A Graph Neural Network model for the reconstruction of particle tracks detected at the MPD experiment of the NICA project

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JINR

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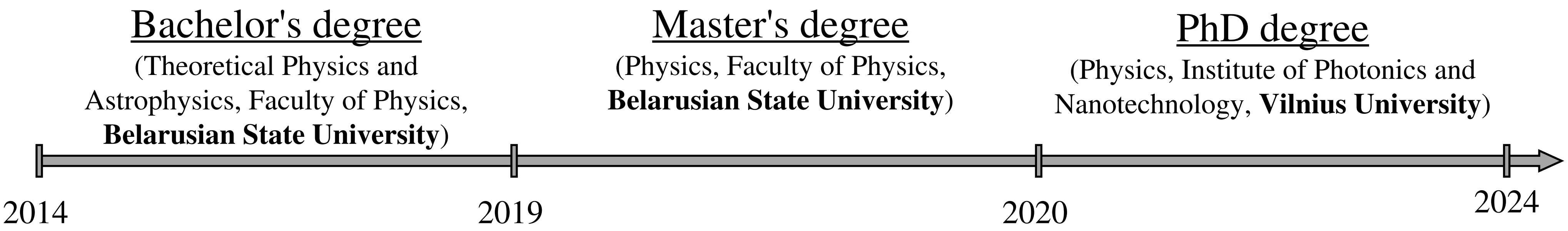
Curriculum Vitae

Education:



Professional experience:

Programing skills:

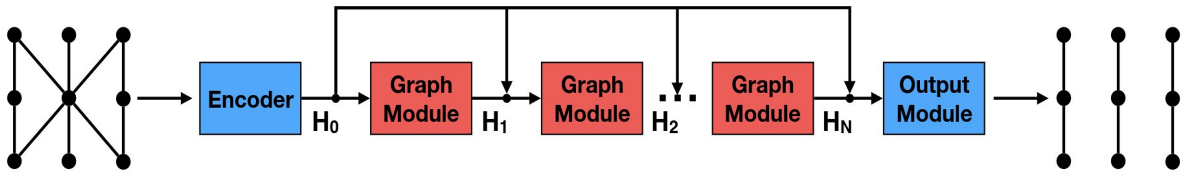
Programing languages	C & C++ (advanced), Phyton (advanced), Wolfram language (advanced), Fortran (basic)
Frameworks, tools & libraries	Qt5, CERN ROOT, OpenMP, CUDA, Eigen3, NumPy, Pandas, NetworkX, PyTorch, Scikit-Learn
Packages	GEANT4 & Quantum Espresso
Own projects	LEPAM

