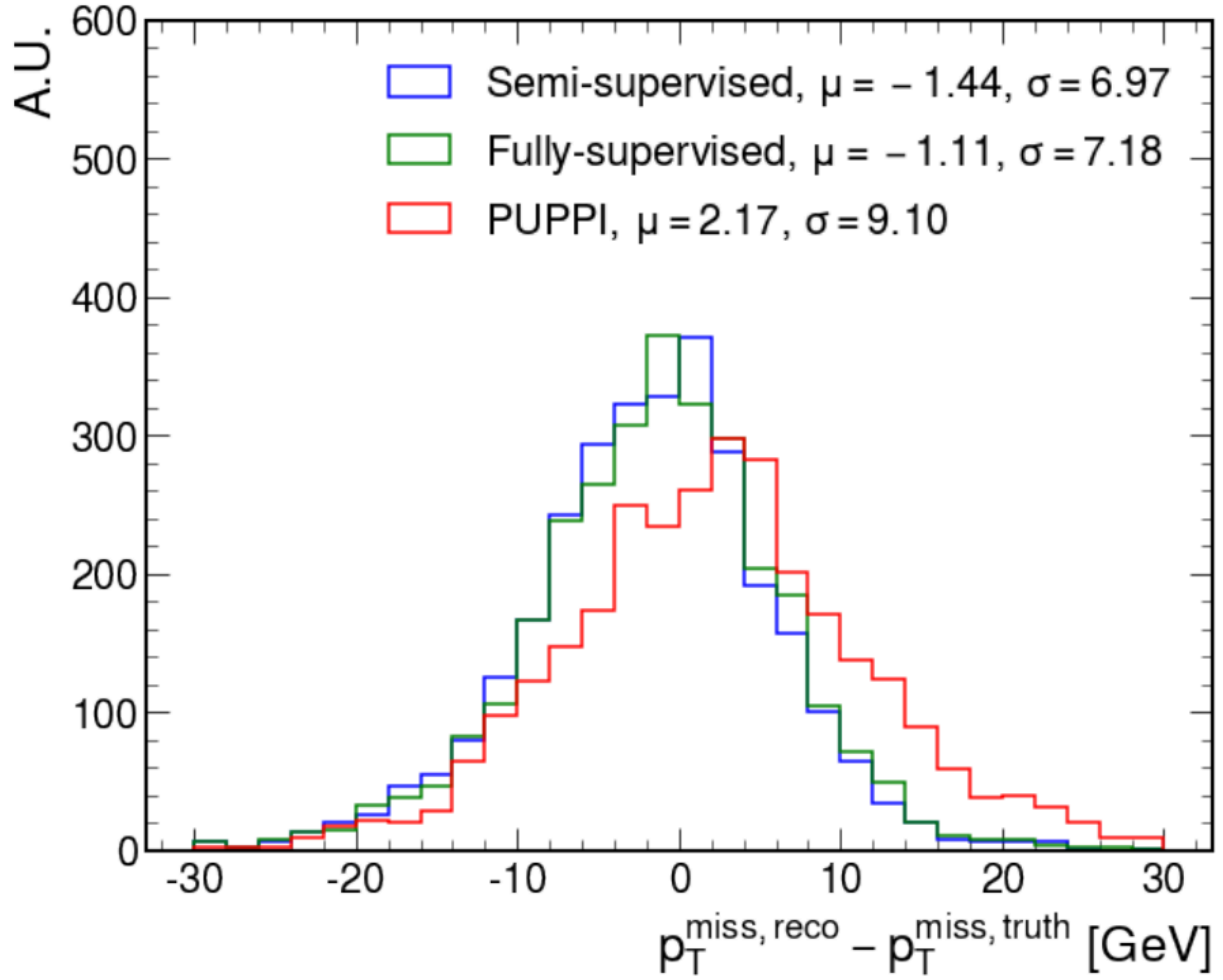
