A Quantum Graph Neural Network Approach to Particle Track Reconstruction

CERN openlab Technical Workshop

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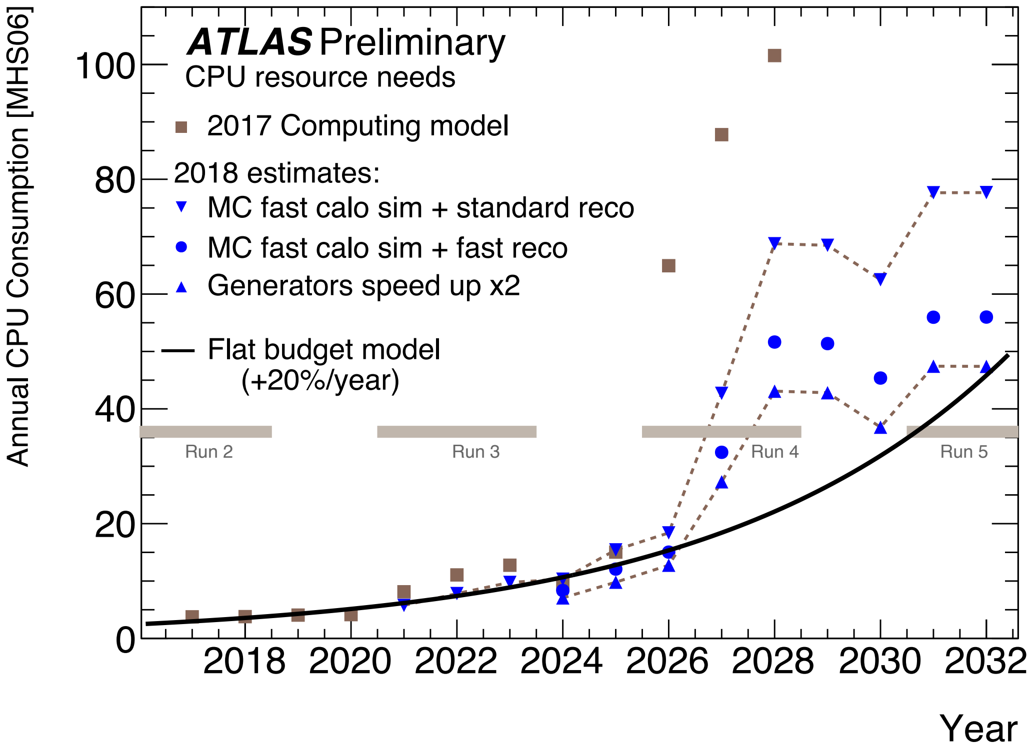
Outline

- Particle Track Reconstruction and TrackML Challenge
- Hep.TrkX Graph Neural Network approach
- Quantum Graph Neural Network approach

High Luminosity LHC

High Luminosity upgrade of LHC brings many computational challenges.



ATLAS computing model projections for Phase-2

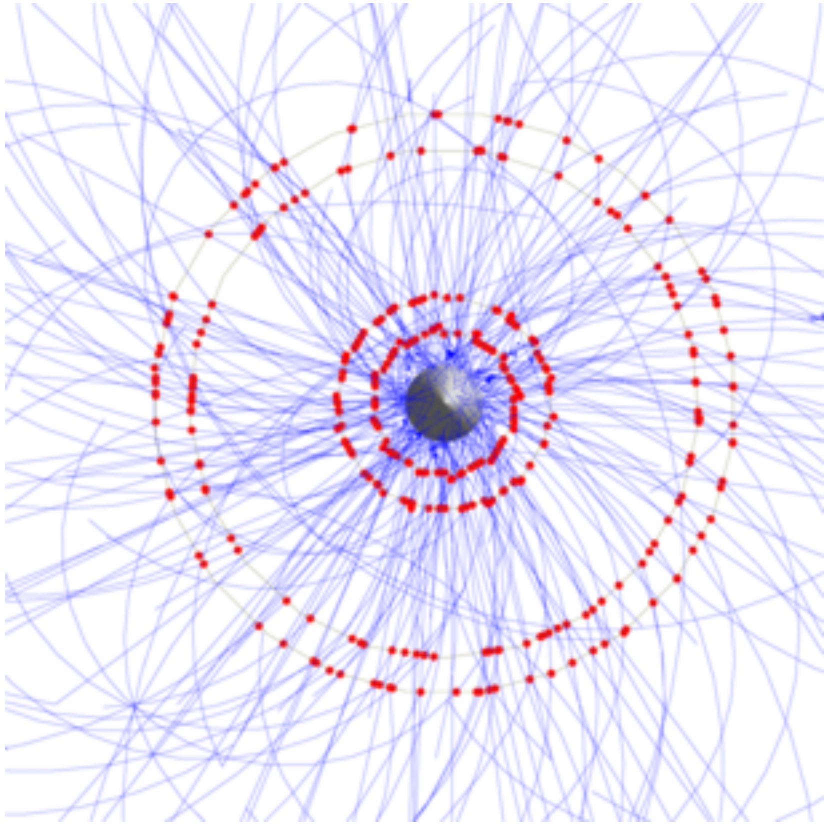
Particle Track Reconstruction

Particle Track Reconstruction becomes much harder!

	Run -1	Run -2	Run -3
μ	21	40	150-200?
Tracks	~280	~600	~7-10k

$\mu: Average\ number\ of\ interactions\ per\ bunch\ crossing$

H. Gray, Track reconstruction in the ATLAS experiment, 2016.

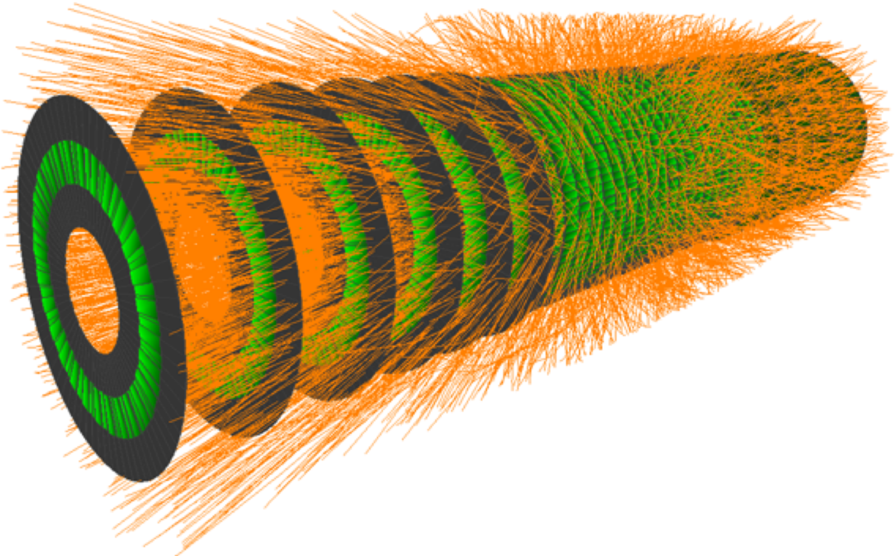


https://agberger.kph.uni-mainz.de/technologies/track-reconstruction/

TrackML Challenge

A Public Machine Learning Challenge for Particle Tracking

https://www.kaggle.com/c/trackml-particle-identification/overview



#	△pub	Team Name	Notebook	Team Members	Score	Entries	Last
1	—	Top Quarks			0.92182	10	1y
2	—	outrunner			0.90302	9	1y
3	—	Sergey Gorbunov			0.89353	6	1y

