

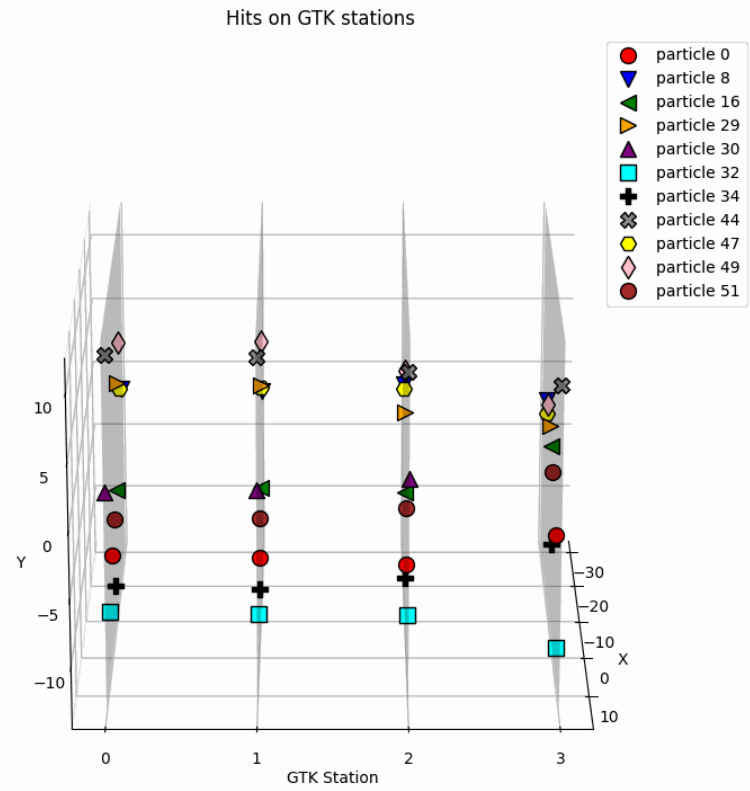
# WIFAI 2024

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National PhD student in Artificial Intelligence  
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[leonardo.plini@lnf.infn.it](mailto:leonardo.plini@lnf.infn.it)

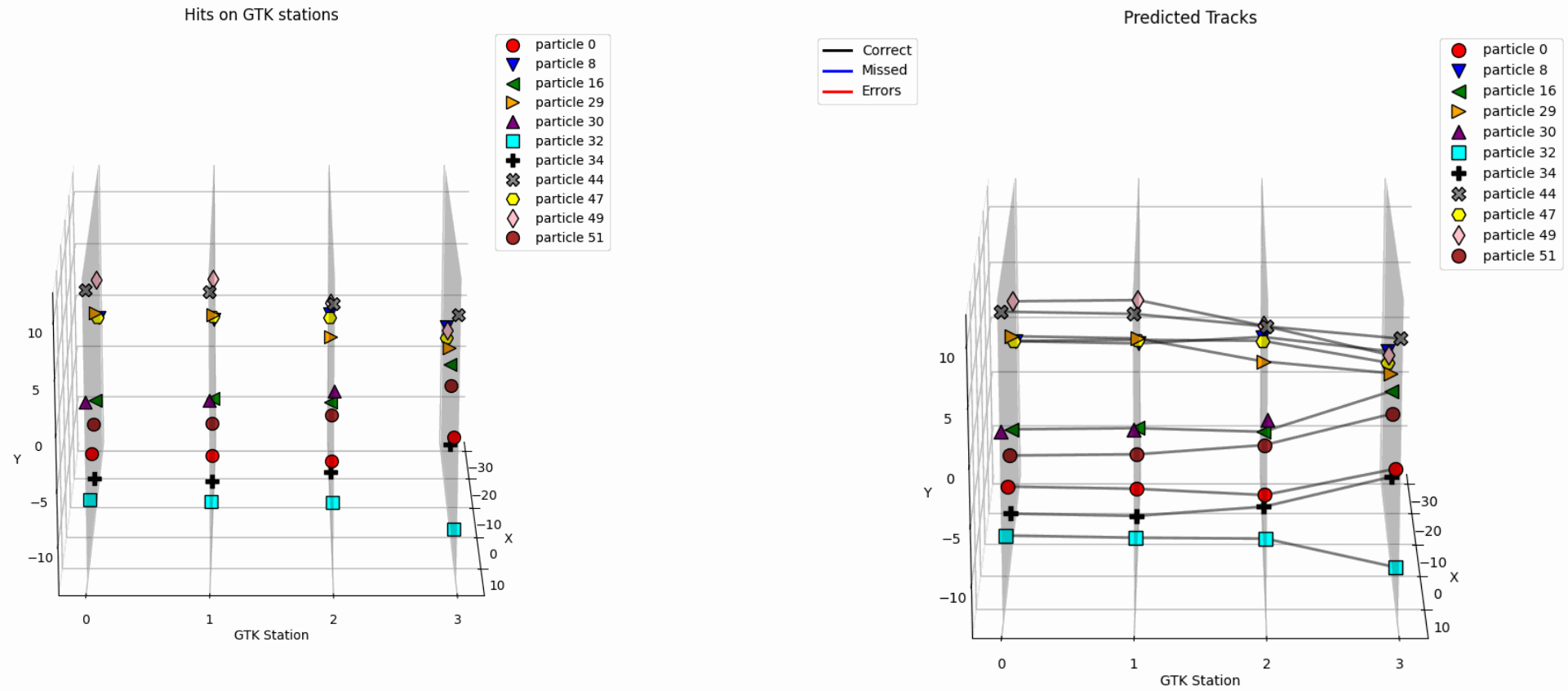


**SAPIENZA**  
UNIVERSITÀ DI ROMA

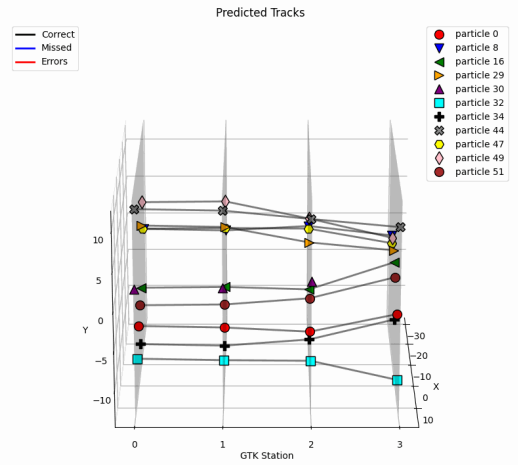
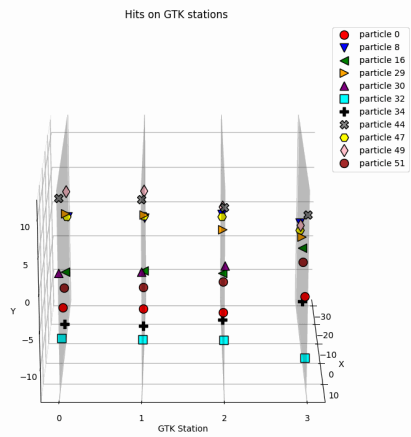
# Particle Tracking



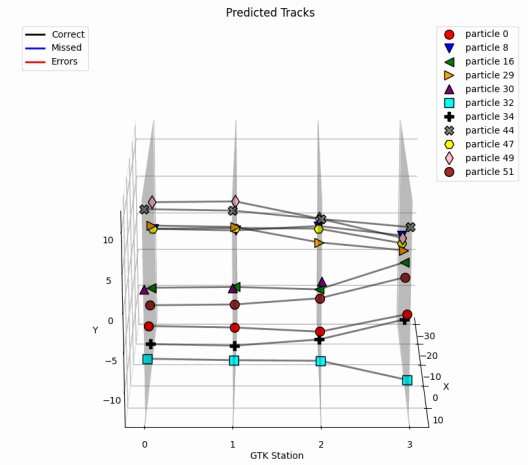
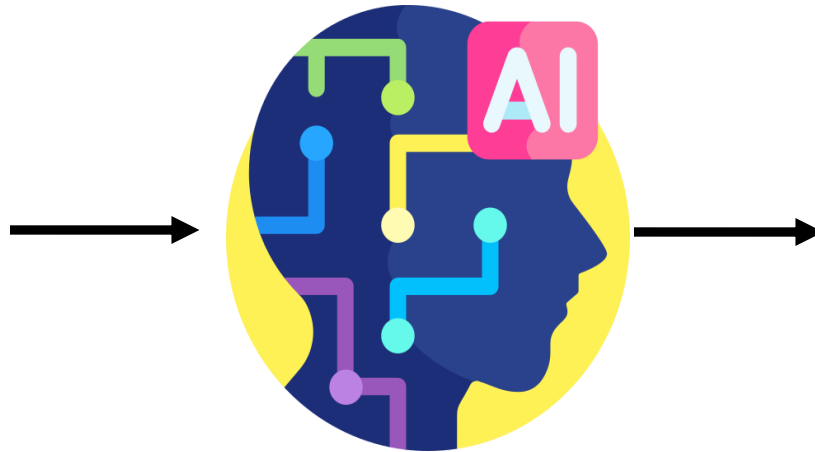
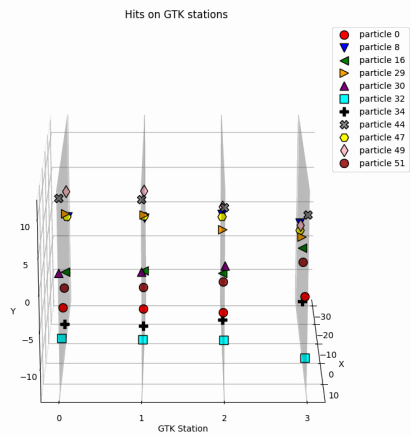
# Particle Tracking



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# Particle Tracking



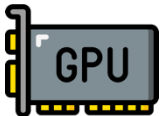
# Motivations



Despite the variety of approaches and theoretical models tested in physical experiments, what they all have in common is the very **large volume of complex data** they produce

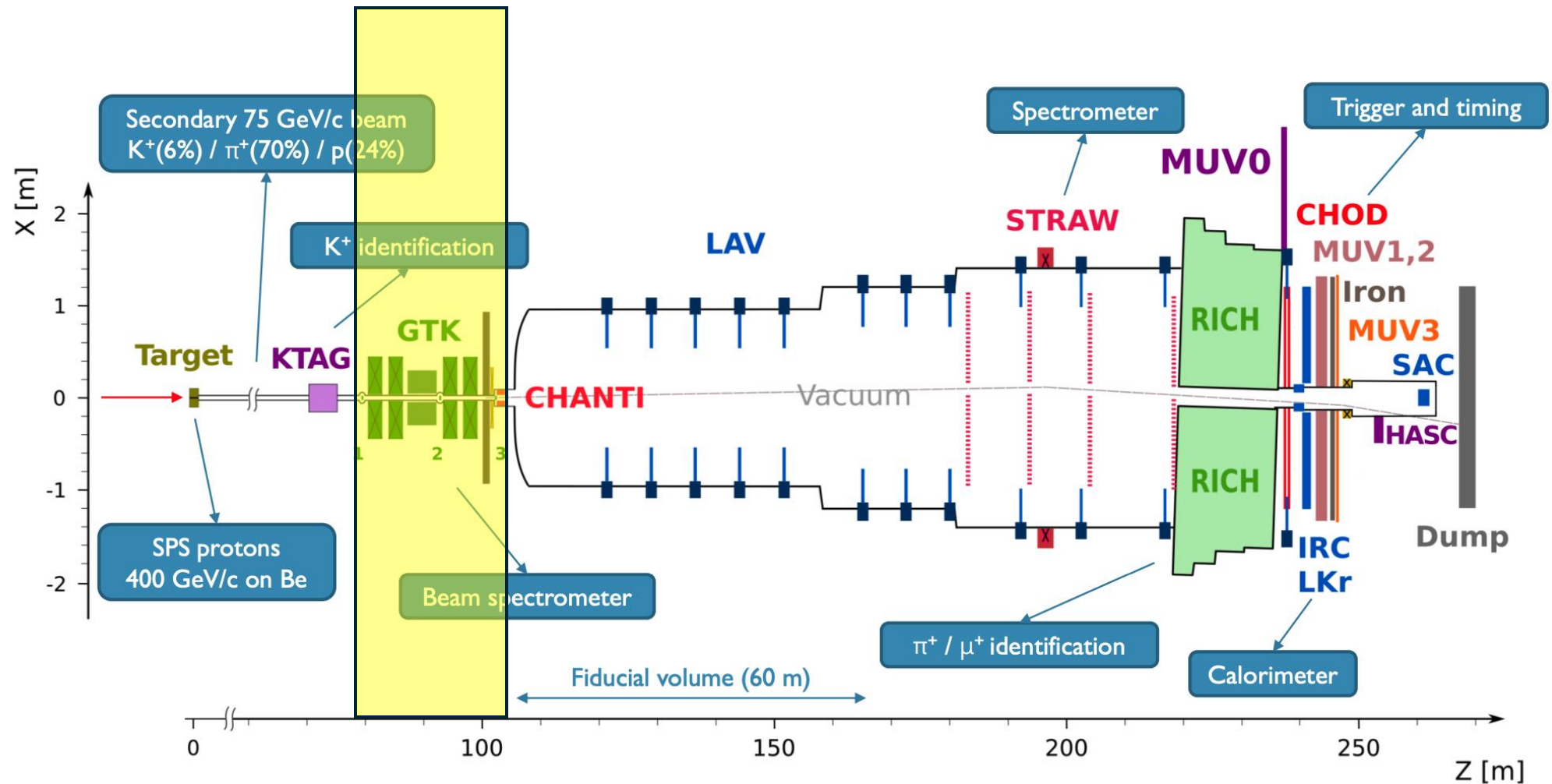


This data challenge calls for powerful computing methods like **Machine Learning** and **Deep Learning**

