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Chinese Academy of Sciences

Status of TOTAL model for Pileup study

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Quantum Computing and Machine Learning Workshop

based on arXiv:2211.02029

Outline

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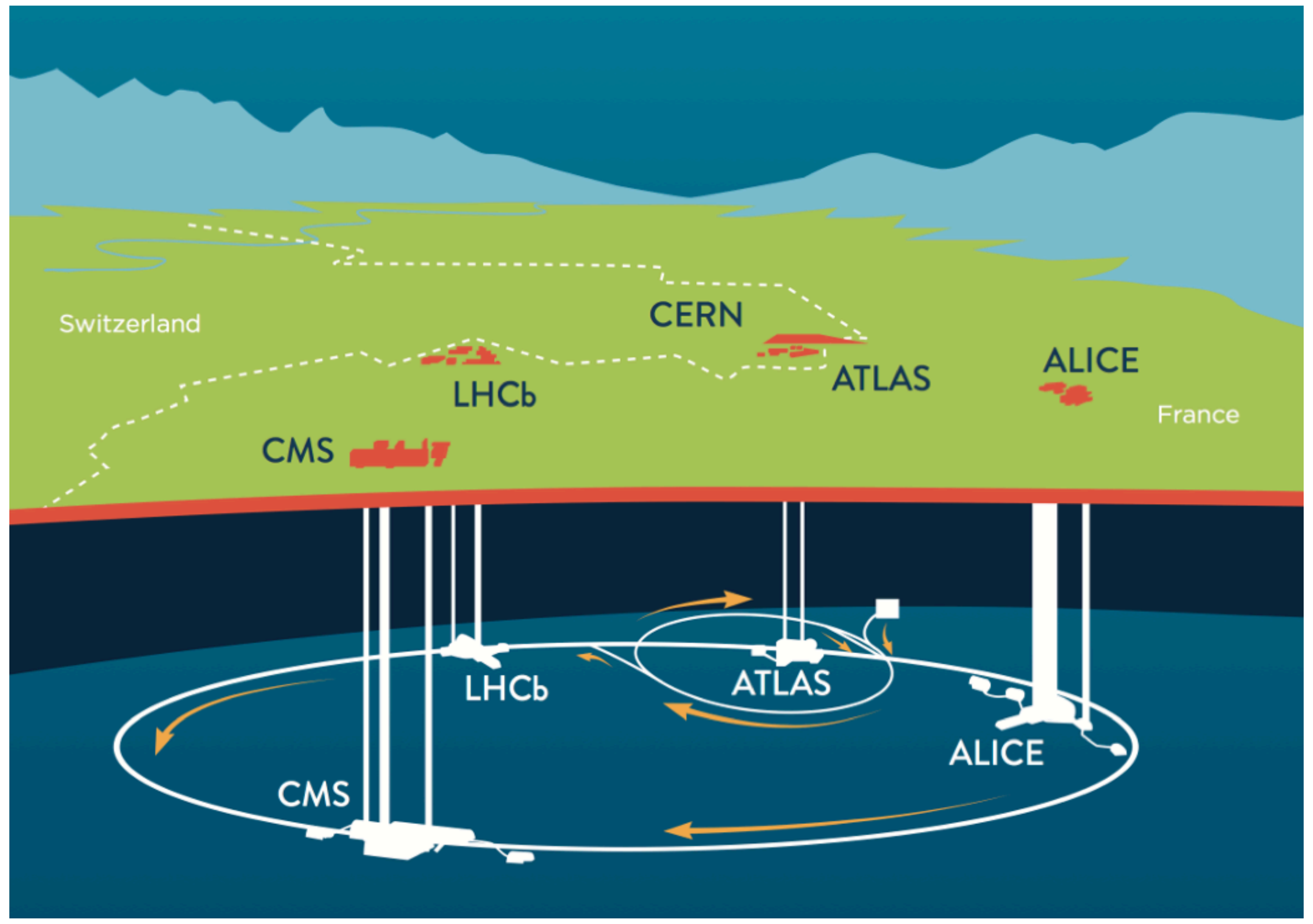
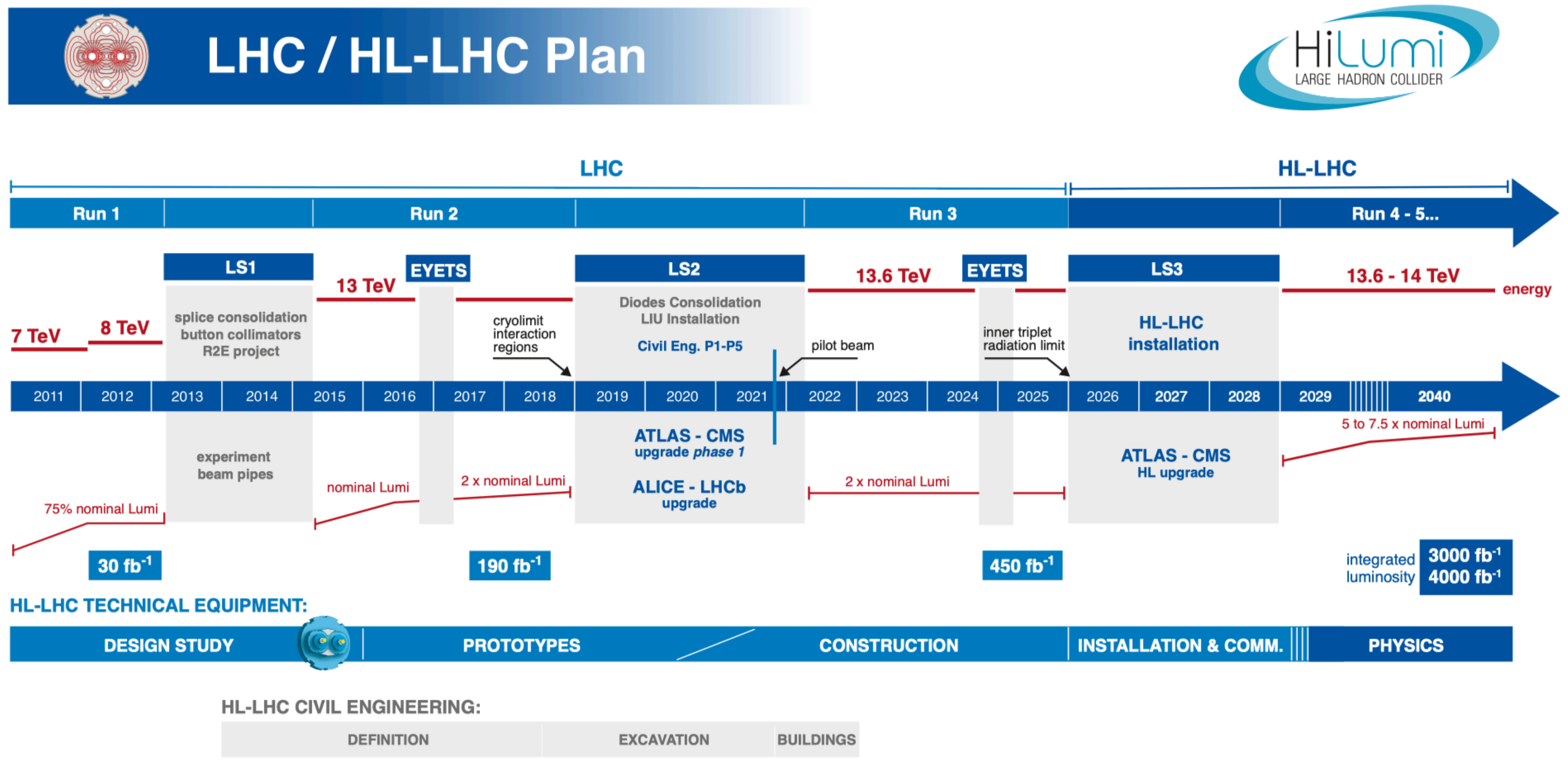
* Pileup in LHC
* TOTAL algorithm
* Performance comparison
* Summary

LHC

- Large Hadron Collider（LHC）：
  - A circular proton collider with a circumference of 27 kilometers, located about 100 meters below the French-Swiss border.
  - 4 Experiments： CMS， ATLAS， LHCb， ALICE
  - Centre of mass energy：
    - First Run（Run1）： 7-8 TeV
    - Second Run（Run2）： 13 TeV
    - Third Run （Run3）： 13.6 TeV
    - Future： 14 TeV
  - Luminosity：
    - First Run（Run1）： 30 fb^{-1}
    - Second Run（Run2）： 190 fb^{-1}
    - Third Run（Run3）： 450 fb^{-1}
    - Future： 3000~4000 fb^{-1}