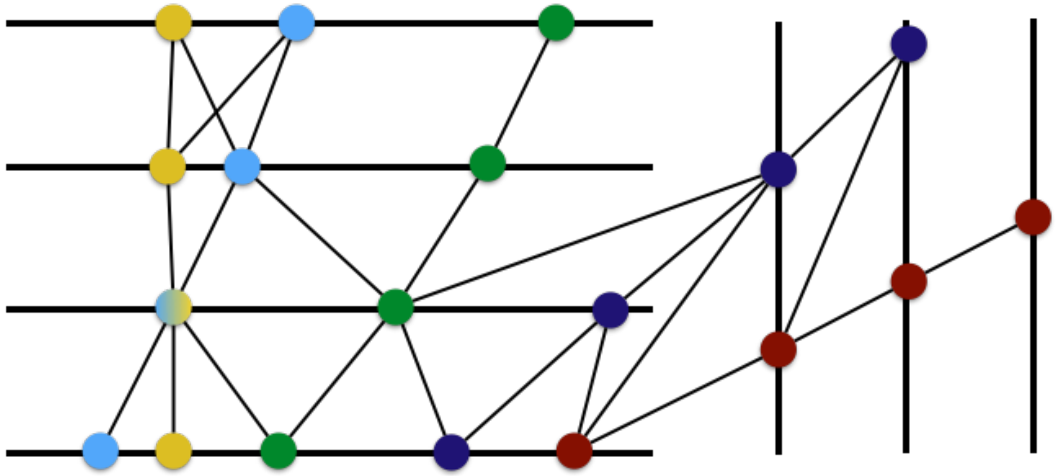
Hep.TrkX GNN

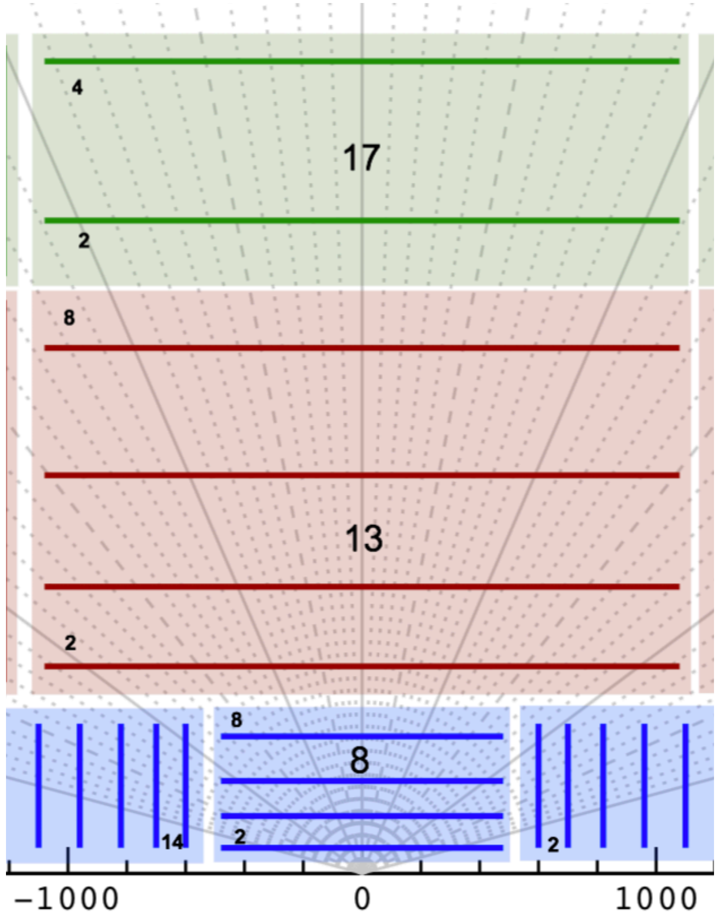
Novel deep learning methods for track reconstruction

Steven Farrell[1,*], *Paolo* Calafiura[1], *Mayur* Mudigonda[1], Prabhat[1], *Dustin* Anderson[2], *Jean-Roch* Vlimant[2], *Stephan* Zheng[2], *Josh* Bendavid[2], *Maria* Spiropulu[2], *Giuseppe* Cerati[3], *Lindsey* Gray[3], *Jim* Kowalkowski[3], *Panagiotis* Spentzouris[3], and *Aristeidis* Tsaris[3]

[1]Lawrence Berkeley National Laboratory
[2]California Institute of Technology
[3]Fermi National Accelerator Laboratory