List of Publications

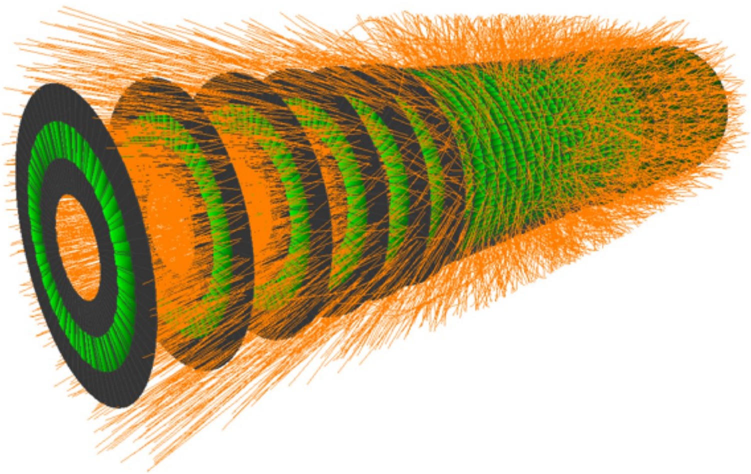
1. **Y. Talochka**, A. Vasil’ev, M. Korzhik, and G. Tamulaitis, *Impact of Compositional Disorder on Electron Migration in Lutetium–Yttrium Oxyorthosilicate Scintillator*, *J. Appl. Phys.*, vol. 132, no. 5, p. 053101, Aug. 2022.
2. **Y. Talochka**, R. Aleksiejūnas, Ž. Podlipskas, J. Mickevičius, G. Tamulaitis, *Evaluation of Ambipolar Diffusion Coefficient in AlxGa1-xN Semiconductor*, *J. Alloys Compd.*, vol. 969, p. 172475, Dec. 2023.
3. **Y. Talochka**, S. Nargelas, Ž. Podlipskas, M. Kucera, Z. Lucenicova, G. Tamulaitis, *Acceleration of emission decay in Ce-doped Gd-containing garnets by aliovalent codoping due to blocking excitation transfer via gadolinium subsystem*, *Radiat. Phys. Chem.*, vol. 218, p. 111589, May 2024.
4. S. Nargelas, **Y. Talochka**, A. Vaitkevičius, G. Dosovitskiy, O. Buzanov, A. Vasil’ev, T. Malinauskas, M. Korzhik, and G. Tamulaitis, *Influence of Matrix Composition and Its Fluctuations on Excitation Relaxation and Emission Spectrum of Ce Ions in (GdxY1-x)3Al2Ga3O12:Ce Scintillators*, *J. Lumin.*, vol. 242, p. 118590, Feb. 2022.
5. G. Dosovitskiy, A. Golutivin, I. Guz, R. Jacobsson, M. Korzhik, V. Mechinsky, **Y. Talochka**, G. Tamulaitis, A. Schopper, and E. Shmanin, *Time and Energy Resolution with SPACAL Type Modules Made of High-Light-Yield Ce-Doped Inorganic Scintillation Materials: Spillover and Background Noise Effects*, *Nucl. Instrum. Methods Phys. Res. Sect. Accel. Spectrometers Detect. Assoc. Equip.*, vol. 999, p. 165169, May 2021.
6. M. Korzhik, K.-T. Brinkmann, V. Dormenev, M. Follin, J. Houzvicka, D. Kazlou, J. Kopal, V. Mechinsky, S. Nargelas, P. Orsich, Z. Podlipskas, V. Sharyy, S. Sykorova, **Y. Talochka**, G. Tamulatis, D. Yvon, H.-G. Zaunick, *Ultrafast PWO scintillator for future high energy physics instrumentation*, *Nucl. Instrum. Methods Phys. Res. Sect. Accel. Spectrometers Detect. Assoc. Equip.*, vol. 1034, p. 166781, Jul. 2022.
7. G. Tamulaitis, S. Nargelas, M. Korjik, V. Mechinsky, **Y. Talochka**, A. Vaitkevičius, A. Vasil’ev, *Transient optical absorption as a powerful tool for engineering of lead tungstate scintillators towards faster response*, *J. Mater. Chem. C*, vol. 10, no. 25, pp. 9521–9529, Jun. 2022.
8. G. Tamulaitis, S. Nargelas, **Y. Talochka**, A. Vaitkevičius, M. Korjik, V. Mechinsky, R. Paramatti, I. Dafinei, M.T. Lucchini, E. Auffray, N. Kratochwil, *Transient Optical Absorption Technique to Test Timing Properties of LYSO:Ce Scintillators for the CMS Barrel Timing Layer*, *Radiat. Phys. Chem.*, vol. 206, p. 110792, May 2023.
9. M. Korzhik, D. Blau, A. Fedorov, A. Bondarau, Y. Borovlev, A. Amelina, I. Komendo, D. Kuznetsova, A. Mikhlin, V. Mechinsky, A. Postupaeva, V. Shlegel, **Y. Talochka**, V. Uglov, *Compositionally disordered tungstate scintillation materials*, *Radiat. Meas.*, vol. 167, p. 106987, Sep. 2023.
10. V. Dubov, D. Kuznetsova, I. Kamenskikh, I. Komendo, G. Malashkevich, A. Ramanenka, V. Retivov, **Y. Talochka**, A. Vasil’ev, M. Korzhik, *On the Quenching Mechanism of Ce, Tb Luminescence and Scintillation in Compositionally Disordered (Gd,Y,Yb)3Al2Ga3O12 Garnet Ceramics*, *Photonics*, vol. 10, p. 615, May 2023.
11. P. Karpyuk, M. Korzhik, A. Fedorov, I. Kamenskikh, I. Komendo, D. Kuznetsova, E. Leksina, V. Mechinsky, V. Pustovarov, V. Smyslova, V.M. Retivov, **Y. Talochka**, D. Tavrunov, A. Vasil’ev, *The Saturation of the Response to an Electron Beam of Ce- and Tb-Doped GYAGG Phosphors for Indirect β-Voltaics*, *Appl. Sci.*, vol. 13, p. 3323, Mar. 2023.
12. V. Retivov, V. Dubov, I. Komendo, P. Karpyuk, D. Kuznetsova, P. Sokolov, **Y. Talochka**, M. Korzhik, *Compositionally Disordered Crystalline Compounds for Next Generation of Radiation Detectors*, *Nanomaterials*, vol. 12, p. 4295, Dec. 2022.
13. S. Nargelas, A. Solovjovas, **Y. Talochka**, Ž. Podlipskas, M. Kucera, Z. Lucenicova, G. Tamulaitis, *Influence of heavy magnesium codoping on emission decay in Ce-doped multicomponent garnet scintillators*, *J. Mater. Chem. C*, vol. 11, pp. 12007–12015, Aug. 2023.
14. V. Dormenev, A. Amelina, E. Auffray, K.-T. Brinkmann, G. Dosovitskiy, F. Cova, A. Fedorov, S. Gundacker, D. Kazlou, M. Korjik, N. Kratochwil, V. Ladygin, V. Mechinsky, M. Moritz, S. Nargelas, R.W. Novotny, P. Orsich, M. Salomoni, **Y. Talochka**, G. Tamulaitis, A. Vaitkevicius, A. Vedda, H.-G. Zaunick, *Multipurpose Ce-doped Ba-Gd silica glass scintillator for radiation measurements*, *Nucl. Instrum. Methods Phys. Res. Sect. Accel. Spectrometers Detect. Assoc. Equip.*, vol. 1015, p. 165762, Nov. 2021.
15. G. Tamulaitis, E. Auffray, A. Gola, M. Korzhik, A. Mazzi, V. Mechinski, S. Nargelas, **Y. Talochka**, A. Vaitkevičius, A. Vasil’ev, *Improvement of the timing properties of Ce-doped oxyorthosilicate LYSO scintillating crystals*, *J. Phys. Chem. Solids*, vol. 139, p. 109356, Apr. 2020.

