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Particle Clustering and Flow Reconstruction for Particle Imaging Neutrino Detectors Using Graph Neural Networks

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ABSTRACT

Machine learning (ML) techniques, in particular deep neural networks (DNNs) developed in the field of Computer Vision, have shown promising results to address the challenge of analyzing data from big, high resolution particle imaging detectors such as Liquid Argon Time Projection Chambers (LArTPCs), employed in accelerator-based neutrino experiments including the Short Baseline Neutrino (SBN) program and the Deep Underground Neutrino Experiment (DUNE). Convolutional neural networks (CNNs) have been the de-facto choice for image feature extraction tasks, and they are particularly powerful for identifying locally dense features. On the other hand, Graph Neural Networks (GNNs) have been studied actively for analyzing correlation features between distant objects. Example applications for LArTPC detectors include identifying signal correlations between two independent detectors (optical detectors and TPCs), reconstructing particle hierarchies (e.g. a primary particle vs. secondary radiation), and clustering particles into interaction in a busy "neutrino pile-up" environment, expected at the DUNE near detector under high neutrino beam intensity. In this talk, we present our work on utilizing GNNs in the context of a full ML-based data reconstruction chain for LArTPC detectors.

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1 Introduction

In recent years, the accelerator-based neutrino physics community in the United States has moved to employ Liquid Argon Time Projection Chambers (LArTPCs) as a central neutrino detection technology [1]. Charged particles that traverse the detector ionize the noble liquid. The electrons so produced are drifted in a uniform electric field towards a readout plane. The location of electrons collected on the anode combined with their arrival time offers mm-scale resolution images of charged particle interactions.

The Short Baseline Neutrino (SBN) program aims at clarifying an anomalous signal observed by the MiniBOONE experiment [2]. The DUNE experiment is a project that will use the LArTPC technology to measure electron neutrino appearance with unprecedented accuracy [3]. It will consist of a near detector (105 t) and a far detector (40 kt). Both of these physics endeavors centrally depend upon the efficient identification and precise reconstruction of electromagnetic (EM) showers. They also rely on the successful clustering and identification of neutrino interactions, which can be piled up with other interactions.

EM showers exhibit an incoherent branching tree structure in LArTPCs. A single electron or photon creates a cascading chain of EM shower fragments that may be far removed from one another in the image. Similarly, a neutrino interaction may produce photons that are seemingly detached from the vertex while other particles originating from it may experience secondary interactions away from the vertex. The recent development of Graph Neural Networks (GNNs) is ideally suited to the clustering of electromagnetic showers and particle interactions in LArTPCs as they may each be represented by a collection of distinct particle objects (the graph nodes) that are correlated through potentially invisible particles (the graph edges). The task thus comes down to identifying the edges that connect fragments within a group.

2 Reconstruction chain

The reconstruction chain is schematically illustrated for the shower clustering task in figure 1 and detailed in [4]. The input set of voxels associated with electromagnetic showers is passed through a density based clustering algorithm that forms dense shower fragments [5]. Each fragment is encoded into a set of node features in a graph connected by arbitrary edges carrying edge features. Edge and node features are updated through a series of message passing composed of edge and node updaters. The updated edge features are used to constrain the connectivity graph and the updated node features to identify shower primaries. The interaction clustering task uses an identical architecture, with particle instances as an input instead of fragments and interaction groups as an output. For the latter task, the node features are not explicitly used.