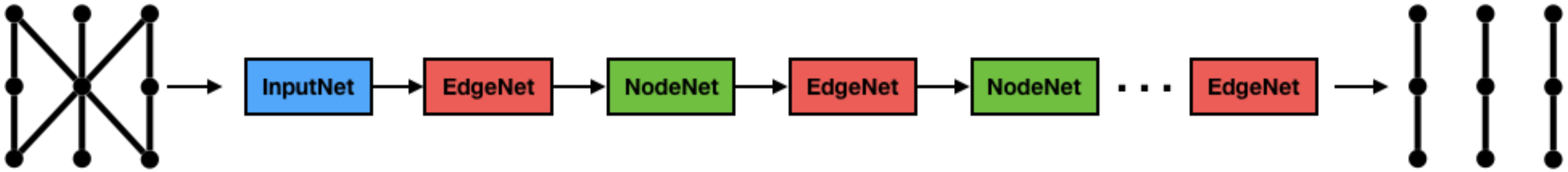
https://arxiv.org/abs/1810.06111

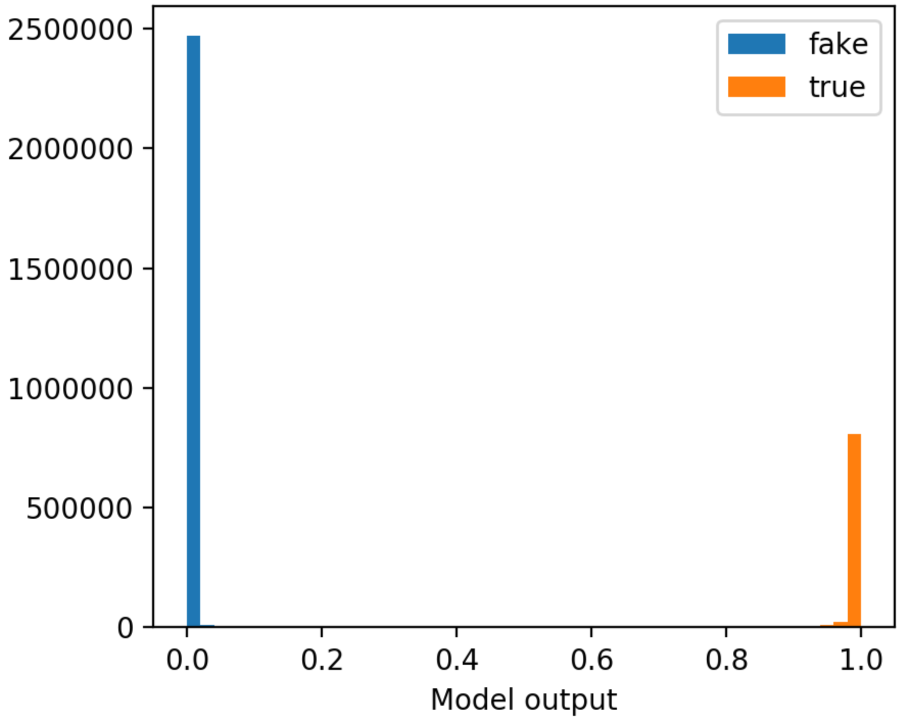


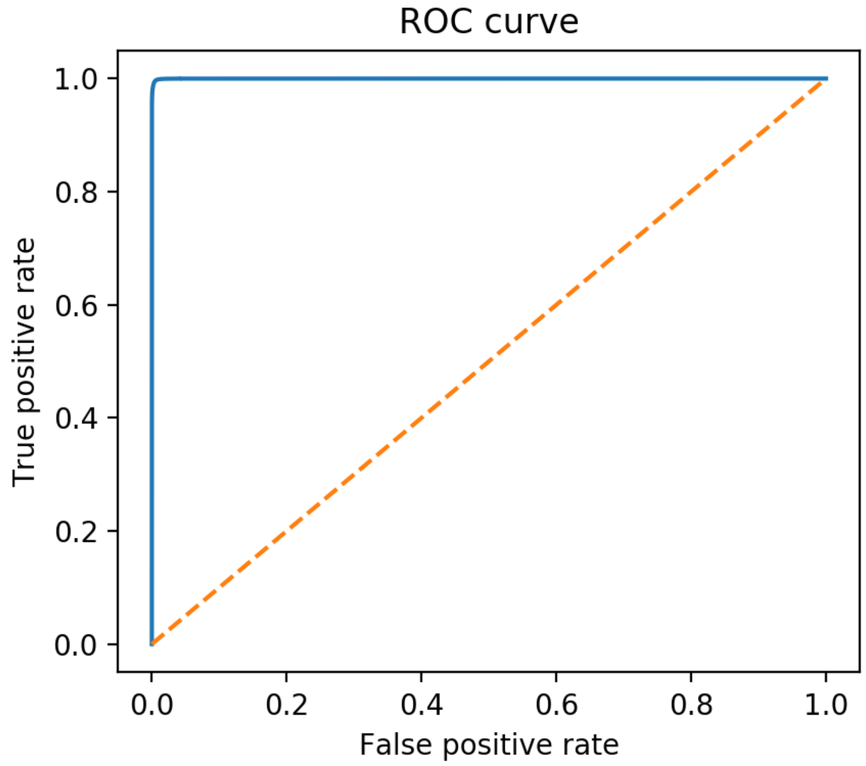


Hep.TrkX GNN

Promising Results



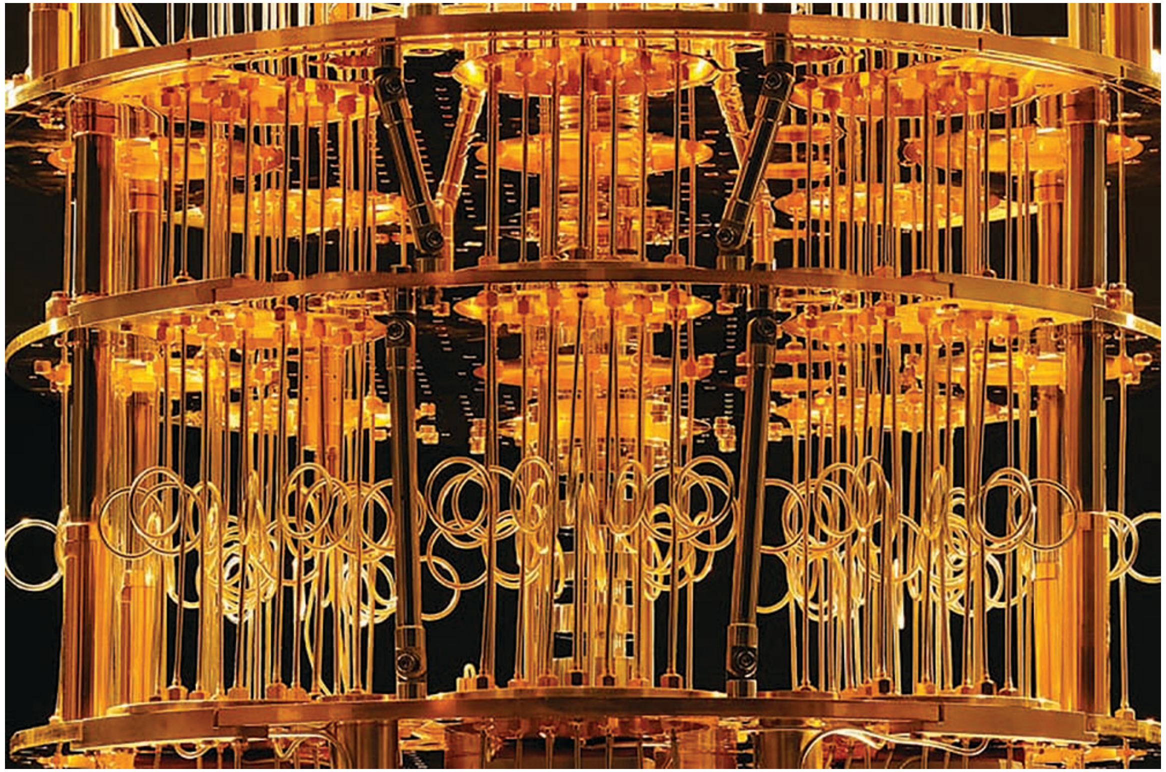




Quantum Computing

Quantum computing allows a new way of computation for certain problems including;

- Prime number factorization
- Solving Linear Equations
- Machine Learning!



Credit: IBM Research

A Quantum Classifier

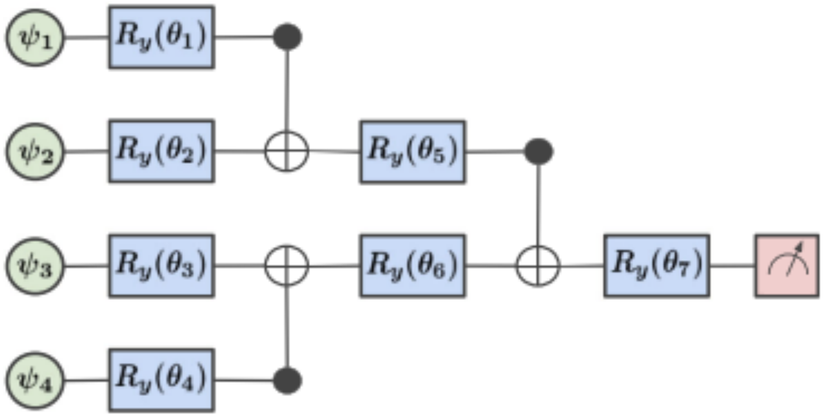
Hierarchical quantum classifiers

Edward Grant[1,2], Marcello Benedetti[1,3], Shuxiang Cao[4,5], Andrew Hallam[6,7], Joshua Lockhart[1], Vid Stojevic[8], Andrew G. Green[6] and Simone Severini[1]

Table 3. Binary classification accuracy on the MNIST dataset

Classifier	Unitaries	Rotations	Is > 4	Is even	0 or 1	2 or 7
TTN	Simple	Real	65.59 ± 0.57	72.17 ± 0.89	92.12 ± 2.17	68.07 ± 2.42
TTN	General	Real	74.89 ± 0.95	83.13 ± 1.08	99.79 ± 0.02	97.64 ± 1.60
MERA	General	Real	75.20 ± 1.51	82.83 ± 1.19	99.84 ± 0.06	98.02 ± 1.40
Hybrid	General	Real	76.30 ± 1.04	83.53 ± 0.21	**99.87** ± 0.02	98.07 ± 1.46
TTN	Simple	Complex	70.90 ± 0.73	80.12 ± 0.64	99.37 ± 0.12	94.09 ± 3.37
TTN	General	Complex	77.56 ± 0.45	83.53 ± 0.69	99.77 ± 0.02	97.63 ± 1.48
MERA	General	Complex	**79.10** ± 0.90	**84.85** ± 0.20	99.74 ± 0.02	**98.86** ± 0.07
Hybrid	General	Complex	78.36 ± 0.45	84.38 ± 0.28	99.78 ± 0.02	98.46 ± 0.19
Logistic	N/A	N/A	70.70 ± 0.01	81.72 ± 0.01	99.53 ± 0.01	96.17 ± 0.01