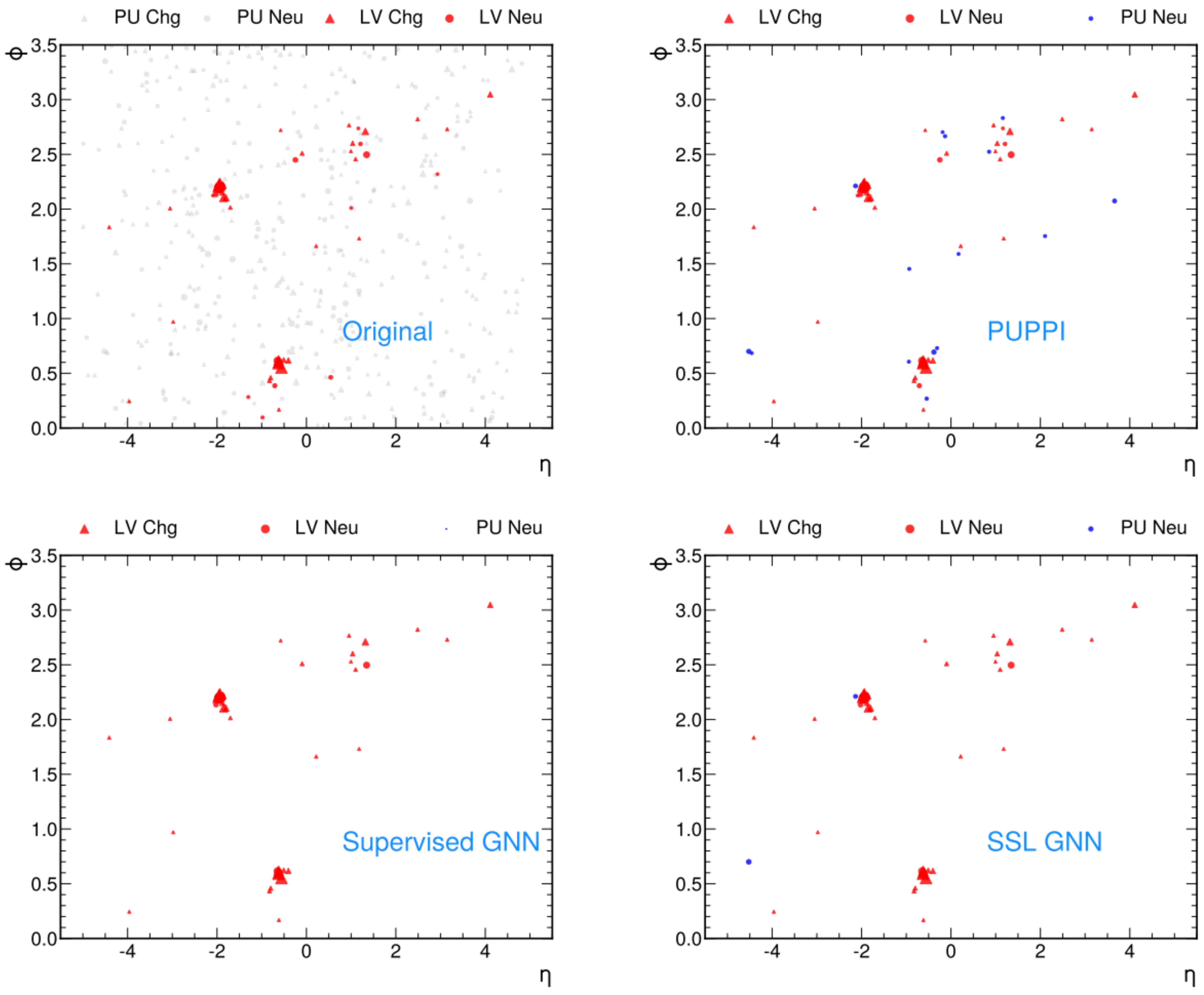