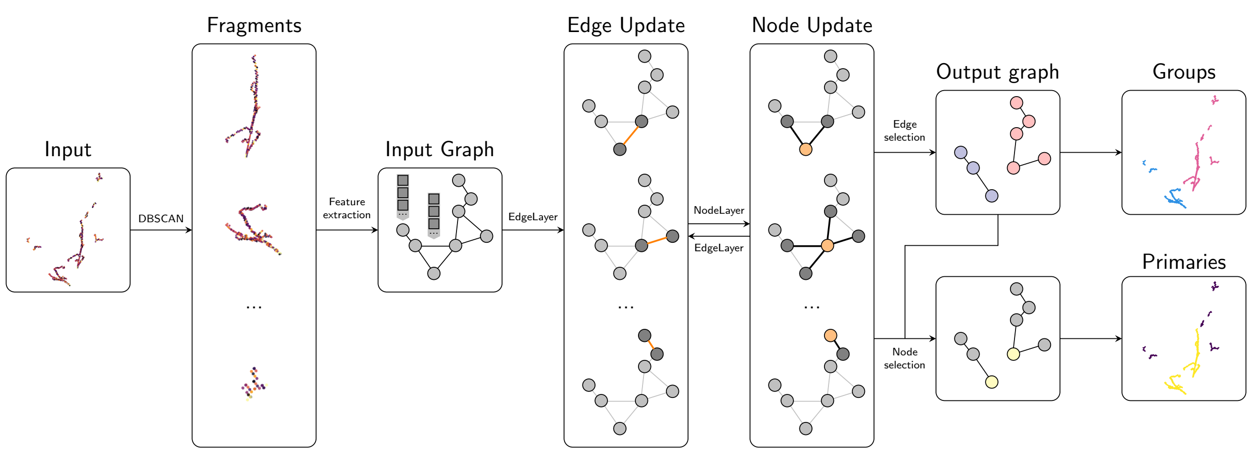


Figure 1: Schematics of the reconstruction chain for shower clustering and primary identification.

2.1 Message passing

The shower fragments are each initially encoded into a set of 22 features: the fragment voxels centroid (3), their covariance matrix (9), its eigenvalues (3), the fragment size (1), the initial point (3) and direction (3). Nodes are connected together by a complete graph in which edges are each given 19 features: the two closest points of approach (6), their displacement vector (3), its outer product (9) and its norm (1).

The node and edge features are updated through message passing [6]. At each step, the edge features are updated by a 3-layer perceptron which combines the edge features with the node features of the two nodes that it connects together. The node features are updated by two successive 3-layer percetrons, one that builds messages by combining source node features with edge features and the other that folds target node features with aggregated messages. After three message passing steps, the number of edge and node features are reduced to two each and passed through the softmax function to produce a *primary* score for shower fragment nodes and an *adjacency* score matrix for edges, S. The ground-truth adjacency matrix, A, is built such that, if two nodes belong to the same group, the edge that connects them is given a label of 1.

2.2 Inference

The network predicts an adjacency score matrix, which does not naturally translate into a node partition. The optimal partition, $\hat{g}$, is built in such a way that it minimizes the cross-entropy loss associated with it, i.e.

$$\hat{g} = \min_g L(S|g) = \min_g \sum_{i,j} \left[\delta_{g_i,g_j} \ln(S_{ij}) + (1-\delta_{g_i,g_j}) \ln(1-S_{ij})\right]. \tag{1}$$

The partition score defined in equation 1 is first calculated for an empty graph in which each node forms its own group. Edges are sequentially added in order of decreasing score, only if the new partition they form improves the partition score. In figure 2, the edge with score 0.6 is not added to the graph because it would put the nodes connected by the edge with 0.1 score in the same group and reduce the partition score.