Mean test accuracy and one standard deviation are reported for TTN, MERA, and hybrid classifiers with five different random initial parameter settings using two different types of unitary parametrization. Hybrid classifiers consist of pre-training a TTN classifier and that transforming it into a MERA classifier by training additional unitaries. Bold values indicate the best result for each classificaiton task



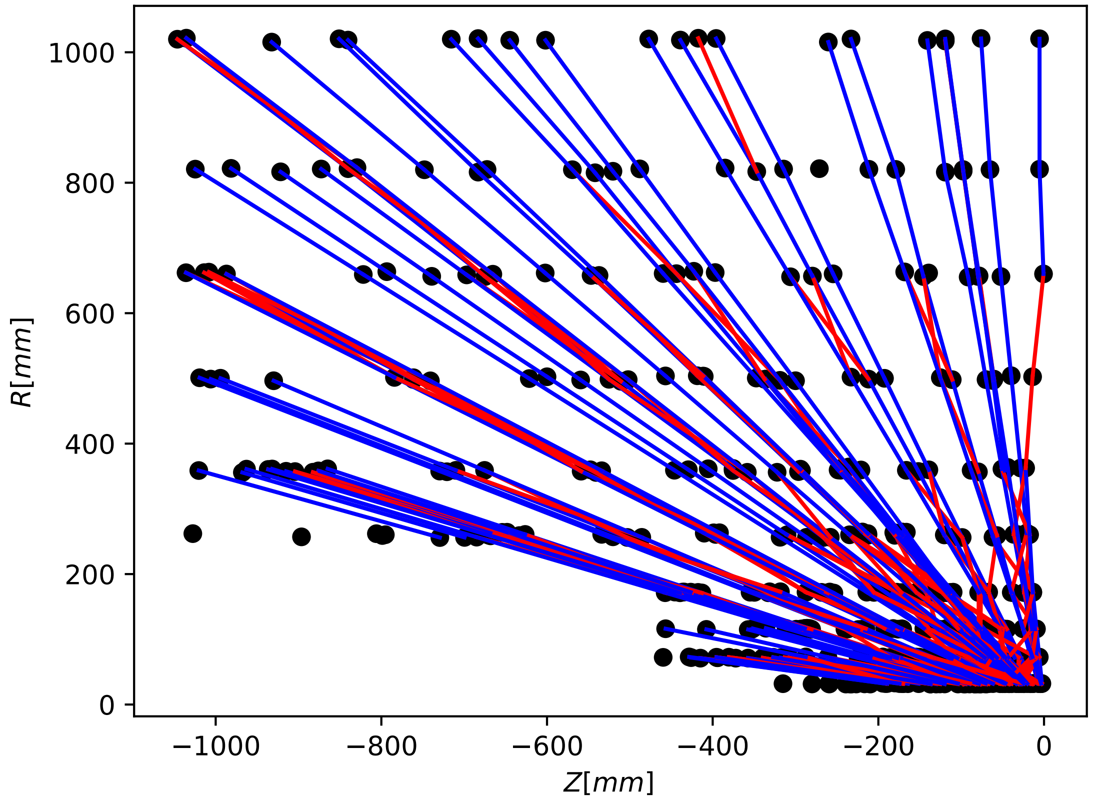
Plotting the Data

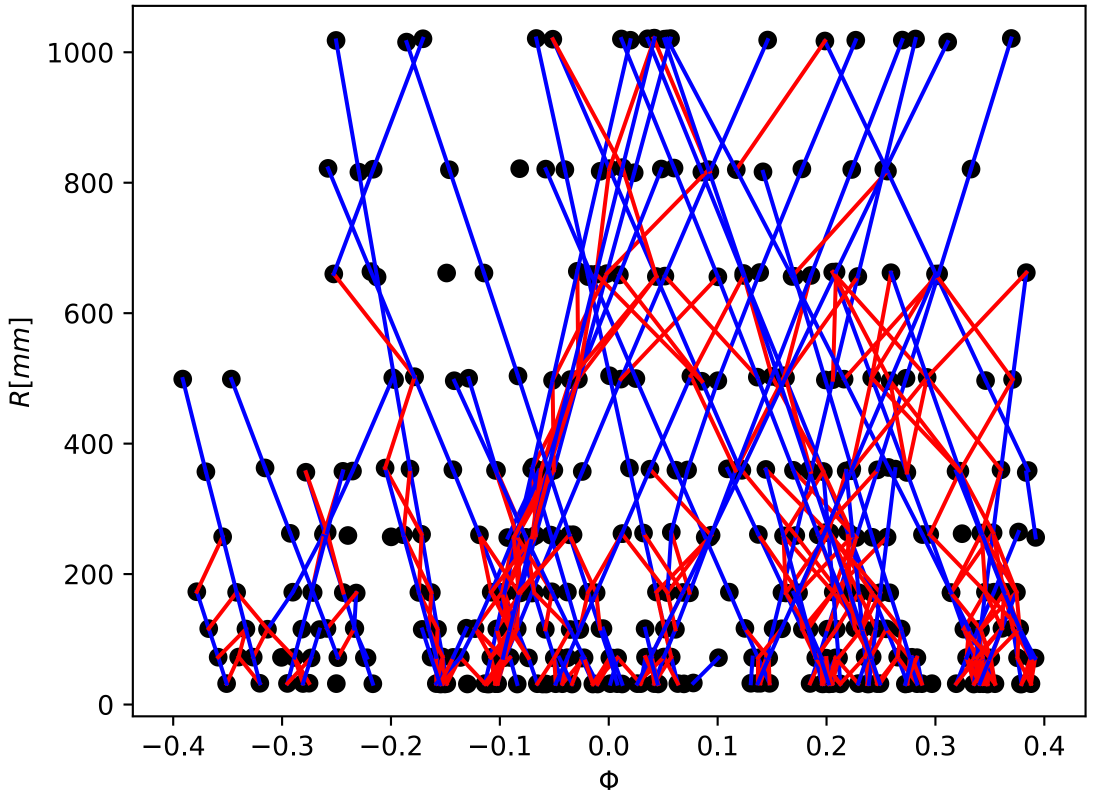
Cylindrical Symmetry → Cylindrical Coordinates

