

IRIS-HEP Summer Fellowship 2021

Accelerating End-to-End Deep Learning using Graph Neural Networks

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Dr. Davide DiCroce

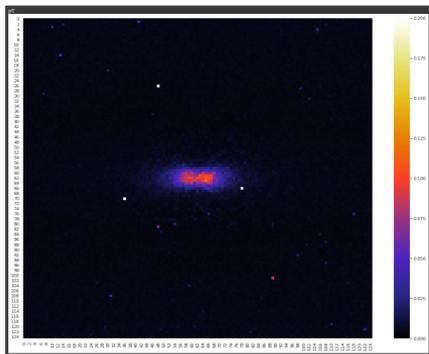


Goals of the project

- Use low-level detector features for high energy particle reconstruction (Taus).
 - Design Graph based deep learning approaches (Graph Neural Networks)
 - Compare their performance with Convolutional Neural Networks.
 - Integrate Tau Tagger with the E2E Framework built within CMSSW (with deep learning inference support using Tensorflow C++ Runtime)
 - Develop a prototype for integration of Graph Neural Networks with E2E Framework.
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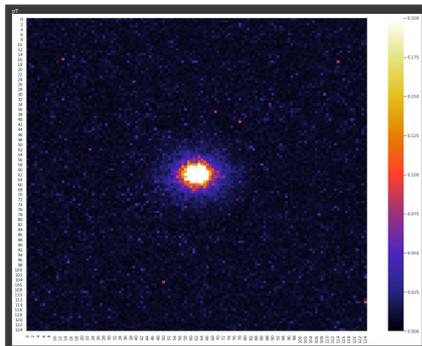
Shower plots

DYTauTau pT



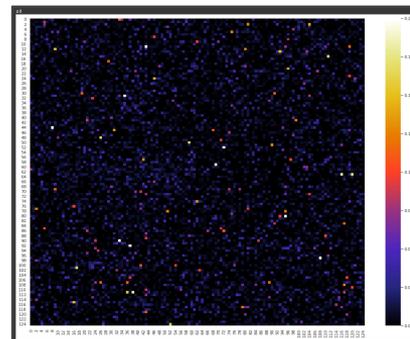
y=1

TTbar pT



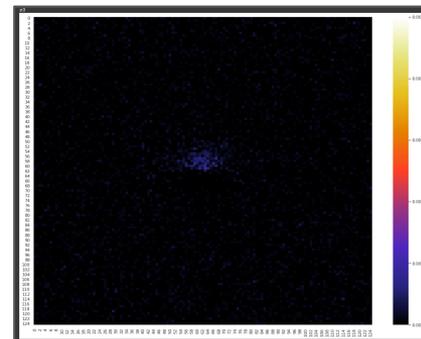
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DYTauTau dz