Current progress

HEPTrkX-presented GNN model



[TrackML dataset](#)

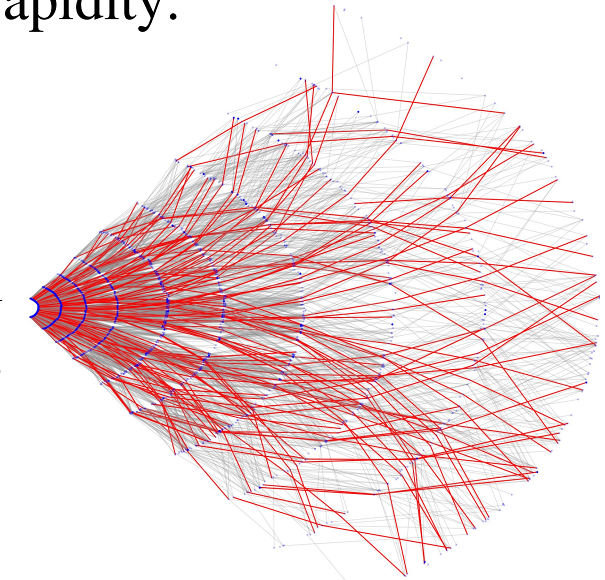


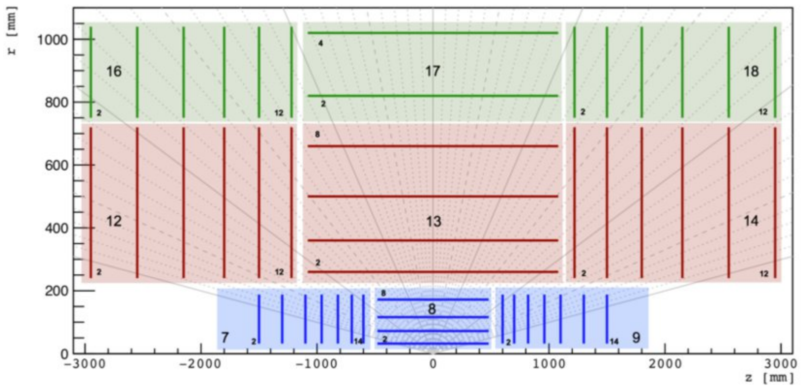
Modules related to the detector groups 8, 13 and 17 were considered in the model.