LHC and 4 experiments



LHC Plan

Pileup in LHC

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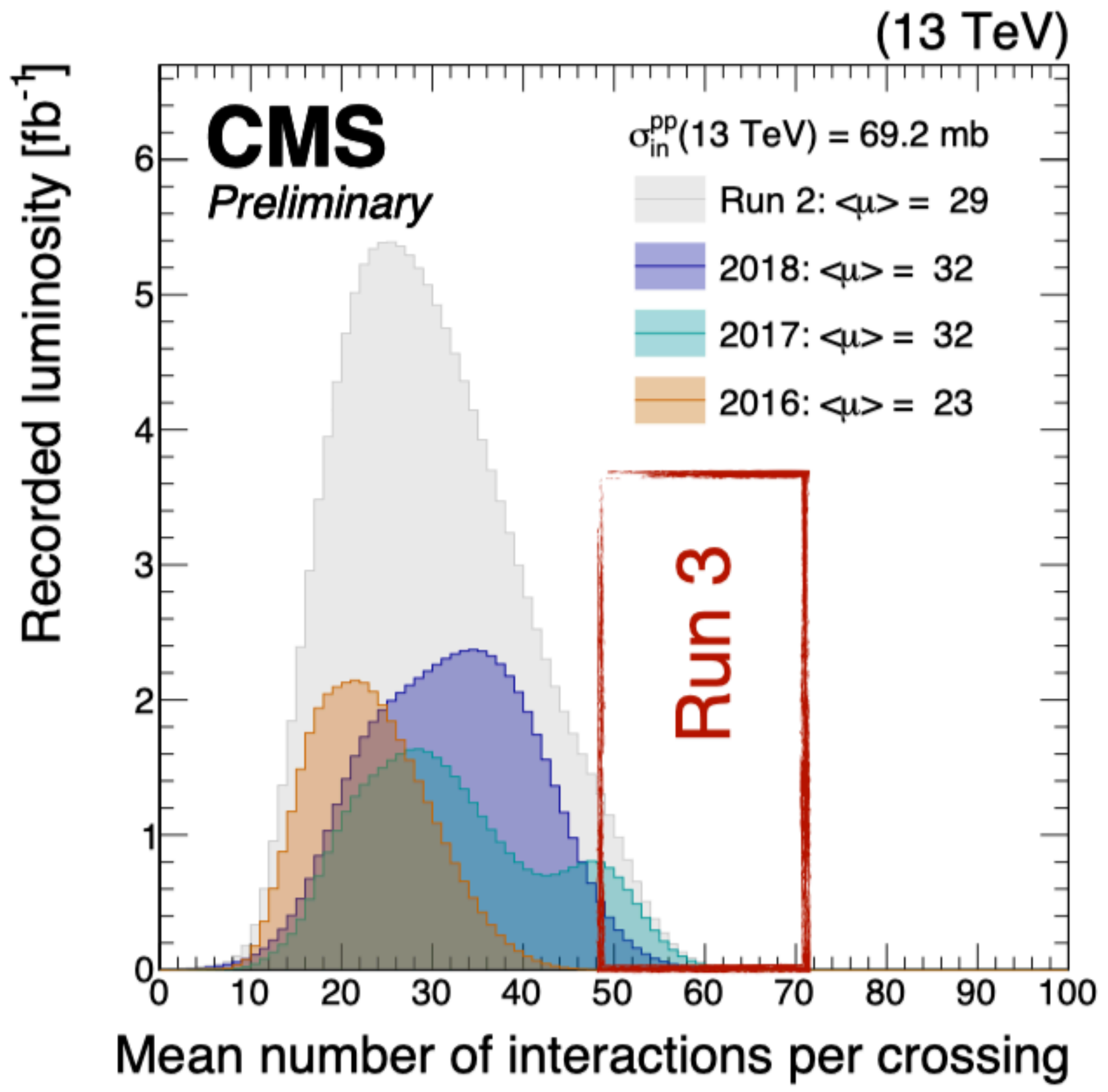

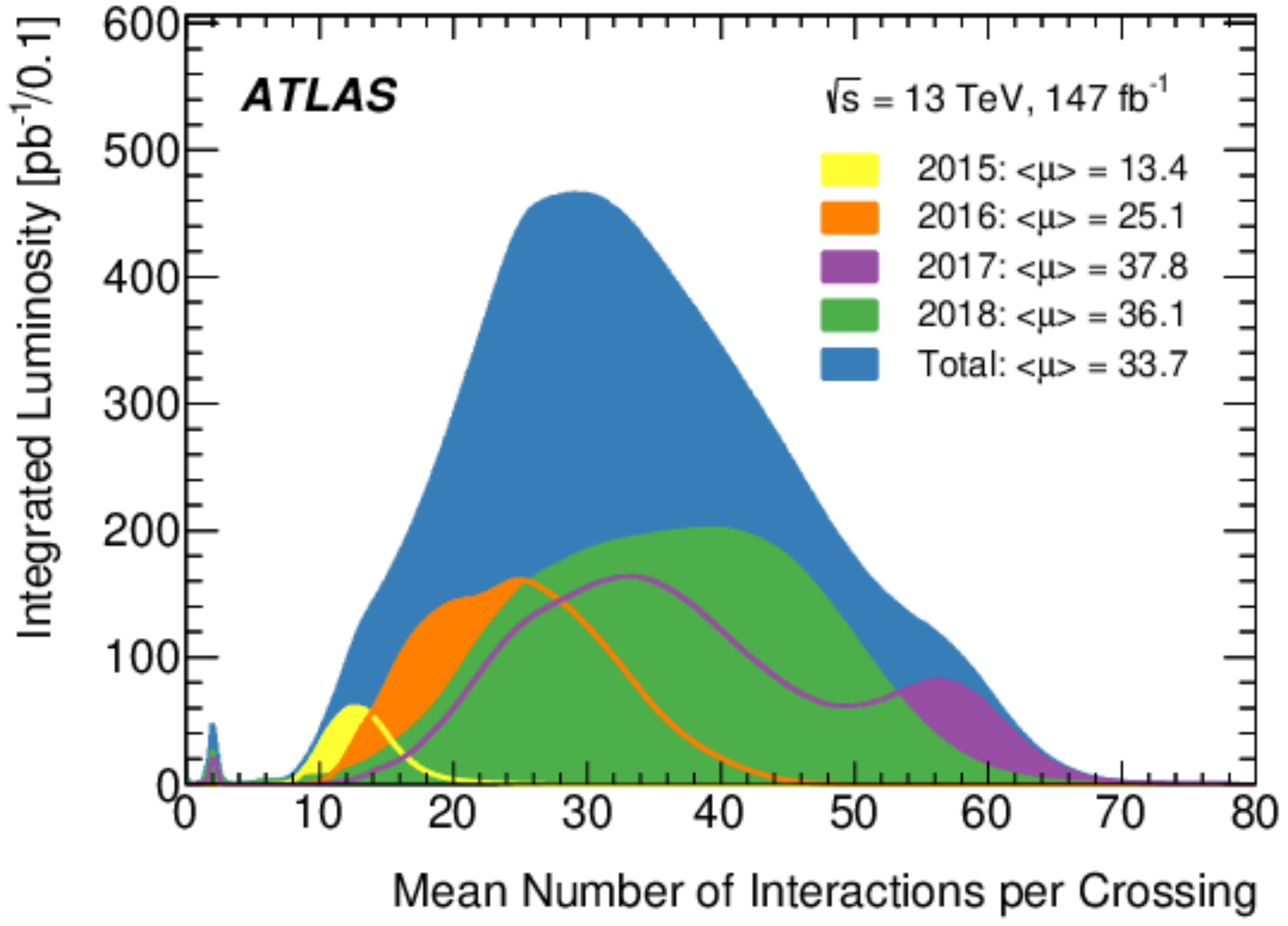

- **Pileup: Additional proton proton collisions at the LHC**
  - The average number of pileup during the Run3 was above 50 (CMS)
  - Average pileup on future high-lumi LHC will be 140
- **Will severely degrade quality of observables (jet multiplicity, jet substructure) if not properly treated**
- **PU mitigation is crucial at hadron colliders**
  - For charged particles, use tracking information to disentangle particles from PU
  - Very challenging for neutral particles

Current PU ID in CMS

- **Pileup Per Particle Identification (PUPPI)**
- **PUPPI is Rule-Based algorithm**
  - Calculates a weight $w \in [0, 1]$ for each particle in the event
    - Encodes the probability for a particle to be leading vertex (LV) or not
    - Weight used to reweight the particle 4-momentum before jet clustering
  - For charged: use tracking information and assign 0 or 1
  - For neutrals: build α variable

$$\alpha_i = \log \sum_{j \neq i, \Delta R_{ij} < R_0} \left(\frac{p_{T,j}}{\Delta R_{ij}} \right)^2 \begin{cases} |\eta_i| < 2.5 & j \text{ are all charged particles from LV} \\ |\eta_i| > 2.5 & j \text{ are all kinds of particles} \end{cases}$$

  - QCD is harder and more collimated than PU, so that α is much higher
  - After some math and assumptions translate α into weight