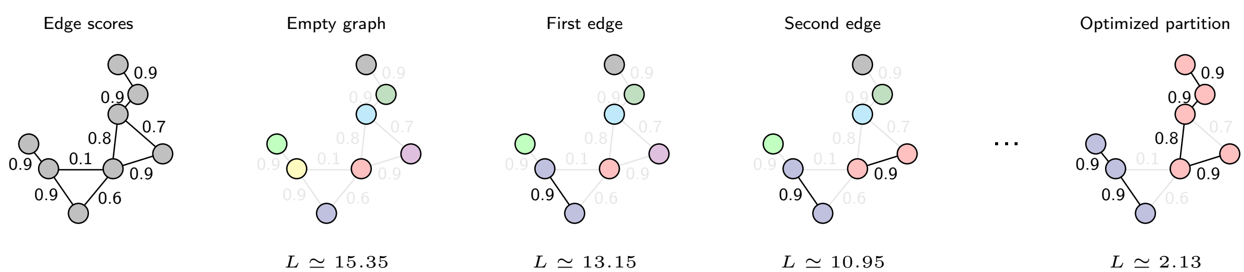


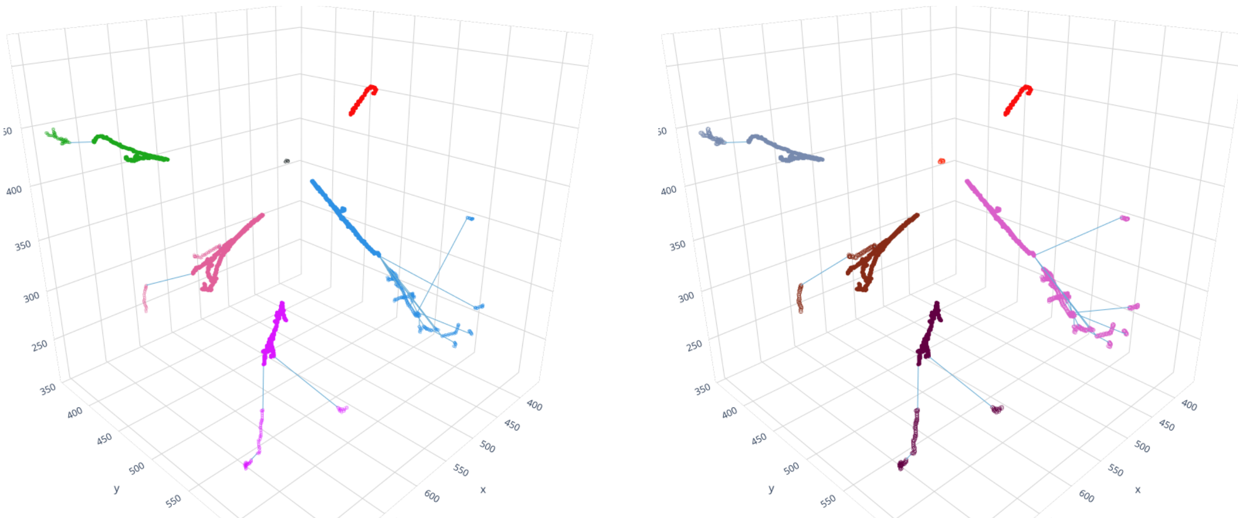
Figure 2: Schematics of the edge selection mechanism at the inference stage.

3 Results

In order to characterize the clustering performance, three metrics are used: efficiency, purity and Adjusted Rand Index (ARI). Efficiency is a measure of underclustering defined as the average fraction of a ground-truth cluster that is mapped to a single predicted cluster. Conversely, purity us a measure of overclustering defined as the average fraction of a predicted cluster that belongs to a single ground-truth cluster. The ARI is a more stringent metric which measures the similarity between two partitions by looking at the fraction of pair of voxels that are correctly either combined or separated, while accounting for random chance [7].

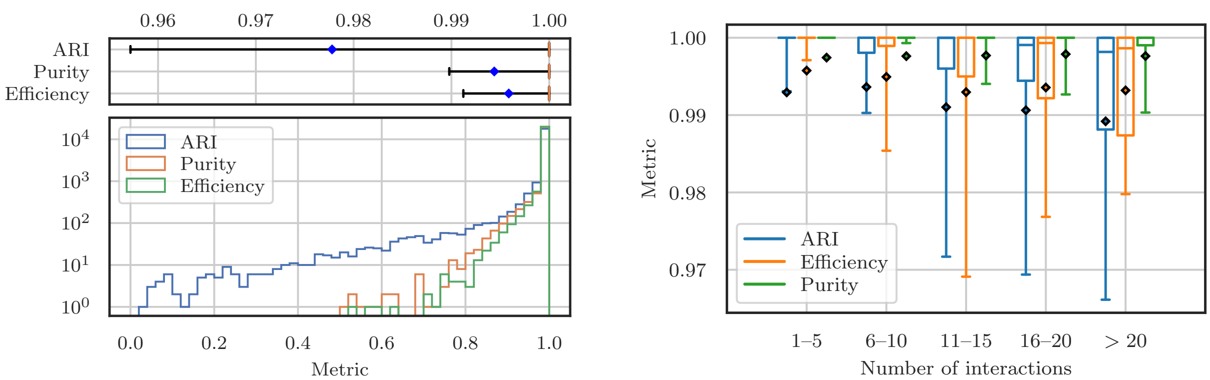
3.1 Shower clustering

Figure 3 shows an example of shower clustering and primary identification produced by the GNN algorithm. The left panel of figure 4 shows the distribution of clustering metrics of the entire test set. The network achieves an average purity of 99.4 %, an average efficiency of 99.6 % and a mean ARI of 97.8 %. The network identifies primaries by selecting the node with the highest primary score in each predicted group, which yields a 99.8 % primary prediction accuracy on this dataset.