Figure 4: Performance on jet mass and jet p_T with different pileup mitigation techniques for $n_{PU} = 80$.

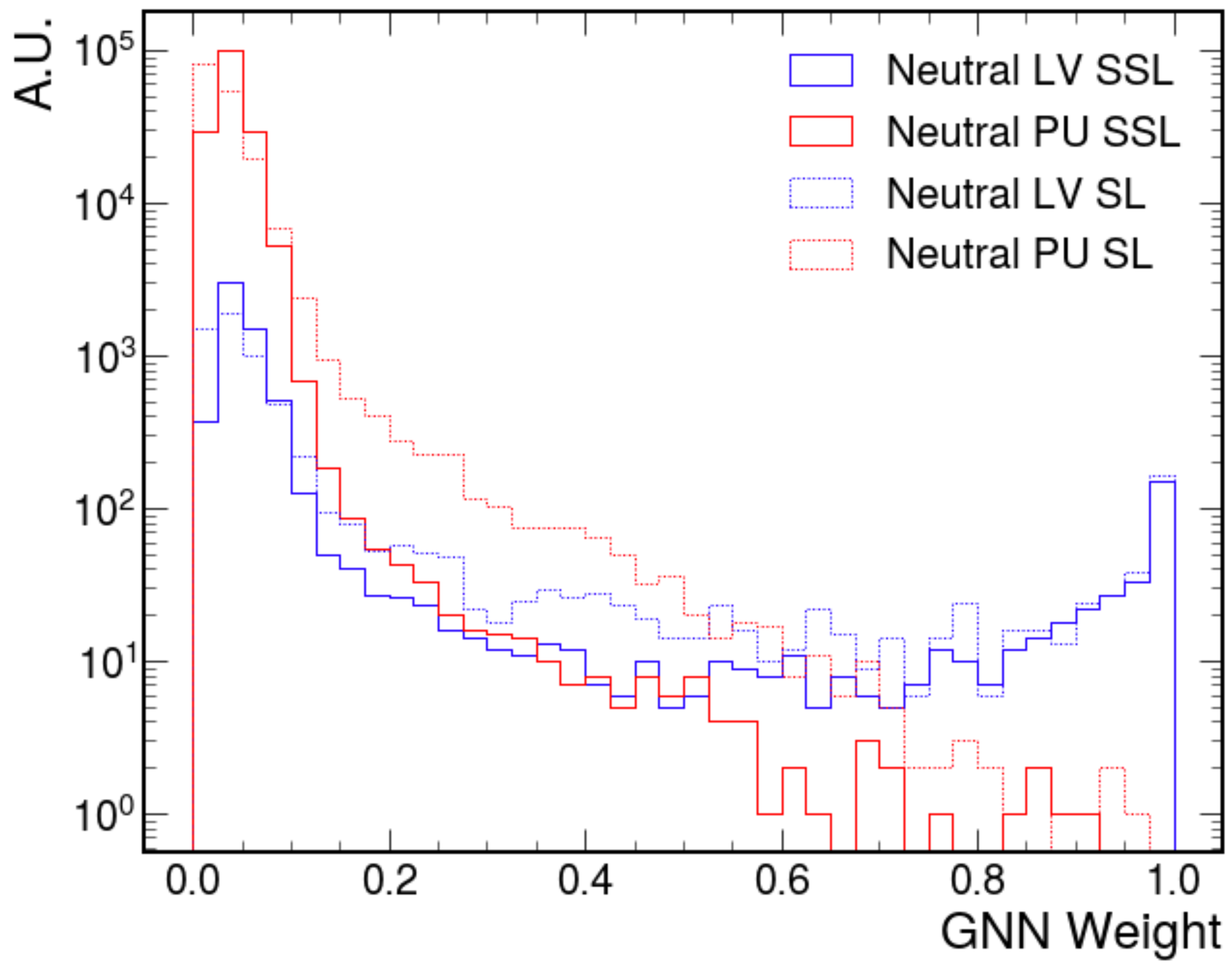
- Similar performances on jets and MET for supervised and semi-supervised; both are better than PUPPI