The detector volume is divided into $n_\varphi \times n_\eta$ segments, where $n_\varphi = 8$ and $n_\eta = 2$, η is the pseudorapidity.

The node features are $\{r, \varphi, z\}$,
the edge features are $\{\Delta\theta, \Delta\varphi, \Delta\varrho, \Delta z\}$.

Here, r, φ and z are the cylindrical coordinates of a hit, θ is its polar angle, $\varrho = \sqrt{\theta^2 + \varphi^2}$.



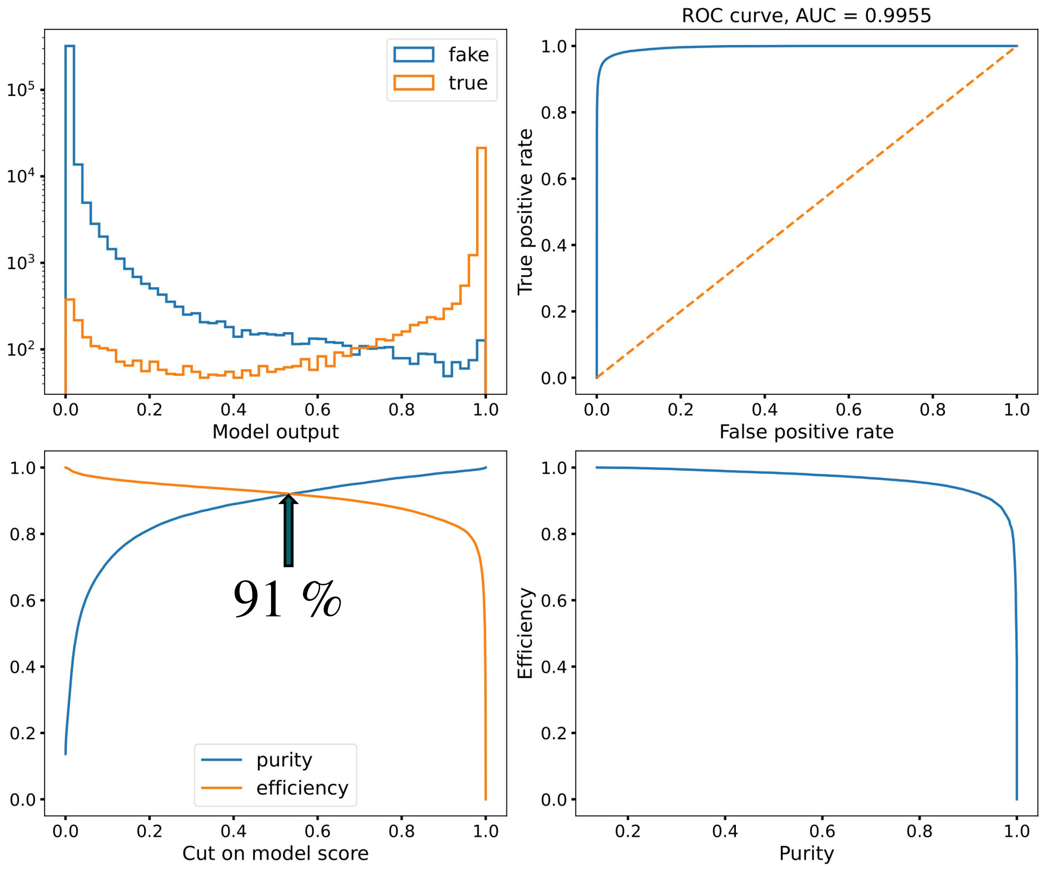


X. Ju et al., "Graph Neural Networks for Particle Reconstruction in High Energy Physics detectors," Mar. 01, 2020. doi: 10.48550/arXiv.2003.11603