ML for pileup mitigation

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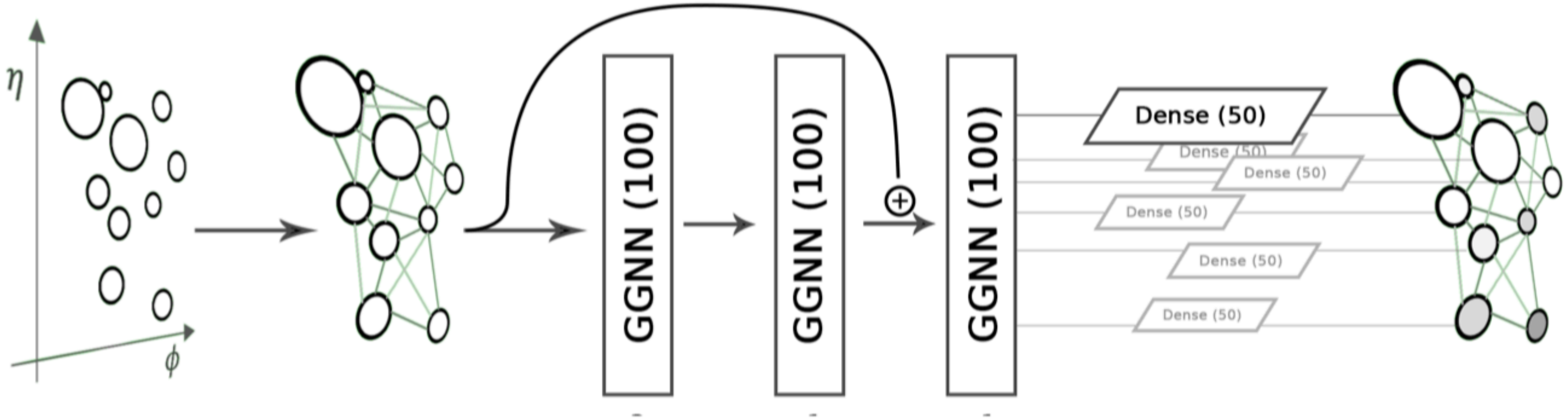
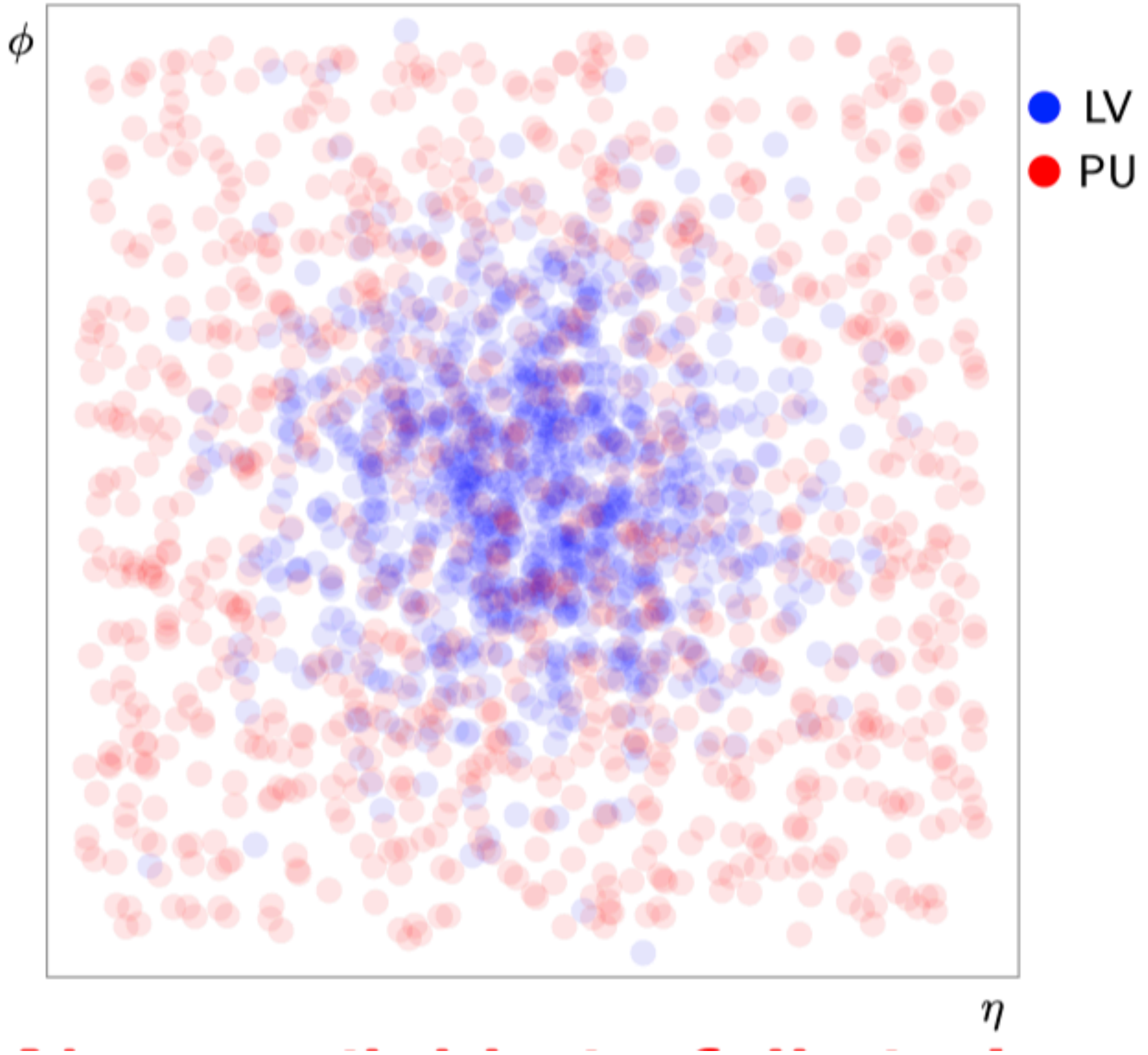
- **Published literature demonstrates that ML can improve over current algorithm [1,2,3]**
- **In particular, GNNs proved to be very effective**
  - Collect info about neighbouring particles in a much more expressive way
- **General strategy in these works: train from a supervised model using Delphes fast-simulation truth labels**
  - A flag set to 1 for charged particles from the LV, -1 for charged pileup and 0 for all neutral particles. This flag provides a simple encoding for weight



Problems in current ML PU algos

- **Critical issue: per-particle labels are not available in Geant4-based full simulations**
  - Marking the source of each particle is not supported
  - Previous approaches can’t be ported to experiments such as ATLAS and CMS
- **Therefore, an algorithm that does not depend on the true labeling of each particle is needed**
  - That's the question this study will solve



Not available in full-sim!

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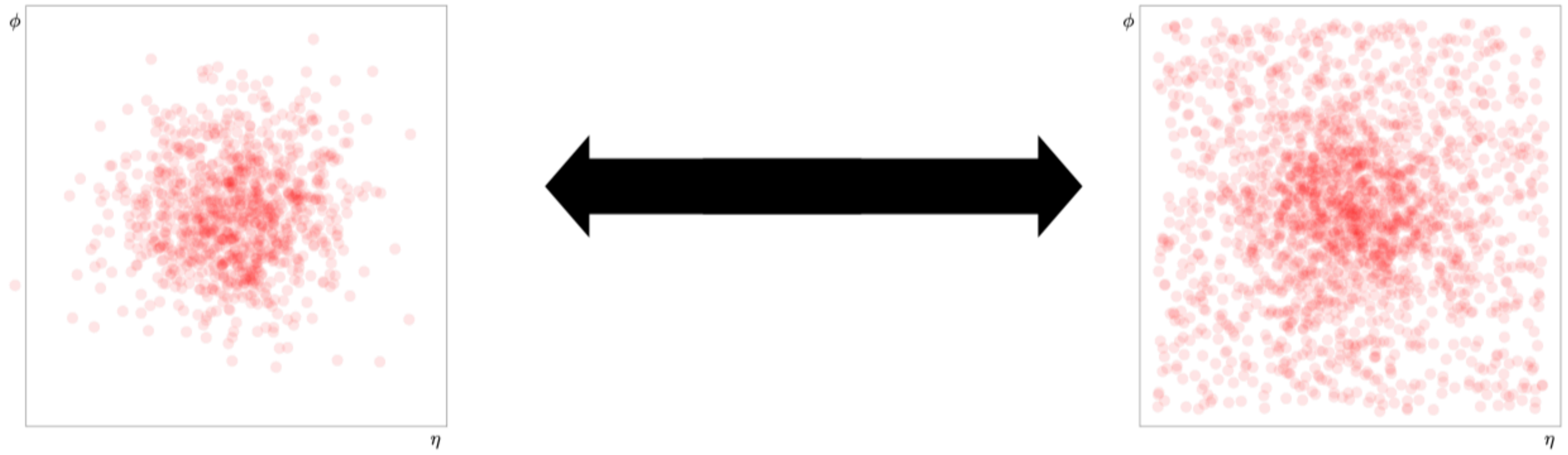
A novel approach in this study

- **At first, we simulate identical proton-proton collisions in two scenarios:**
  - Only the hard interaction is simulated: no-PU sample (X_{no-PU})
  - Pileup is superimposed to the hard interaction: PU sample (X_{PU})
- **Train network to learn differences between the two samples**



  - Network choice: Attention-Based Cloud Network (ABCNet)

TOTAL algorithm

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- **Used optimal transport，OT to design loss function**
  - Optimal transport (OT) can measure the “distance” between probability distributions
- **Network output：per-particle weights** w
  - Used to mitigate PU （PU particles are close to 0, LV particles are close to 1)
- **During training, weight PU sample（**X_{PU}**）by the weights** w
- **Tweak weights to minimize the distance between** X_{no-PU} **and** $w{\cdot}X_{PU}$
- **No need for per-particle labels in this setup**

TOTAL algorithm

- **Sliced Wasserstein Distance （SWD）**
  - A "distance" measure for multidimensional variable distributions based on optimal transportation
  - No guarantee that energy is conserved between the two
- **Add an event-level MET constraint term to the loss**
  - Enforce energies in no-PU and PU events to be similar
- **Final loss function:**
  - $\mathcal{OT} = \mathrm{SWD}(\omega \cdot \mathbf{X}_{\mathrm{PU}}, \mathbf{X}_{\text{no-PU}}) + \lambda \times \mathrm{MSE}\left(\mathrm{MET}(\omega \cdot \mathbf{X}_{\mathrm{PU}}), \mathrm{MET}(\mathbf{X}_{\text{no-PU}})\right)$
- **Call this Training Optimal Transport with Attention Learning: TOTAL**