Blue: After preprocessing with Hep.TrkX methods

Red: Ground Truth

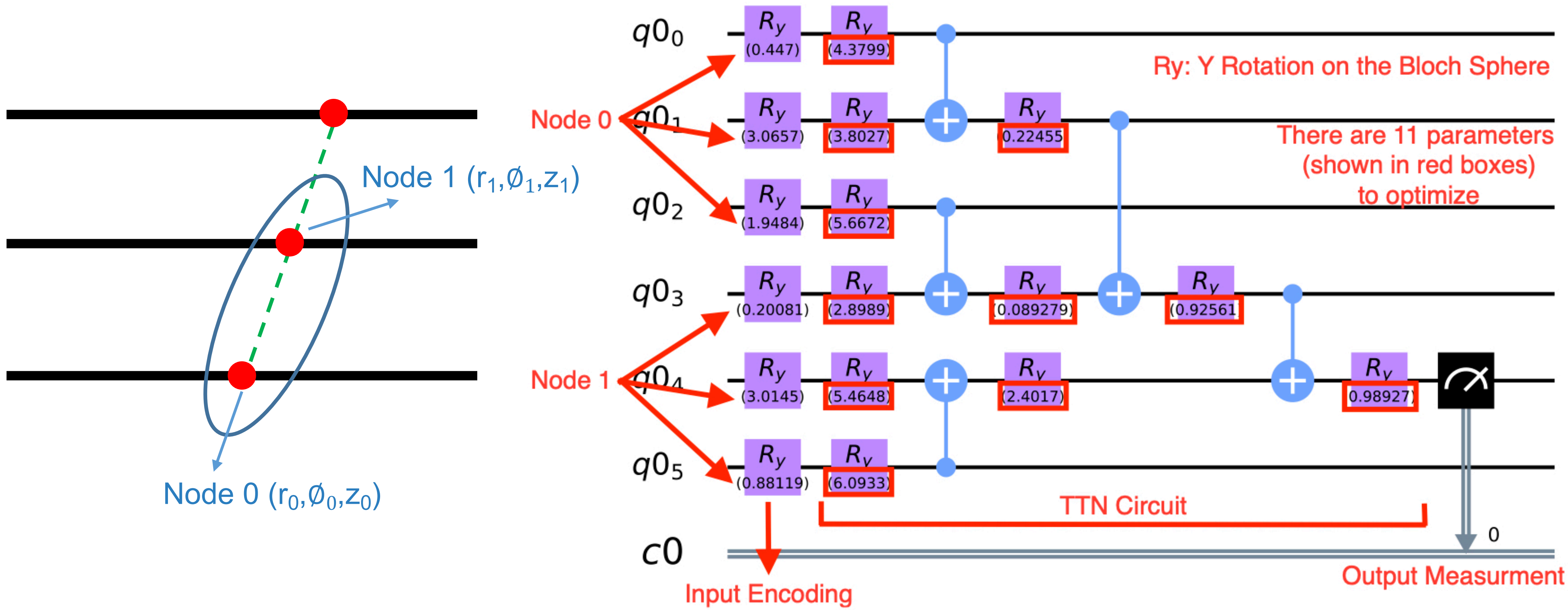
1/16 of an event





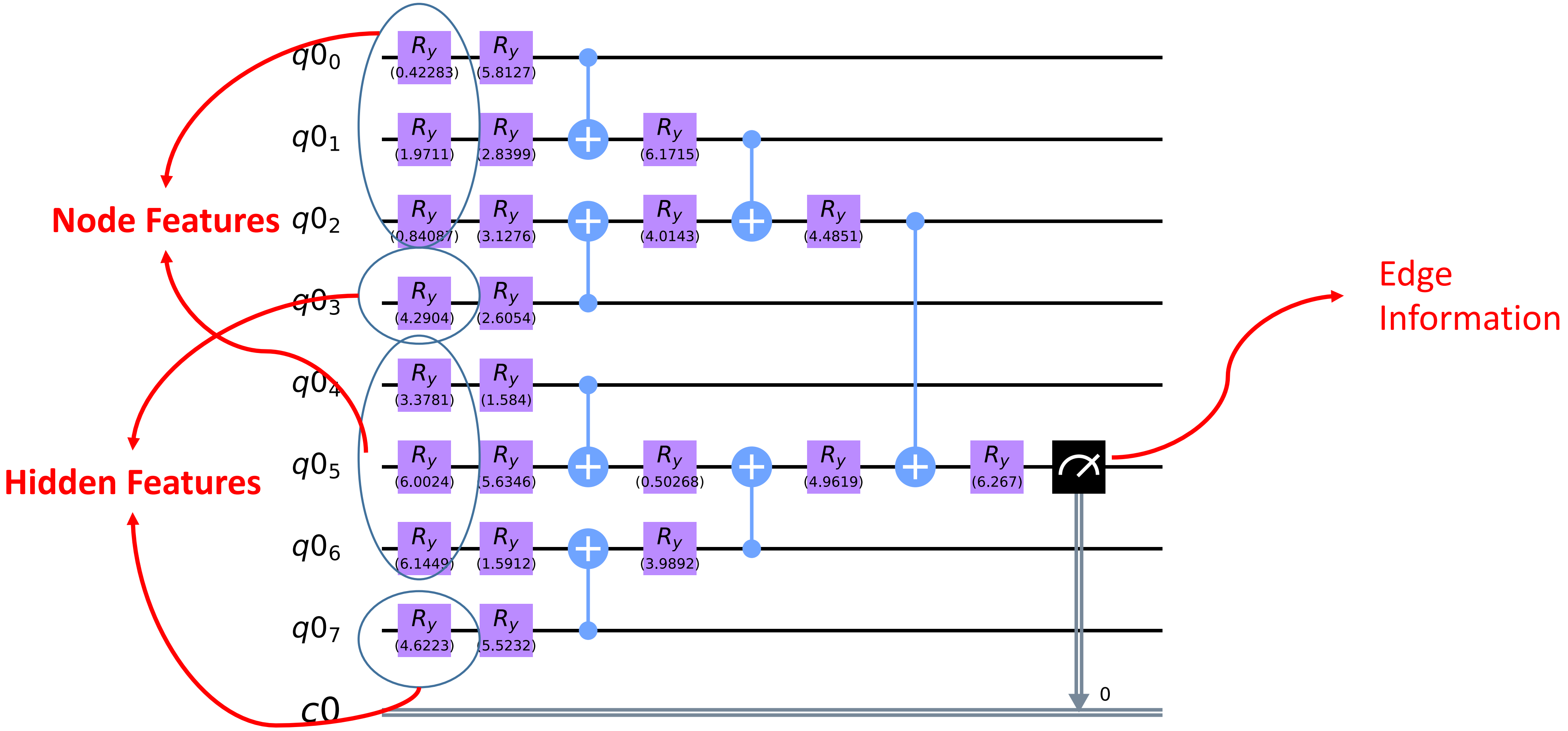
A Quantum Classifier

How does it work?