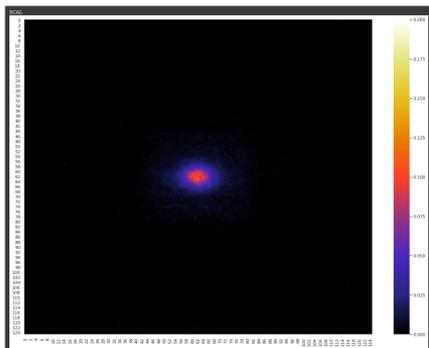


y=1

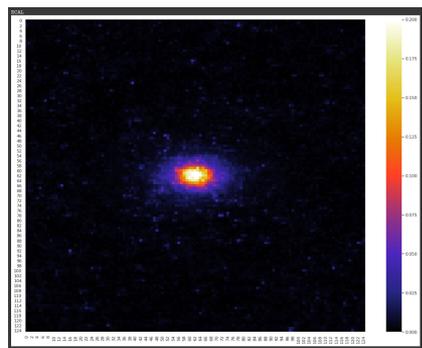
TTbar dz



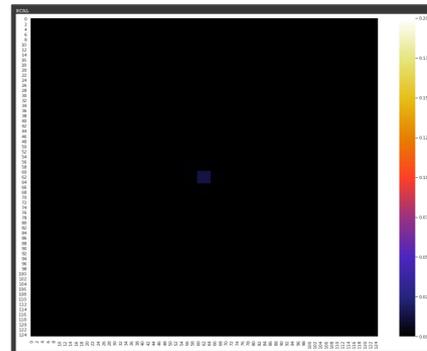
y=0



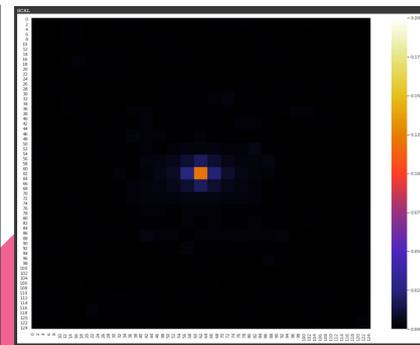
DYTauTau ECAL



TTbar ECAL

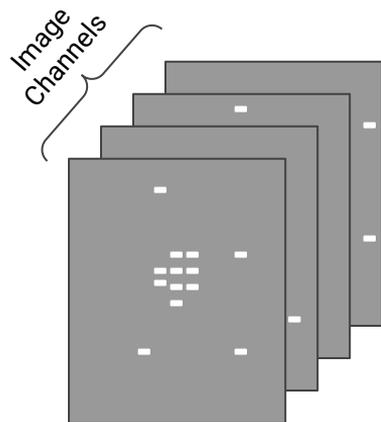


DYTauTau HCAL

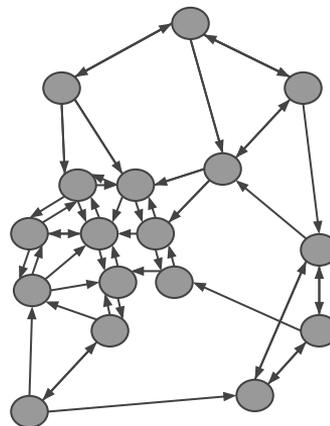


TTbar HCAL

Data preparation & preprocessing



Multichannel
Image



Graph (k=3)

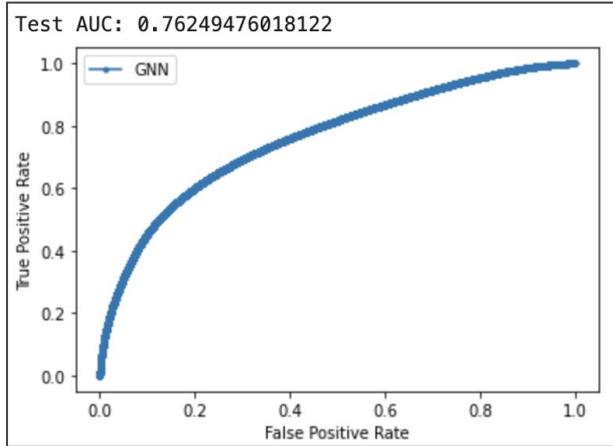
- All the nonzero pixels of the images are used to construct the graph.
- The edges are constructed using the euclidean distance and knn graph clustering fashion based on the image coordinates.
- The node features are the nonzero pixels of the image channels.

Graph Neural Network

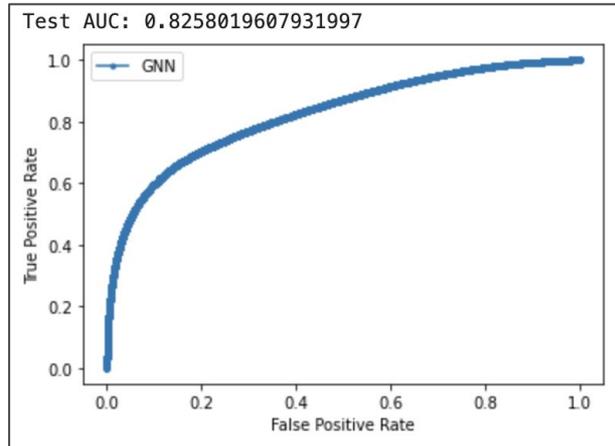
Trained on Tesla P100 GPU and Intel(R) Xeon(R) CPU E5-2690 v3 @ 2.60GHz