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- LHC and CMS experiment
- Pile Up in CMS
- TOTAL algorithm
- **Performance comparison**
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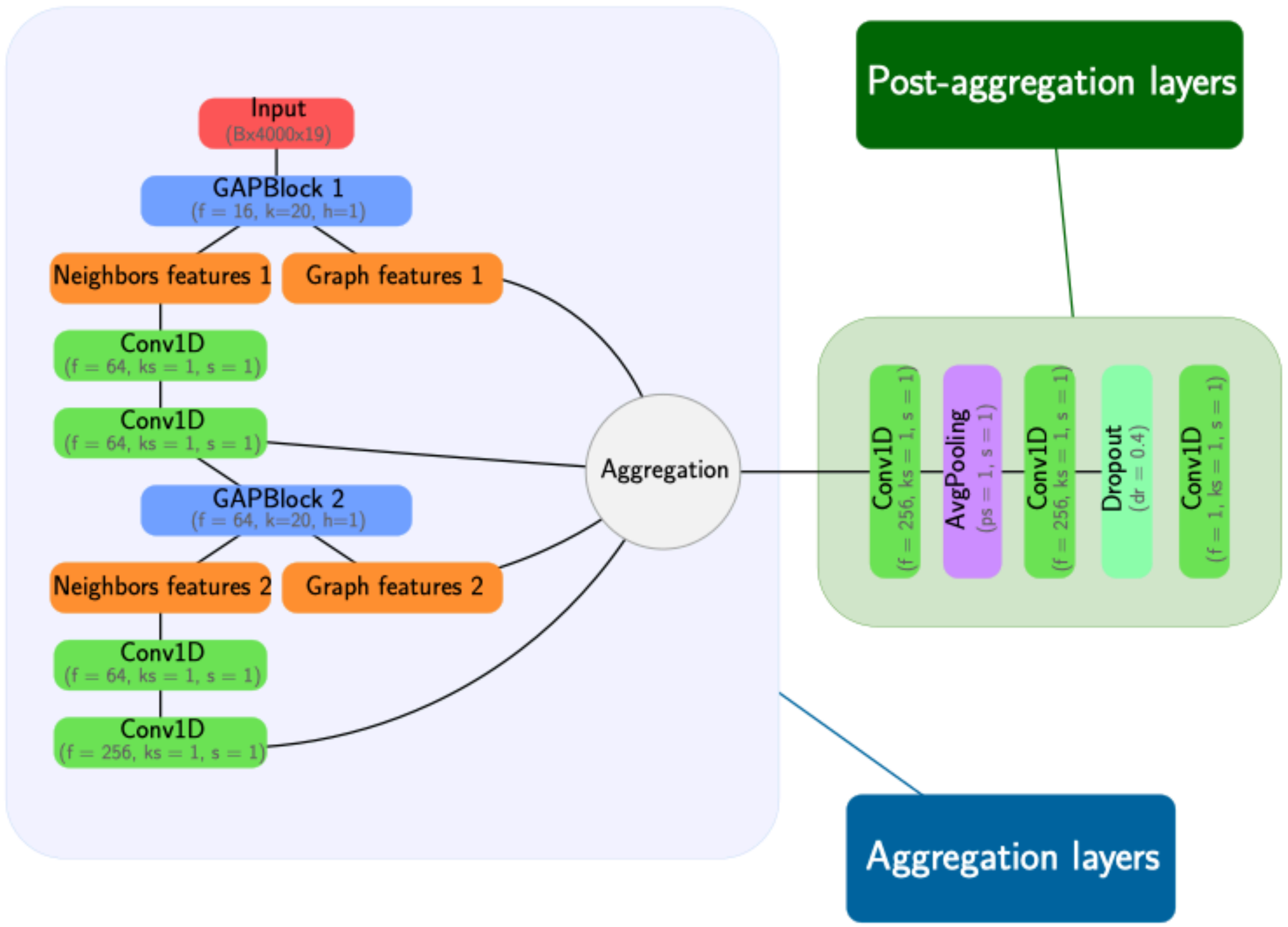
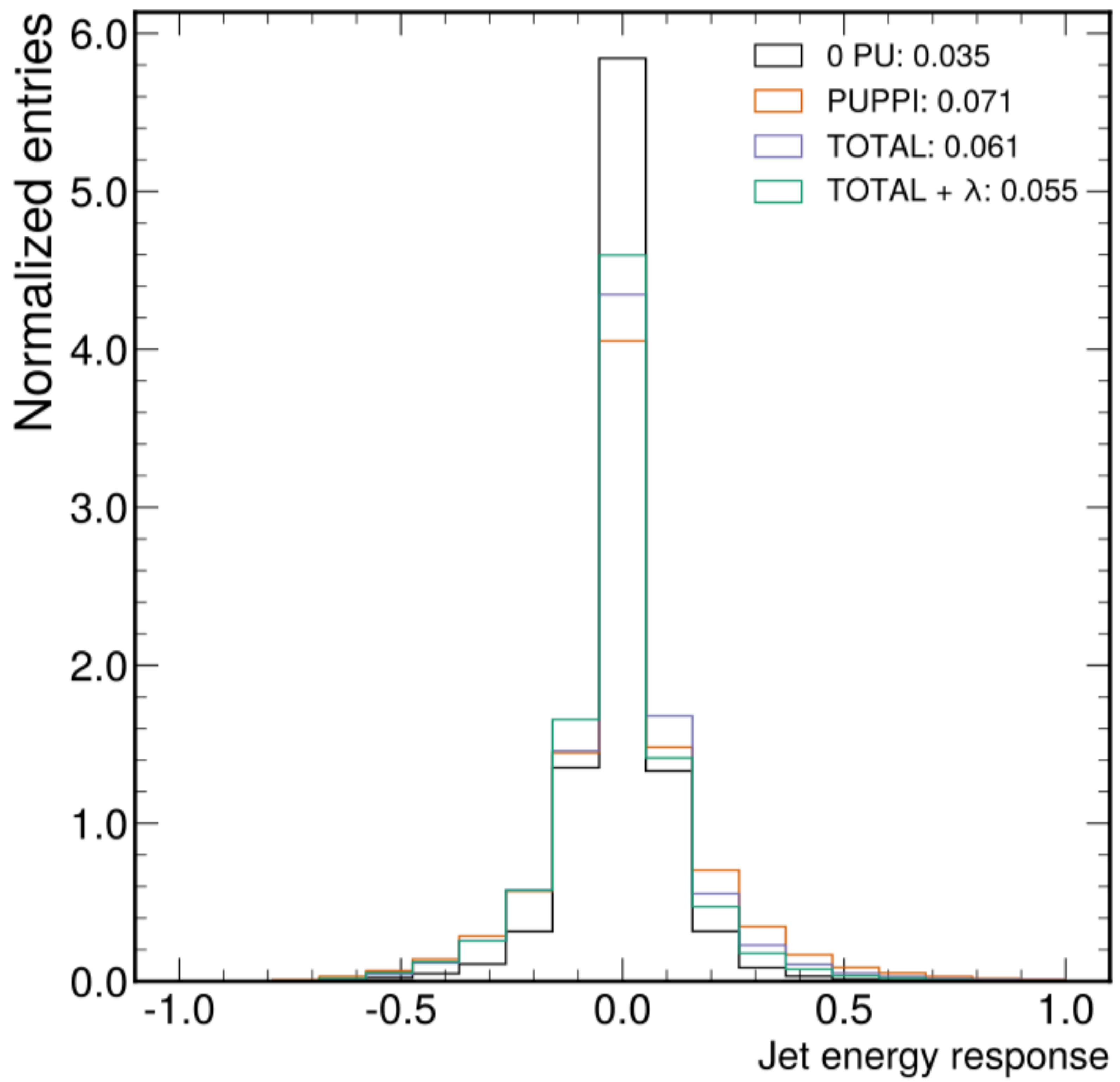
The Model



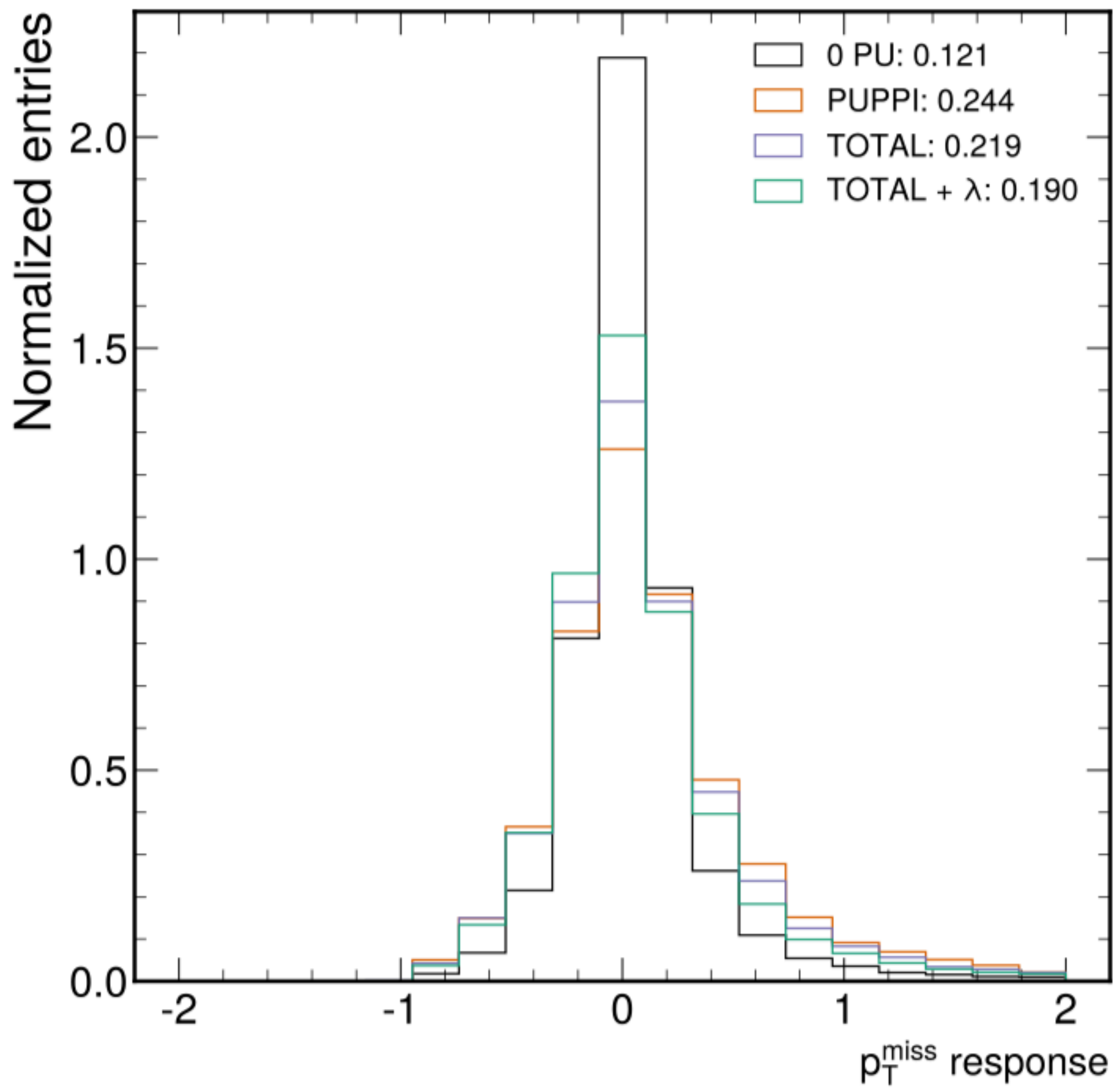
- Compare TOTAL with PUPPI and no-PU scenario
- Reweight each particle's 4-momentum by the network weight
- Cluster TOTAL jets and TOTAL MET
- Define the resolution as:
  - $$\delta = \frac{q_{75\%} - q_{25\%}}{2}$$
  - where q is the X-th quantile of the considered response distribution

