## ML tracking **IRIS-HEP** fellowship project presentation

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## Agenda

#### Project description Graph Neural Networks Data analysis Data preprocessing Train overview Results Acknowledgment





Project description



#### Particles collision data Simulated by sPHENIX project

- After beams' collision
- Detection
- Analysis





#### **Detection** MVTX & INTT detectors

- Complex detector geometry
- High dimensionality (9k x 9k x 3)
- Variational input data
- Solutions: models with flexible data dimensionality + reduction of the useless data

![](_page_4_Figure_5.jpeg)

![](_page_4_Picture_6.jpeg)

![](_page_4_Picture_7.jpeg)

#### Tracks

#### & their representations

![](_page_5_Figure_2.jpeg)

- Tracks ~ graphs
- Geometrical constraints:  $\delta(\phi) \leq \frac{\pi}{4}, \ \delta(z) \leq 300 \text{ mm}$
- With each iteration we find more relevant tracks and automise the process of matching the hits into graphs

z, mm

![](_page_6_Figure_1.jpeg)

# Graph Neural Networks

![](_page_7_Picture_1.jpeg)

### **GINN idea** G = F(N, E)

![](_page_8_Figure_1.jpeg)

- Predictions: node level, edge level, graph-level
- Hyper parameters: Embedding size, MPL amount.
- Python lib for working with GNN - PyG (PyTorch geometrical)

#### Graph Convolutional Network graph level prediction

![](_page_9_Figure_1.jpeg)

![](_page_9_Picture_2.jpeg)

![](_page_10_Figure_0.jpeg)

# Data analysis + preprocessing

## Raw data

#### Simulated by sPHENIX project

- Generated json samples containing events
- Each event consist of: metadata, detectors data/positions/ids, points ids/pixel data/position/chip info, particles energy/momentum info, ground truth about vectors (containing particle ids etc.)

```
"Events" : [
"MetaData": {
    "Description": "These are meta data for this event. Not intended to use in ML algorithm"
    "EventID": 0,
    "Unit": "cm",
    "CollisionVertex": [
        0.0026662557331342347,
        0.0025958270878951186,
        -10.565255027683989
    ],
    "Layer_Count": 3,
    "PixelHalfLayerIndex_Count": 6,
    "Layer0": {
        "PixelPhiIndexInLayer_Count": 6144,
        "PixelPhiIndexInHalfLayer_Count": 3072,
        "PixelZIndex_Count": 9216,
         "HalfLayer_Count": 2,
        "Stave_Count": 12,
        "Chip_Count": 9,
        "Pixel_Count": 524288
    },
    "Layer1": {
        "PixelPhiIndexInLayer_Count": 8192,
        "PixelPhiIndexInHalfLayer_Count": 4096,
        "PixelZIndex_Count": 9216,
        "HalfLayer_Count": 2,
        "Stave_Count": 16,
        "Chip_Count": 9,
        "Pixel_Count": 524288
    },
    "Layer2": {
        "PixelPhiIndexInLayer_Count": 10240,
        "PixelPhiIndexInHalfLayer_Count": 5120,
        "PixelZIndex_Count": 9216,
         "HalfLayer_Count": 2,
         "Stave_Count": 20,
```

![](_page_12_Picture_6.jpeg)

#### Preprocessing part **Goals and steps**

Main steps should be:

1) unpack json raw data2

2) read carefully points data by ids

3)concatenate points from INTT and MVTX

4) reconstruct tracks from ground truth

- 5) cluster points on 1 detector
- 6)calculate cylindrical coordinates

7)segment possible edges by geometrical constraints

- 8) scale features
- 9) save in appropriate format.

#### Clustering

Collect all nearby points -> calculate mean euclidian (center) -> save center coordinates and number of pixels

0	1	0	0	0
1	1	1	1	0
0	1	1	0	0
0	0	0	0	0
0	0	1	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0

![](_page_13_Figure_14.jpeg)

![](_page_13_Figure_15.jpeg)

#### Preprocessed data **Before training**

Preprocessed data (per event), which can be considered to serve as input for the model, consist of next characteristics:

- 1) Scaled geometrical data: r vector value, phi angle value, z coordinate across cylindrical axe, amount of pixels on chip used in clustering
- 2) Possible edge combinations between point ids
- 3) Ground truth each track consist of some points

# Train process overview

![](_page_15_Picture_1.jpeg)

#### **Technology stack for training** Tools and technologies

- Remote developing, ssh, linux, conda3
- Python software engineering (OOP) for constructing training class, data loaders and models
- Torch, PyTorch geometrical, numpy, distributed programming
- Utils: wandb for experiment tracking.

#### **Training overview** Optimizer and model

- Optimizer Adam, with 1e-4 learning rate, weight\_decay 1e-4, and Ir decay schedule, starting from 60th epoch with 0.1 factor + I1+I2 regularisation
- Model: Graph Neural Network, consisting of MLP + Edge + Node networks (num of parameters = 753 and 2,5k)
- Loss: Binary cross-entropy
- Accuracy: precision (correctly predicted edges/all edges)
- Data: 800 training events + 200 validation (2000, 400)

#### **Training results Process and performance**

• 700 parameters, 800 training events ->

![](_page_18_Figure_2.jpeg)

![](_page_18_Figure_3.jpeg)

![](_page_18_Figure_4.jpeg)

![](_page_18_Figure_5.jpeg)

![](_page_18_Figure_6.jpeg)

#### **Example picture** Inference track reconstruction

![](_page_19_Figure_1.jpeg)

![](_page_19_Picture_2.jpeg)

![](_page_19_Picture_3.jpeg)

### Ideas for improving **Training and data preprocessing**

- Any scaling of the raw parameters should be applied in the initial layers of the network, since scaling parameters can harm feature importance and should be fine-tuned by the model to maximise the performance
- Energy and momentum are not counted right now in the pipeline, which can be a significant improve in results, because of extra input information.
- Hyperparameters tuning
- Models increasing + dataset expanding

## Conclusion

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- I learned Graph Neural Networks models from zero and implemented some of their variations in the new library PyTorch geometrical
- I met new people, who taught me a lot on coding, data analysis, physics context overview and nuclear physics itself.
- I expanded my thoughts about international scientific cooperation, by directly participating in it.
- It is an honour to be a part of such interesting and cutting-edge project, which combines classical scientific subjects, such as physics, together with machine learning engineering.

# Acknowledgment

![](_page_23_Picture_1.jpeg)

- I would like to acknowledge help of Dantong Yu in providing working resources and inviting me for his project.
- Also I would like thanks Tingting Xuan for helping with pipeline and sharing ideas of the implementation.

## Thanks for attention

![](_page_25_Picture_1.jpeg)