Shower Reconstruction in Liquid Argon Time Projection Chambers using Graph Neural Networks

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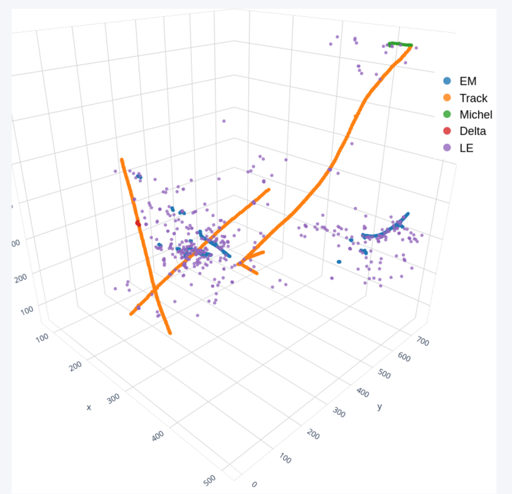
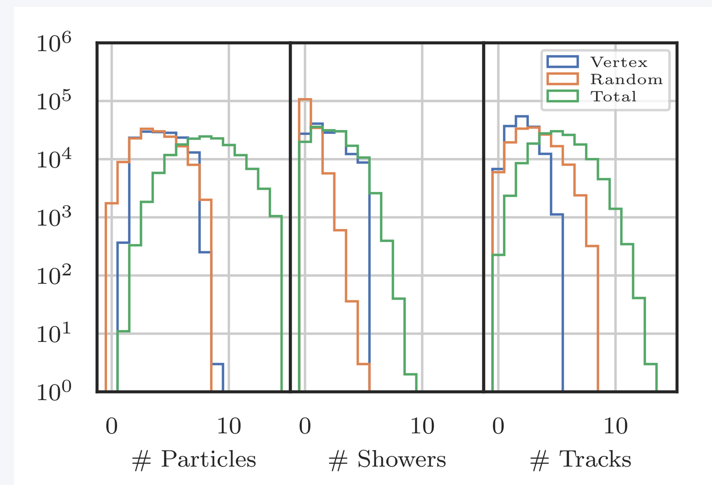
1. Input data

Simulation of generic particle interactions in liquid argon (LAr):

- 768^3 voxels images ($\sim 12\,\mathrm{m}^3$ of LAr, $3 \times 3 \times 3\mathrm{mm}^3$ voxels)
- One `particle bomb' per image (tracks + showers from common vertex)
- Cosmic muons + random showers overlayed

Only EM shower voxels are part of this study. See poster ID 373 to find out how classification is done using a the so-called U-ResNet architecture.





3. Feature extraction

Fragment i encoded in geometric features, $\boldsymbol{x}_i$:

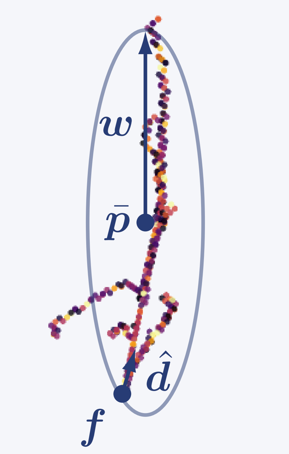
- Centroid, $\bar{\boldsymbol{p}}$
- Covariance matrix and its eigenvalues, $\boldsymbol{w}$
- Size in number of voxels
- Start point, $\boldsymbol{f}$, start direction estimate, $\hat{\boldsymbol{d}}$

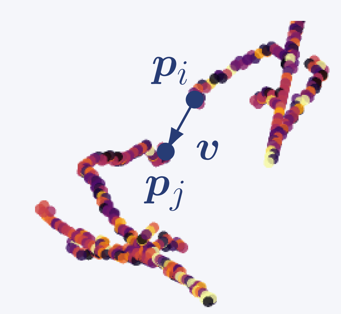
Start point optained using the Point Proposal Network described in poster ID 319