Energy response

- The improvement in Jet energy response is about 23% relative to PUPPI and 22% for missing transverse momentum



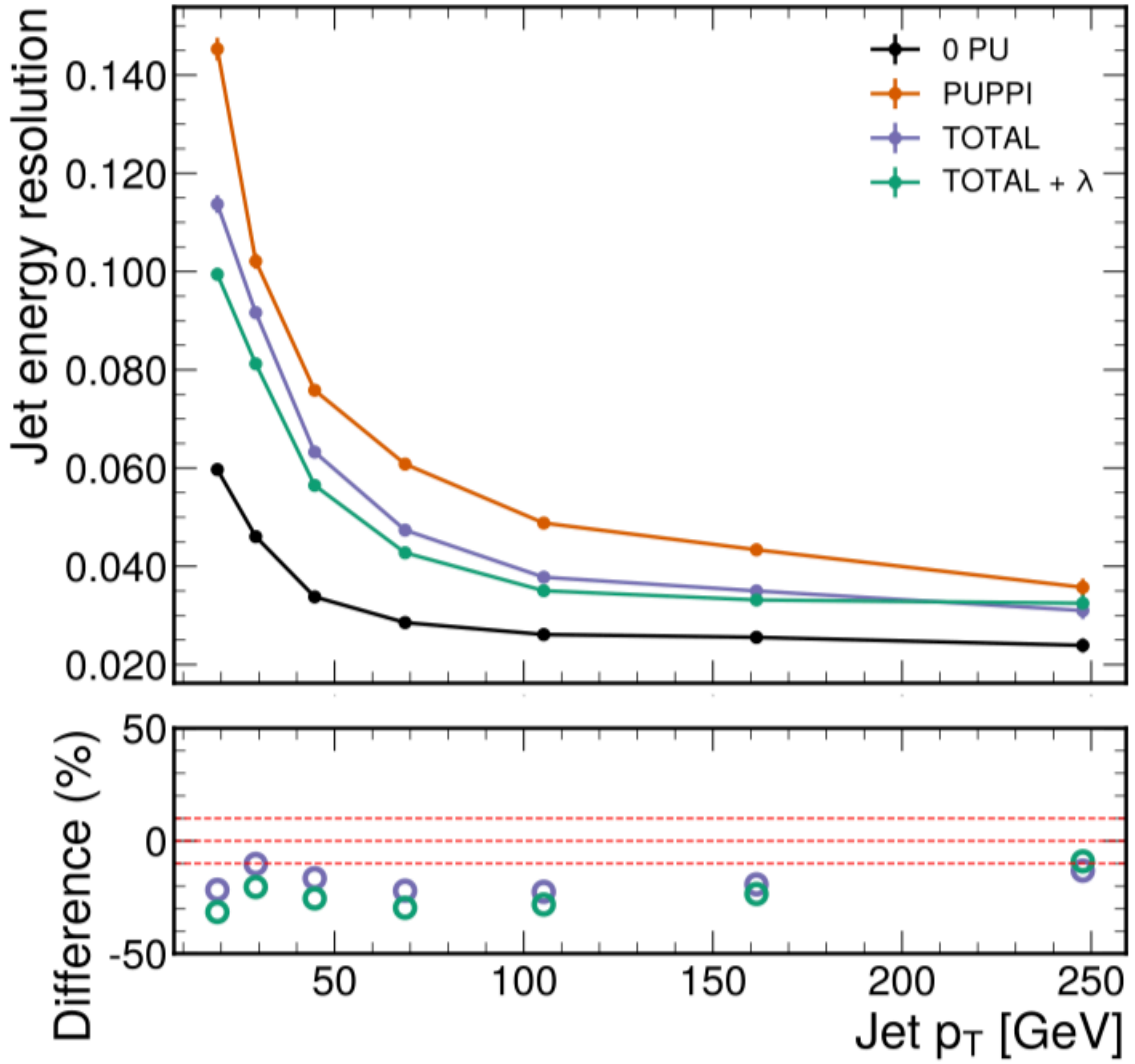
喷注能量响应



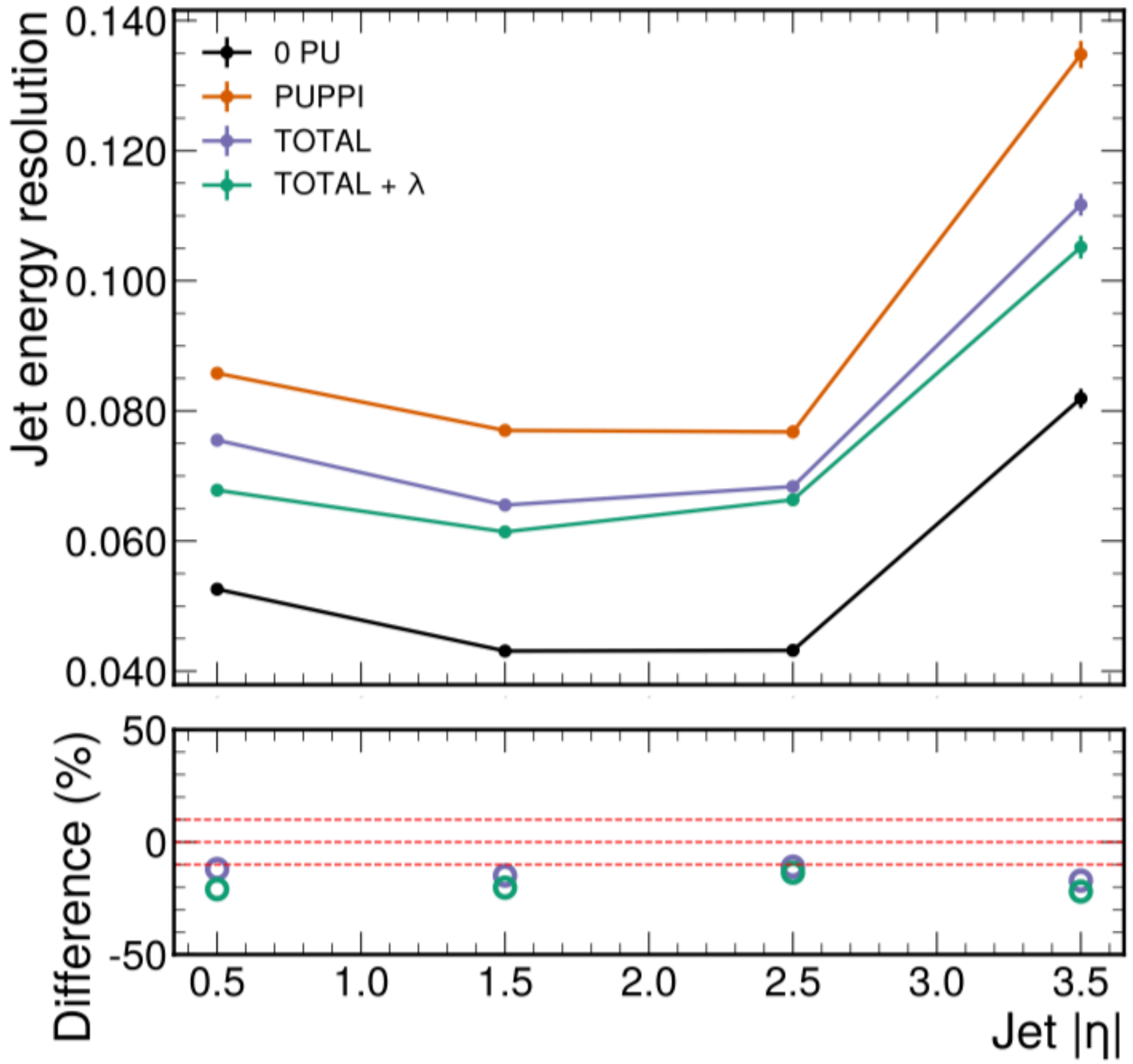
缺失横动量响应

Jet differential resolutions

- **Improvement of Jet energy resolution relative to PUPPI: 20～30%**



Injection energy resolution varies with injection energy



Variation of injection energy resolution with η

Robustness

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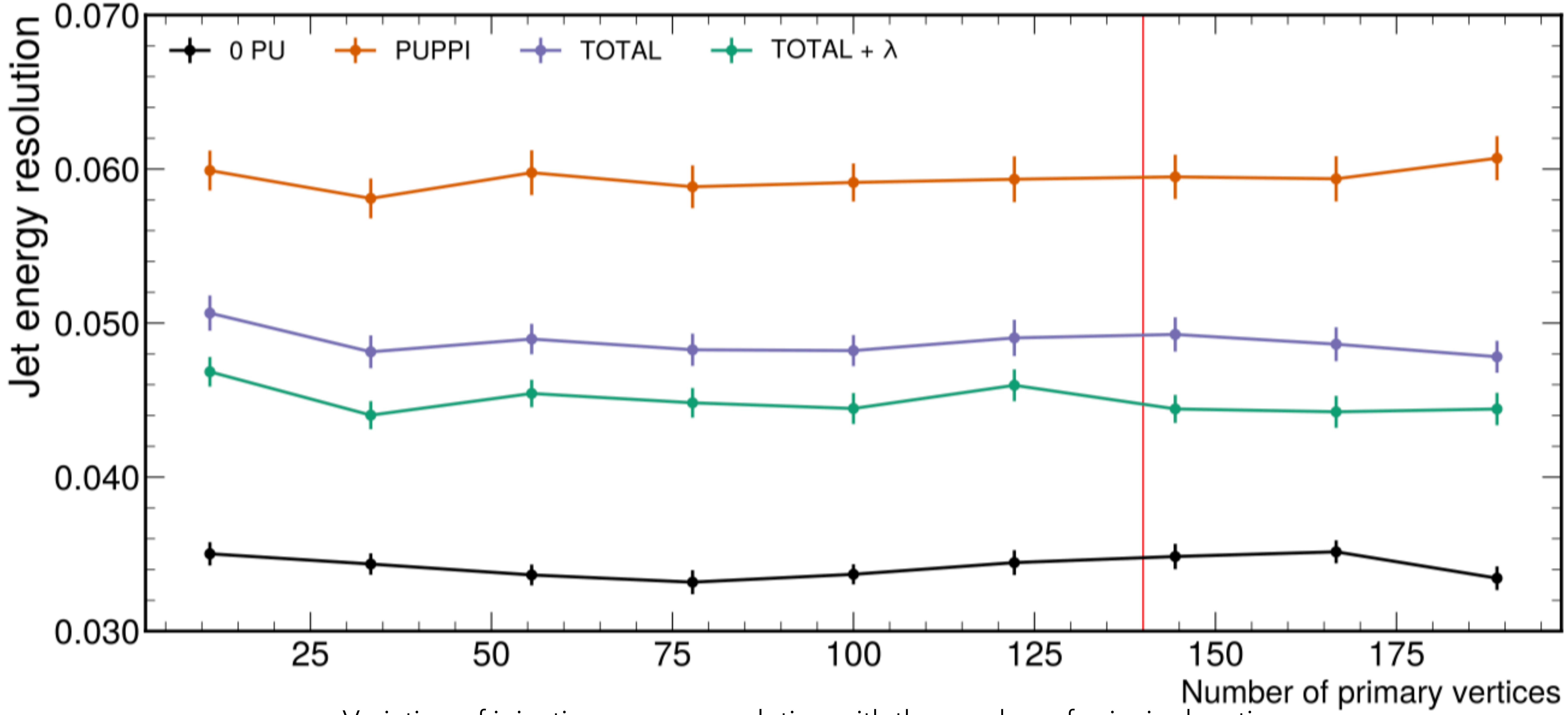
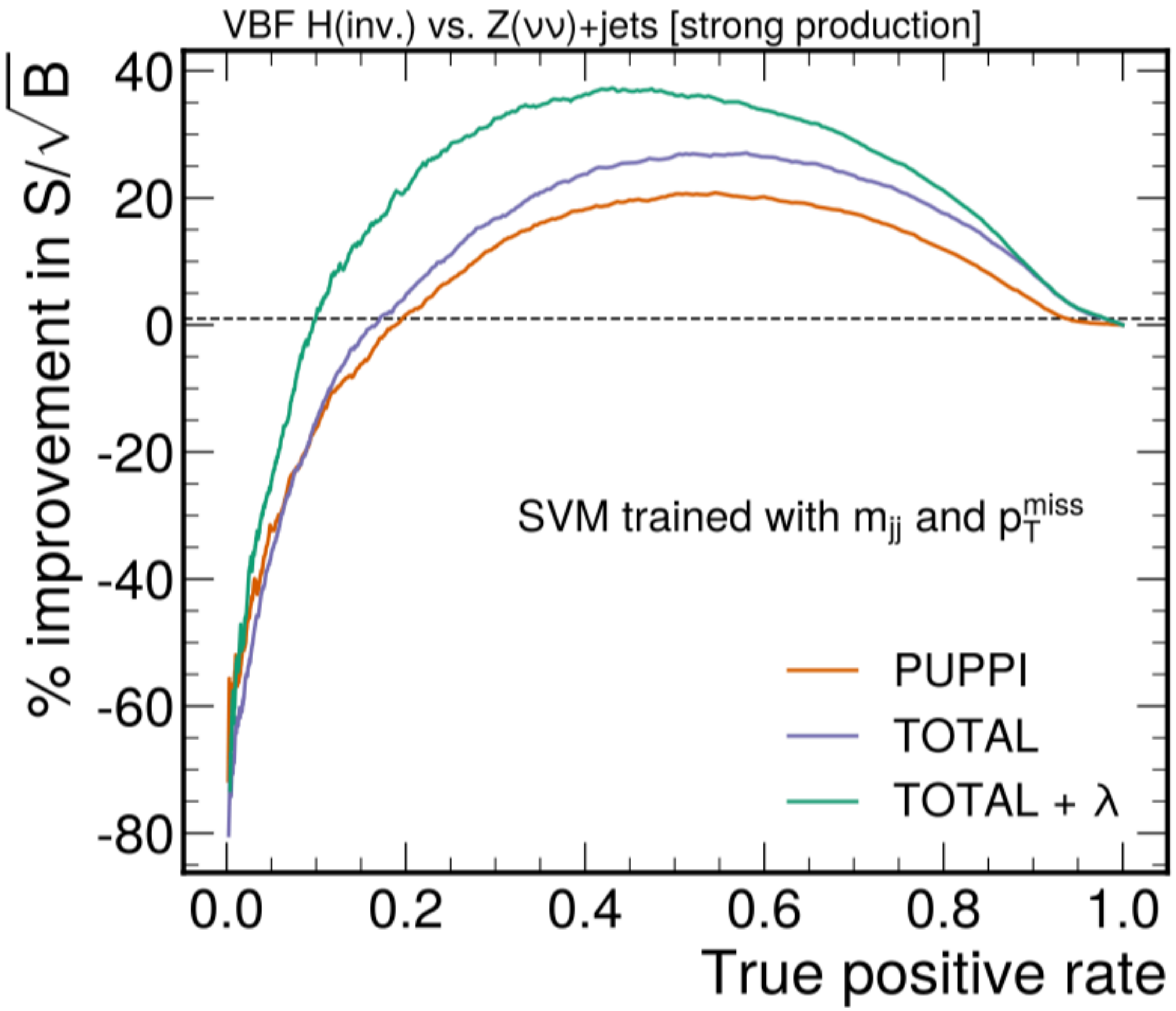
- **The model in this study was trained based on 140 primary vertices, but it still works for 200 vertices with little change**



Variation of injection energy resolution with the number of principal vertices

Physics impact

- Study impact of TOTAL on LHC searches:
  - Search for BSM VBF H(inv.)
- Signal signature: pair of forward jets and MET
