Graph Generative Models for Fast Detector simulations in Particle Physics

Authors: Ali Hariri[1], Darya Dyachkova[2], Sergei Gleyzer[3]

[1] American University of Beirut, Beirut, Lebanon, aah71@mail.aub.edu

[2] Minerva Schools at KGI, San Francisco, CA, US, darya.dyachkova@minerva.kgi.edu

[3] University of Alabama, Tuscaloosa, AL, US, sgleyzer@ua.edu

1. Abstract

Accurate and fast simulation of particle physics processes is crucial for the high-energy physics (HEP) community. Simulating the particle showers and interactions in the detector is both **time consuming** and **computationally expensive**. To address that, classical **fast simulation** approaches based on non-parametric approaches map the events from the generation level directly to the reconstruction level. That improves the speed of the full simulation but suffers from lower levels of fidelity. As an alternative, we introduce a **graph neural network-based autoencoder model** that provides effective reconstruction of calorimeter deposits using the **earth mover distance metric**.

2. Motivation

- Deep generative models show great ability to learn complex representations for image reconstruction and segmentation.
- Most of the existing work on supervised and unsupervised deep learning for HEP simulation relies to Euclidean data structures.
- We explore **Graph Neural Networks** that learn on non-Euclidean, point cloud data mapped into graphs for the purpose of Fast Detector Simulation.

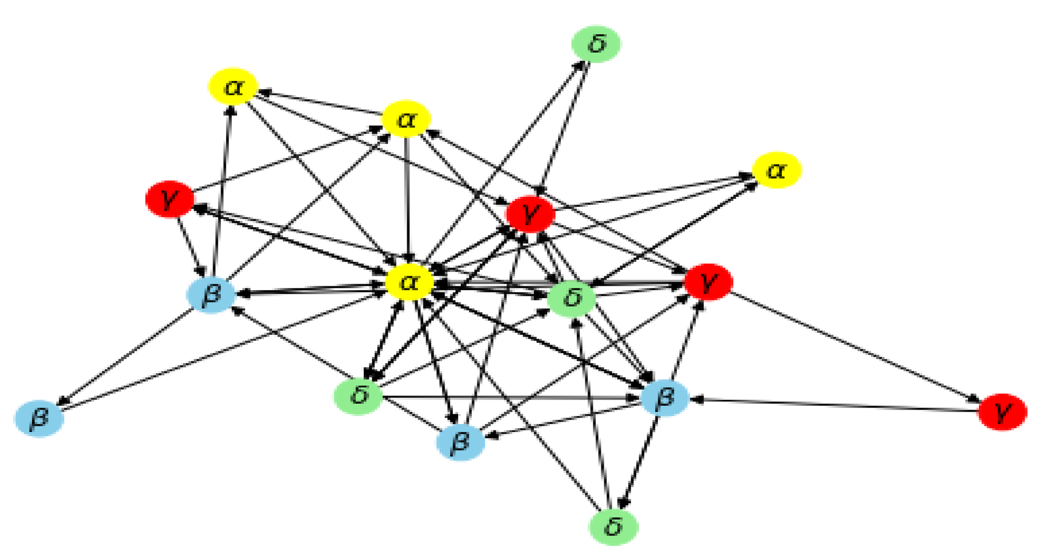

Figure 1

3. Data

- We use **top quark simulation events** produced using Pythia 6 generator, available through CMS Open Data release [1].
- 30000 samples of 3x125x125 arrays representing the 3 sub-detectors: Tracker, Electromagnetic calorimeter (ECAL) and Hadronic Calorimeter (HCAL).
- Here, we focus on the electromagnetic calorimeter (ECAL) signatures of jets.
- The non-zero hits within the 125x125 array correspond to the deposited and reconstructed hit energies.

4. Model architecture and metrics

We developed a Graph Variational Autoencoder (GVAE) architecture, where the encoder embeds the node features into the latent space through **Dense GraphSAGE** layers and compresses them into smaller dimensions using **spectral graph pooling**. Next, a decoder performs decoding of the latent space compressed nodes to obtain upsampled feature matrix X and adjacency matrix A, S being a learned cluster assignment matrix:

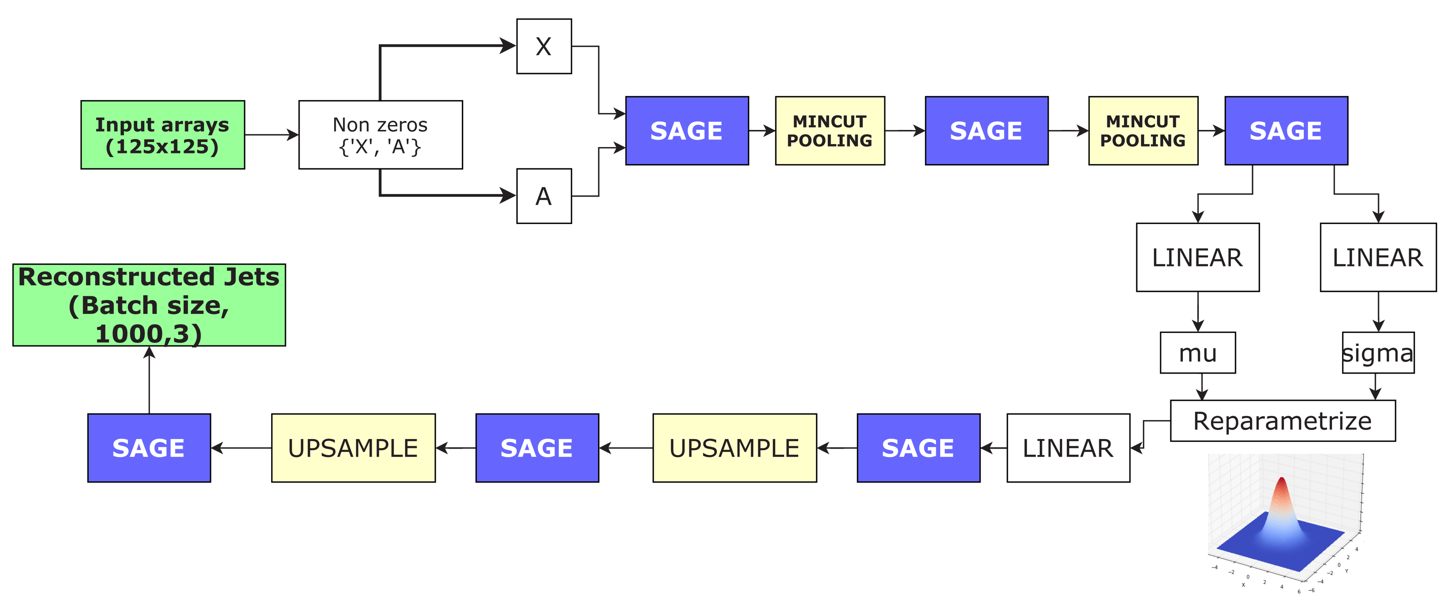

Figure 2

$$X^{rec} = SX^{Pooled}; A^{rec} = SA^{Pooled}S^T \quad (1)$$

We choose k=4 as the number of nearest neighbours to be connected to each node and the Adam optimizer with the learning rate of 0.001. The loss function includes the **MSE** loss between node features together with the **KL divergence** between the latent space and the real P(z|x) distribution. We split our dataset into 70% training, 20% validation, 10% testing. To further evaluate our data, we use the **Earth Mover Distance (EMD)** metric, which provides the cost associated with moving a point cloud distribution to a reference distribution.

5.1 Results

- Fig.3 displays the reconstruction output for several simulated jets from our GVAE model, displaying accurate reconstruction in terms of location and energy values.
- Figure 4 shows the EMD values corresponding for 4800 reconstructed jets; low EMD values imply a high-level of similarity between the jets. We train on a Tesla V100 GPU. During inference, the GVAE model spends a total of 0.1235 seconds on a batch of 64 jets, which is orders of magnitude faster than full simulation. (Fig. 5).