(a) (b)

Figure 3: (a) Ground-truth shower group labels and particle edges, (b) predicted shower group labels and edges. The filled circle correspond to voxels that belong to the primary fragment.

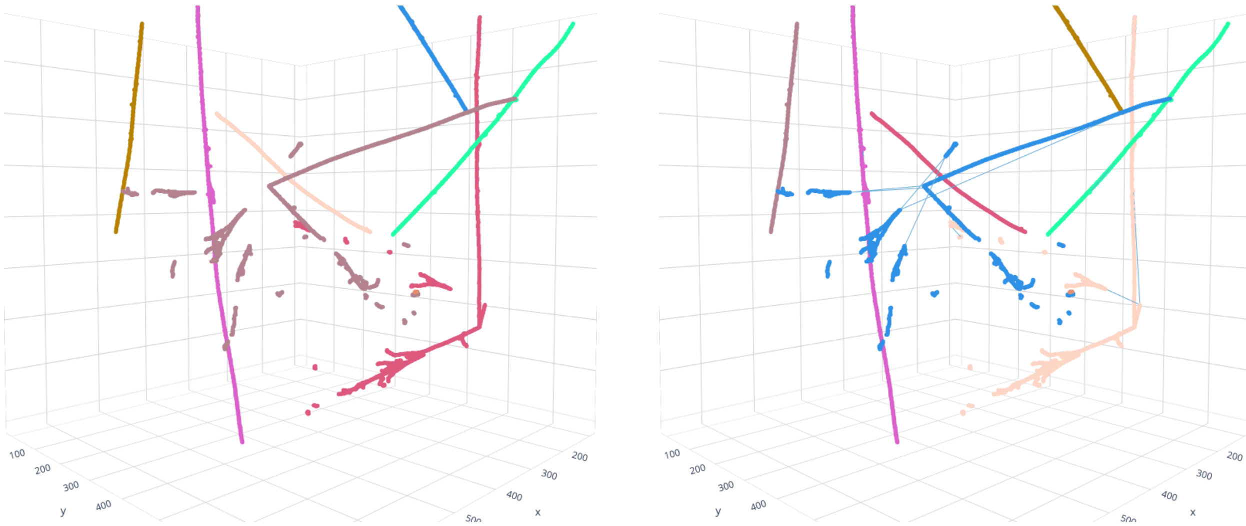


(a) (b)

Figure 4: (a) Distribution of shower clustering metrics. (b) Box plot distribution of interaction clustering metrics as a function of the number of interactions in the image. The diamonds represent the means, the lines the medians, the boxes the interquartile ranges and the whiskers extend from 10^{th} to the 90^{th} percentile.

3.2 Interaction grouping

Figure 5 shows an example of interaction clustering produced by the GNN algorithm on an image with seven interactions. The right panel of figure 4 shows the distribution of clustering metrics of the entire test set for different number of interactions in the image. For a realistic density of 5–10 interactions per image, the network achieves an average purity of 99.8 %, an average efficiency of 99.5 % and a mean ARI of 99.4 %.



(a) (b)

Figure 5: (a) Ground-truth interaction labels, (b) predicted interaction labels and edges.

4 Conclusions

Graph Neural Networks (GNNs) are an ideally suited method to tackle the clustering of spatially detached objects in Liquid Argon Time Projection Chambers (LArTPCs). A GNN-based reconstruction chain was developed to cluster electromagnetic showers and particle interactions. This paper studied its performance on a generic 3D sample of particle interactions in liquid argon and demonstrated a clustering efficiency and purity all above 99 % for both tasks. This method will be part of an end-to-end machine learning reconstruction chain developed at SLAC for all LArTPCs.

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