Graph Generative Models for Fast Detector Simulations in Particle Physics

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1 About me

I am a Machine Learning Engineer having recently defended my Master's thesis in a collaboration between the American University of Beirut and the CMS experiment at CERN. My academic thesis shed light on the application of graph neural networks in High Energy Physics. More specifically, I was selected for the 2020 Google Summer of Code where I developed a Graph Variational Auto-Encoder (GVAE) that learns the latent space representation of boosted top quark jets and eventually reconstructs them. In this work jet showers are mapped into graphs connected by means of K-nearest neighbours. This model uses the GraphSAGE algorithm for spatial convolution operations on the nodes [1] and the Mincut pooling technique for graph size reduction [2]. Moreover, I was selected for the 2020 Helmholtz GPU hackathon where I optimized my code and scaled the graph model to multiple GPUs obtaining 2.76x speedup. Throughout this period, I have gained skills in using frameworks such as PyTorch, Tensorflow and CUDA in addition to coding graph model for deep learning training and acquiring extensive knowledge in graph theory and the application of different types of graph neural networks (Spatial/spectral/spatio-temporal).

My publication record throughout this thesis work includes a NeurIPS workshop paper on ML in the Physical Sciences, an upcoming talk at the GPU Technology Conference in April and two accepted conference papers at the Computing in High Energy Physics Conference. Moreover, my work has recently been accepted to the ICLR Workshop on Deep Learning for Simulation.

On this proposed IRIS-HEP project I intend to work with Prof. Sergei Gleyzer (University of Alabama), Prof. Harrison Prosper (Florida State University) and Prof. Michelle Kuchera (Davidson College). This work is intended to be open-source and has a potential to impact many researchers who rely onparticle simulations for physics studies.

2 Abstract

The Large Hadron Collider (LHC) at CERN is the world's highest energy particle accelerator, delivering the highest energy proton-proton collisions ever recorded in the laboratory, permitting a detailed exploration of elementary particle physics at the energy frontier. Simulating the particle showers and interactions in the LHC detectors is both time consuming and computationally expensive. Present fast simulation approaches based on non-parametric techniques can improve the speed of the full simulation chain but suffer from lower levels of fidelity. For this reason, alternative methods based on machine learning can provide faster solutions, while maintaining a high level of fidelity. The main goal of a fast simulator is to map the events from the generation level directly to the reconstruction level. The recent rise of deep generative models paved the way for novel AI-based simulation methods. These are characterized by a high ability to learn complex data features in a high dimensional space as probability distributions to reconstruct or simulate new samples from those data. Hence, generative models make great candidates for the representation learning of particle collision events. The most used generative architectures are Generative Adversarial Networks [3] and Variational Auto-Encoders [4]. Given the non-Euclidean nature of jet events data, we aim to investigatethe efficiency of graph generative models in simulating event reconstructions in a given detector.

3 Graph Variational Auto-Encoders

Variational Autencoders (VAEs) have shown great success in reconstruction Euclidean types of data such as images and audio [4]. Yet, numerous data structures are non-Euclidean in reality such as social networks and molecular structures. In this project we shed light on the ability of autoencoders to operate on graph structures as defined in [5]. A graph is defined by an adjacency matrix A defining the connections between the nodes of the graph i.e the graph topology and a feature matrix X assigning nodes to their specific features. A has the shape $N \times N$ while X has the shape $N \times F$ where N is the total number of nodes within the graph and F is the number of node features. Similar to images, graphs in neural networks undergo convolution operations either through spectral operations in the Laplacian domain or using spatial convolutions.

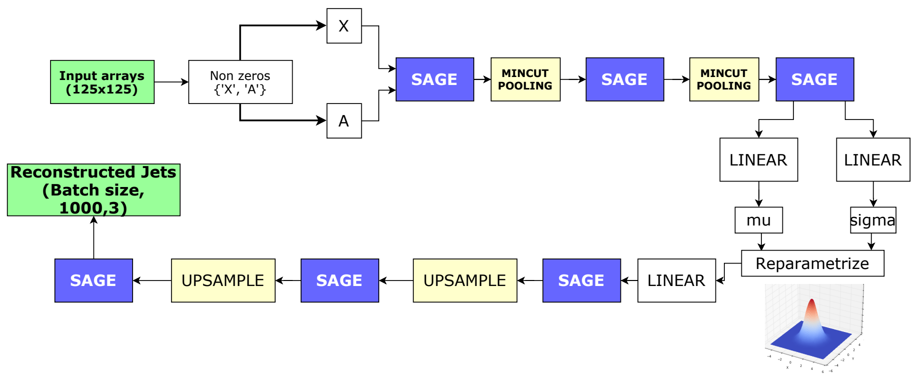

Figure 1: Model architecture of the Graph Variational Autoencoder showing Graph-SAGE layers and pooling blocks [6]

