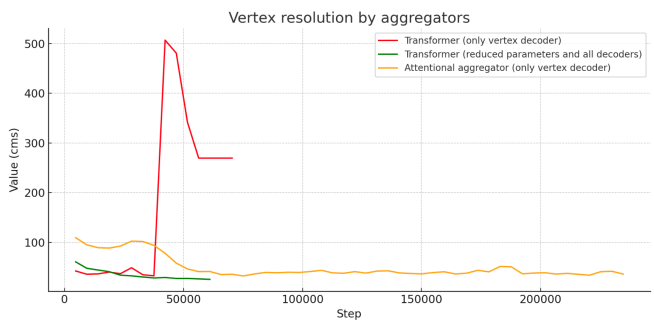
Winter Data Clinic 2024: Fermilab Graph Neural NetworkVertex Detection Optimization

Neutrinos are the most abundant particles with mass in the universe and are an area of active physics research. However, because neutrinos weakly interact with other particles, it is difficult for physicists to create neutrino detection data for research projects.

Currently Fermilab is building a model to simulate these neutrino interactions through a graph neural network (GNN) machine learning model, which is built on data from a physics detector called a 'Liquid Argon Time Projection Chamber'. The model is designed to identify the presence of neutrinos from noise in the chamber and estimate the paths of the particles within the detector. This quarter, Data science clinic students optimized the dimensions of Fermilab's GNN model, which will help Fermi researchers better label neutrino interactions and increase the amount of overall neutrino detection data available for future experimental applications.

This team was assigned the responsibility of analyzing the location predictor aspect of the model and applied a variety of machine learning configurations in their training instances to measure tradeoffs in resources, runtime, and accuracy. The location predictor is a part of the model that estimates the 3D coordinates of the neutrino behavior. They leveraged the University of Chicago's computing cluster, a powerful remote server, to train computationally intensive configurations of their model. This setup allowed them to experiment with various model architectures and examine how different message aggregation methods in Graph Neural Networks (GNNs) influence the accuracy of predicting neutrino interaction locations. Message aggregation in GNNs equips each node with the contextual information of other nodes, enriching the network's understanding and performance. This task required knowledge of the distributed computing architecture to access these resources in a way that minimizes user interaction throughout the model training. This was achieved through writing a queuing bash script that automated the model training, enabling the students to train models beyond the 12-hour resource bound. The students also visualized their findings by logging the training sessions on the Tensorboard, as shown below.



Finding the optimal aggregation method improves the convergence rate and performance of the vertex decoder. With a more accurate model, Fermi researchers will be able to measure neutrino interactions better, contributing to research that applies to a wide range of topics, from speeding up global communication to detecting the presence of nuclear weapons. Throughout the clinic process, the students documented their process and code base in a GitHub repository for the next quarter of Data Clinic students to contribute to and continue the Fermilab project.