- Main background: strongly produced Z($\nu\nu$) + Jets
- Perform toy analysis by training a linear classifier (SVM) using dijet mass and MET
- Observe the change in significance (S/$\sqrt{B}$) with signal efficiency:
  - TOTAL is about a 15% improvement over PUPPI



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Summary

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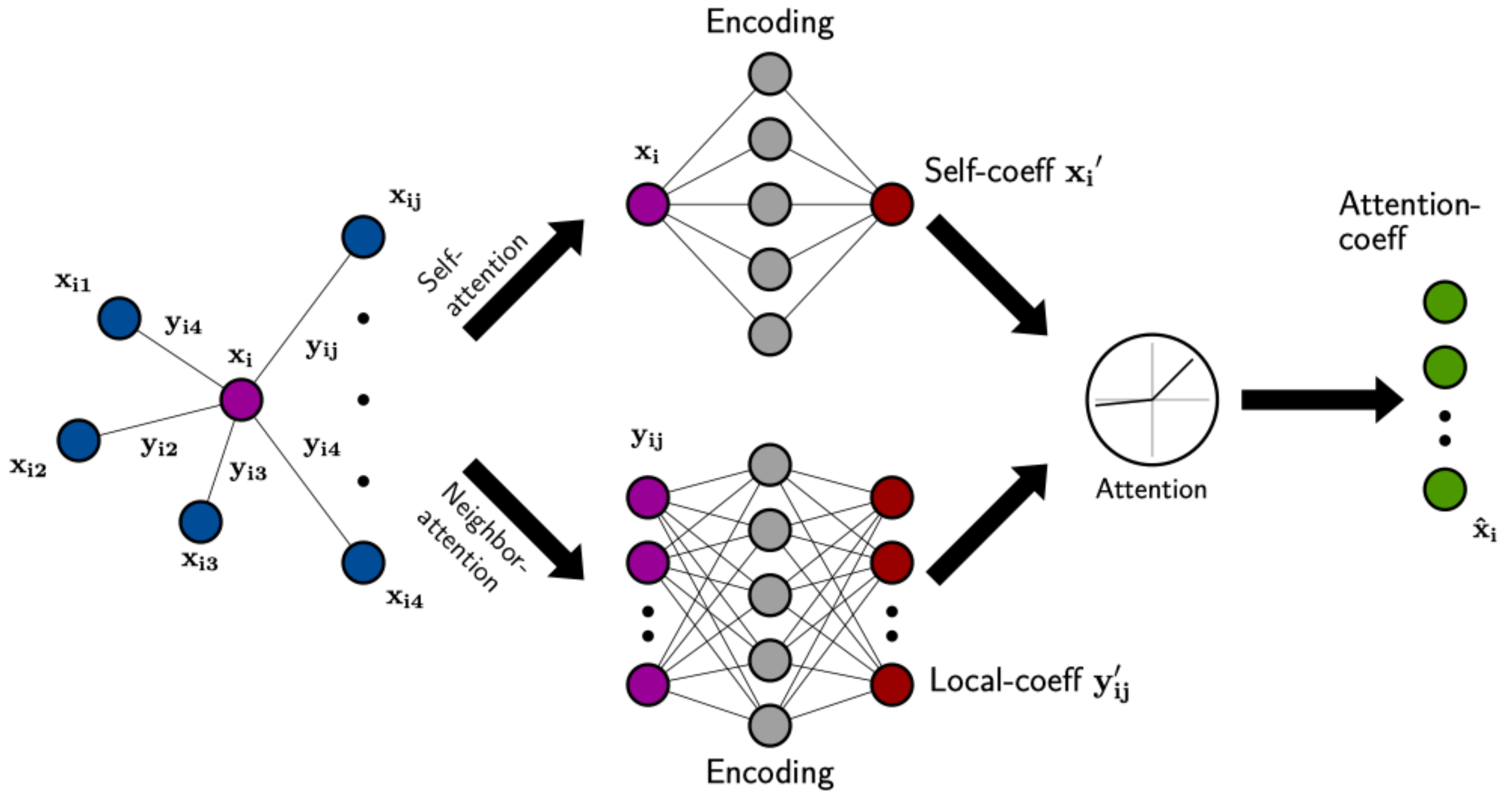
- **We presented novel algorithm to reject PU particles at high-intensity hadron colliders**
  - Trained and tested on Delphes simulation of Phase2 CMS detector
- **We are Training Optimal Transport with Attention Learning: TOTAL**
- **We solved the longstanding problem of neutral labels in PU mitigation**
- **We do not rely on explicit, per-particle labelling**
- **Such an algorithm will be crucial at the High-Luminosity LHC, where much harsher data-taking conditions are expected**
- **Our approach can be generalized to a wide range of denoising problems**