Build complete undirected graph which connects all fragments with all other fragments

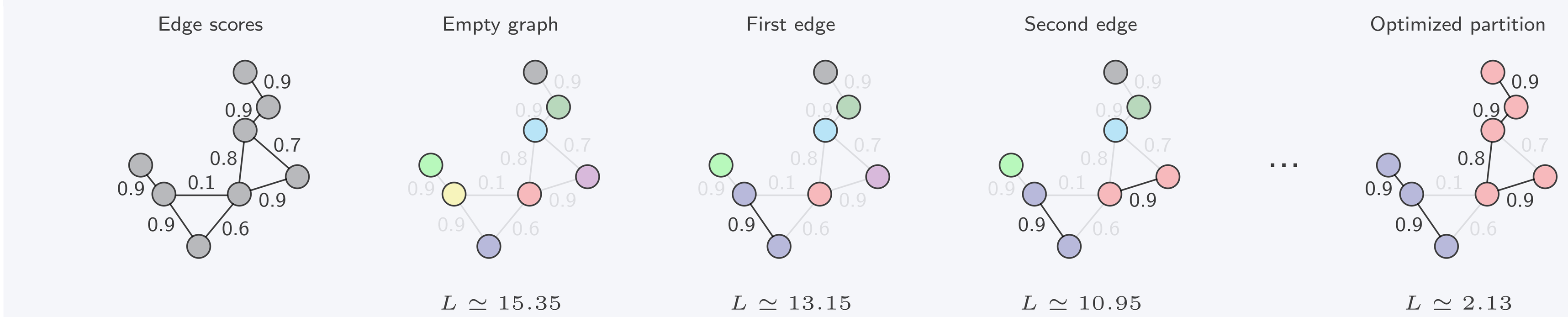
Graph edge (i, j) provided with features, $\boldsymbol{e}_{ij}$

- Closest points of approach, $\boldsymbol{p}_i$, $\boldsymbol{p}_j$
- Displacement vector, $\boldsymbol{v} = \boldsymbol{p}_j - \boldsymbol{p}_i$
- Outer product and norm of $\boldsymbol{v}$





5. Shower grouping



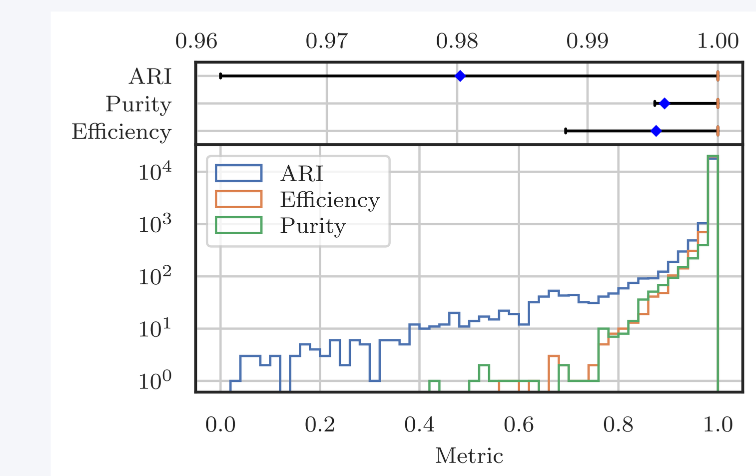
GNN infers adjacency score, s_{ij}^e, for each edge (i, j)

Optimize fragment partition, $\boldsymbol{g}$, to minimize CE loss:

$$L = \frac{1}{N_e} \sum_{(i,j) \in E} \delta_{g_i, g_j} \ln(s_{ij}^e) + (1 - \delta_{g_i, g_j}) \ln(1 - s_{ij}^e)$$

Clustering metrics:

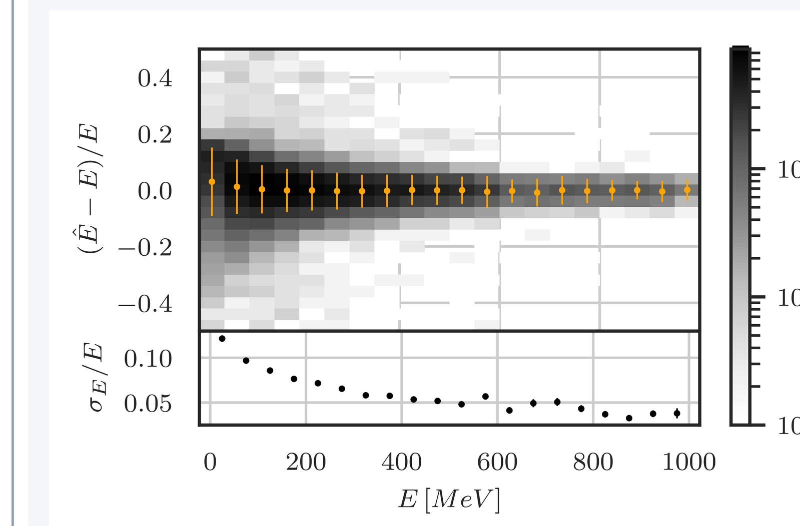
- Purity = 1 if predicted groups do not mix labels
- Efficiency = 1 if true groups are not split
- ARI stringent measure of partition similarity



7. Neutral pion reconstruction

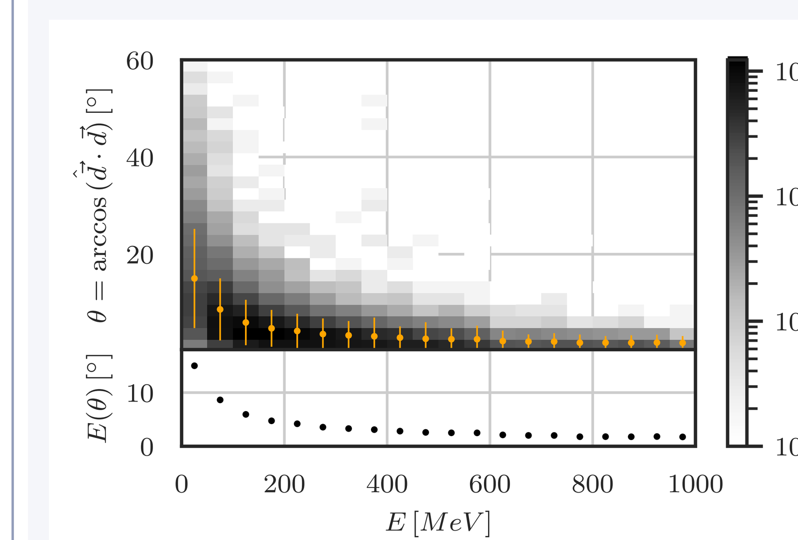
Shower grouping used to reconstruct shower energy by summing voxel energies in group

- $\sim 5\,\%$ energy resolution for $E > 500$ MeV
- Uncertainty driven by fragment selection



Shower direction estimated by taking mean primary direction w.r.t. to start point

- $\sim 2°$ angular resolution for $E > 500$ MeV



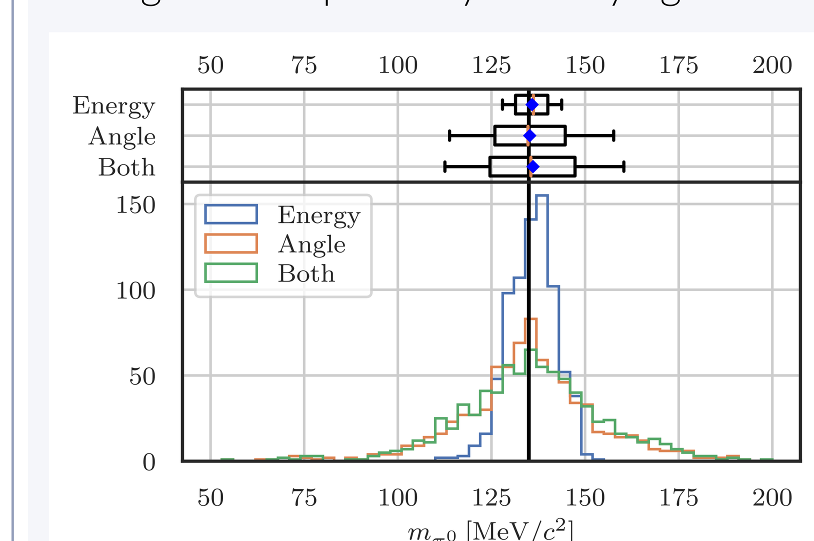
Neutral pions typically immediatly decay to two gamma rays whose kinematics verify