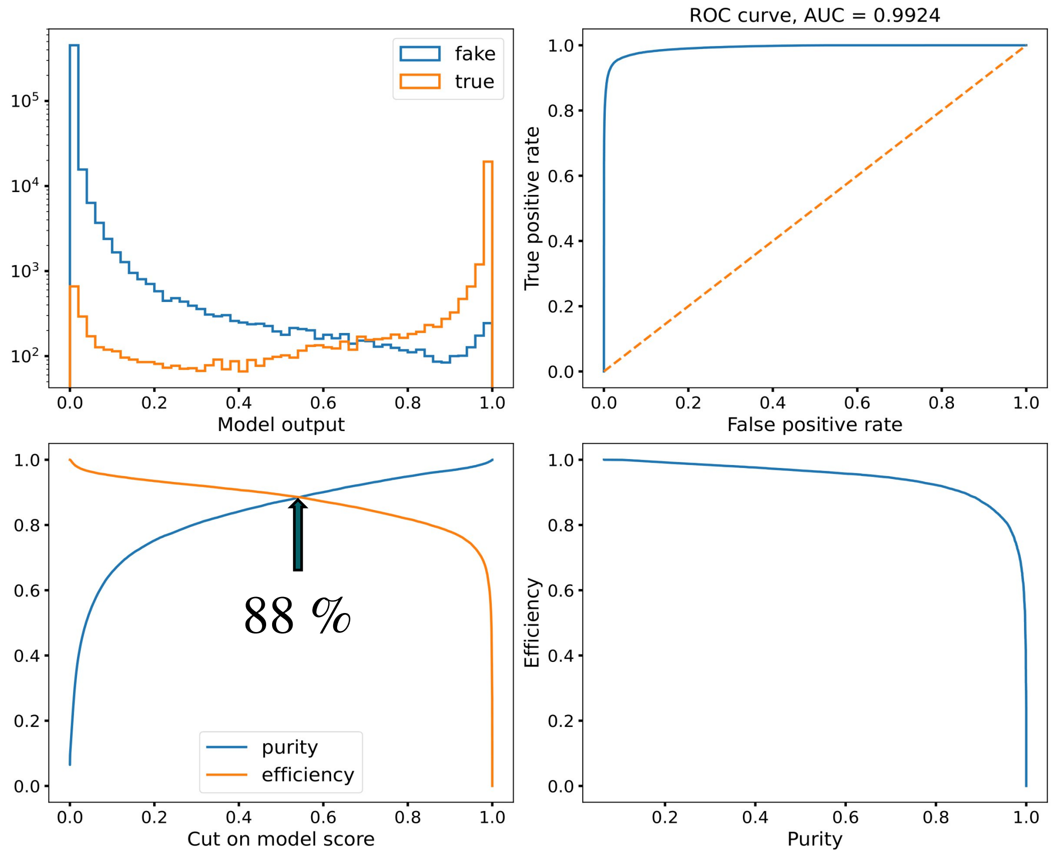
Adaptation of the GNN model and its efficiency

- Noise in the dataset was taken into account.

w/o noise

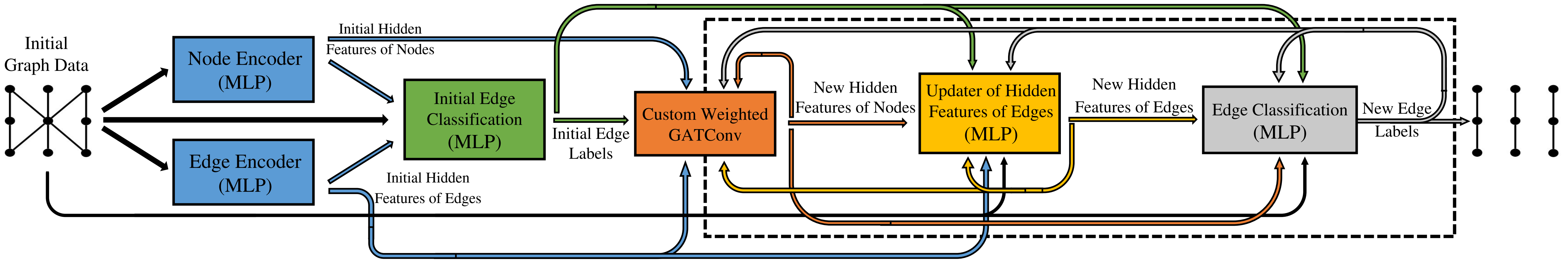


19.5% of noise



CPU-RAM usage up to 16 GB ← That is a significant problem which should be solved to exploit the GNN model for datasets from the MPD in the future.