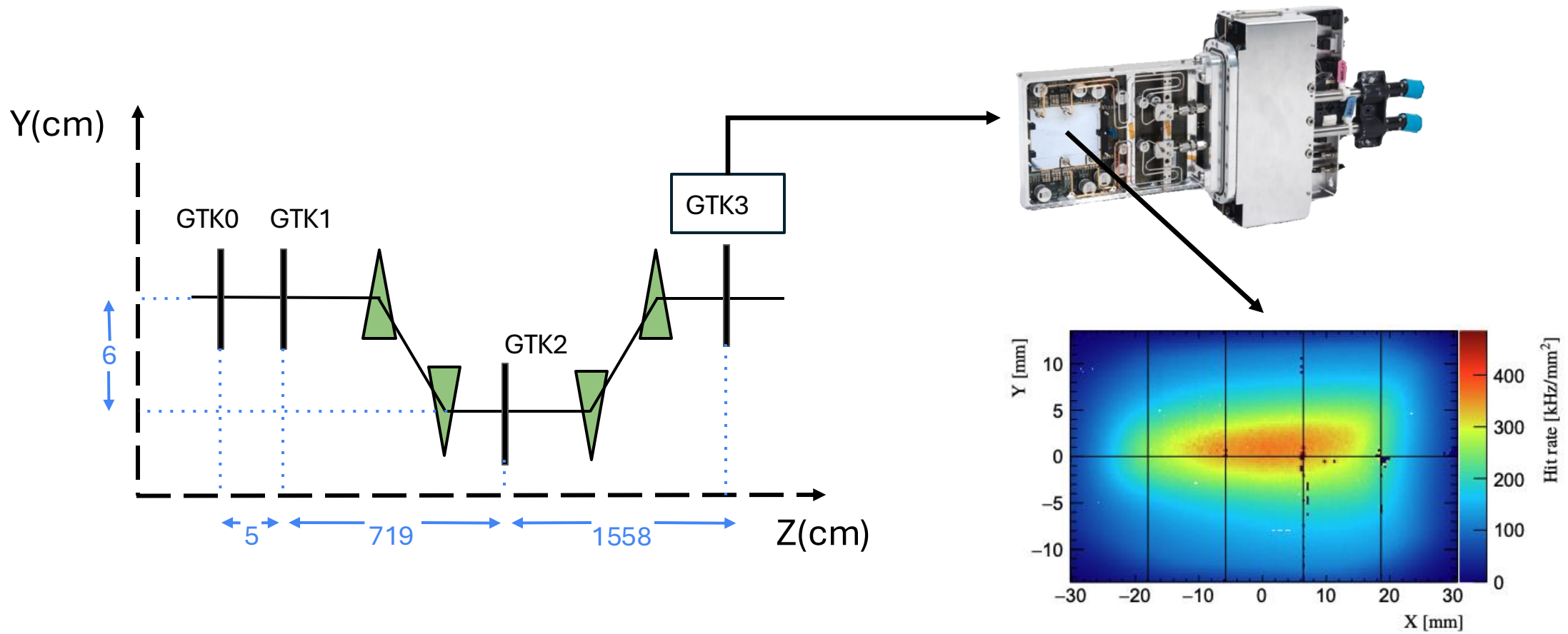


GPU parallelization and memory capacity allow to drastically reduce computational time

# Introduction: NA62 experiment



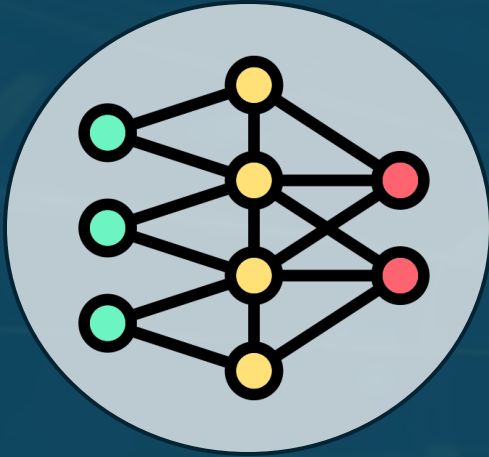
# Introduction: Giga Tracker Stations





# Proposal

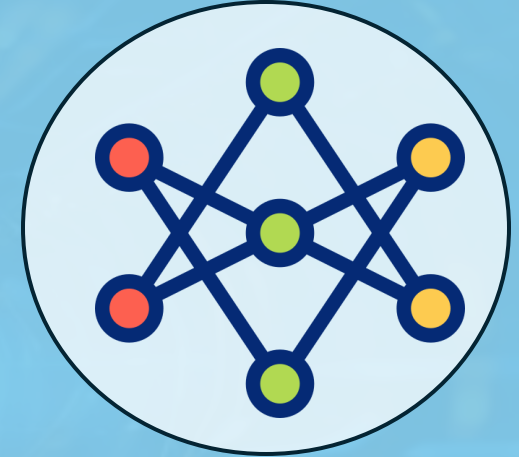
A futuristic, glowing blue and orange tunnel with a bright light at the end, symbolizing a proposal or a path forward. The tunnel is composed of many parallel lines that converge towards a bright blue light source at the far end. The walls of the tunnel are made of a grid-like structure of blue and orange lines, creating a sense of depth and perspective. The overall atmosphere is one of high-tech and innovation.



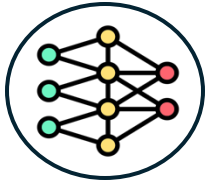
Multi-Layer Perceptron



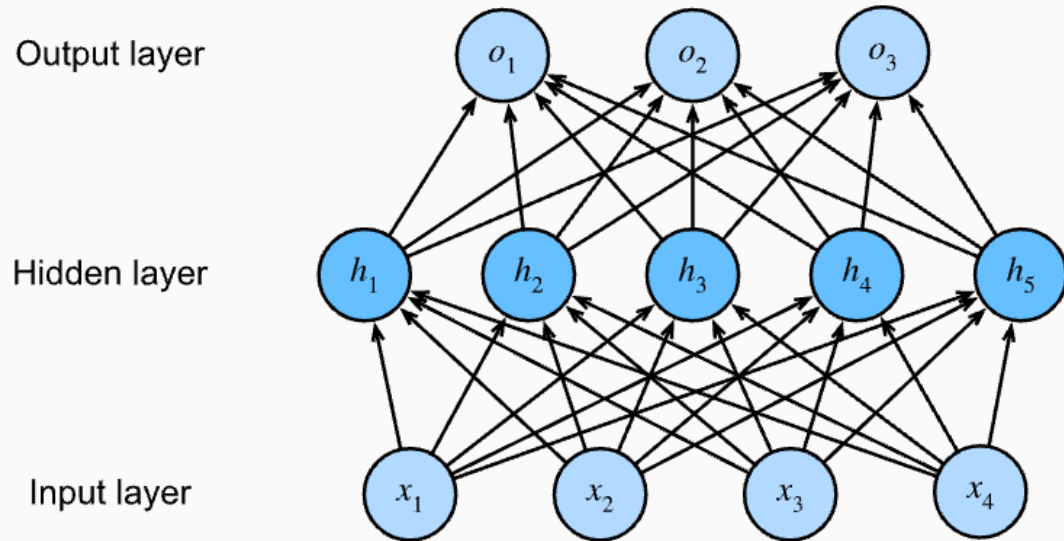
Transformer



Graph Neural Network



# Multi-Layer Perceptron

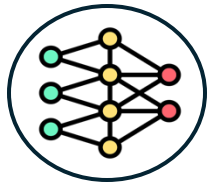


MLP is an architecture made up of composable and differentiable layers that optimizes its weights ( $W, b$ ) by means of **Back-Propagation** to minimize a loss function  $L$ .

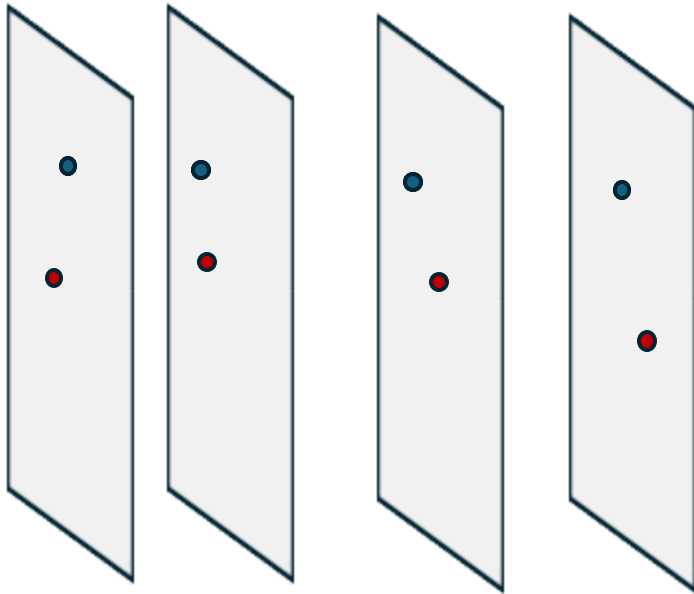
$$\hat{o} = f(x) = \sigma_2(W_2 \sigma_1(W_1 x + b_1) + b_2)$$

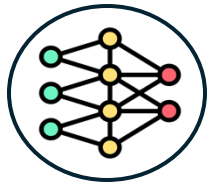
$$W^*, b^* = \operatorname{argmin} L(o, \hat{o})$$