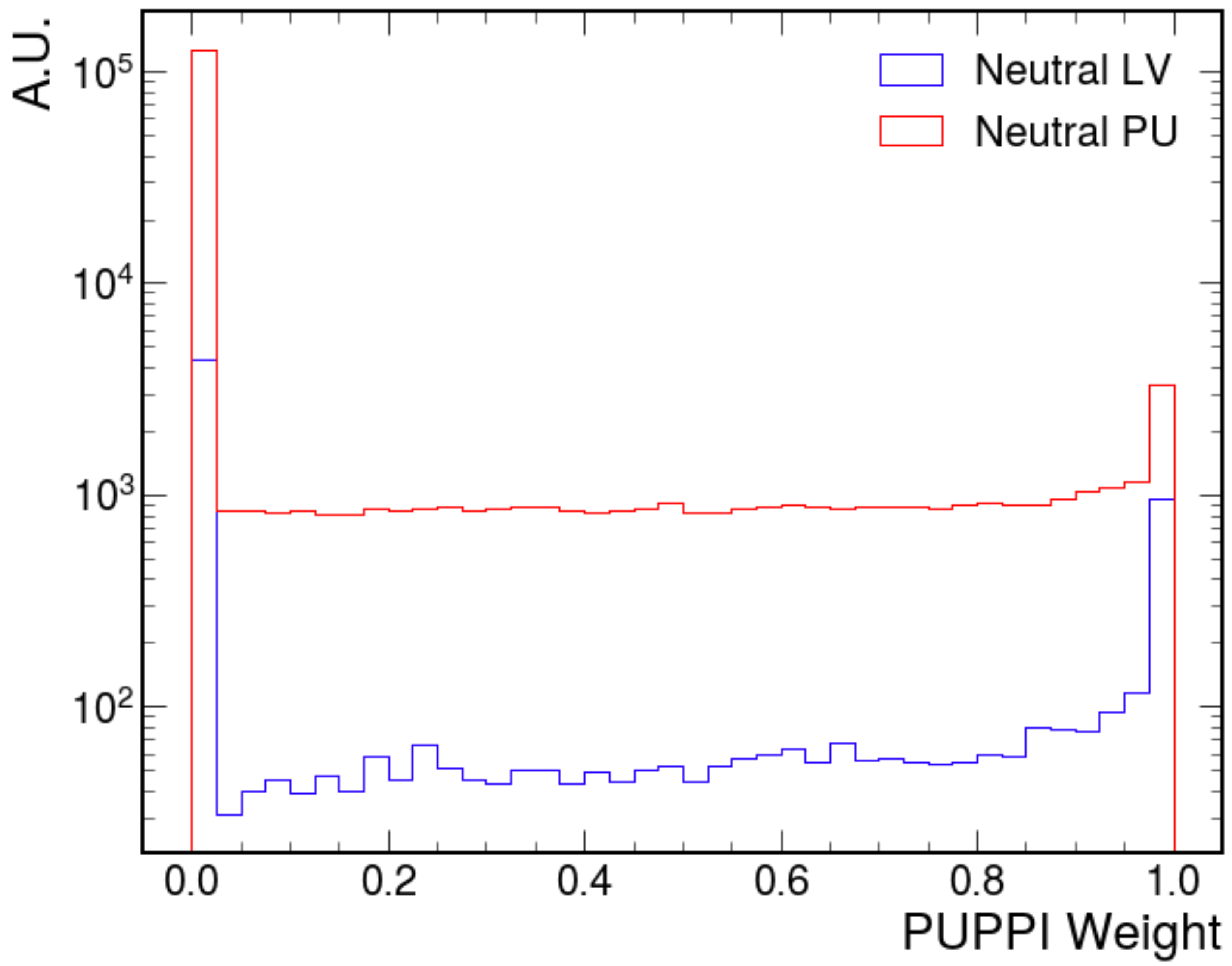
Event Display



- One event display example
- Supervised and Semi-supervised clean the pileup more effective than PUPPI
- Supervised and semi-supervised are similar

GNN Weights on Neutral Particles





- GNN Weights of neutral particles from the LV (blue) and pileup (red) on the left; right plot is the PUPPI weight distribution as a reference
- Much smaller fraction of particles get a weight around 1.
- Compared with Supervised training, the semi-supervised training seems to tend to have fewer particles in the middle weight range

Summary

- Presented the study of applying semi-supervised training for pileup mitigation with GraphNN, where the training is done on charged particles, and the inference is on neutral particles

- Results look very promising
  - Better ROC curve and resolutions on jet mass and MET for both supervised training and semi-supervised training
  - No significant performance drop going from supervised to semi-supervised