Upgraded GNN model

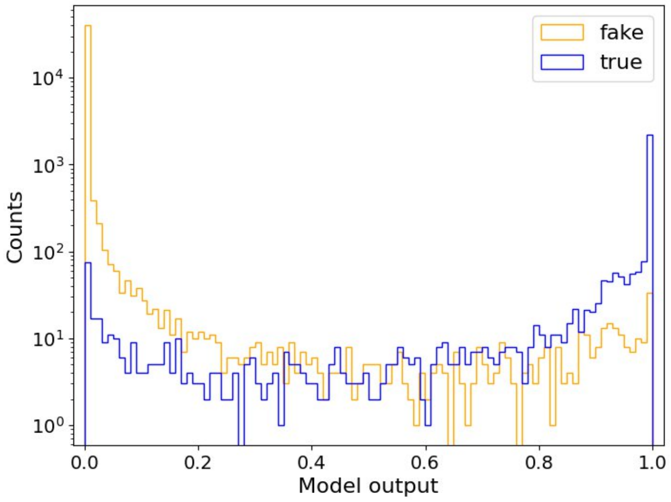


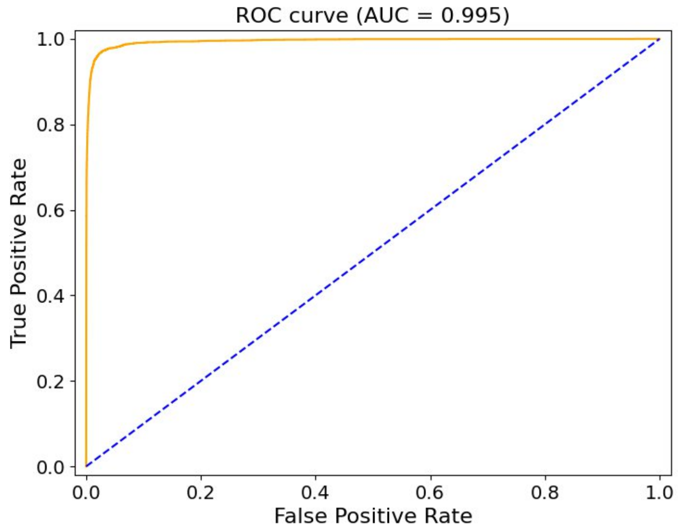
PyTorch Geometric → MessagePassing

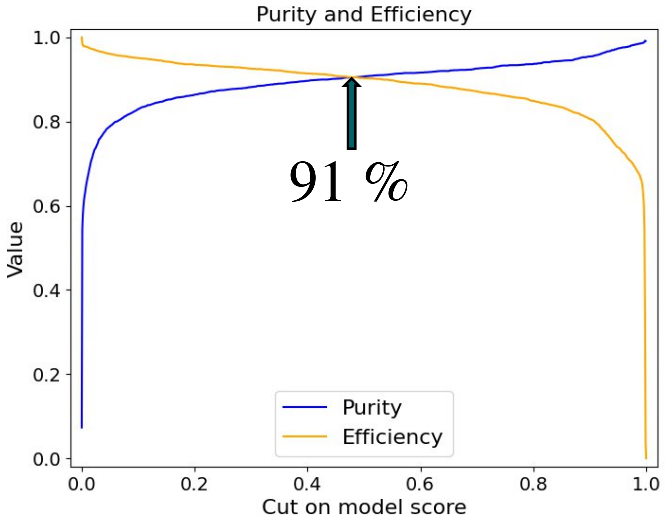
```
class CustomWeightedGATConv(MessagePassing):
    def __init__(self, node_feature_dim, hidden_dims, output_dim, edge_feature_dim, activation=torch.nn.Tanh(), end_activation = None, dropout = torch.nn.Dropout(0.1)):
        super(CustomWeightedGATConv, self).__init__(aggr='add')
        self.mlp = CustomMLP(2 * node_feature_dim + edge_feature_dim, hidden_dims, output_dim, activation, end_activation, dropout)

    def forward(self, x, edge_index, edge_attr, edge_weight):
        return self.propagate(edge_index, x=x, edge_attr=edge_attr, edge_weight=edge_weight)

    def message(self, x_j, edge_attr, edge_weight):
        return edge_weight.view(-1, 1) * torch.cat([x_j, edge_attr], dim=-1)

    def update(self, aggr_out, x):
        out = torch.cat([x, aggr_out], dim=-1)
        return self.mlp(out)
```