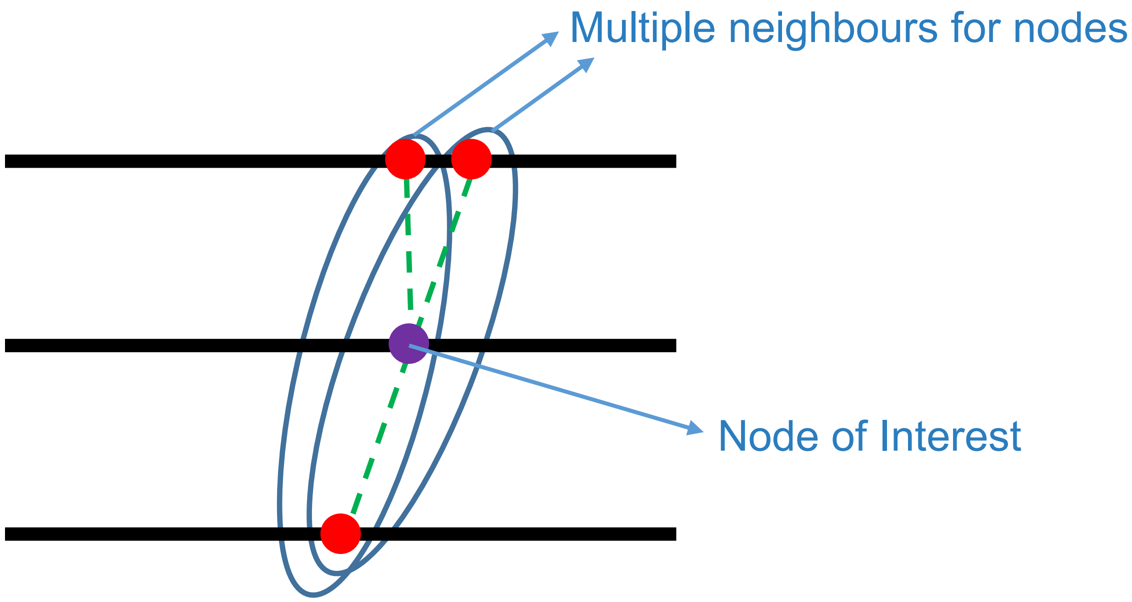
Quantum Networks

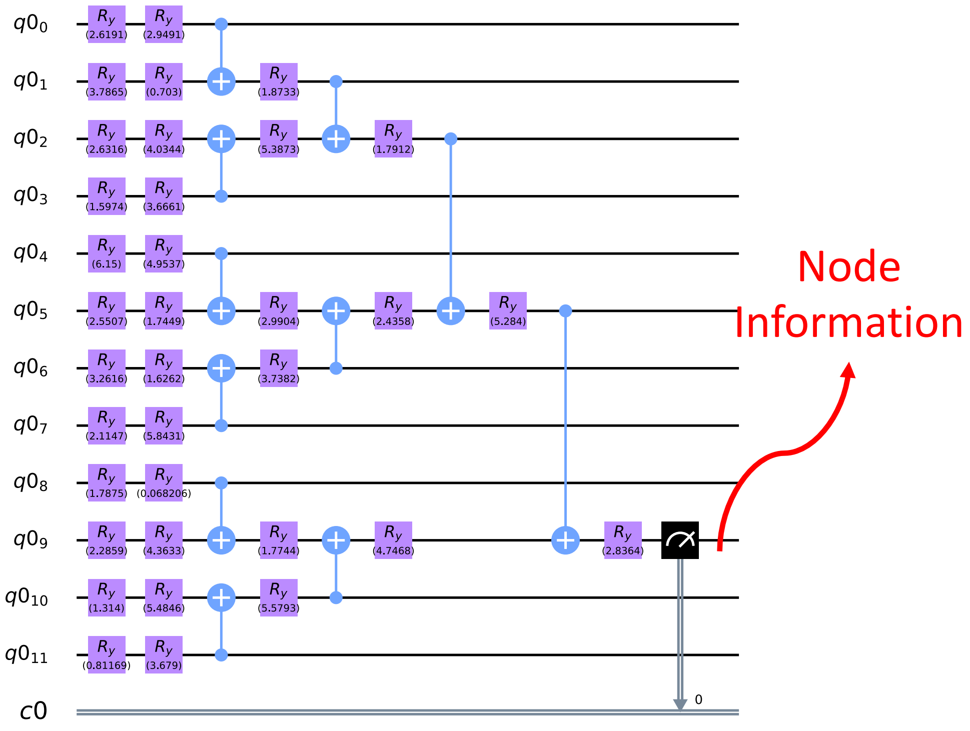
QuantumEdgeNetwork

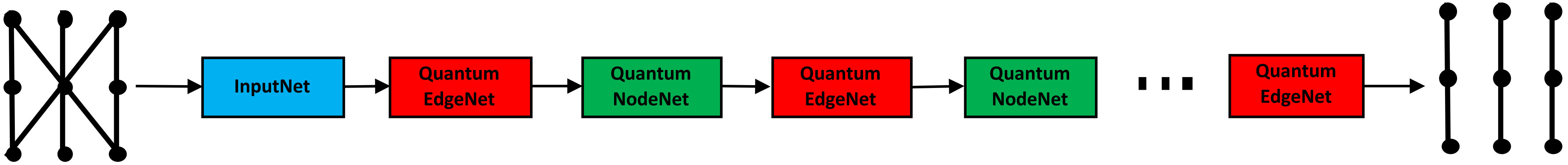


Quantum Networks

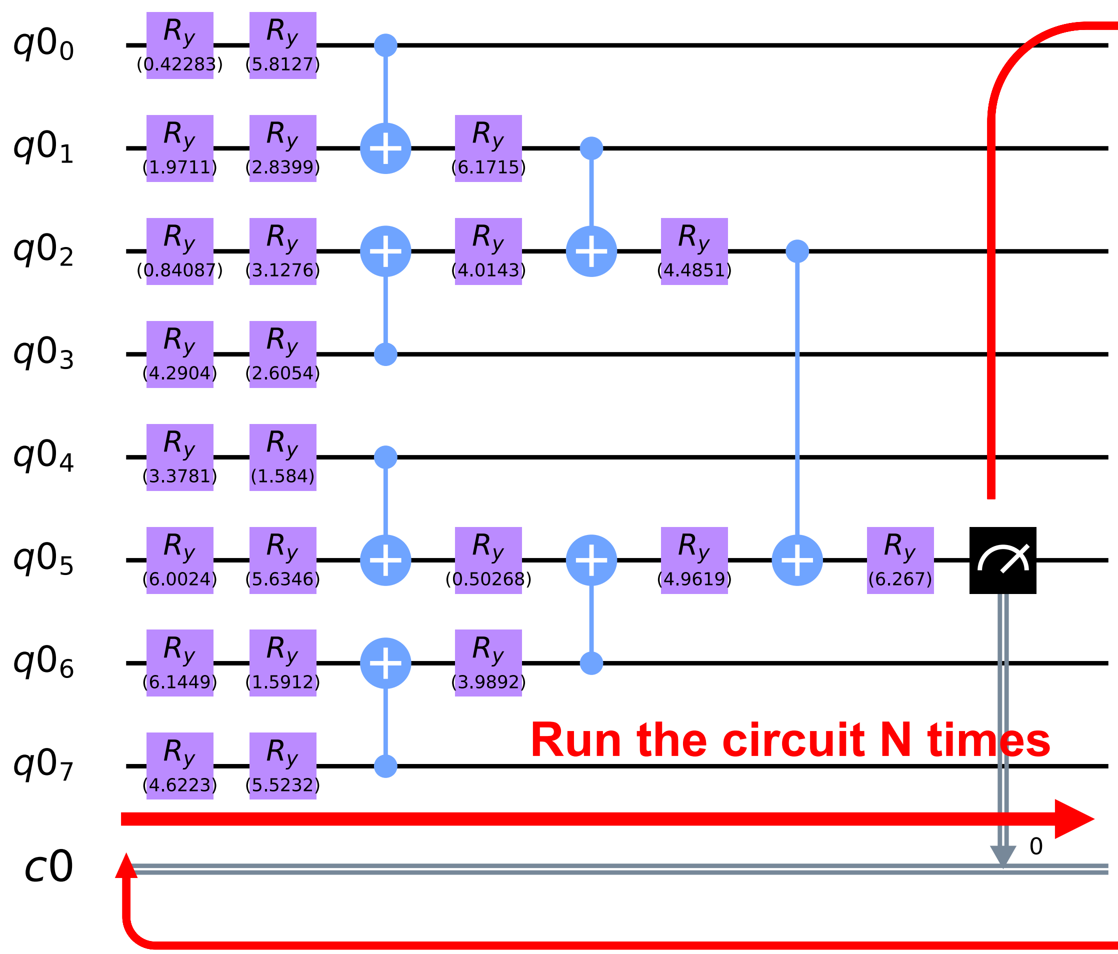
QuantumNodeNetwork







Training the Network



Averaging the measurement outcomes gives a probability of being an edge.

Calculate an error from the ground truth data.

Calculate the gradients of the parameters.