| Channels | Validation ROC AUC scores |
|--|---------------------------|
| BPIX * 4 | 0.697 |
| pT + ECAL | 0.856 |
| pT + ECAL + HCAL | 0.864 |
| pT + ECAL + HCAL + dz + d0 | 0.870 |
| pT + ECAL + HCAL + dz + d0 + BPIX *4 + TIB*2 + TOB*2 | 0.887 |

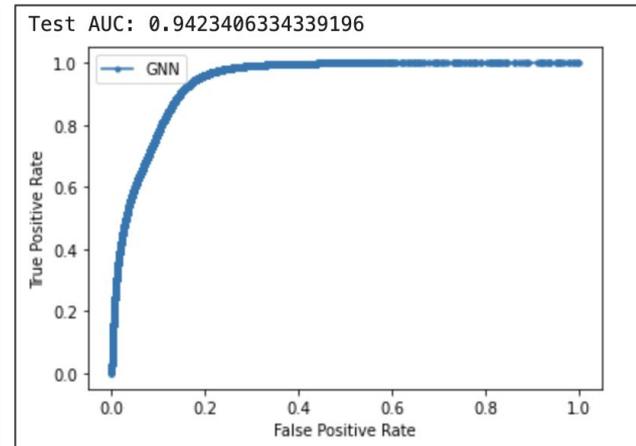
Model Performance for low momentum jets (DYTauTau)



DYTauTau vs Wjets
($p_T + \text{ECAL} + \text{HCAL} + dz + d_0$)



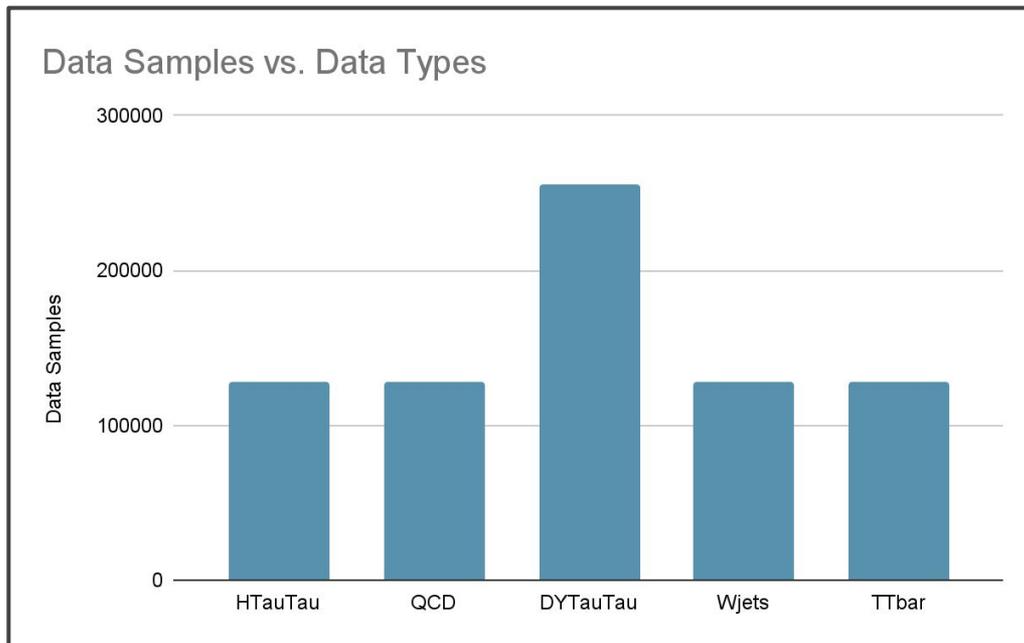
DYTauTau vs QCD
($p_T + \text{ECAL} + \text{HCAL} + dz + d_0$)