Upgraded GNN model

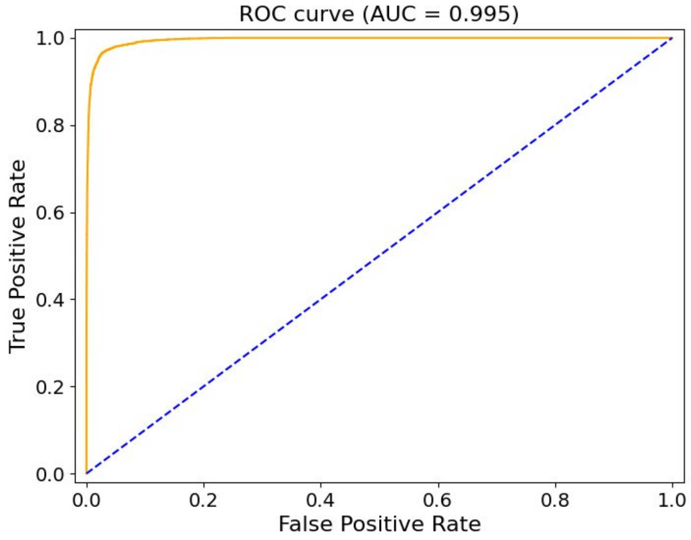
w/o noise

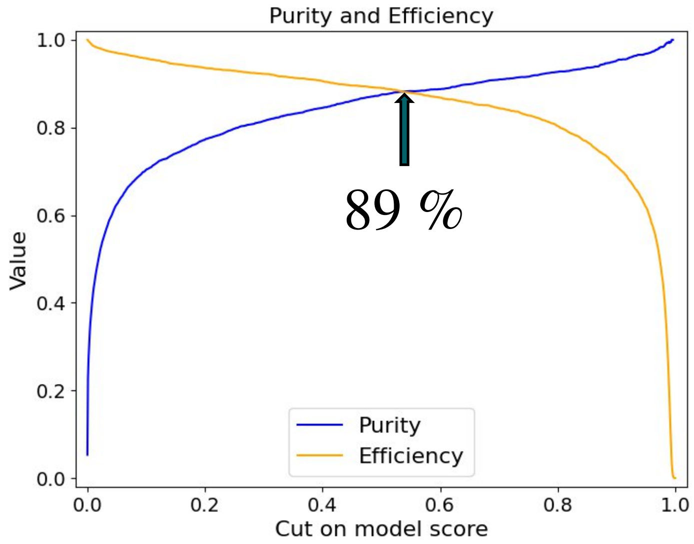


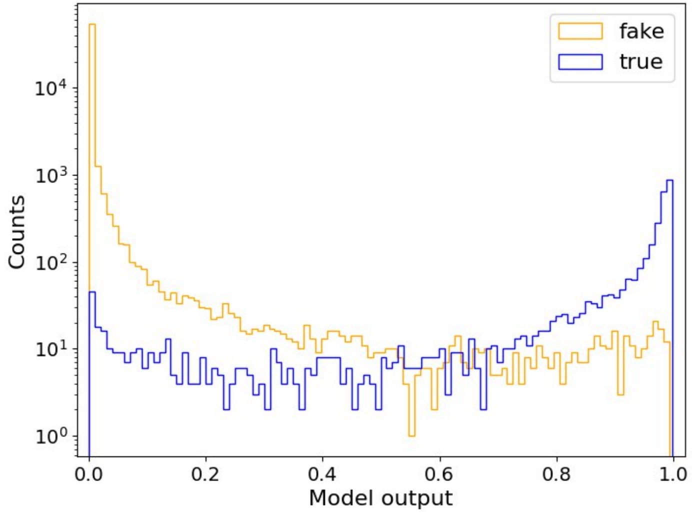




19.5% of noise







CPU-RAM usage up to 3 GB and GPU-RAM usage up to 5 GB

How does it work?