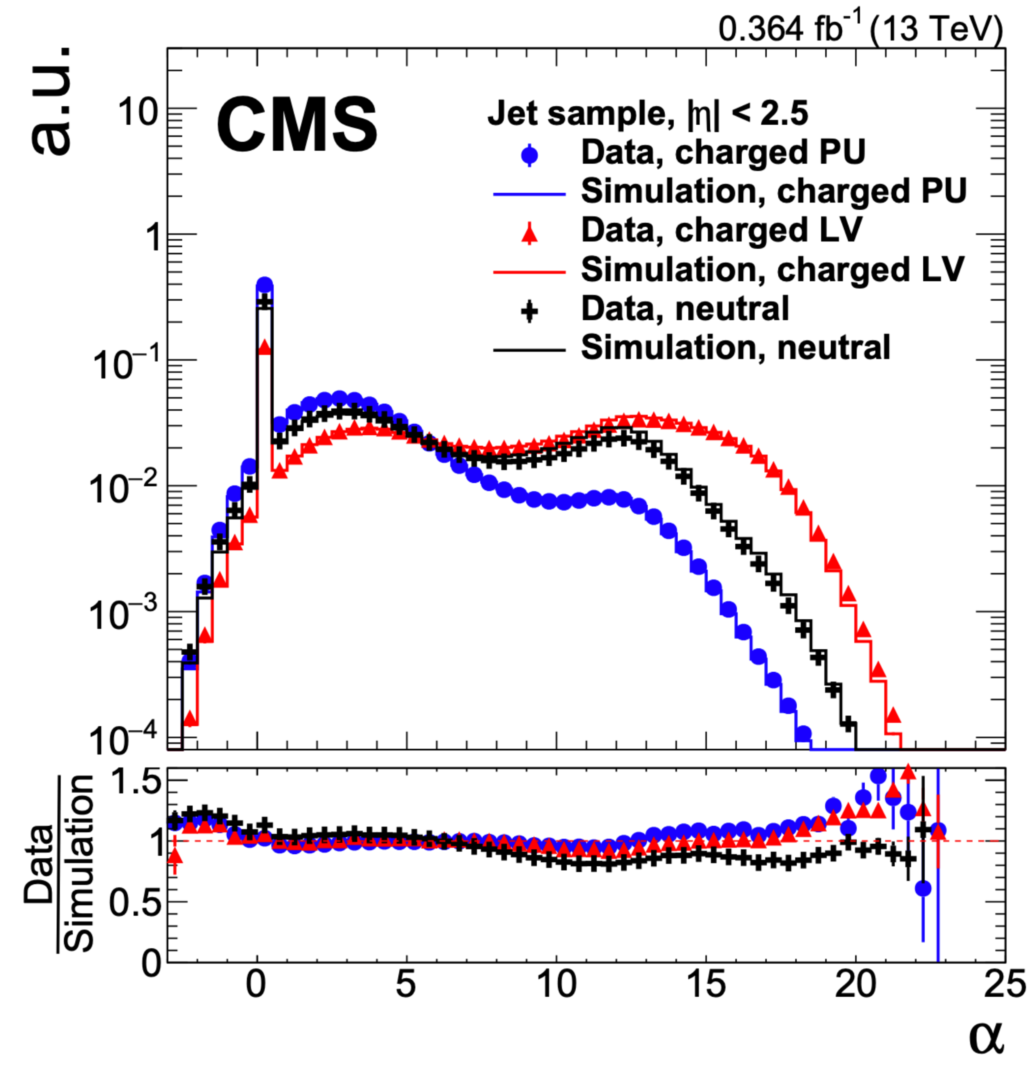
- Working on the evaluations on the CMS full-simulations; more features to explore; more realistic conditions and challenges to handle.