DYTauTau vs TTbar
($p_T + \text{ECAL} + \text{HCAL} + dz + d_0$)



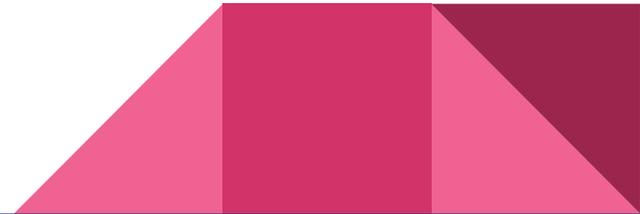
Training Data Distribution



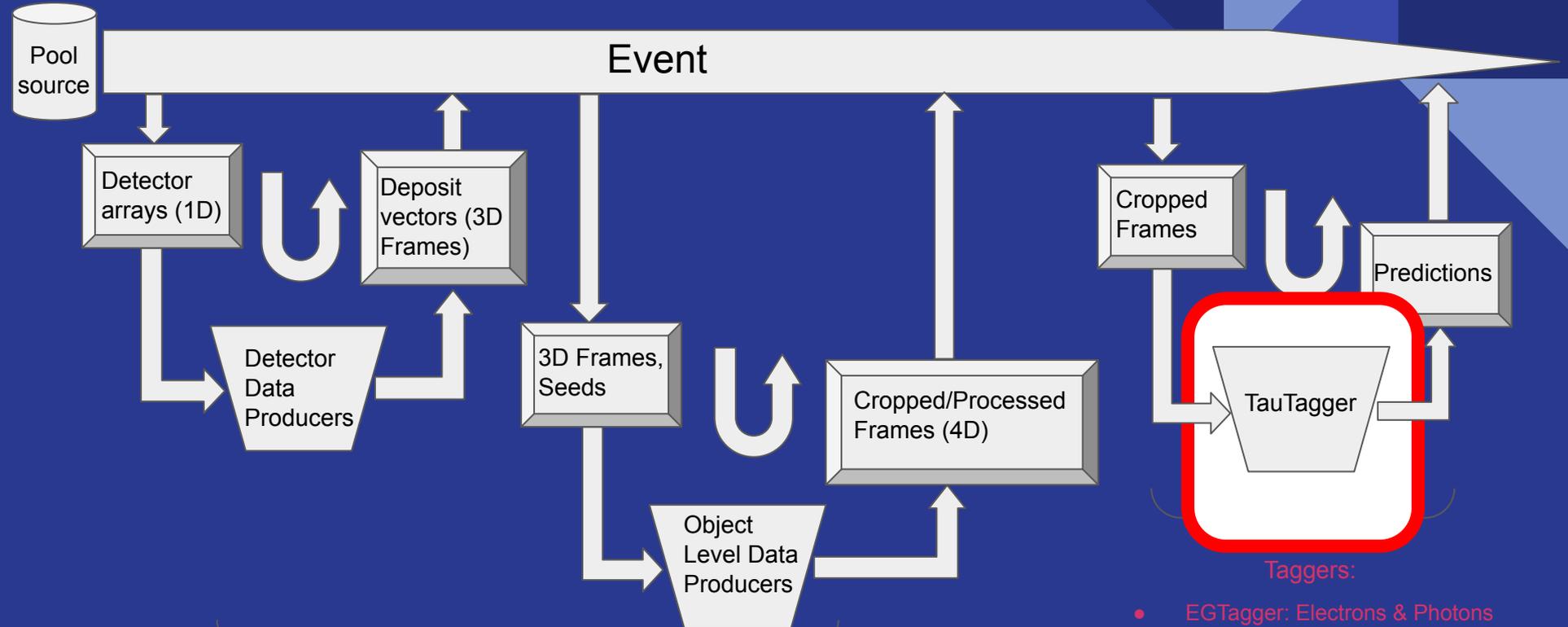
Comparison with CNN

| Channels | GNN | CNN |
|--|-------|-------|
| pT + ECAL + HCAL + dz + d0 | 0.87 | 0.798 |
| pT + ECAL + HCAL + dz + d0 + BPIX*4 + TIB*2 + TOB*2 | 0.887 | 0.864 |