Update the parameters:

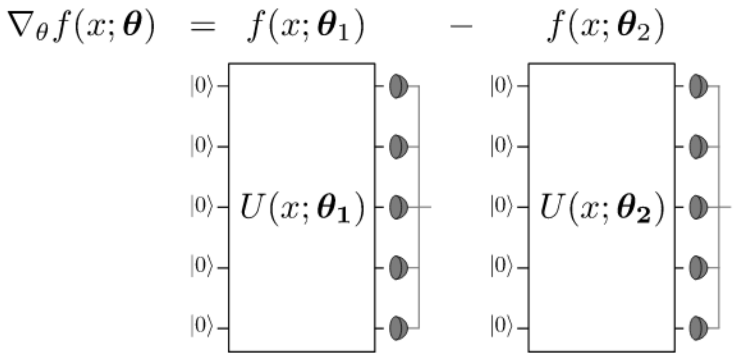
$$\boldsymbol{\theta} = \boldsymbol{\theta} - \eta \, \nabla_{\theta} \mathcal{J}(\theta)$$

Repeat!

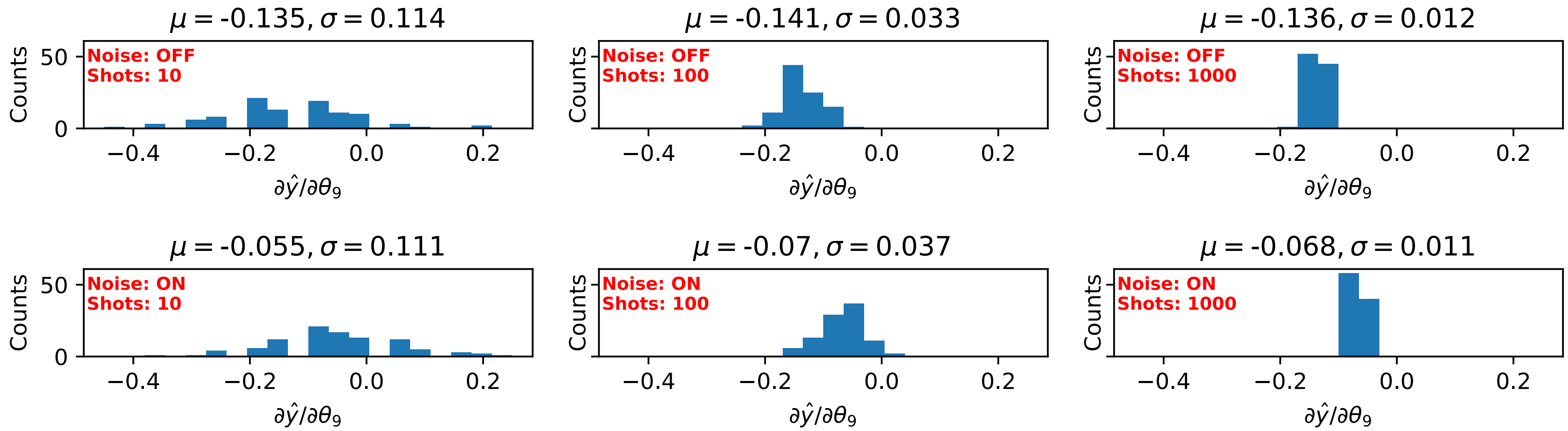
Taking Gradients of a Q. Circuit

Gradient taking operation can be composed as 2 Quantum Circuits.

Pennylane is a software that supports automatic differentiation of quantum circuits.

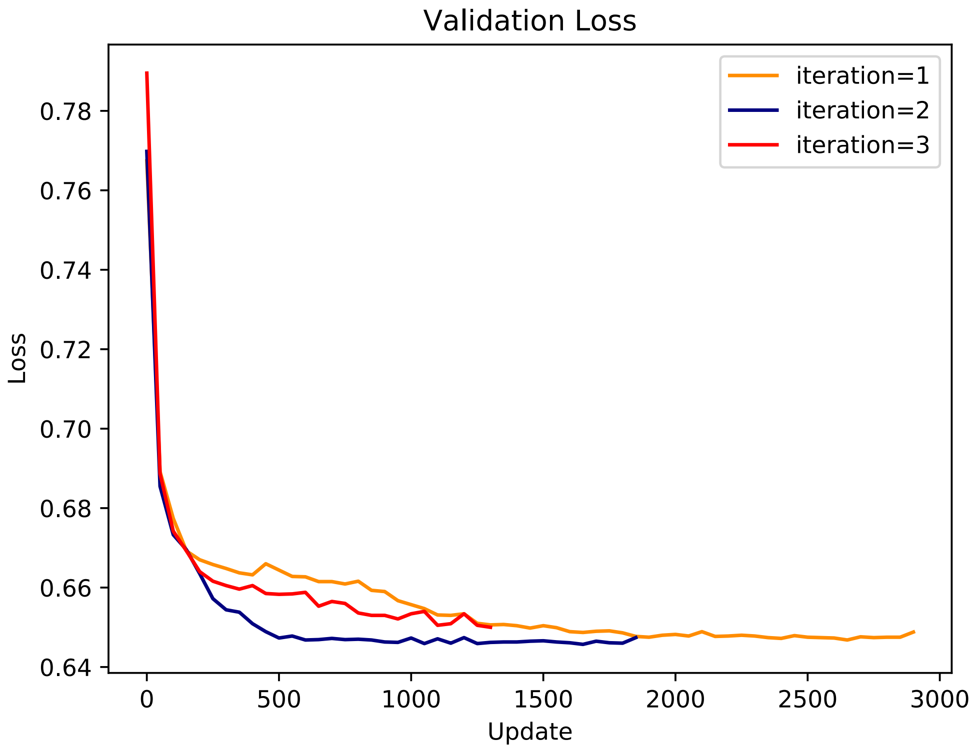


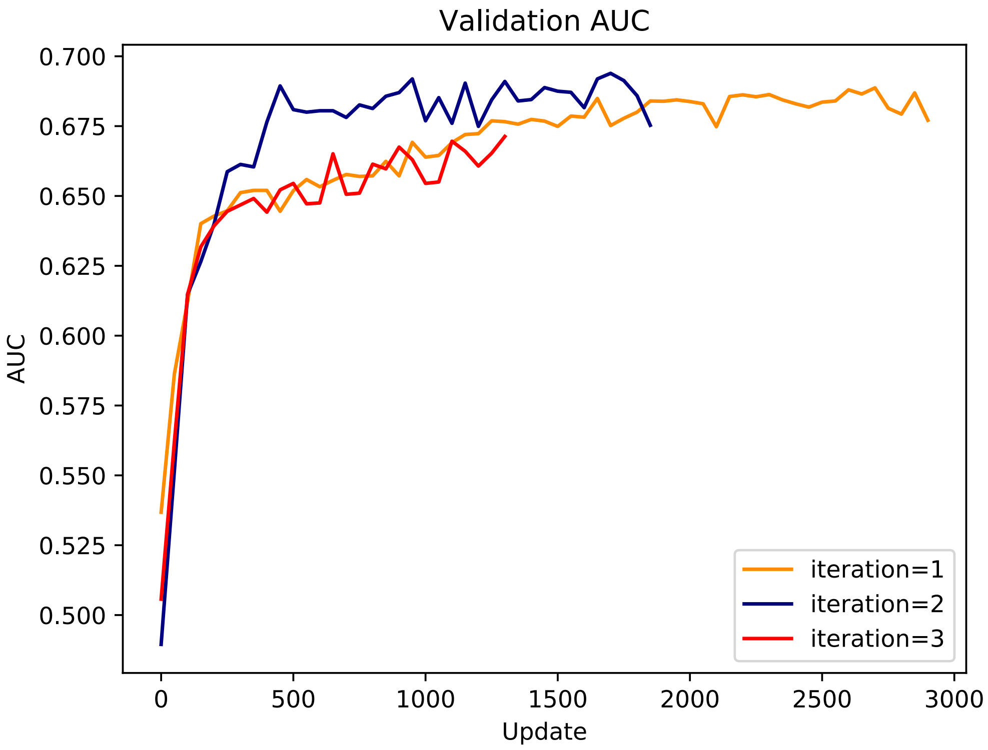
https://pennylane.ai/



Noisy simulations are promising!