where  $\sigma$  is an activation function

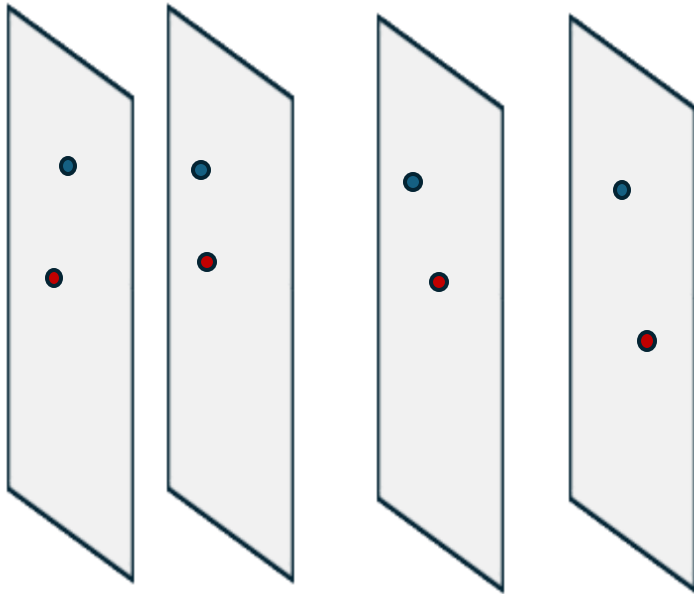


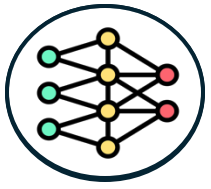
# Multi-Layer Perceptron



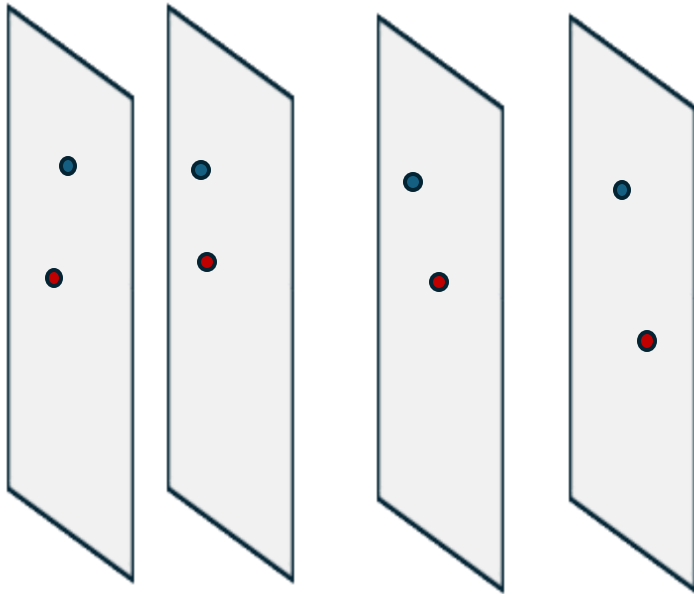


# Multi-Layer Perceptron

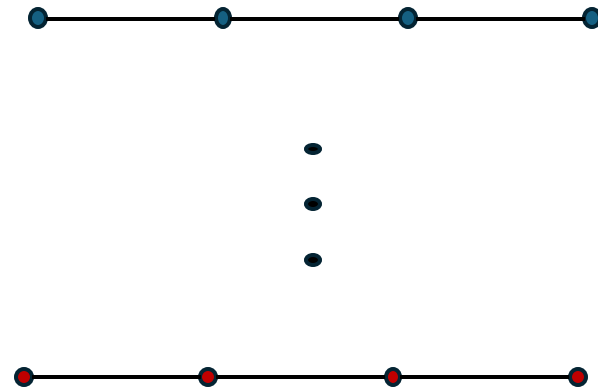


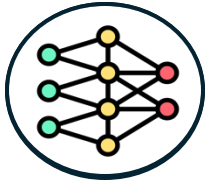


# Multi-Layer Perceptron

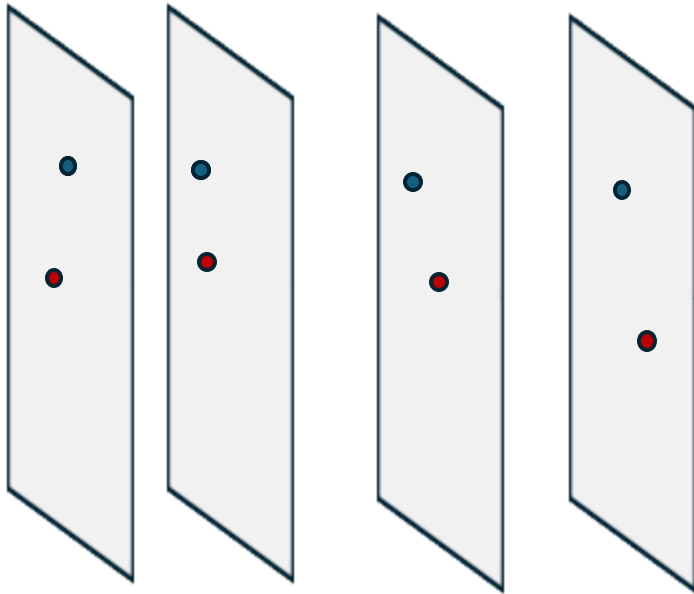


Admissible track combinations

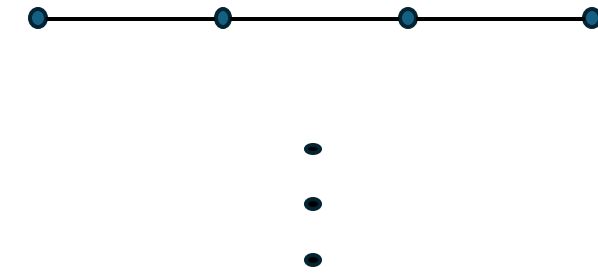




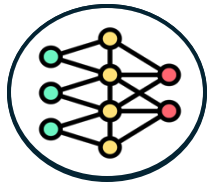
# Multi-Layer Perceptron



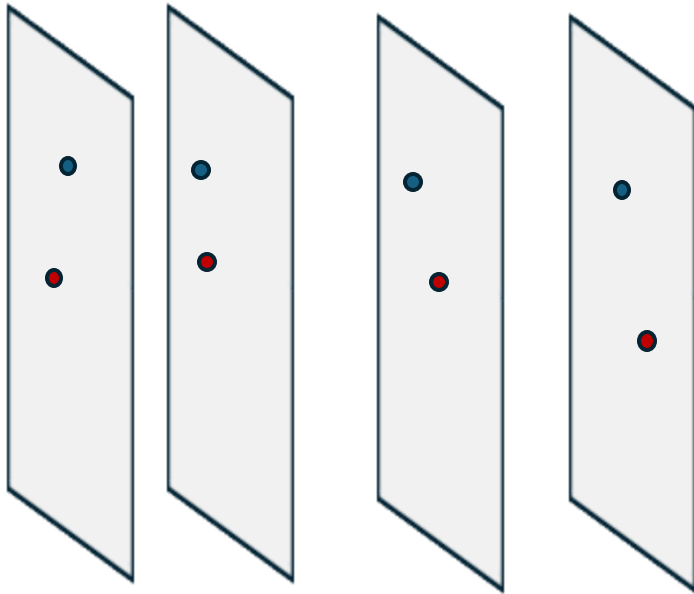
Admissible track combinations



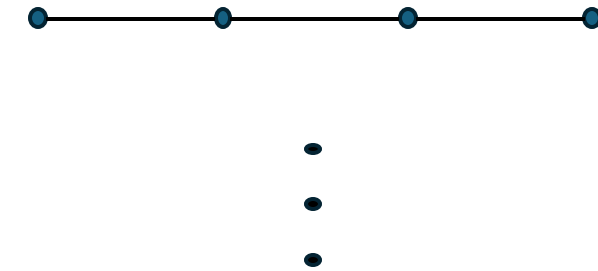
Not admissible track combination



# Multi-Layer Perceptron



Admissible track combinations



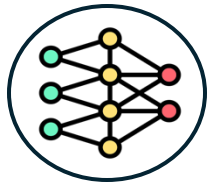
⋮



Not admissible track combination

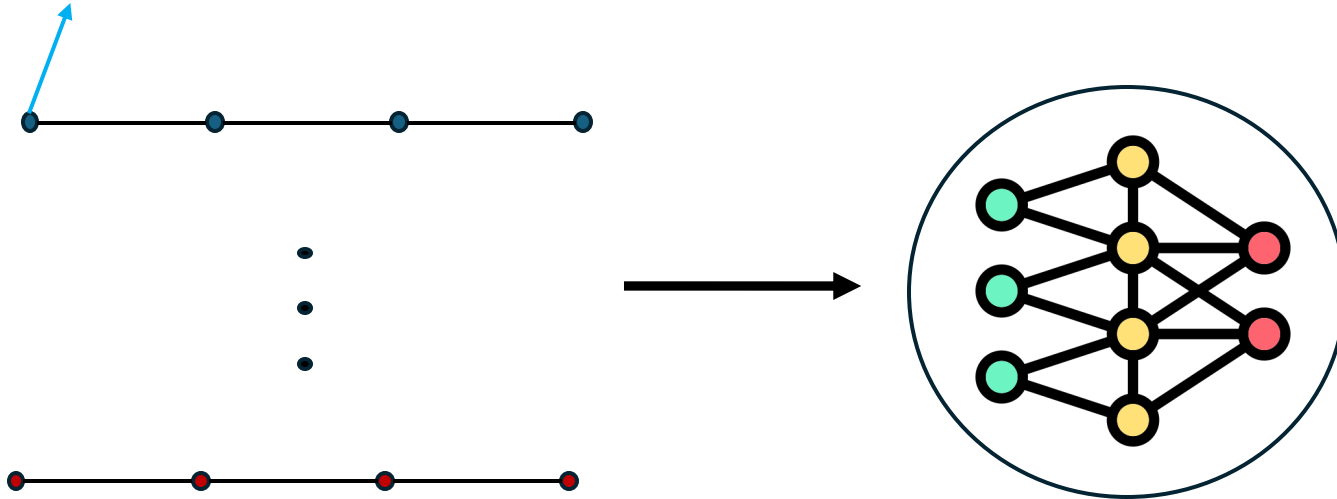


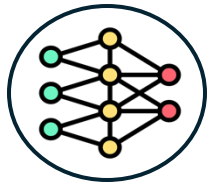




# Multi-Layer Perceptron

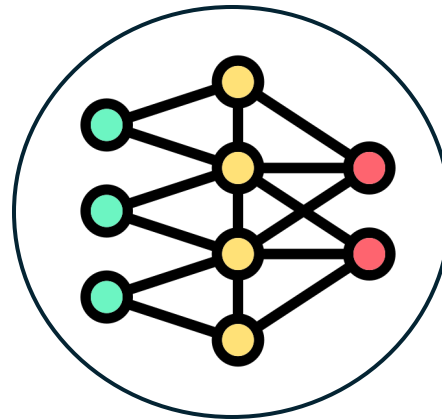
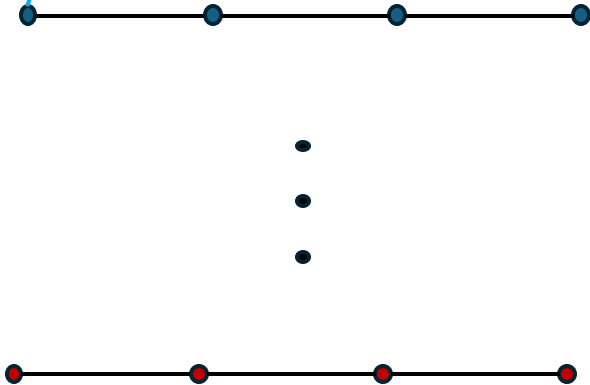
[ x, y, z, time ]





# Multi-Layer Perceptron

[ x, y, z, time ]

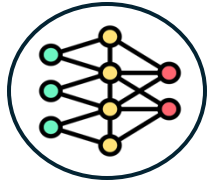


Existence Score

1- Existence Score

0.76	0.24
...	...
...	...
0.13	0.87
0.94	0.06





# Multi-Layer Perceptron: results



$$\text{Efficiency} = \frac{\# \text{ correctly predicted tracks}}{\# \text{ total true tracks}}$$



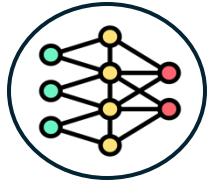
$$\text{Purity} = \frac{\# \text{ correctly predicted tracks}}{\# \text{ total predicted tracks}}$$



$$\text{Fake Tracks} = \frac{\# \text{ wrongly predicted tracks}}{\# \text{ total true tracks}}$$

- NA62 MC reproducing the datataking condition in 2022
- 200156 events  $\{-10 \text{ ns}, +10 \text{ ns}\}$  wrt KTAG reference time
- The models were implemented on an RTX 3060Ti Trio with 8 GB equipped with a Ryzen 7 3700X CPU
- 60% Train, 20% Validation, 20% Test
- Training on Train Set
- Hyper-parameters using Validation Set
- Results on Test Set

Efficiency	Purity	Fake Tracks
70.06 %	92.3 %	39.45 %



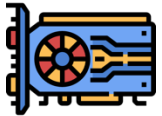
## Multi-Layer Perceptron: conclusion



- Local awareness



- Poor Performances



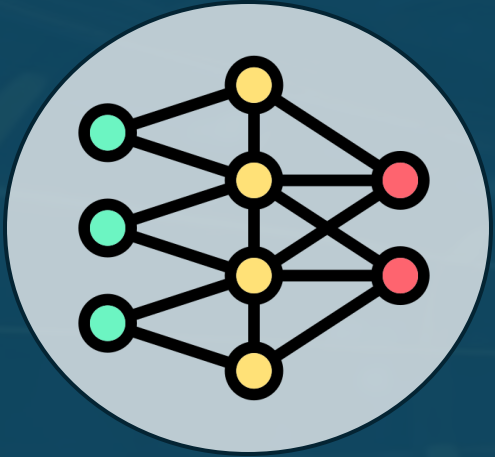
- Big GPU memory needed to store all admissible combinations



- Slow computations



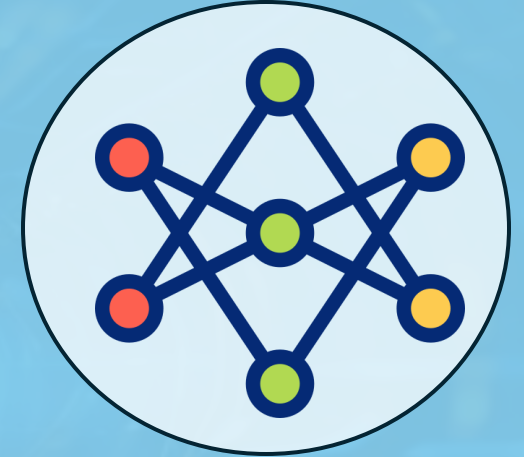
- **Class Imbalance**



Multi-Layer Perceptron



Transformer



Graph Neural Network



# Transformer

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## Attention Is All You Need