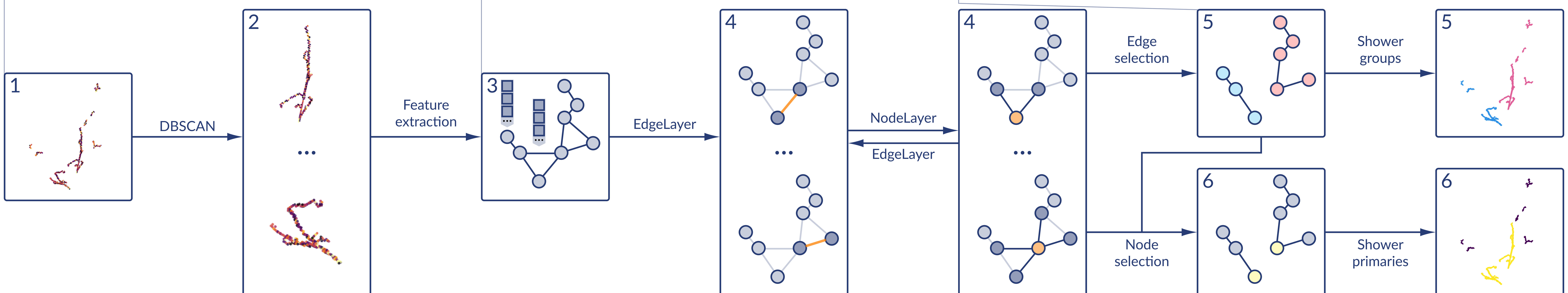
$$m_{\pi^0} = \sqrt{2E_1 E_2 (1 - \hat{\boldsymbol{d}}_1 \cdot \hat{\boldsymbol{d}}_2)},$$

with E_1, E_2 the reconstructed energies and $\hat{d}_1$, $\hat{d}_2$ the estimated directions of the showers

Impact of the shower energy and angular resolution on π^0 mass resolution is studied:

- π^0 selection done using truth information
- Mass resolution: $136.1 \pm 20.4\,\mathrm{MeV}/c^2$
- Angle can improve by identifying vertex





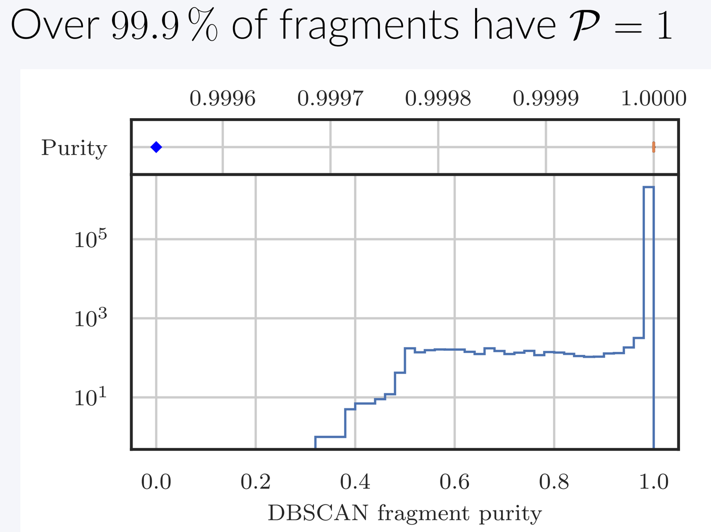
2. Fragment clustering

Dense fragments clustered using DBSCAN

- Distance scale $\epsilon = 1.999$, min points: 1

Fragment purity, $\mathcal{P}$, defined as fraction of fragment that belongs to one shower group

