Graph Neural Networks for End-to-End Particle Identification with the CMS Experiment

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To ML4SCI

1. Introduction

Graph-structured data are a natural way to represent many complex systems, and occur in many engineering settings. Graph Neural Nets implement a system where information is propagated across a graph so as to perform node-level, edge-level, and graph-level predictions efficiently.

The choice of architecture for the GNN model largely depends upon the ratio of the number of training samples to the dimensions: for smaller values of the ratio, much simpler architectures such as Simplified Graph Convolutions (SGC) [1] and Approximate personalized propagation of neural predictions (APPNP) [2] are found to perform better [3], but for more training samples per dimension we require Graph Convolutional Networks, and hence this is the architecture I propose to build during my internship at GSoC.

First introduced in the paper [4], Graph Convolutional Networks consist of layers each of which applies 1. Graph convolution, 2. A linear layer, and finally 3. Non-linear activation. A network of these layers scales very well while training on GPUs or TPUs due to its high parallelizability.

Particle identification is the process of analysing the information from a particle detector to identify the particle that passed through it. It is done by reducing backgrounds from data collected from the detector. [5] Tau particles, specifically, are identified by classifying the jet (a spray of stable particles that has stemmed from the particle decaying and interacting with other particles) produced by “the hadronic decay of the tau from ordinary quark jets”. In this project proposal I present a method to perform tau particle identification using a Graph Neural Network.

2. Why I Want to Work on this Project

I am fascinated by how instinctively GNNs can map graph data problems. On creation of a network by putting multiple GN blocks together, very complex and long-range computations become feasible by the propagation (and processing) of information through the graph.

It excites me to learn that deep learning is being applied to particle identification: I read papers on the topic and that convinced me of the power that GNNs hold over particle physics.

Moreover, I think this is the right project for me because I have experience working with GNNs in PyTorch and PyTorch-Geometrical, along with other libraries like NumPy, Dask, H5py that we might need, as well as an immense interest in deep learning.

3. Objective

Goal: Jet classification through a GNN for identification of tau particles, and reconstruction using the CMSSW engine

- Discussing Graph Neural Network architectures with the mentors and coming up with a structure that can efficiently map our graph data to another graph or summary output.
- The model should be able to generalise well to new graphs; this is a characteristic of GNNs, since training is performed on and node- and edge-level.
- Discerning the strengths and weaknesses of the formulated architecture by testing out the model on new graph data samples.

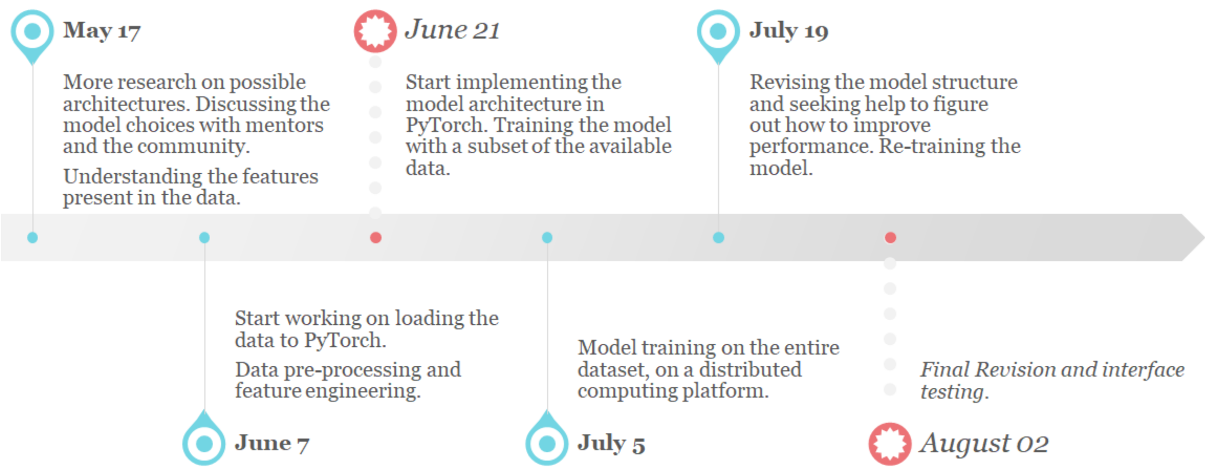
4. Implementation

According to [5], identification of b-jets is made possible by the large lifetime of b-hadrons. The process is called b-tagging; by using neural networks, b-tagging can be generalised to the identification of jets coming from other particles, including tau particles. [6]