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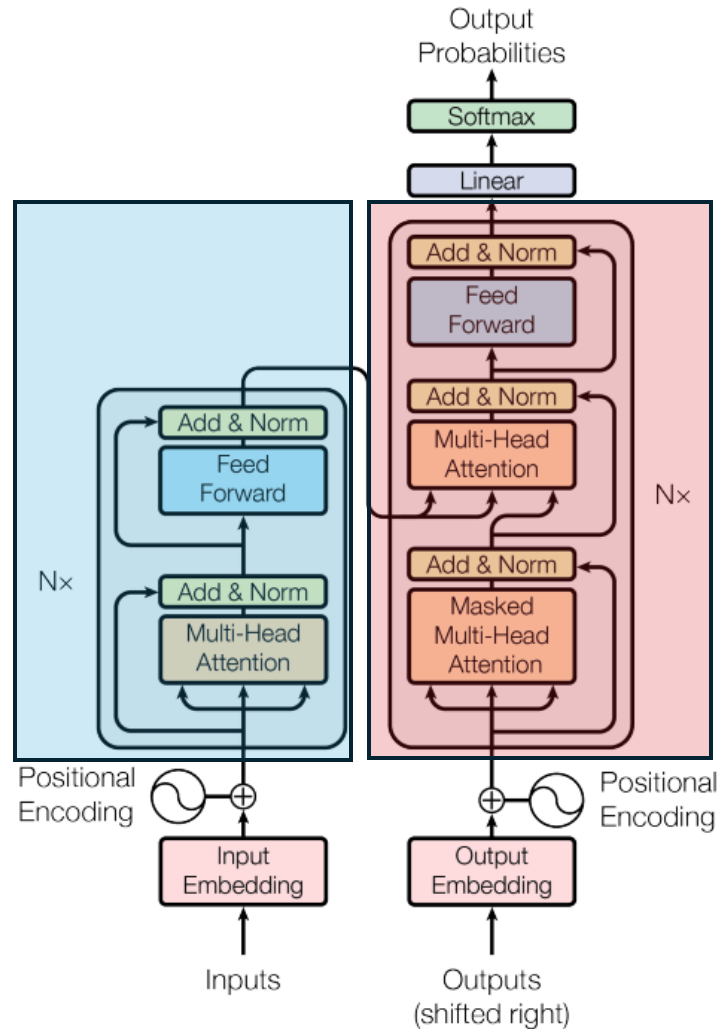
**Illia Polosukhin\* †**  
illia.polosukhin@gmail.com

Presented in 2017 and now widely adopted due to their incredible performances and parallelization.

They represented a revolution in Natural Language Processing, Computer Vision and Multimodal Learning



# Transformer



**Encoder:** processes the input sequence by applying self-attention to capture relationships between all tokens in the sequence. It then passes the resulting representations through feed-forward layers to create a context-aware representation of the input data

**Decoder:** uses this representation to generate the output sequence, often performing tasks like translation or text generation

Note: we used only the Encoder



# Transformer



Local awareness



If we have  $n$  hits per station, we will create:

- $n^4$  (GTK0-GTK1-GTK2-GTK3)
- $n^3$  (GTK0-GTK2-GTK3)
- $n^3$  (GTK1-GTK2-GTK3)

Total:  $n^4 + 2n^3$



Global awareness with  
Transformer

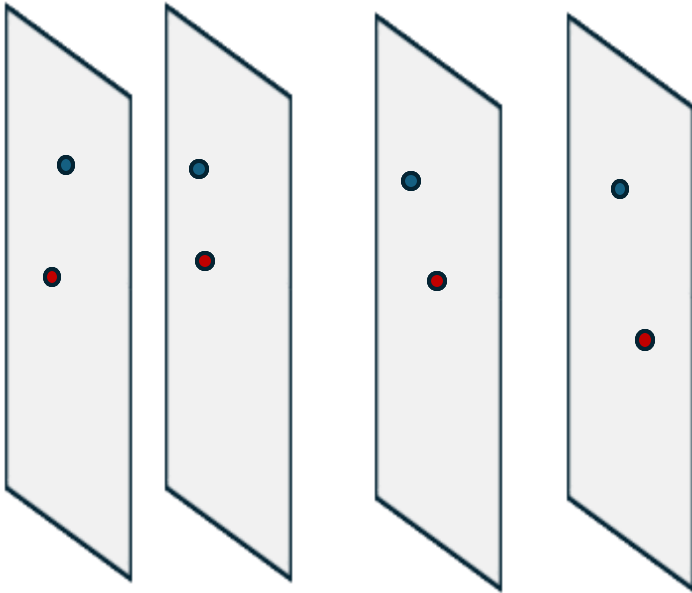


What if move the problem from tracks to  
edges?

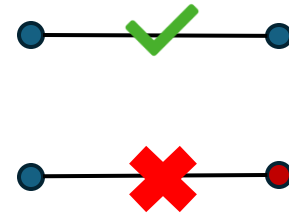




# Transformer



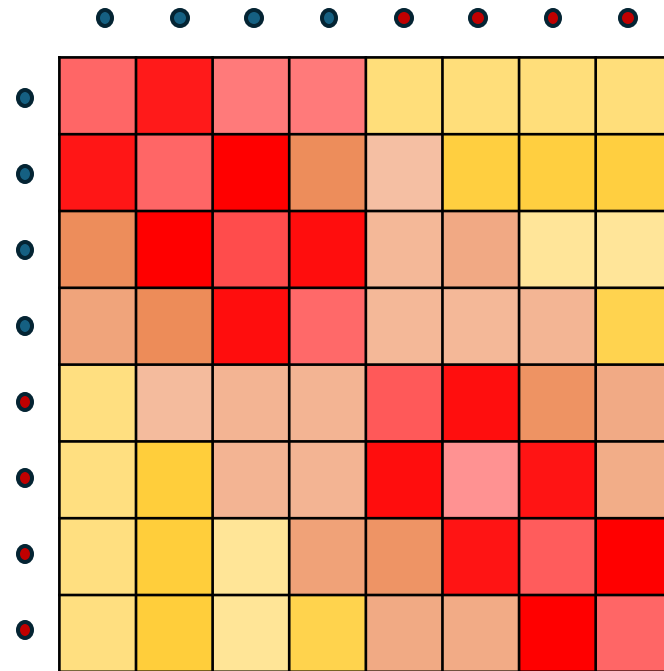
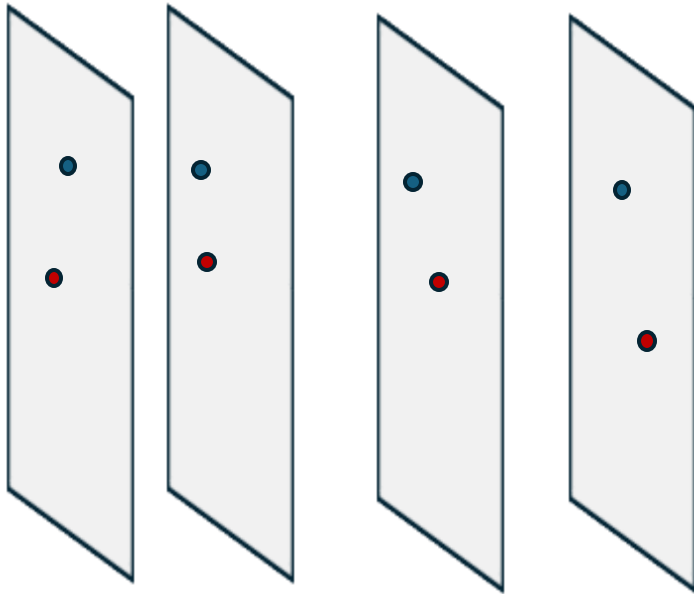
## Binary Classification



The number of candidates we need to evaluate is  $(4n)^2 = 16n^2 \ll n^4 + 2n^3$

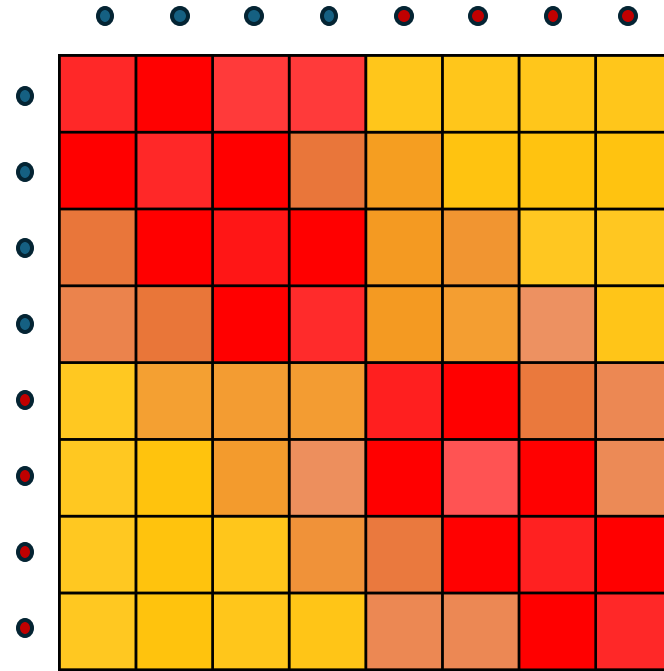
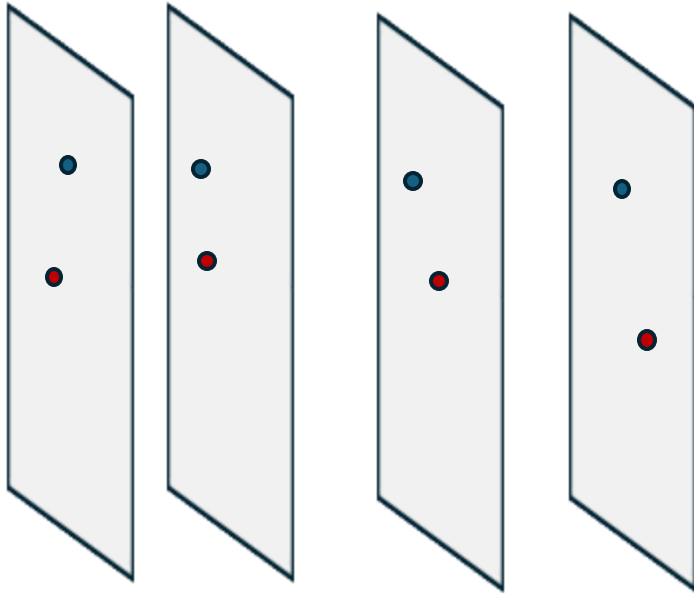


# Transformer



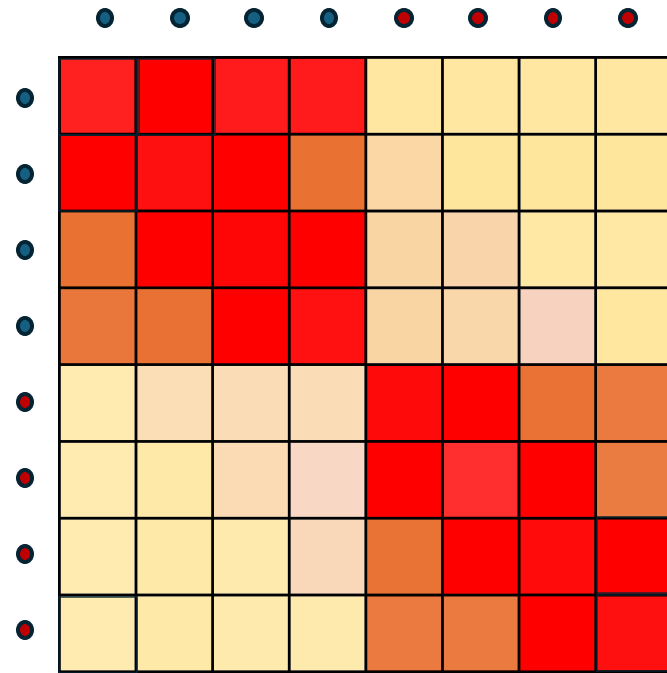
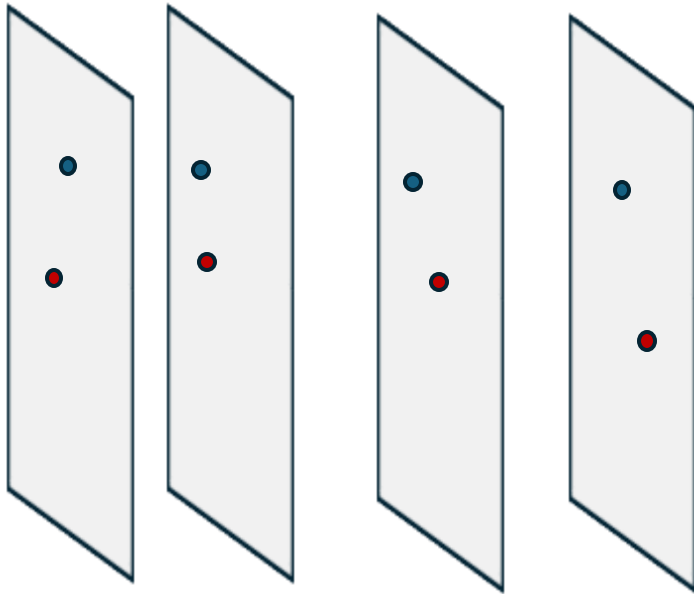