Integration of Tau Reconstruction with E2E Pipeline



Current Pipeline:



FrameProducer package:

- EGFrameProducer: Electrons & Photons
- JetFrameProducer: Quarks, Gluons, Top Jets & Taus

Taggers:

- EGTagger: Electrons & Photons
- QGTagger: Quarks & Gluons
- TopTagger: Top Jets
- TauTagger: Taus

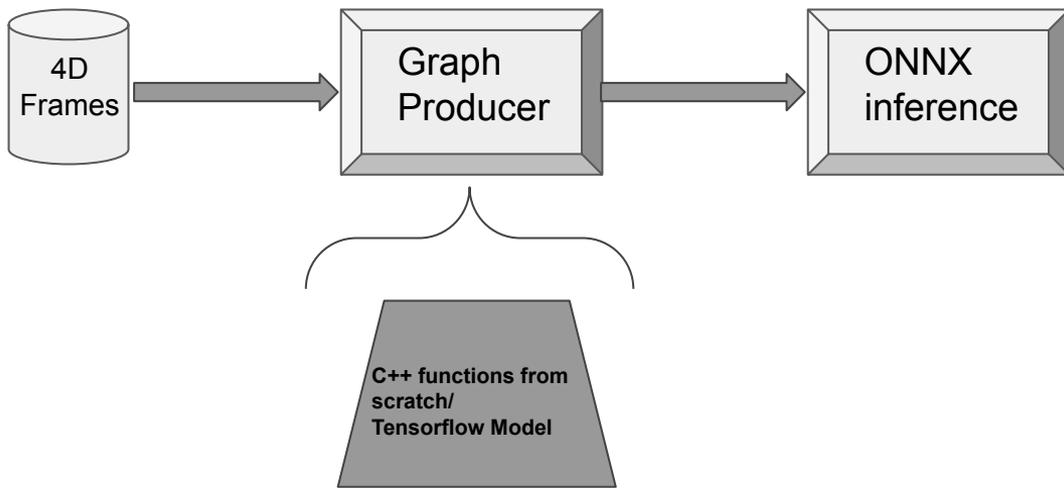
GNN with CMSSW

Available tools:

- MXNet
- SonicTriton (using Nvidia Triton Server)
- ONNX
 - Open format built to represent Machine Learning (ML) models.
 - Consists of common set of operators and common file format to enable the use of ML/DL models with a variety of frameworks, tools, runtimes and compilers.



E2E GNN Framework



- ONNX exporter does not support PyG knn_graph function for graph definition.

ONNX Runtime Input Space

A grid representing the ONNX Runtime Input Space. The columns are labeled "eta", "phi", "pT", "ecal", "hcal", and "pix". The rows are grouped into "Batch1" (rows 1-5) and "Batch2" (rows 6-8). The bottom-right portion of the grid is shaded in pink.

| | eta | phi | pT | ecal | hcal | pix |
|--------|------|-----|----|------|------|-----|
| Batch1 | N | | | | | |
| | o | | | | | |
| | n | | | | | |
| | z | | | | | |
| | e | | | | | |
| Batch2 | r | | | | | |
| | o | | | | | |
| | pix | | | | | |
| | vals | | | | | |