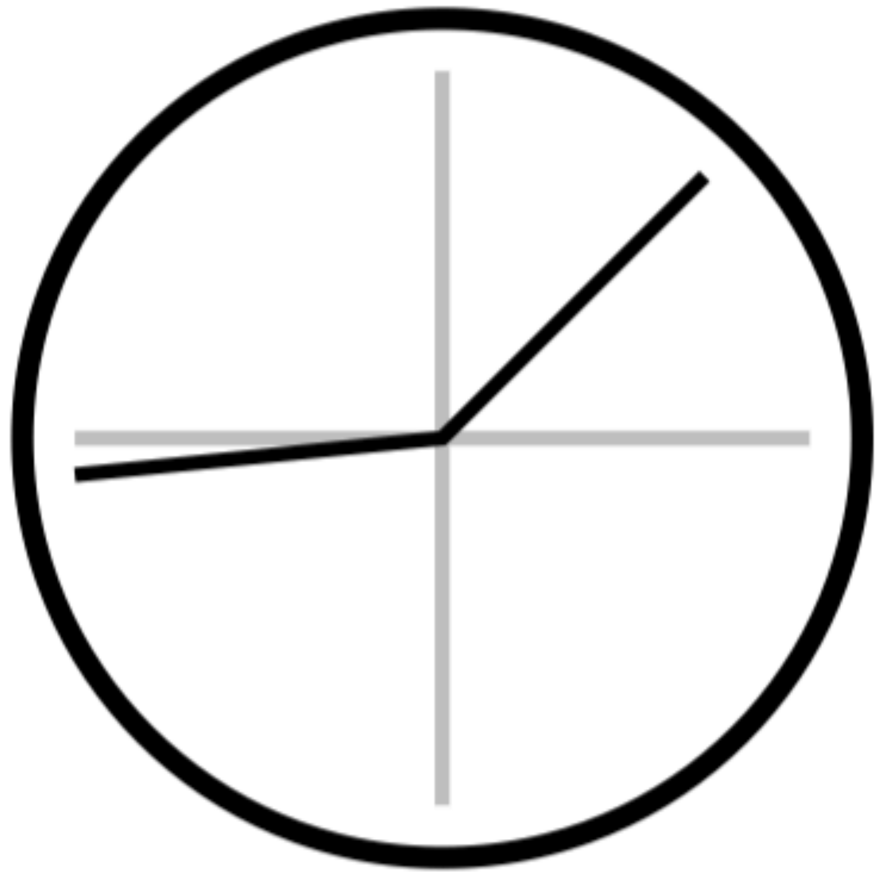
Backup

Attention Based Cloud Network

- **ABCNet is an graph neural network enhanced with attention mechanisms**
  - Treat particle collision data as a set of permutation-invariant objects
  - Attention mechanisms filter out the particles that are not relevant for the learning process
  - Implemented inside custom graph attention pooling layers (GAPLayers)



Attention mechanism



Attention

- Add together self- (x_i') and local- (y_{ij}') coefficients and apply non-linearity

$$c_{ij} = \text{LeakyRelu}(x_i' + y_{ij}')$$

- Align coefficients c_{ij} by applying SoftMax

$$c_{ij}' = \frac{\exp(c_{ij})}{\sum_k \exp(c_{ik})}$$

- Get attention coefficients by multiplying y_{ij}' by c_{ij}'

$$\hat{x}_i = \text{Relu}\left(\sum_j c_{ij}' y_{ij}'\right)$$

Efficient OT

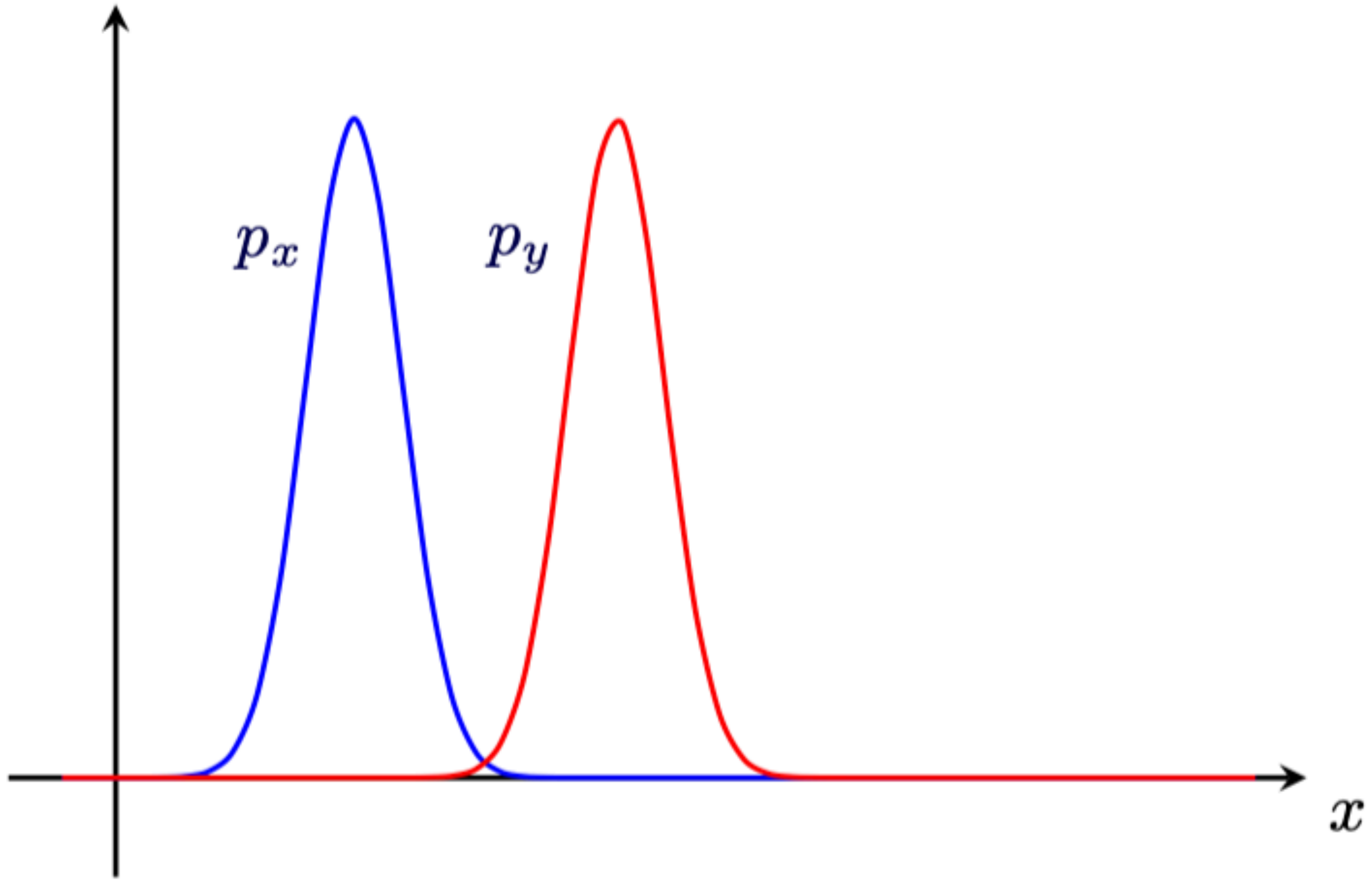
- **The optimal transport problem has a closed form for 1D problems:**