Back Up

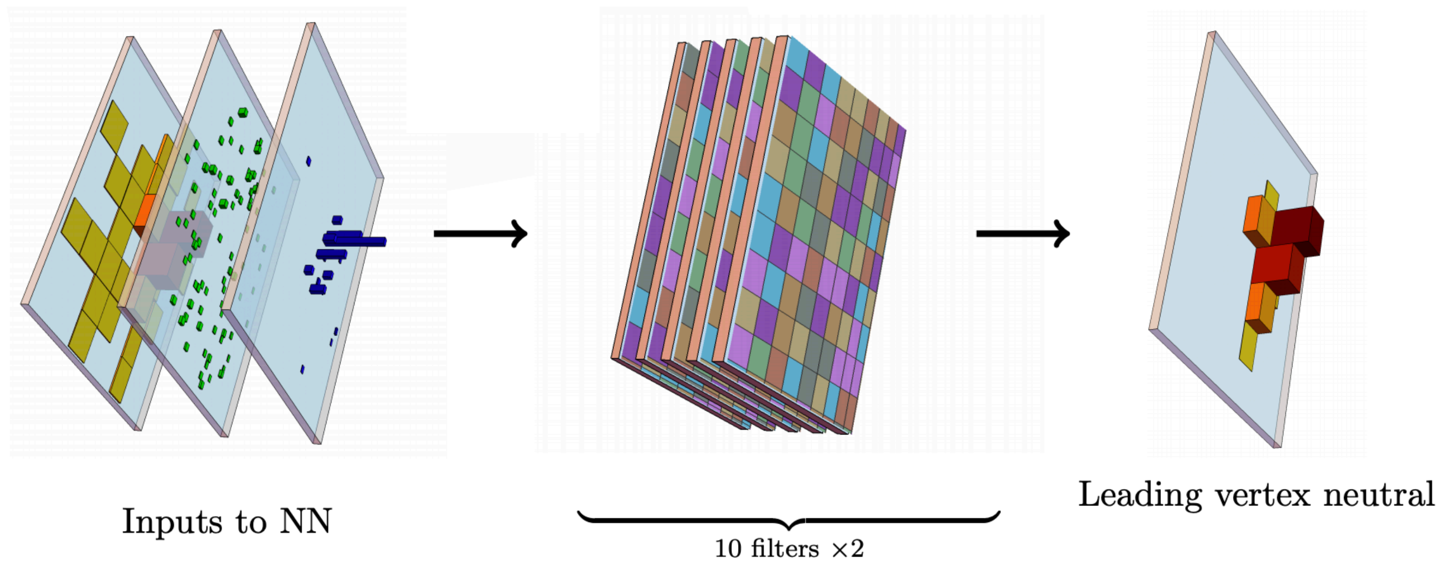
Introduction: Pileup Mitigation Studies

- Most charged leading vertex (LV) and pileup (PU) particles can be identified (Charged hadron subtraction, CHS)
- Particle self features: PU particles have lower-pT -> SoftKiller
- Particle neighboring features: PUPPI. A local shape variable α is defined and PUPPI weights are calculated based on α

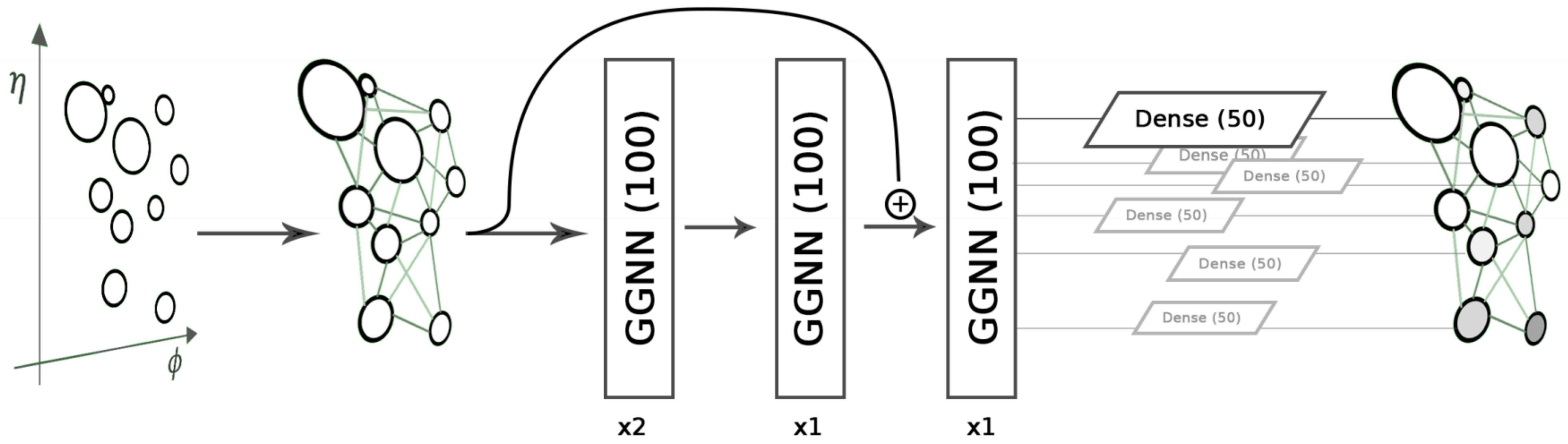
$$\alpha_i = \log \sum_{j \in \text{event}} \xi_{ij} \times \Theta(R_{\min} \leq \Delta R_{ij} \leq R_0), \quad \text{where } \xi_{ij} = \frac{p_{Tj}}{\Delta R_{ij}}.$$



- Pileup Mitigation with ML (PUMML, arxiv 1707.08600): Convolutional neural network on jet image



- Gated Graph Neural Network for PUPPI (PUPPIML, arxiv.1810.07988): GGNN on particle graph
- Other graph/attention models: (ABCNet, arxiv.2001.05311), (PUMA: with transformer, arxiv.2107.02779)



More Event Display

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