4 Graph Generative Models in Particle Physics

4.1 Jet reconstruction

In our recent work on "Graph Generative Models for Fast Detector Simulations in High Energy Physics", we present a geometric deep learning-based approach for the representation learning of particle physics data [6]. We develop a Graph Variational Autoencoder to reconstruct the boosted top quark jets data. The first step consisted of mapping sparse particle hits into graphs whose nodes contain 3 features: x location, y location and particle momentum. To proceed, we perform message passing within the nodes by means of the GraphSAGE algorithm to learn high-dimensional space representation of those nodes. The latter are then compressed into a smaller cluster using the mincut graph pooling technique. A latent space distribution of the events is obtained and characterized by vectors mu and sigma. Eventually, the original jet data are gradually reconstructed through the decoder. A visual description of our model can be found in Figure 1.

4.2 Performance Studies

Apart from the reconstruction efficiency in terms of topology and energy scale, another aspect to consider when developing any deep learning is the time it takes for the training and inference on the model. As more detector channels are encoded into the deep learning model, we need to monitor the computational and memory cost associated with the corresponding upgrade. Such channels include the Electromagnetic Calorimeter (ECAL), the Hadronic Calorimeter (HCAL) and the Tracks projected to the ECAL surface. To proceed, jet image data will be pre-processed into graphs connected by means of k-nearest neighbors approach and will be sent as mini-batches to training using Parquet's lazy-loading technique.

On the other hand, we will try different spatial convolution techniques for message passing (Graph Attention, GraphSAGE, etc) and compare the corresponding runtimes (training and inference). Moreover, the numerous architectures will be investigated for their complexity when operating on larger numbers of detector channels. Finally, the scalability of the most optimal model will be investigated, potentially using distributed deep learning libraries such as Horovod. In fact, scalability is a crucial characteristic to take advantage of in a model given the compute resources under disposal for simulation operations and the efficiency obtained by distributing the algorithms to execute in parallel on these hardware resources.

4.3 Comparison of Classical and Quantum Machine Learning Approaches

Several studies so far shed light on the ability of neural networks in learning on high energy physics data. Yet, the potential of neural networks combined with quantum algorithms is still under-explored. Quantum computing is a rising field with promising aspects with regards to the acceleration of several machine learning applications due to exponentially reduced time and memory relative to classical methods. This has been shown in numerous fields, mainly cryptography [7] and financial forecasting [8]. In High Energy Physics, the potential of Quantum Machine Learning (QML) has been recently investigated in a set of applications including particle tracking [9] and event classification [10].

In this work we suggest to encode particle physics data into quantum states in a Hilbert space to be learned upon by a quantum graph variational autoencoder. In [11], Khoshaman et.al develop a Quantum Variational Autoenconder (QVAE) to operate on the MNIST dataset by sampling from large Quantum Boltzman Machines (QBMs) in the latent space to reconstruct the MNIST images. We propose to develop a Quantum Graph Variational Autoencoder to reconstruct particle physics events. Quantum Graph Neural Network architectures have been previously developed for graph isomorphism classification and unsupervised graph clustering [12], but quantum graph generative models remain under-explored, especially in High Energy Physics.

5 Project Timeline

- **Weeks 1 & 2:** Decide on the data to be simulated (Boosted top quarks,electrons,etc). After visualizing and pre-processing the data, reproduce it using the Graph VAE obtained in [6] while tuning model hyperparameters. These results would be the baseline for future comparisons.
- **Weeks 3 to 6:** Gradually upgrade the channels to be studied. Within this timescale experiments should cover at least tracks, ECAL and HCAL. During this period further literature is to be done on recent quantum neural network models that could be helpful.
- **Weeks 7 to 10:** Upgrade the existing channels to cover the tracker and pixel layers. The computational complexity and scaling should be noted. If time al-

lows, perform training and validation of a quantum graph generative model for the reconstruction of particle physics data.

- **Weeks 11 & 12:** Document the codes and the numerous architectures that have been tried. Compare the Quantum model to the classical one and interpret the results.

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