- Over $99.9\,\%$ of fragments have $\mathcal{P} = 1$

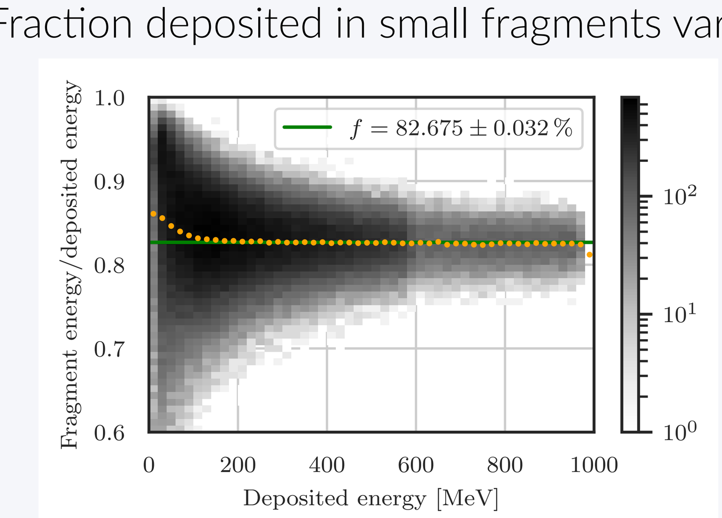


Fragments selected to have > 10 voxels

- Ensures fragments have direction
- Simplifies clustering task

Introduces an uncertainty on shower energy

- Fraction deposited in small fragments varies



4. Message passing

Message passing used to communicate in a graph (arXiv:1806:01261)

At each EdgeLayer, the edge features of edge (i, j) are updated through:

$$\boldsymbol{e}_{ij}^{s+1} = \psi_{\boldsymbol{\Theta}}(\boldsymbol{x}_i^s, \boldsymbol{x}_j^s, \boldsymbol{e}_{ij}^s)$$

Messages are then built to carry information from fragment j to i:

$$\boldsymbol{m}_{ji}^{s+1} = \phi_{\boldsymbol{\Theta}}(\boldsymbol{x}_j^s, \boldsymbol{e}_{ji}^{s+1})$$

Messages received by fragment i are aggregated to update its features

$$\boldsymbol{x}_i^{s+1} = \chi_{\boldsymbol{\Theta}}(\boldsymbol{x}_i, \square_{\mathcal{N}(i)} \boldsymbol{m}_{ji}^{s+1})$$

Functions $\psi_{\boldsymbol{\Theta}}$, $\phi_{\boldsymbol{\Theta}}$, $\chi_{\boldsymbol{\Theta}}$ and $\square$ are arbitrary. In this study:

- $\psi_{\boldsymbol{\Theta}}$, $\phi_{\boldsymbol{\Theta}}$ and $\chi_{\boldsymbol{\Theta}}$ are learnable 3-layer perceptrons outputting 64 features
- $\square$ takes the mean of the incoming messages
- Message passing is performed thrice

6. Primary identification

GNN infers a primary score, s_i^p, for each fragment i, correlated to the likehood of a fragment to have initiated a shower

- For true primaries, $s_i^p > 0.5$ in $98.83\,\%$ of events
- For true secondaries, $s_i^p < 0.5$ in $99.86\,\%$ of events

Primary identification improved by using grouping information

Given inferred shower groups, select fragment with highest primary score in each group

- Yields $99.77\,\%$ accuracy

Without prior knowledge of fragment start points, algorithm maintains $99.00\,\%$ accuracy