hits.csv

↓

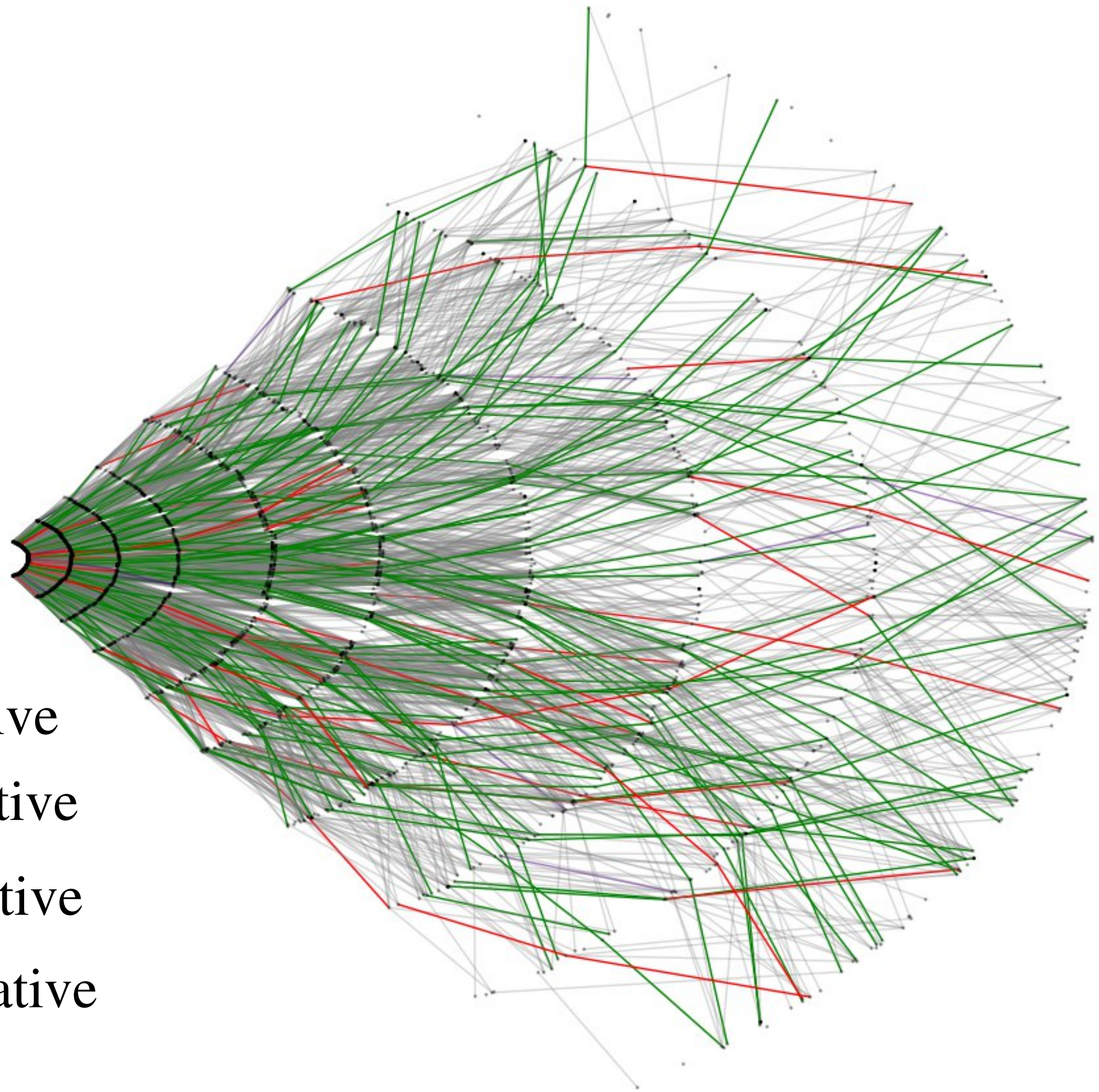
preprocessing_of_data.py

↓

graph.npz

↓

Evaluate_graph.py →



- True Positive
- False Positive
- True Negative
- False Negative

Outlook

- Adapting the GNN model to datasets obtained from the MPD experiment of the NICA project, taking into account their specifics, is the next step in the current study.

Thank you for attention!