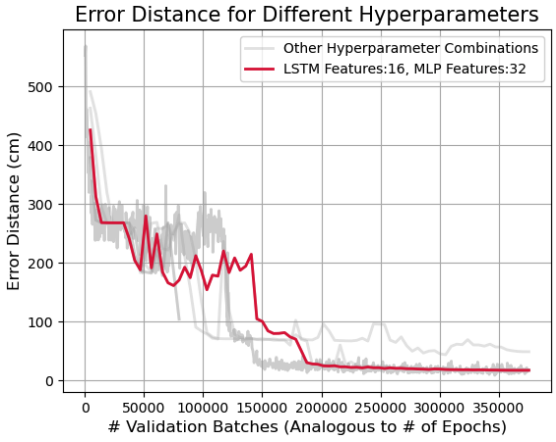
Fermilab Graph Neural Network Vertex Detection Optimization

Neutrinos are abundant in the universe with properties of remarkable interest. Yet, their properties render detecting neutrinos a longstanding experimental challenge for physicists, limiting access to novel data that can inform new physics.

Data science clinic students spent the quarter improving Fermilab's graph neural network (GNN), which analyzes data from a specialized detector called a 'Liquid Argon Time Projection Chamber'. The machine learning model distinguishes neutrinos from background noise and reconstructs their trajectories through the detector.

This team was tasked with improving the vertex decoding accuracy, a piece of the model which estimates the 3D coordinates of the neutrino interaction after the GNN has been trained. They used the University of Chicago's high-performance computing resources to conduct experiments on model architecture, aiming to identify the optimal model parameters for accurate prediction of neutrino interaction location. This task required significant research and effort to determine how to run code on the computing resources, and do so in an iterable way to minimize user interaction throughout the search process. Students also developed a Bayesian Optimization method, which adaptively selects sets of hyperparameters based on the outcomes of previous sets, rather than completely randomly, leading to greater confidence in reaching the optimal set when it is inefficient to test all parameters.

The identification of optimal hyperparameters improves the convergence and the final resolution on the vertex decoder, as shown in the figure. This will allow scientists to measure neutrino interactions more accurately, contributing to research questions in a broad range of fields from the nature of dark matter to Earth's internal structure.



Throughout the clinic process, the students documented set-up and operation procedures in the repository for the use of future students on the project to more easily build upon their work.