# Transformer



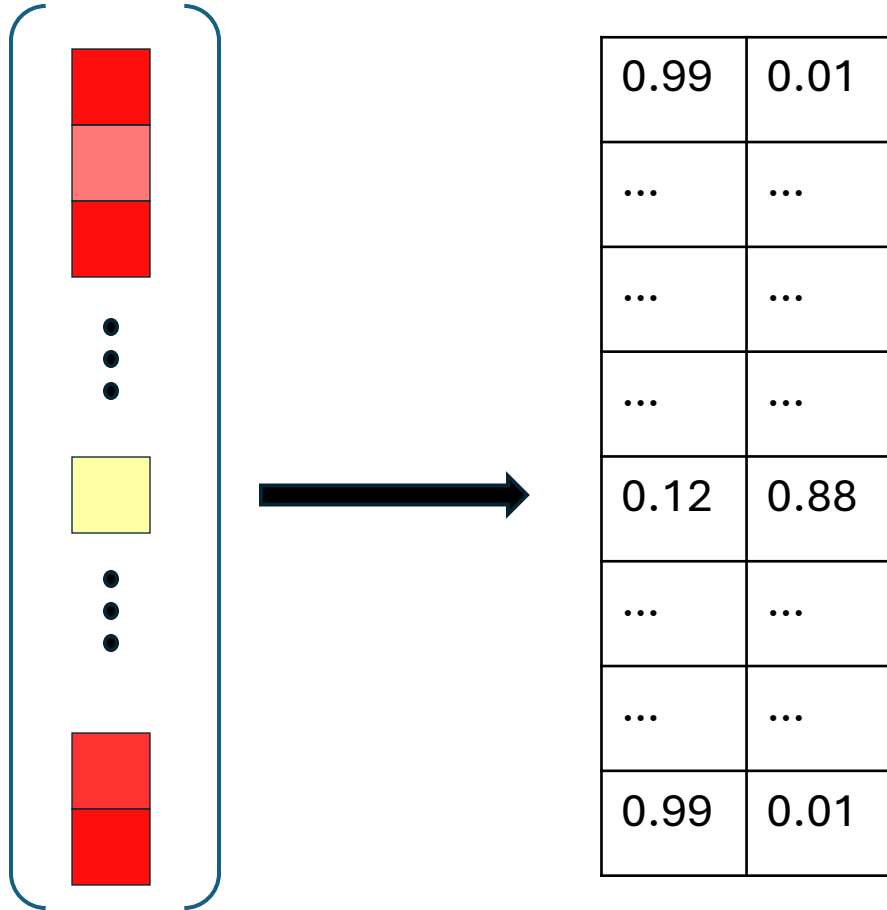


# Transformer



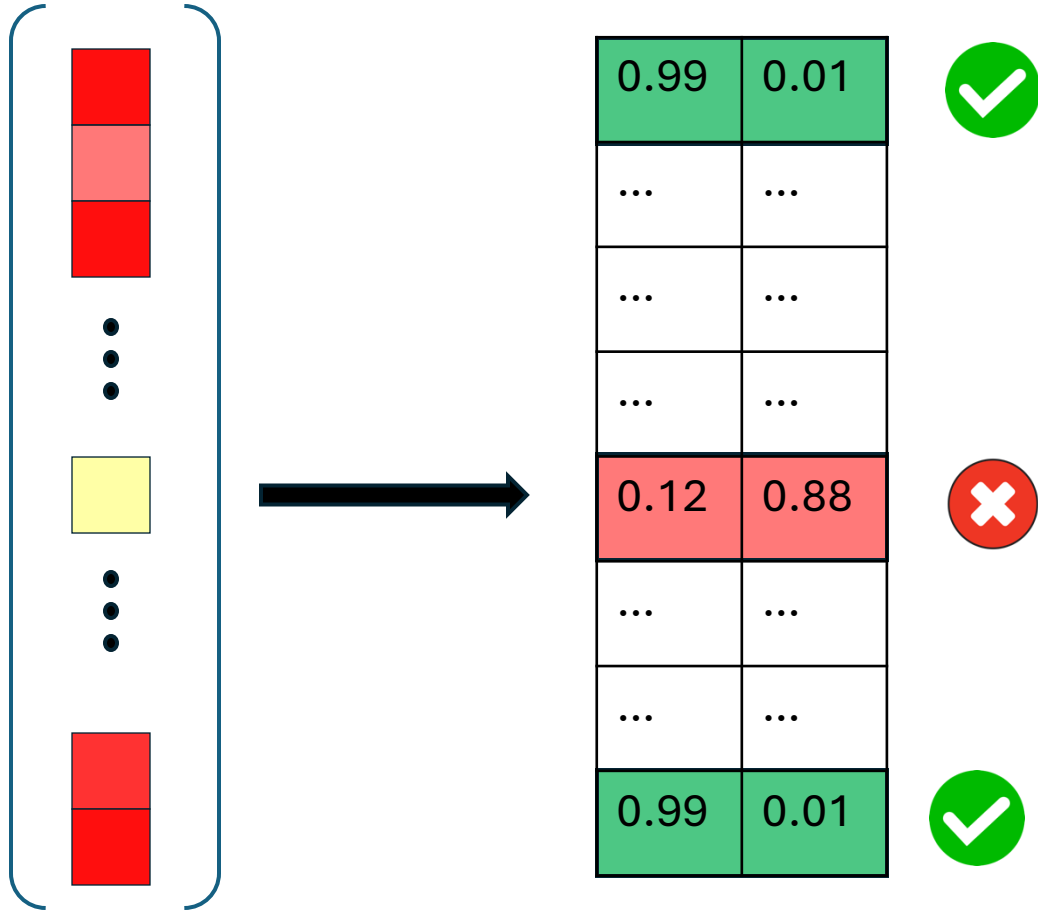


# Transformer



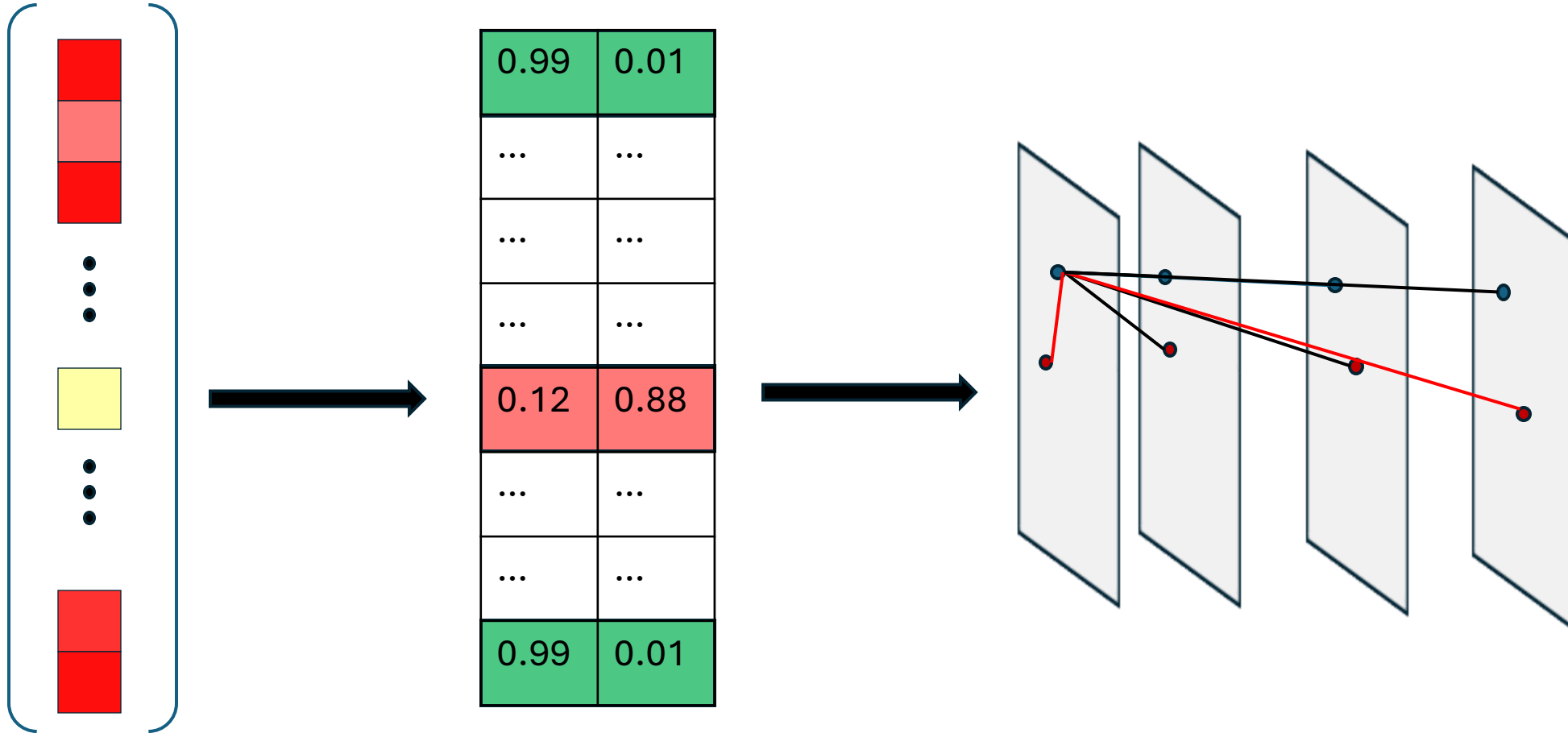


# Transformer





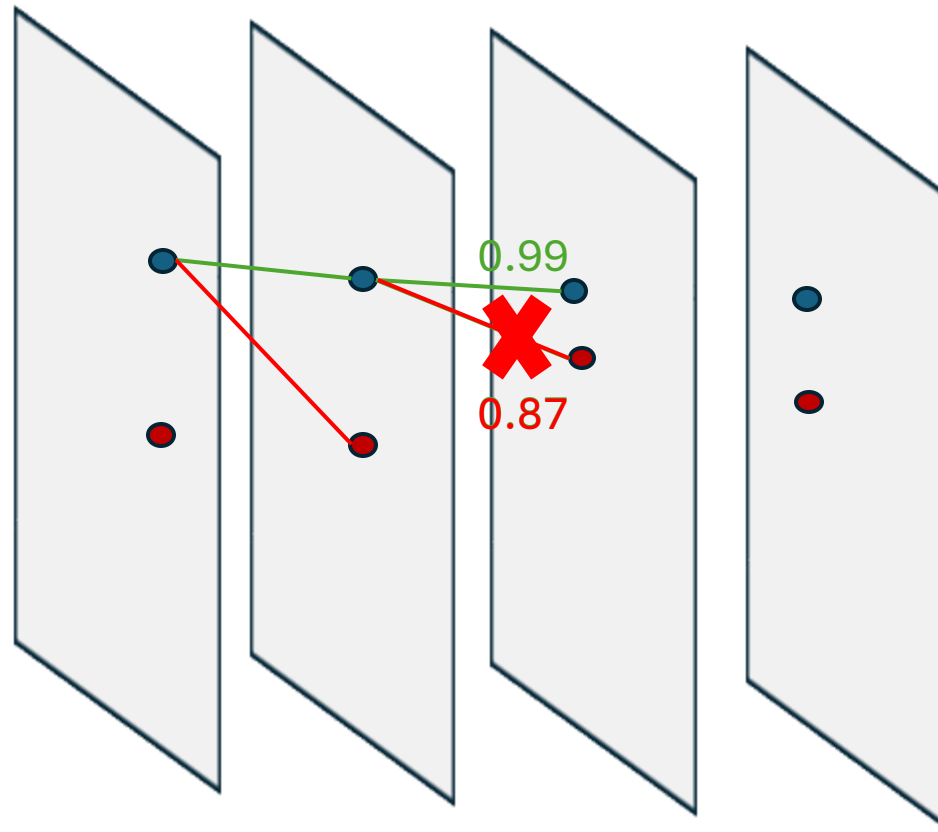
# Transformer





# Transformer

## Max Edge selection







# Transformer



$$\text{Efficiency} = \frac{\# \text{ correctly predicted tracks}}{\# \text{ total true tracks}}$$



$$\text{Purity} = \frac{\# \text{ correctly predicted tracks}}{\# \text{ total predicted tracks}}$$



$$\text{Fake Tracks} = \frac{\# \text{ wrongly predicted tracks}}{\# \text{ total true tracks}}$$