Much of the background to b-jets is constituted by QCD jets which originate from pure hadronic interaction. I intend to perform a method similar to [7], to represent the collection of particles in a graph data structure. The paper implements “the edgeconv method”, which is used to derive a point-cloud architecture of the graph data. The node neighbourhoods are computed to give the connectivity of this graph. The authors of [7] implement this model to classify whether a certain jet is originating from a quark or a gluon, outperforming previous architectures. [8] again implements this architecture on semi-visible jet originating from “the cascade decay of hypothetical dark hadrons”. This architecture again performs better than novel neural nets.

I am also quite interested in the methods described in [9] and [10]: these implement attention graph networks. [9] proposes the attention-based cloud net (ABCNet), which 1. creates a point cloud interpretation and implements an attention mechanism, which enhances the local information extraction, and 2. uses direct connections for global input features to learn the global information. [9] also demonstrates how we can improve upon the stability of our model using a multi-head mechanism. [10] compares graph attention networks and GCNs, building upon the computational efficiency of the model. I would also like to propose research on the comparative performance of these two methods on our data, measured against our novel GCN implementation.

5. Project Timeline



5.1 Deliverables for the First Evaluation

PyTorch Implementation of the GNN architecture that is discussed with the mentors and finally decided upon. The model will be able to perform jet classification and discern whether

5.2 Deliverables for the Final Evaluation

Thoroughly revised implementation of the GNN architecture, along with an interface for physicists to input their graph data for tau particle identification.

6. Related Work and Bibliography

[1] Simplifying Graph Convolutional Networks
Felix Wu, Tianyi Zhang, Amauri Holanda de Souza Jr., Christopher Fifty, Tao Yu, Kilian Q. Weinberger

[2] Predict then Propagate: Graph Neural Networks meet Personalized PageRank
Johannes Klicpera, Aleksandar Bojchevski, Stephan Günnemann

[3] On the Choice of Graph Neural Network Architectures
Clément Vignac, Guillermo Ortiz-Jiménez, Pascal Frossard

[4] Spectral Networks and Deep Locally Connected Networks on Graphs
Bruna et al

[5] Review of Particle Physics. Phys. Rev. D
M. Tanabashi et al.

[6] Graph Neural Networks in Particle Physics
Jonathan Shlomi, Peter Battaglia, Jean-Roch Vlimant

[7] Particlenet: Jet tagging via particle clouds
Huilin Qu and Loukas Gouskos.

[8] Casting a graph net to catch dark showers.
Elias Bernreuther, Thorben Finke, Felix Kahlhoefer, Michael Kr¨amer, and Alexander M¨uck.

[9] Abcnet: An attention-based method for particle tagging
Vinicius Mikuni and Florencia Canelli.

[10] Graph Attention Networks
Petar Veliˇckovi´c, Guillem Cucurull, Arantxa Casanova, Adriana Romero, Pietro Li`o, and Yoshua Bengio.

6.1. Related Work

End-to-End Physics Event Classification with CMS Open Data
Applying Image-Based Deep Learning to Detector Data for the Direct Classification of Collision Events at the LHC
M. Andrews, M. Paulini, S. Gleyzer, B. Poczos

End-to-End Jet Classification of Quarks and Gluons with the CMS Open Data
M. Andrews, J. Alison1 S. An,, B. Burkle, S. Gleyzer, M. Narain, M.Paulini, B. Poczos, E. Usai

Graph Neural Networks: Architectures, Stability and Transferability
Luana Ruiz, Fernando Gama, Alejandro Ribeiro

Semi-Supervised Classification with Graph Convolutional Networks
Thomas N. Kipf, Max Welling

Energy Flow Networks: Deep Sets for Particle Jets
Patrick T. Komiske, Eric M. Metodiev, and Jesse Thaler

8. About me

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