Fast detector simulation and anomaly detection using Graph variational autoencoders

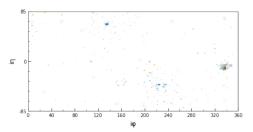
December 7, 2023

Collisions at the LHC

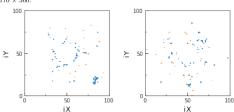
- ► In the CMS and ATLAS detectors at LHC, opposing proton beams are smashed[3]
- By products are measured using various sub-detectors
- Trackers track the trajectories of photons and charged particles
- ► ECAL measures the transverse momenta of electrons/photons and cylindrical coordinates
- ► HCAL measures the transverse momenta of hadrons and cylindrical coordinates

The generated image

lacktriangle From hits in a subdetector, we get "images" wrt ϕ and $\eta[2]$

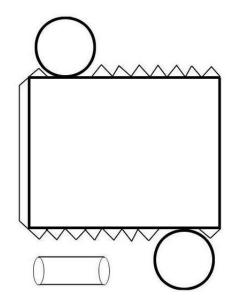


(a) Barrel section of composite image in ECAL-centric geometry. Image resolution: $170\,\times\,360.$

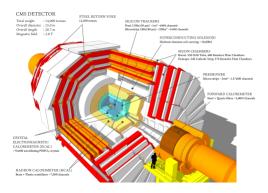


(b) Endcap sections of composite image in ECAL-centric geometry. Image resolution: 100×100 .

Imagine making a (finite) cylinder out of paper



Cross section of the CMS detector



Simulating the collisions

- Hard(core) scattering
- Secondary collisions
- Decays and radiative correction
- Hundreds of different processes, everything Monte Carlo!

Hard scattering

- ► The moments right after the primary collision...
- Modeled using perturbative QCD- cross sections are given by Feynman diagrams
- ➤ The initial/final states are not eigenstates of unperturbed theory, unlike QED
- ► Higher order loops with IR divergences require very precise Monte Carlo or analytical estimates

Secondary collisions/processes

- Non-relativistic QCD and semi-classical appromations for decay processes
- Highly empirical, sometimes benchmarked by detector calibrations
- ▶ Factorization theorems and Parton Distribution functions
- General purpose libraries- PYTHIA, SHERPA[7]

Detector effects and ML models

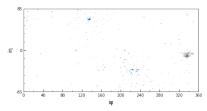
- ► GEANT4 has extremely precise models of detector interaction with final product states[1]
- ► The entire simulation pipeline can take days to run on supercomputers, for sufficient hits/samples
- Non ML alternatives to GEANT4 (like DELPHES) tradeoff precision for speed[4]
- ML models fit precise data to well-behaved functions- similar to variational inference of energy eigenstates in quantum systems

Generative ML for end to end simulation

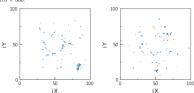
- ► Particle hit images are inherently probabilistic- so ML models approximate probability distributions on the data
- Dominant Generative ML paradigms- VAE, GAN, NF
- Popular implementations use convolution layers to generate pixel by pixel
- Downside- detector hits are highly sparse which limit applicability of convolutions



Sample detector image



(a) Barrel section of composite image in ECAL-centric geometry. Image resolution: $170\times360.$



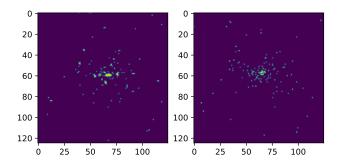
(b) Endcap sections of composite image in ECAL-centric geometry. Image resolution: 100 × 100.

Graph modeling and message passing convolutions

- ▶ Number of non-zero pixels << Total number of pixels [6]
- ▶ We model non-zero hits alone, and their positions
- Assume each hit depends on nearest neighbor hits
- Graph message passing implements precisely this[5]
- Output invariant of order of nodes or their neighbors- similar to translation invariance in CNNS

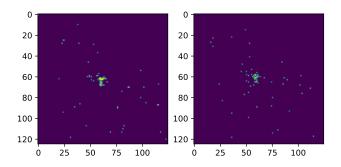
Some initial results

Quark jet



An anomaly

Gluon jet



```
while questions:
attempt_to_answer()
print("Thank you and peace out!")
```

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