8. References

[1] CERN Open Data Portal: http://opendata.cern.ch

5.2 Figures

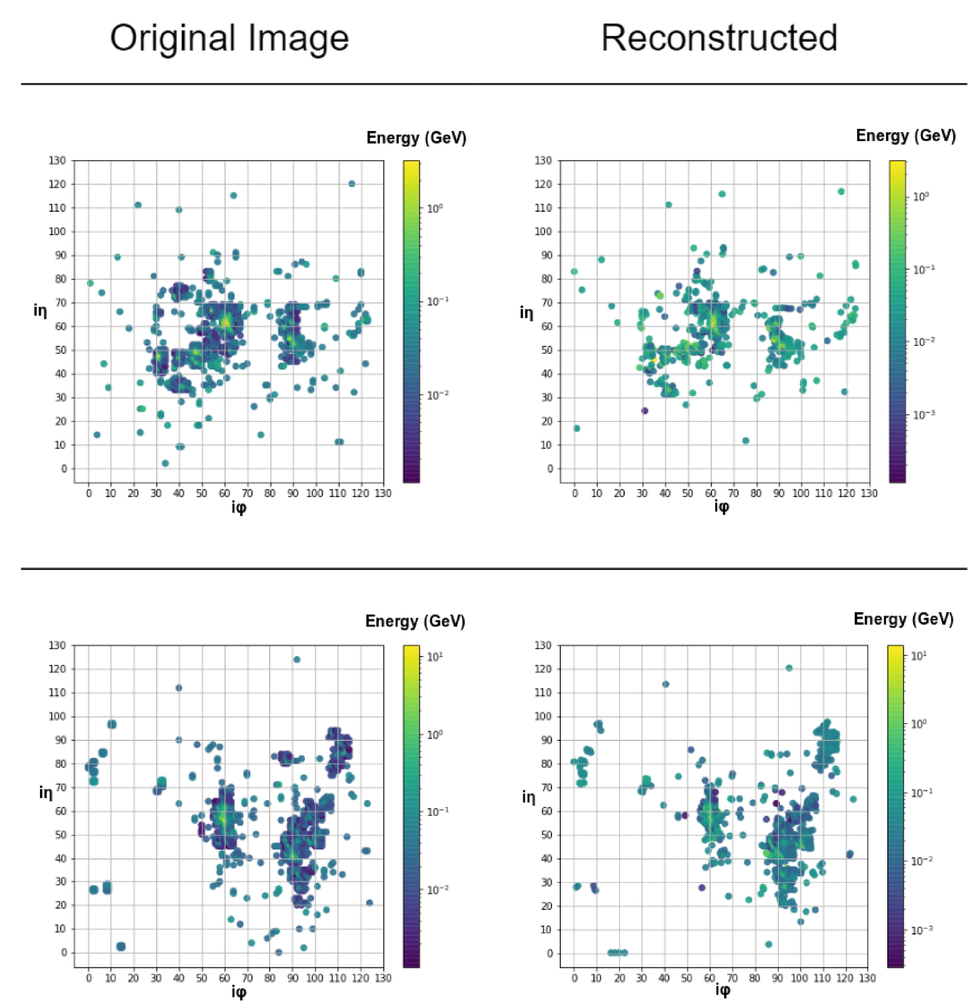

Figure 3

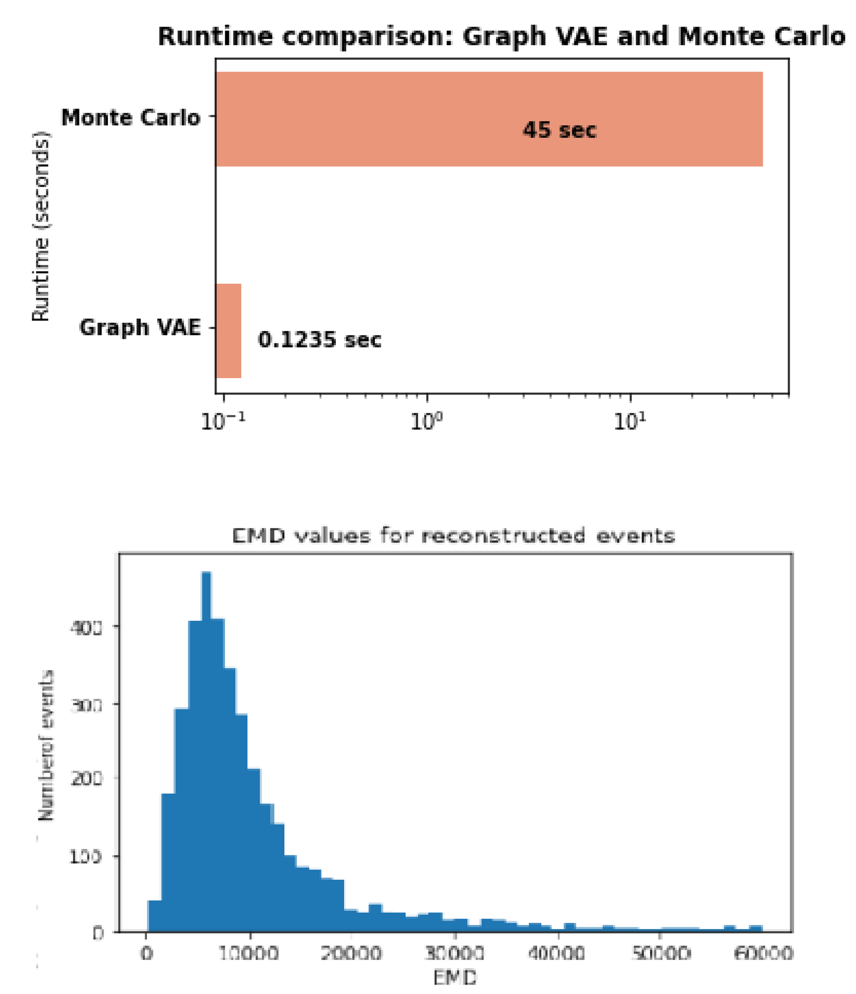

Figure 4 (bottom) and Figure 5 (top)

6. Conclusions

In this work we find that the graph variational autoencoder model is promising for learning the representation of high-energy particle physics events, and we explore its potential for next-generation of fast simulators at the Large Hadron Collider.

7. Broader Impact

- This work is an open-source project, and has a potential to impact many researchers who rely on particle physics simulations.
- The computational efficiency provided by the generative model presented in this work allows to overcome computational constraints.
- In absence of adequate computational resources, this type of simulation allows speedup in obtaining the results.

We thank NVidia Corporation for access to a Tesla V100 Cluster used to train the GVAE models.