Multi-Layer Perceptron

Efficiency	Purity	Fake Tracks
70.06 %	92.3 %	39.45 %

Transformer

Efficiency	Purity	Fake Tracks
95.95 %	98.62 %	1.22 %



# Transformer



Solved class imbalance



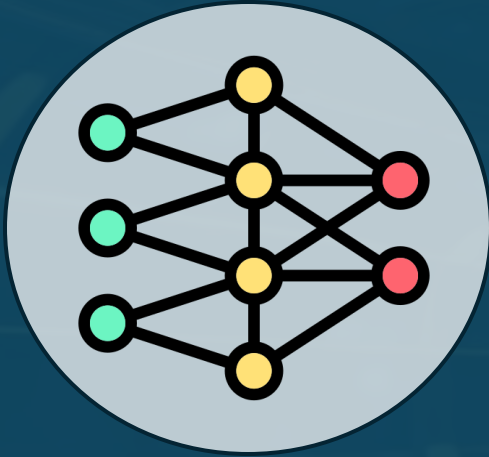
Global awareness



Efficient computations



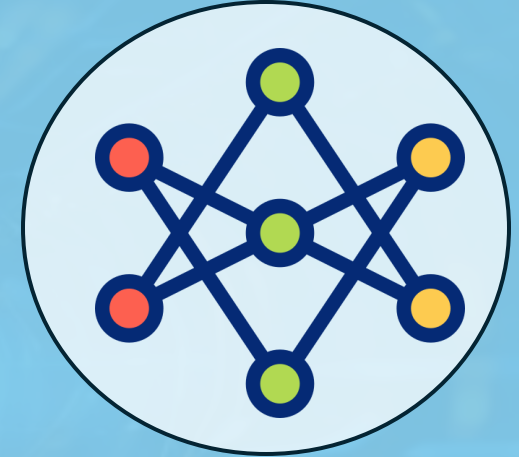
Many computations to consider all the connections



Multi-Layer Perceptron



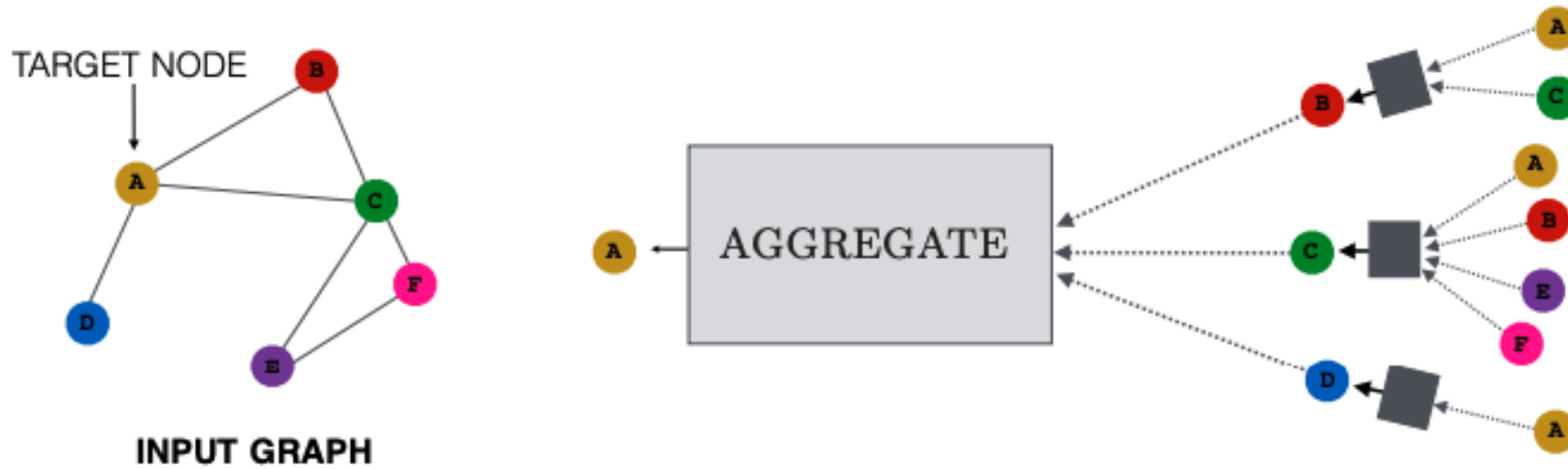
Transformer



Graph Neural Network



# Graph Neural Network



Graph Neural Networks are a type of neural network designed to work with graph-structured data.

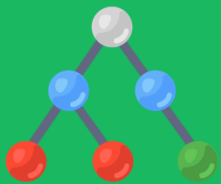
They **propagate** and **aggregate** information across nodes and edges in a graph, allowing them to learn representations that capture the relationships and structure within the data



# Graph Neural Network



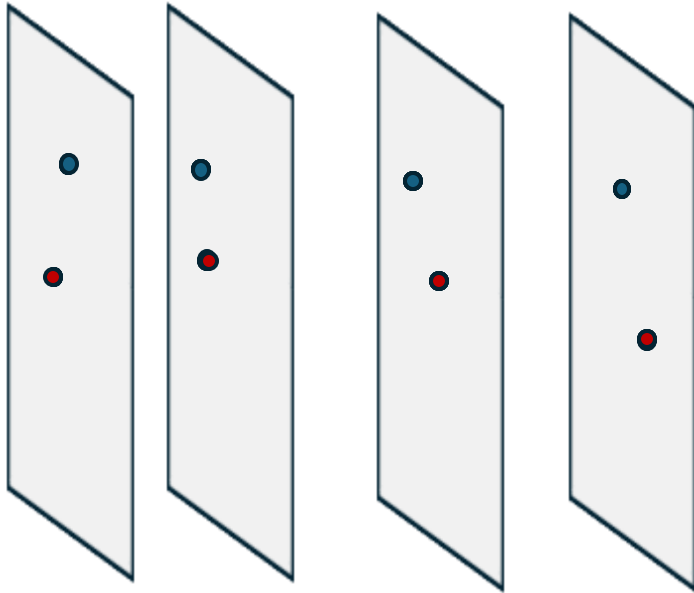
Many computations to consider all the connections



Graphs allow to decide the topology (e.g. the connections between nodes)

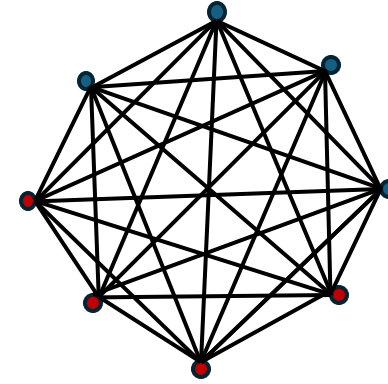
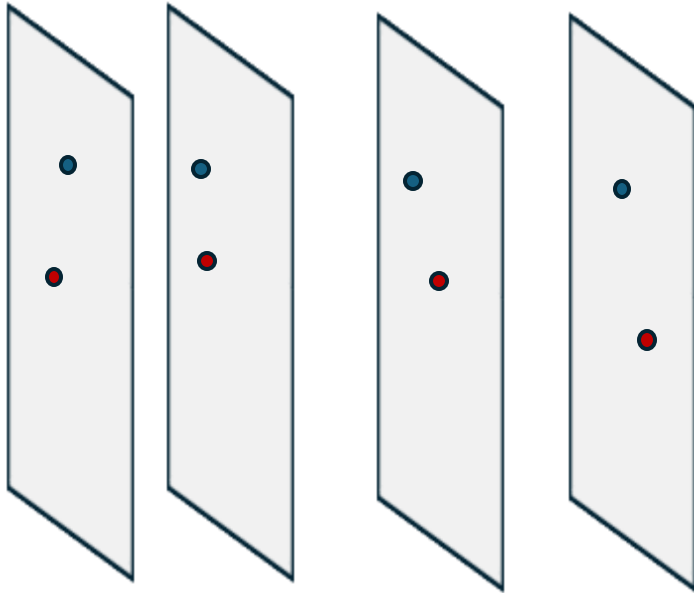


# Graph Neural Network

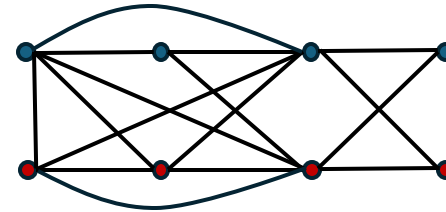




# Graph Neural Network



**Complete Graph**



**Sparse Graph**

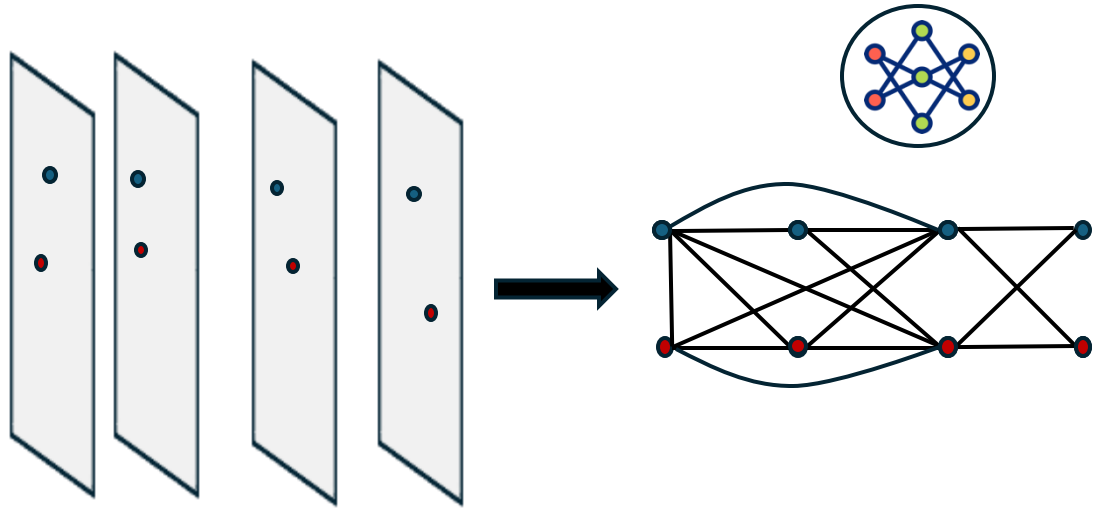
If we consider possible edges between hits:

- $2n^2$  (GTK0-GTK1 and GTK0-GTK2)
- $n^2$  (GTK1-GTK2)
- $n^2$  (GTK2-GTK3)