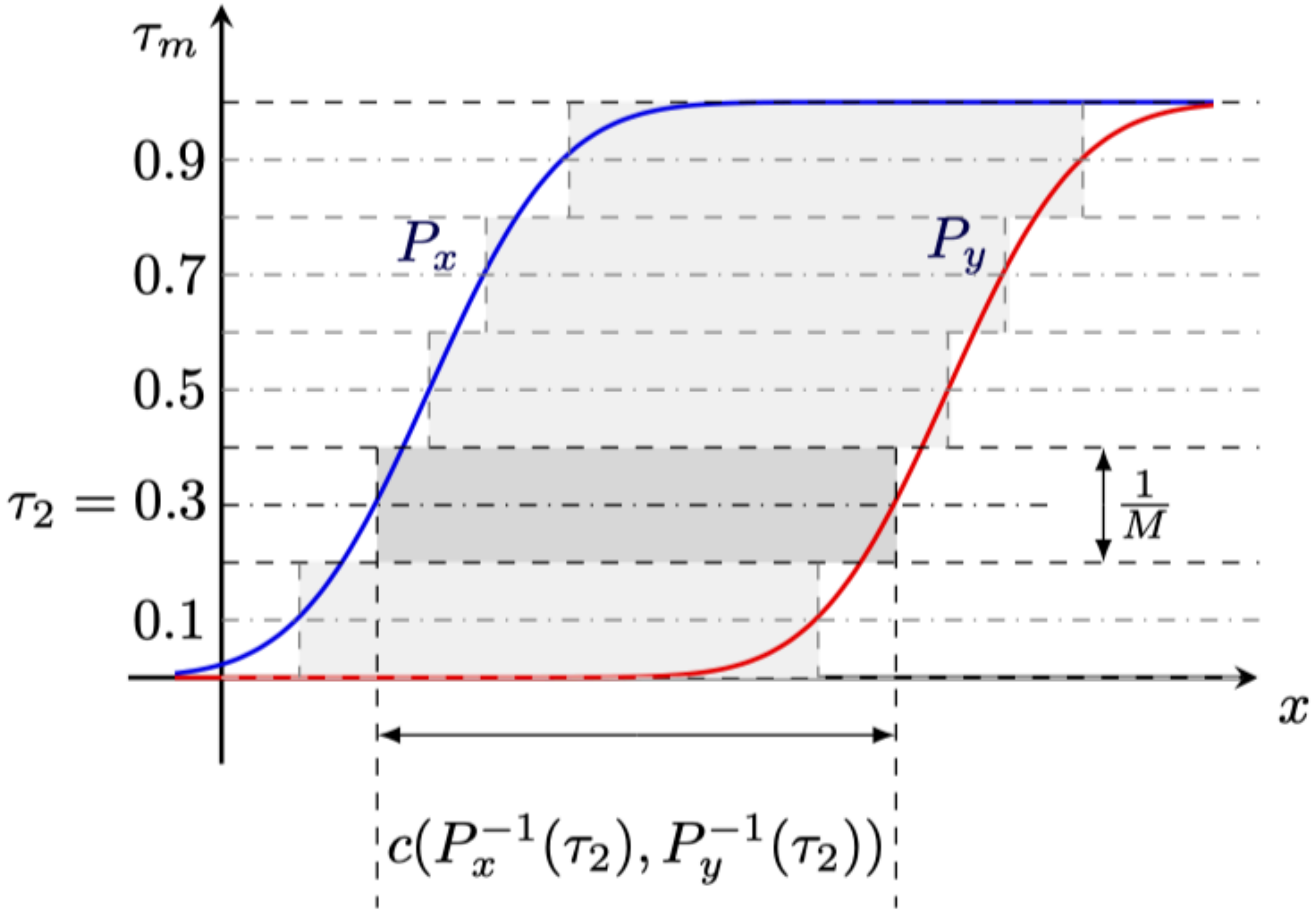
$$W_c(p_X, p_Y) = \int_0^1 c\left(P_X^{-1}(\tau), P_Y^{-1}(\tau)\right) \mathrm{d}\tau$$

- where pX , pY are 1D PDFs, $PX^{-1}(\tau)$, $PY^{-1}(\tau)$ are the respective CDFs and c(·, ·) is the transportation cost function
- No guarantee that the integral is solvable
- The integral can always be approximated by the finite sum

$$\frac{1}{M}\sum_{m=1}^{M} c\left(P_X^{-1}(\tau_m), P_Y^{-1}(\tau_m)\right), \qquad \tau_m = \frac{2m-1}{2M}$$

Example: M=5

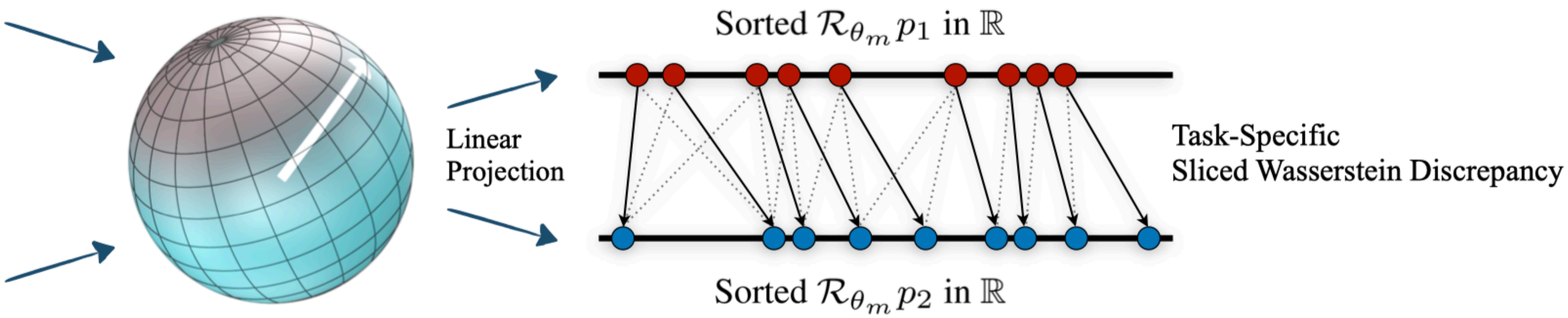




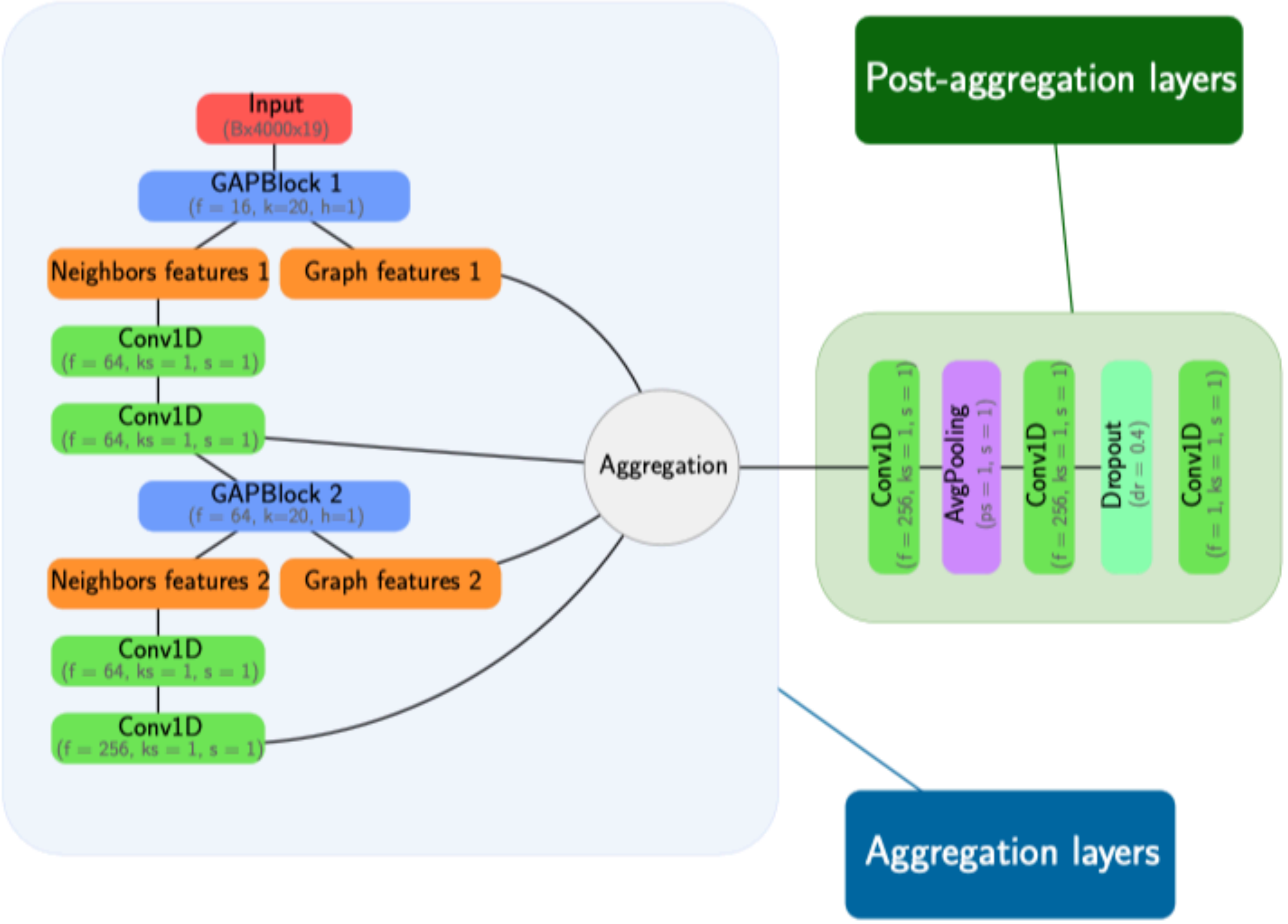
- $m \in \{1,2,3,4,5\} \implies \tau_m = \frac{2m-1}{2M} \in \{0.1, 0.3, 0.5, 0.7, 0.9\}$

sliced Wasserstein distance (SWD)

- Each particle is a sample from a n-D feature space
- **SWD**: take n-D feature space and **project (slice)** it **to 1D**
- Project on a vector belonging to S^{n-1}
- For robustness, take **multiple random slices**
- Now can **solve the 1D OT problem for each slice**
- **Sort particles by slice**
- The **average on all slices and particles** becomes the **loss function**



The model



- **9 input features**:
  - (p_T, η, ϕ, E)
  - Charge
  - PDG ID
  - dXY & dZ impact parameters
  - Vertex association (for charged)
- **Loss**: $\mathrm{SWD}(\vec{x}_p \cdot \vec{\omega}, \vec{x}_{np}) + \mathrm{MET}$ constraint
- **Cost function**: squared distance
- **Sliced features**: (p_T, η, ϕ, E)
- **Output**: per-particle weight $\vec{\omega}$

- Train on **300k events**, equally split between QCD multijet, $t\bar{t}$ dileptonic and VBF Higgs(4ν) processes
- Consider **9000 particles per event** (zero-padding included)
- Gather the **20 *k*-nearest neighbors** for each particle when building graph