Issues with ONNX exporter & Solutions

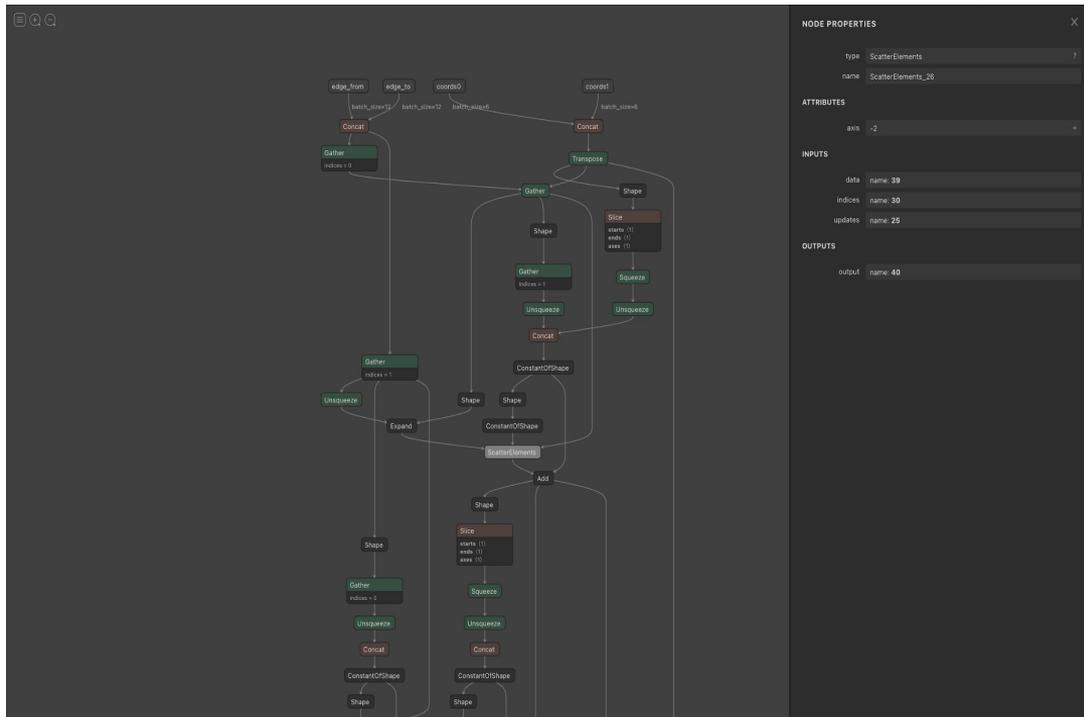
- The PyTorch to ONNX exporter is currently not mature enough to convert graph neural networks defined in PyTorch to ONNX.
- Hence, the exporter fails when multiple inputs with different sizes are used in the graph neural network model.
- The core problem seems to be with the message passing class of the *torch_geometric* (PyG) library due to which the exporter is not able to parse multiple sized inputs correctly.
- To develop the prototype, we wrote the GNN code from scratch without using *torch_geometric* library. Using this strategy we were able to deploy small sized GNN layers. (Work in progress)



More on issue with PyG



PyTorch Model Without PyG



NODE PROPERTIES

Type: ScatterElements 7

name: ScatterElements_26

ATTRIBUTES

axis: -2

INPUTS

data: name: 39

indices: name: 30

updates: name: 25

OUTPUTS

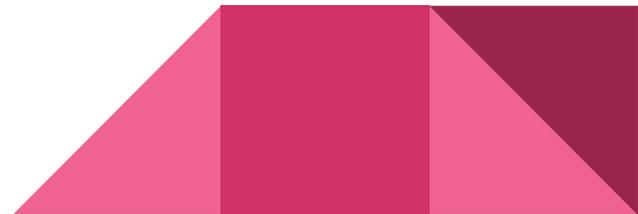
output: name: 40

PyTorch Model With PyG

Relevant Github Issues raised: <https://github.com/pytorch/pytorch/issues/65138>
<https://github.com/pytorch/pytorch/issues/64769>

Future Goals

- Continue the development of ONNX interface
- Implement several other architectures (attention based) to achieve even better than state of the art performance



THANK YOU