Total:  $4n^2 < 16n^2$



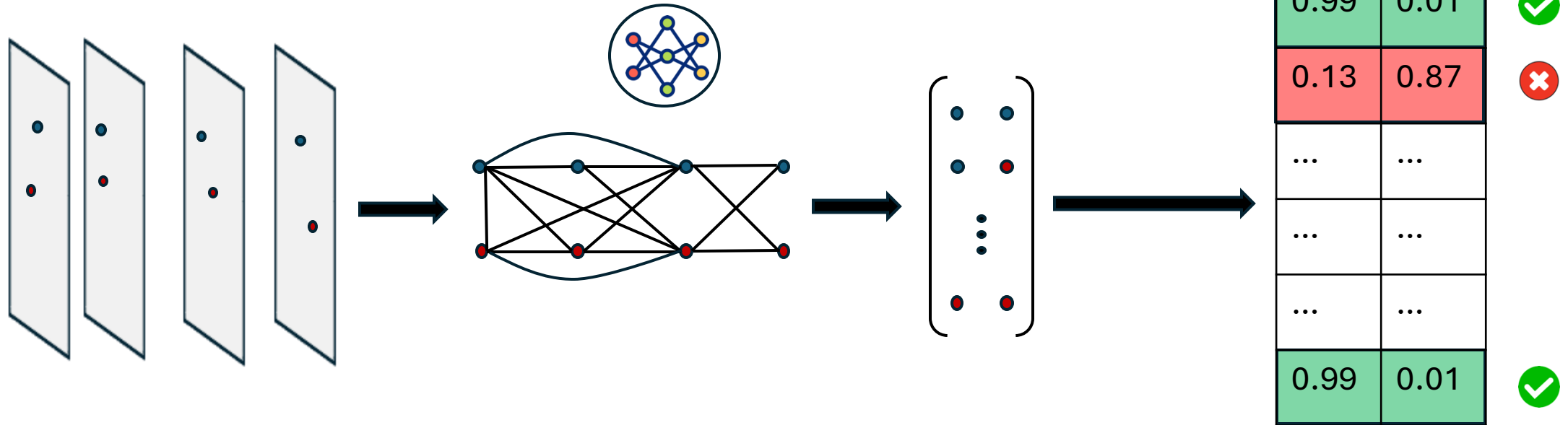
# Graph Neural Network





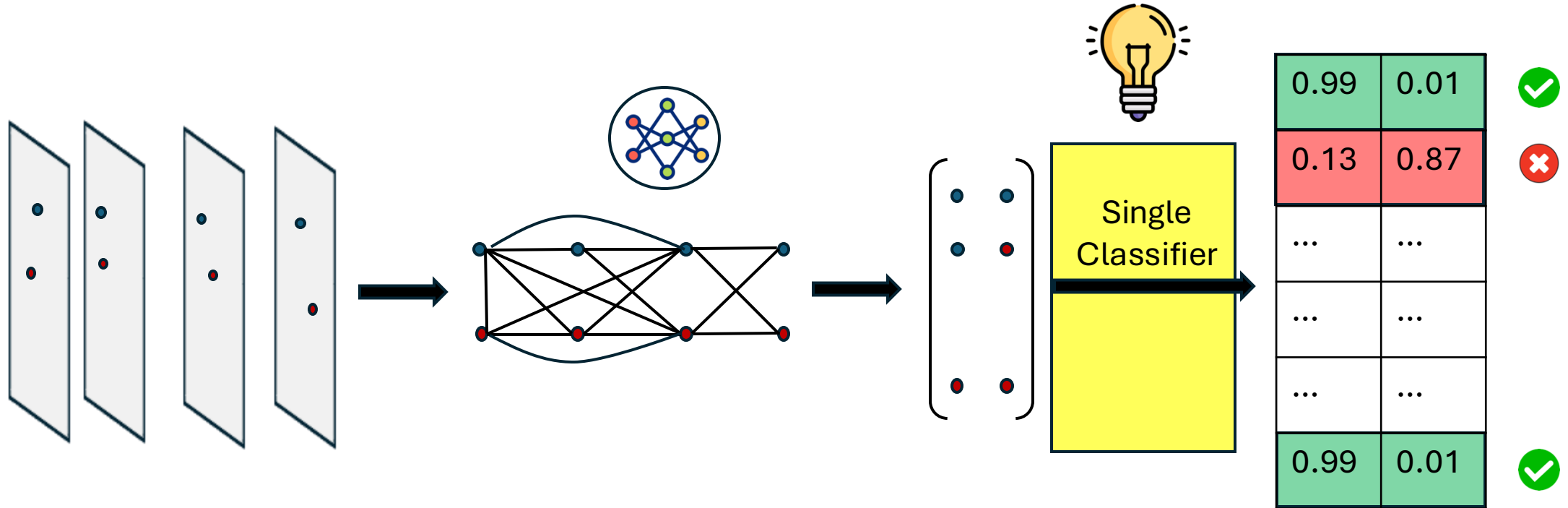


# Graph Neural Network



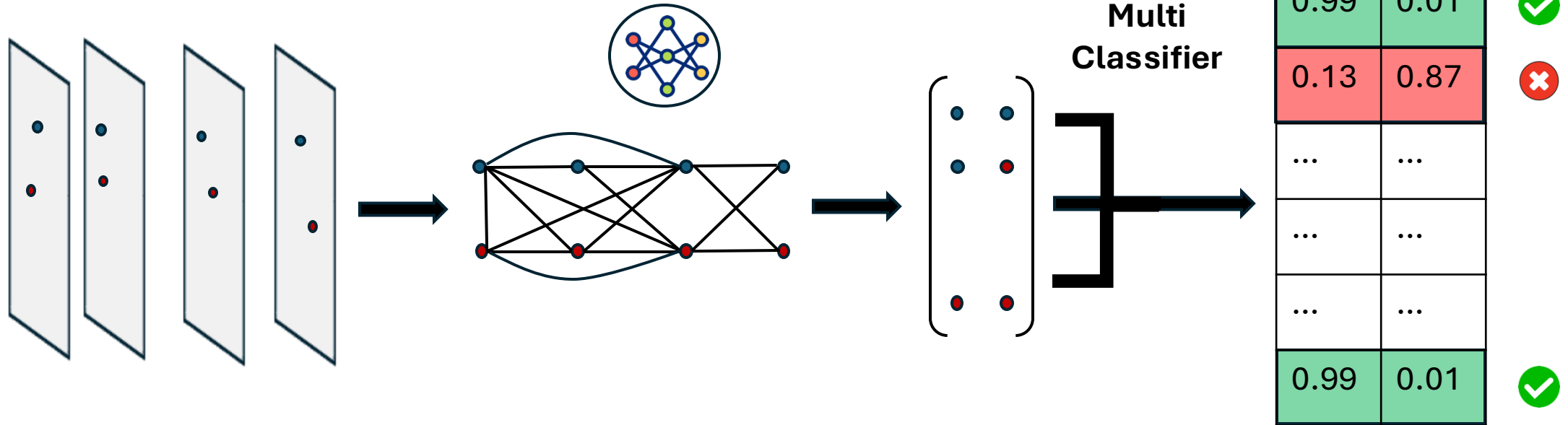


# Graph Neural Network



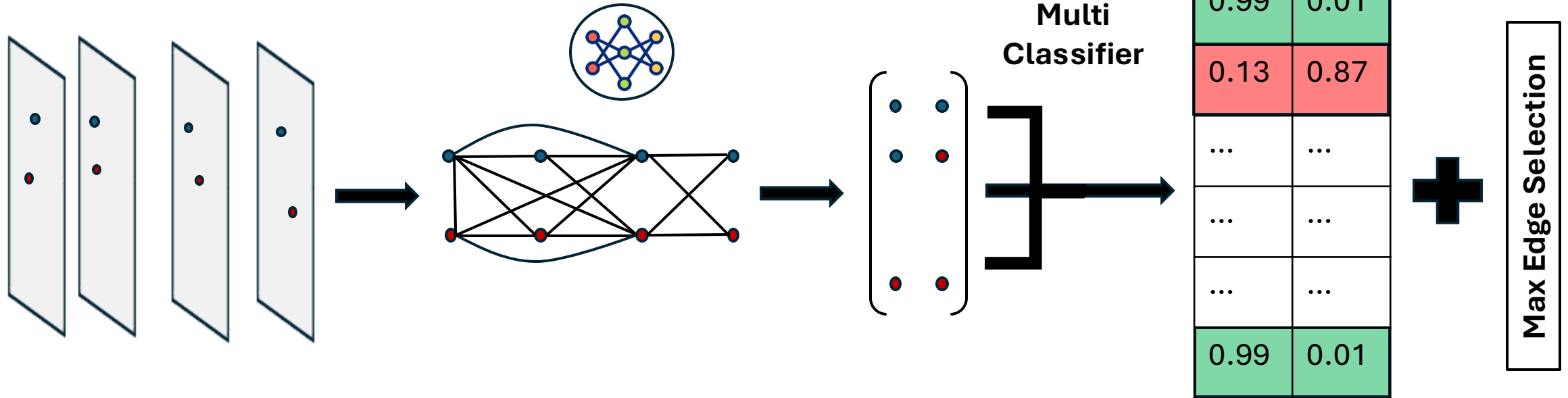


# Graph Neural Network





# Graph Neural Network





# Graph Neural Network



$$\text{Efficiency} = \frac{\# \text{ correctly predicted tracks}}{\# \text{ total true tracks}}$$



$$\text{Purity} = \frac{\# \text{ correctly predicted tracks}}{\# \text{ total predicted tracks}}$$



$$\text{Fake Tracks} = \frac{\# \text{ wrongly predicted tracks}}{\# \text{ total true tracks}}$$

## Multi-Layer Perceptron

Efficiency	Purity	Fake Tracks
70.06 %	92.3 %	39.45 %

## Transformer

Efficiency	Purity	Fake Tracks
95.95 %	98.62 %	1.22 %

## Graph Neural Network\*

Efficiency	Purity	Fake Tracks
94.78 %	99.78 %	0.21 %

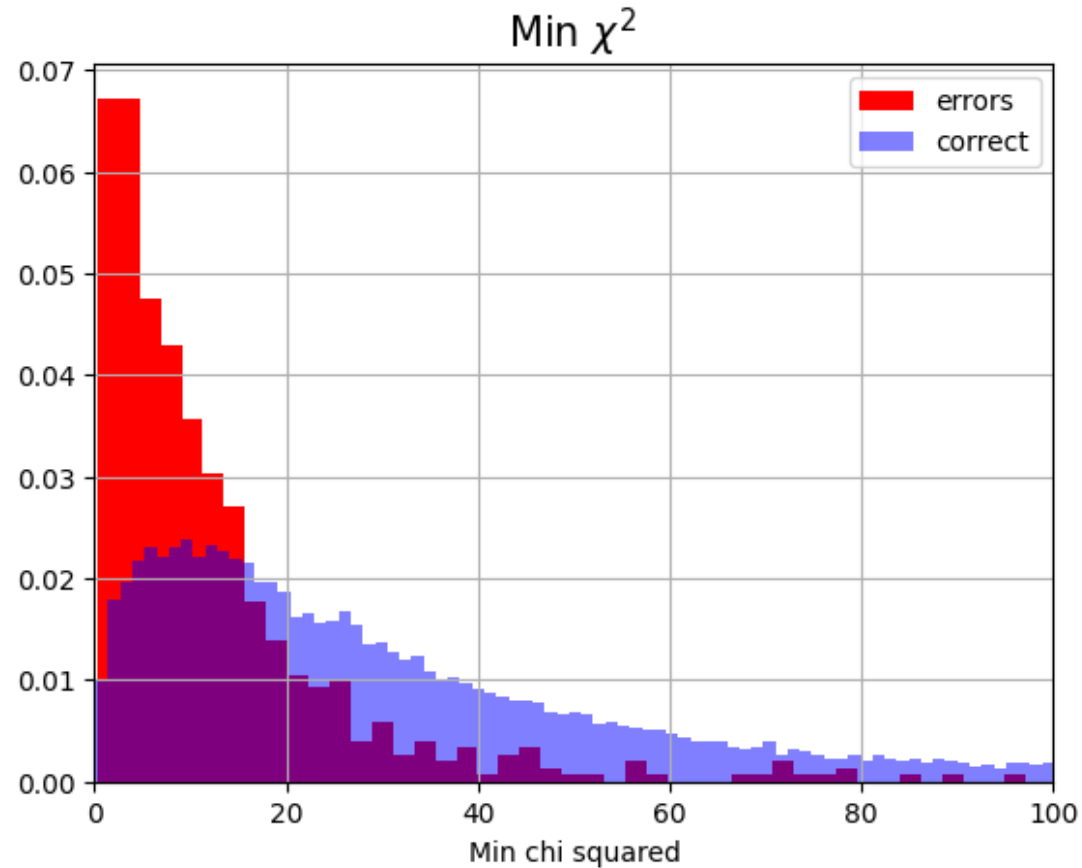
\* Direct, Fully-connected graph with Graph Convolutional Network and Multi-Classifer



# Graph Neural Network

## Difficulty Score

$$\chi^2 = \min_{k=0,1,2,3} \left( \min_{1 \leq i < j \leq n} [(x_{i,k} - x_{j,k})^2 + (y_{i,k} - y_{j,k})^2 + (t_{i,k} - t_{j,k})^2] \right)$$

