12th April, 2022

Equivariant Graph Neural Networks for Particle Tracking

Ameya Thete (BITS Pilani – K.K. Birla Goa Campus)
PIs: Dr. Savannah Thais (Princeton University), Dr. Daniel Murnane (LBNL)
Area: Innovative Algorithms

1 Introduction

At the CERN Large Hadron Collider (LHC), specialized tracking devices (or trackers) provide high-precision kinematic measurements of particles produced near a collision event. Charged particles produced in these events move in helical trajectories and generate energy deposits called hits within the tracker. The task of track reconstruction involves clustering these hits to trace out trajectories of the charged particles. Current tracking algorithms at the LHC implement combinatorial Kalman Filters which scale quadratically — or even worse — with detector occupancy [1]. The High-Luminosity upgrades to the LHC (HL-LHC) underline the need for better tracking algorithms exhibiting competitive perfomance in high-pileup environments.

In recent years, there has been a tremendous progress in the use of machine learning methods for solving problems in high-energy physics [1, 2], with a growing focus on geometric deep learning (GDL) which generalizes deep neural models to non-Euclidean data like graphs and manifolds. Graphs are a much more natural representation of tracker energy deposits compared to images or time series formats, as the hits can be mapped to nodes of a graph and the track segments between two hits to (directed) edges between these nodes. Consequently, Graph Neural Networks (GNNs) are well-suited to particle tracking applications. Aside from the relational inductive biases that GNNs carry, they may also relieve the large computational burden for big data HEP experiments. By leveraging greater parallelism, GNN-based algorithms might exeute faster with a smaller computational footprint than their traditional extant counterparts. This speedup is particularly vital at low-level layers like trackers that have to process millions of hits in a fraction of a second.

Most modern GNN architectures are permutation-invariant; however, there has not been much study into explicitly enforcing other forms of equivariance into GNN architectures, particularly for particle physics applications. Typical GNN models are resource-intensive and time-consuming to develop, and often contain a large number of parameters or require the construction of complex graphs [3]. Incorporating physically meaningful symmetries into the GNN can reduce the number of parameters and potentially reduce training and inference times for the model, while retaining their expressive power.

2 Proposed Project

In this project, we propose to develop an equivariant graph neural network for charged particle tracking by extending the work developed in [3] and [4]. We would ideally like to modify the VecNet architecture presented in [3] to support an edge-classification task for particle tracking. The VecNet architecture consists of repeated applications of convolution blocks that can be tuned to a desired degree of equivariance, followed by a KNN-aggregation step. We posit that we can explicitly incorporate $E(3)$ equivariance into the model by modifying the distance metric used in the aggregation step, as in [5]. Once an equivariant model is developed, we would like to benchmark its performace against other tracking algorithms (such as the Interaction Network GNN) on three major metrics: edge classification accuracy as formulated in [4] at the edge classification step; LHC match efficiency and Double-majority efficiency at the track building step; and model inference time — all for a range of $p_T^{\min}$ thresholds. We expect the equivariant network to exhibit competitive performance, if not outperform its counterparts while also requiring fewer number of trainable parameters. This project will be conducted remotely under the supervision of Dr. Savannah Thais and Dr. Daniel Murnane.

3 Timeline

I propose to work on this project over a 12-week period in the summer, from 06 June 2022 to 29 August 2022. I do not have any academic obligations during the fellowship period; however, I anticipate a brief commitment around mid-July for about a week. This interruption will be compensated by working for a few extra hours over the next couple of weeks.

Week(s)	Tasks
1 – 2	**Project Setup** • Review existing implementations of GNNs, particularly [3, 5] and allied works. • Replicate results from [3] to familiarize myself with equivariant GNNs.
3 – 4	**Dataset Curation** • Identify dataset candidates — TrackML is a potential choice. • Study symmetries in the dataset that can be incorporated into the model.
5 – 7	**Constructing the GNN** • Begin constructing the GNN model. Start with a baseline from [3] and add dataset- and symmetry-specific modifications.
Midsummer Review	Review the progress made so far in the project, and adjust the timeline and goals accordingly.
8 – 11	**Training and Comparative Analysis** • Continue implementation of the GNN model, following the design-build-test-learn cycle. • Benchmark the equivariant GNN against other geometric and non-geometric tracking models.
12	**Documentation and Wrapping Up** • Prepare the results, document code and upload it to a publicly visible repository, and submit a final report to the mentors. • Present the results in an IRIS-HEP topical meeting.

4 Deliverables

The primary deliverables of this project include an equivariant graph neural network for particle tracking along with a detailed analysis of its performance, including a benchmarking study comparing it to other contemporary tracking algorithms. All code written during the course of this project will be open-source and publicly available on a code repository like GitHub.

References

[1] J. Duarte and J.-R. Vlimant, *Graph neural networks for particle tracking and reconstruction*, in *Artificial Intelligence for High Energy Physics*, pp. 387–436, World Scientific (2022), DOI [2012.01249].

[2] S. Farrell, P. Calafiura, M. Mudigonda, Prabhat, D. Anderson, J.-R. Vlimant et al., *Novel deep learning methods for track reconstruction*, 2018 [1810.06111].

[3] D. Murnane, S. Thais and J. Wong, *Semi-equivariant GNN architectures for jet tagging*, [2202.06941].

[4] G. DeZoort, S. Thais, J. Duarte, V. Razavimaleki, M. Atkinson, I. Ojalvo et al., *Charged particle tracking via edge-classifying interaction networks*, *Computing and Software for Big Science* **5** (2021) 26.

[5] V.G. Satorras, E. Hoogeboom and M. Welling, *E(n) equivariant graph neural networks*, in *Proceedings of the 38th International Conference on Machine Learning, ICML 2021*, vol. 139 of *Proceedings of Machine Learning Research*, pp. 9323–9332, PMLR, 2021, http://proceedings.mlr.press/v139/satorras21a.html.