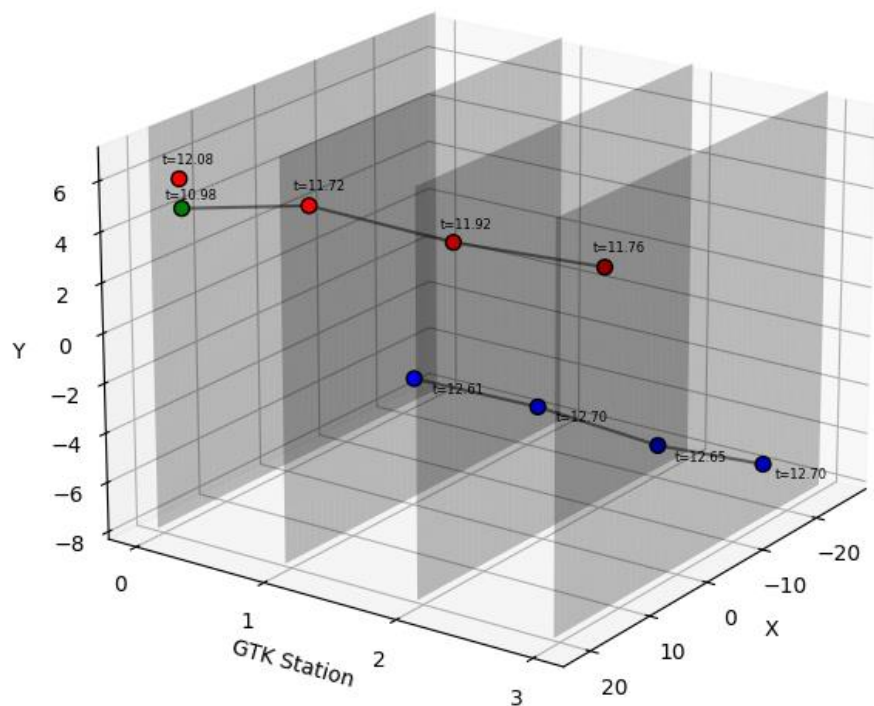




# Graph Neural Network

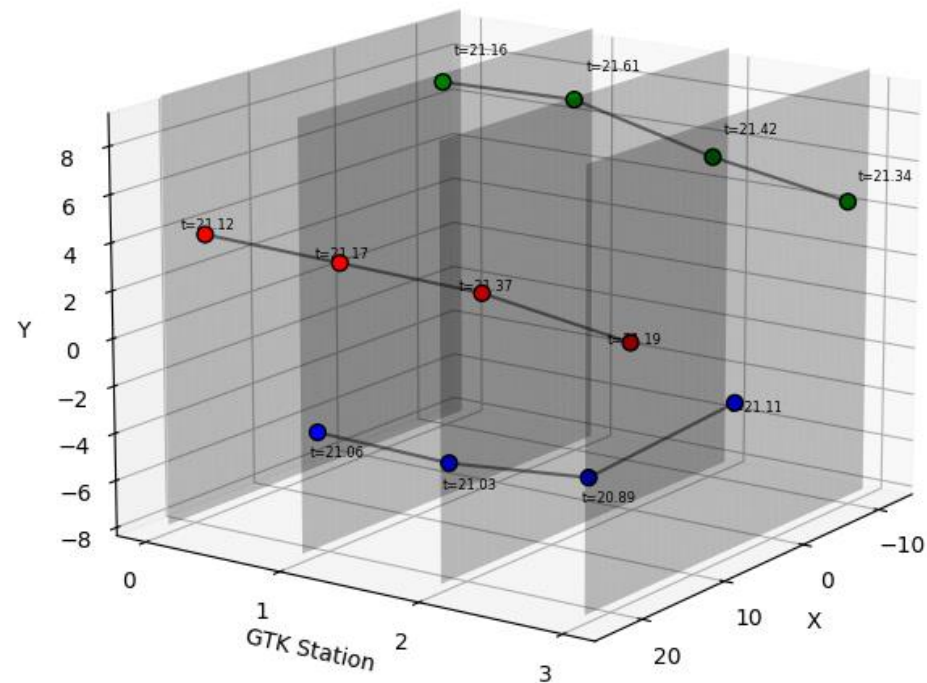
Example of an error

- particle 0
- particle 20
- particle 31



Example of a good prediction

- particle 0
- particle 42
- particle 55





# Graph Neural Network



Solved class imbalance



Global awareness



Computationally Efficient

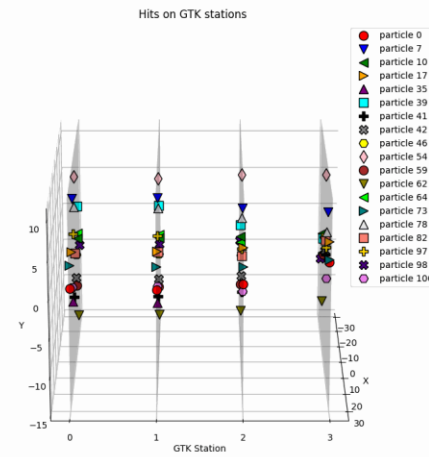
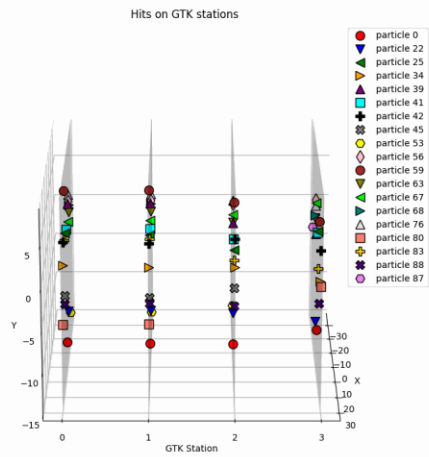


Flexible Topology



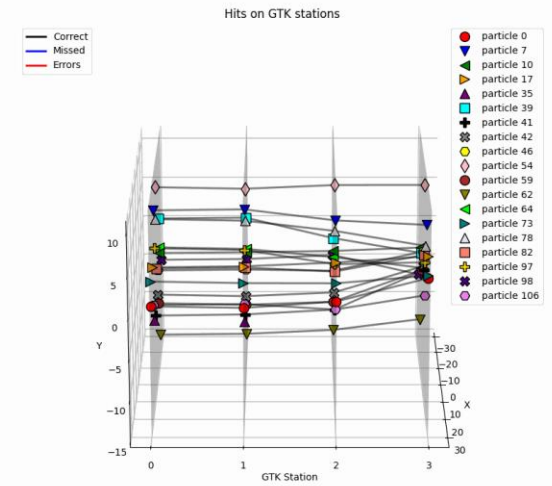
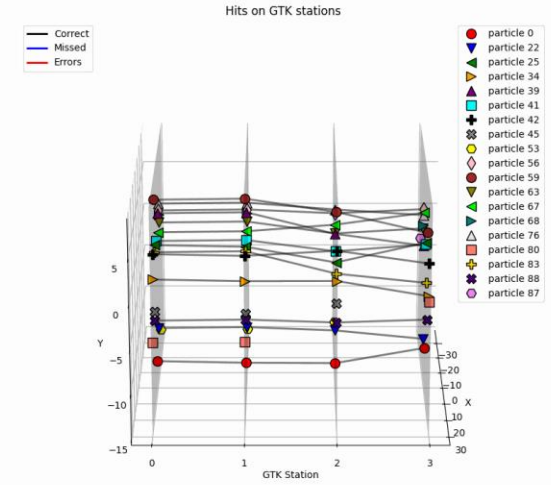
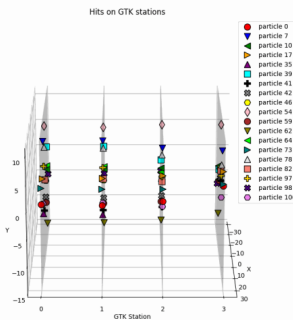
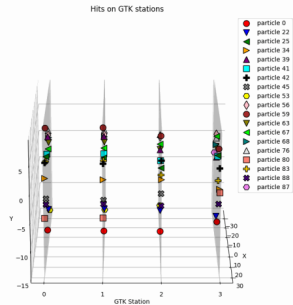


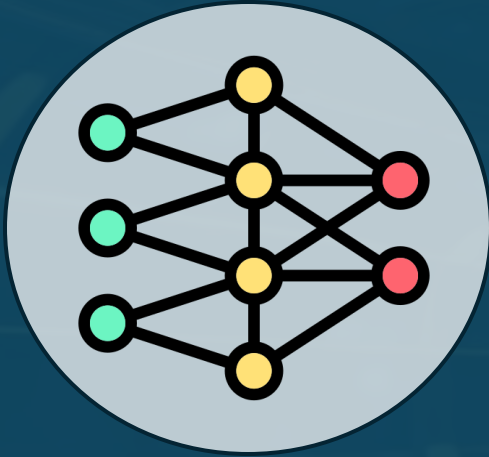
# Graph Neural Network





# Graph Neural Network

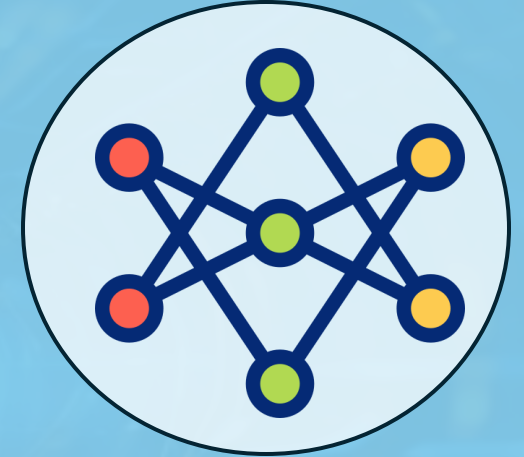




Multi-Layer Perceptron

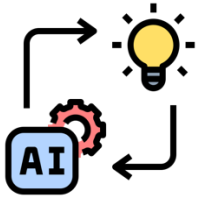


Transformer

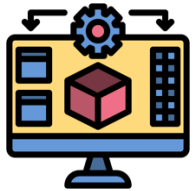


Graph Neural Network

# Conclusions



- Machine Learning algorithms can be used to track particles



- 3 different algorithms were proposed ( MLP, Transformer, Graph Neural Network)

# Acknowledgments

This project was based on Monte Carlo simulations kindly provided by the NA62 Collaboration.

# References

- [1] B. Denby. Neural networks and cellular automata in experimental high energy physics. *Computer Physics Communications*, 49(3):429–448, 1988.
- [2] Alexander Radovic, Mike Williams, David Rousseau, Michael Kagan, Daniele Bonacorsi, Alexander Himmel, Adam Aurisano, Kazuhiro Terao, and Taritree Wongjirad. Machine learning at the energy and intensity frontiers of particle physics. *Nature*, 560(7716):41–48, August 2018.
- [3] Bourilkov D. Machine and deep learning applications in particle physics. *International Journal of Modern Physics A*, 34(35):1930019, December 2019.
- [4] M. Feickert and B. Nachman. A living review of machine learning for particle physics, 2021.
- [5] M. Bronstein, J. Bruna, Y. LeCun, A. Szlam, and P. Vandergheynst. Geometric deep learning: Going beyond euclidean data. *IEEE Signal Processing Magazine*, 34(4):18–42, July 2017.
- [6] F. Scarselli, M. Gori, A. C. Tsoi, M. Hagenbuchner, and G. Monfardini. The graph neural network model. *IEEE Transactions on Neural Networks*, 20(1):61–80, Jan 2009.
- [7] T. Gaudet and et al. Utilizing graph machine learning within drug discovery and development. *Briefings in Bioinformatics*, 22(6):bbab159, 05 2021.
- [8] F. Liu, S. Xue, J. Wu, C. Zhou, W. Hu, C. Paris, S. Nepal, J. Yang, and P.S. Yu. Deep learning for community detection: Progress, challenges and opportunities. In *Proceedings of the Twenty-Ninth International Joint Conference on Artificial Intelligence, IJCAI-PRICAI-2020. International Joint Conferences on Artificial Intelligence Organization*, July 2020.
- [9] Z. Zhang, P. Cui, and W. Zhu. Deep learning on graphs: A survey, 2020..
- [10] Z. Wu, S. Pan, F. Chen, G. Long, C. Zhang, and P. S. Yu. A comprehensive survey on graph neural networks. *IEEE Transactions on Neural Networks and Learning Systems*, 32(1):4–24, January 2021.
- [11] J. Zhou, G. Cui, S. Hu, Z. Zhang, C. Yang, Z. Liu, L. Wang, C.Li, and M. Sun. Graph neural networks: A review of methods and applications, 2021.
- [12] S. Farrell et al. Novel deep learning methods for track reconstruction, 2018.
- [13] X. Ju and et al. Graph neural networks for particle reconstruction in high energy physics detectors, 2020.
- [14] I. Henrion, J. Brehmer, J. Bruna, K. Cho, K. Cranmer, G. Louppe, and G. Rochette. Neural message passing for jet physics. 2017.
- [15] J. Shlomi, S. Ganguly, E. Gross, K. Cranmer, Y. Lipman, H. Serviansky, H. Maron, and N. Segol. Secondary vertex finding in jets with neural networks. *The European Physical Journal C*, 81(6), June 2021.
- [16] J. A. Martinez, O. Cerri, M. Pierini, M. Spiropulu, and J. Vlimant. Pileup mitigation at the large hadron collider with graph neural networks, 2019.
- [17] E. Cortina Gil. et al. The beam and detector of the na62 experiment at cern. *Journal of Instrumentation*, 12(05):P05025, may 2017.
- [18] Rinella et al. The na62 gigatracker: a low mass high intensity beam 4d tracker with 65 ps time resolution on tracks. *Journal of Instrumentation*, 14(07):P07010–P07010, July 2019.
- [19] A. Tsaris and et al. The hep.trkx project: Deep learning for particle tracking. *Journal of Physics: Conference Series*, 1085(4):042023, sep 2018.
- [20] Exa.TrkX Collaboration. Exa.trkx. <https://exatrxx.github.io/>.
- [21] S. Caillou, P. Calafiura, S. Farrell, X. Ju, D. Murnane, C. Rougier, J. Stark, and A. Vallier. ATLAS ITk Track Reconstruction with a GNN-based pipeline. Technical report, CERN, Geneva, 2022.
- [22] X. et al. Ju. Performance of a geometric deep learning pipeline for hl-lhc particle tracking. *The European Physical Journal C*, 81(10), October 2021.
- [23] M. Kiehn and et al. The trackml high-energy physics tracking challenge on kaggle. *EPJ Web of Conferences*, 214:06037, 01 2019.
- [24] S. Thais and et al. Graph neural networks in particle physics: Implementations, innovations, and challenges, 2022.
- [25] V. Mikuni and F. Canelli. ABCNet: an attention-based method for particle tagging. *The European Physical Journal Plus*, 135(6):463, 2020.
- [26] R. Liu, P. Calafiura, S. Farrell, X. Ju, D. Murnane, and T. Pham. Hierarchical graph neural networks for particle track reconstruction, 2023.
- [27] G. DeZoort, S. Thais, J. Duarte, V. Razavimaleki, M. Atkinson, I. Ojalvo, M. Neubauer, and P. Elmer. Charged particle tracking via edge-classifying interaction networks. *Computing and Software for Big Science*, 5(1), November 2021