Training Results of the QGNN





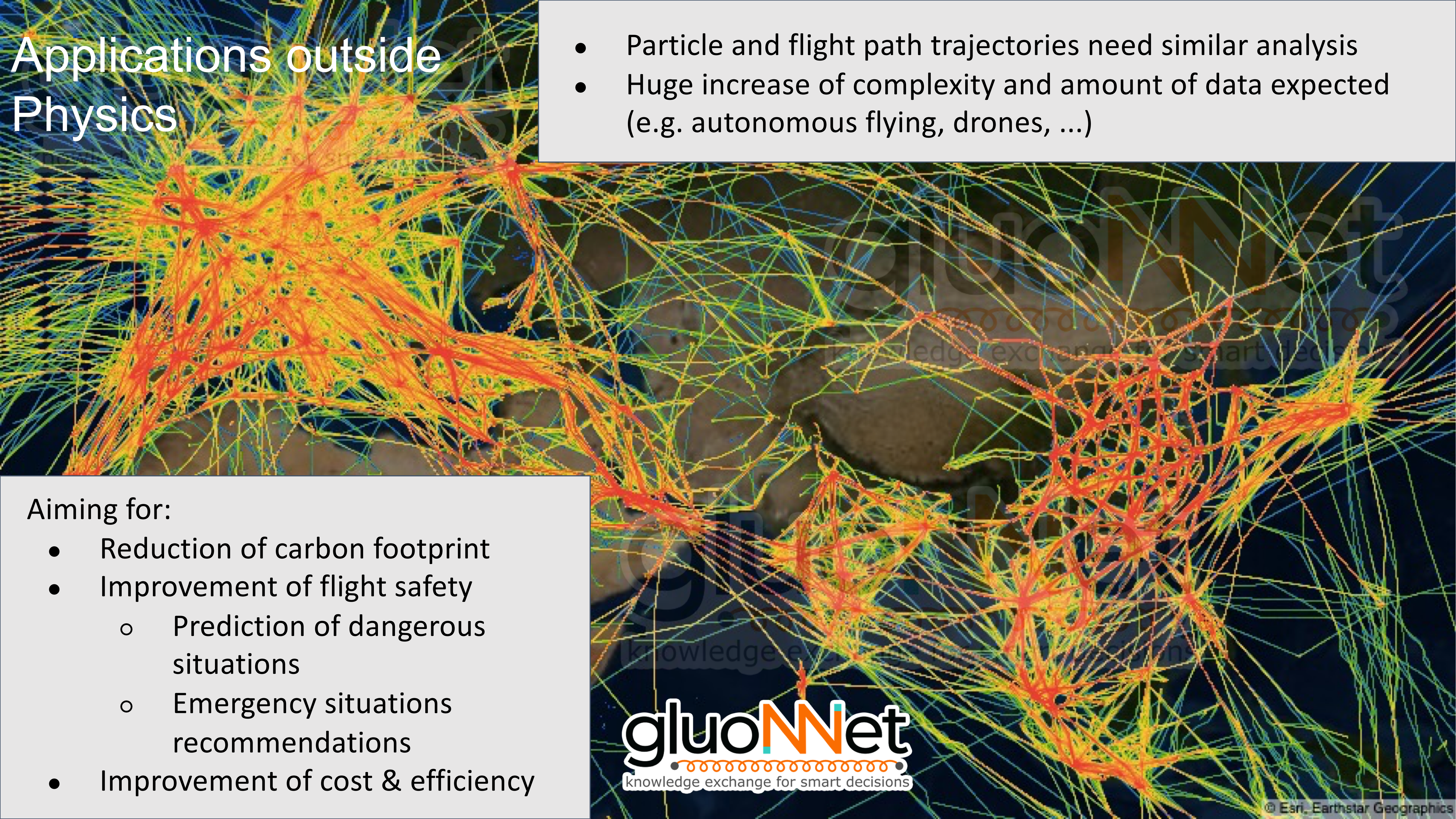
Training set: 1450 subgraphs, Validation set: 150 subgraphs,
using ADAM, binary cross entropy, lr = 0.01, shots =1000

Applications outside Physics

- Particle and flight path trajectories need similar analysis
- Huge increase of complexity and amount of data expected (e.g. autonomous flying, drones, ...)

Aiming for:

- Reduction of carbon footprint
- Improvement of flight safety
  - Prediction of dangerous situations
  - Emergency situations recommendations
- Improvement of cost & efficiency



gluoNNet
knowledge exchange for smart decisions

Conclusion

First results are promising. With this approach we are optimistic to get better results.

There are things to explore;

- More layers(iterations)
- More hidden features(qubits)
- Different Quantum Networks/Architectures

Contributors

C. Tüysüz[1], F. Carminati[2], B. Demirköz[1], D. Dobos[3], F. Fracas[2], K. Novotny,[3] K. Potamianos[3,4], S. Vallecorsa[2], J.R. Vlimant[5]

[1]Middle East Technical University, Ankara, Turkey, [2]CERN, Geneva, Switzerland, [3]gluoNNet, Geneva, Switzerland, [4]DESY, Hamburg, Germany, [5]California Institute of Technology, Pasadena, California, USA

Special thanks to:
Oral Okan, Egemen Sert from STB

QUESTIONS?

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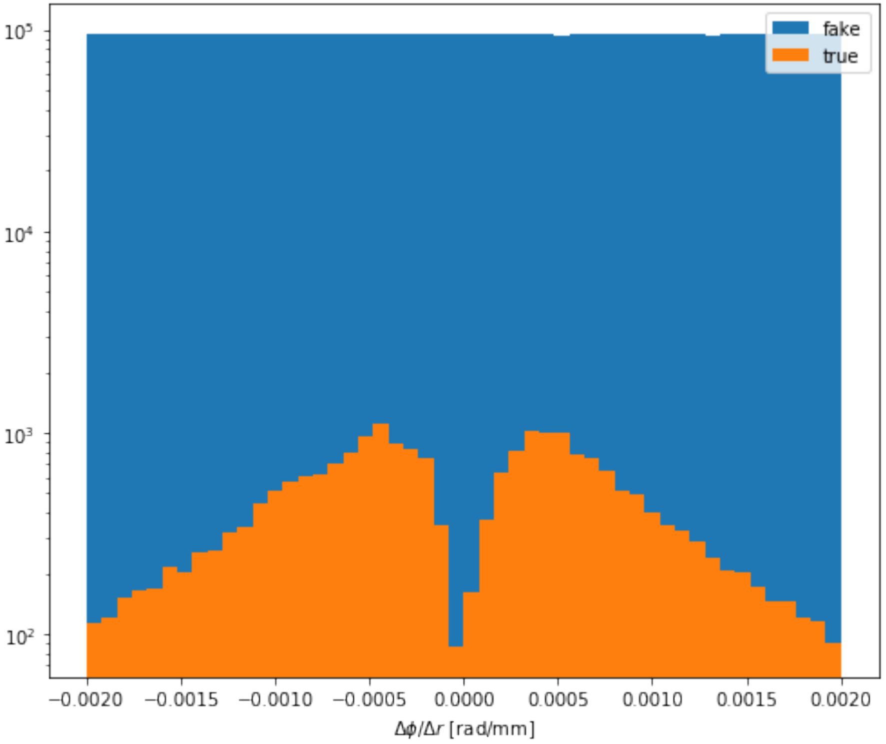
github.com/cnktysz/heptrkx-quantum

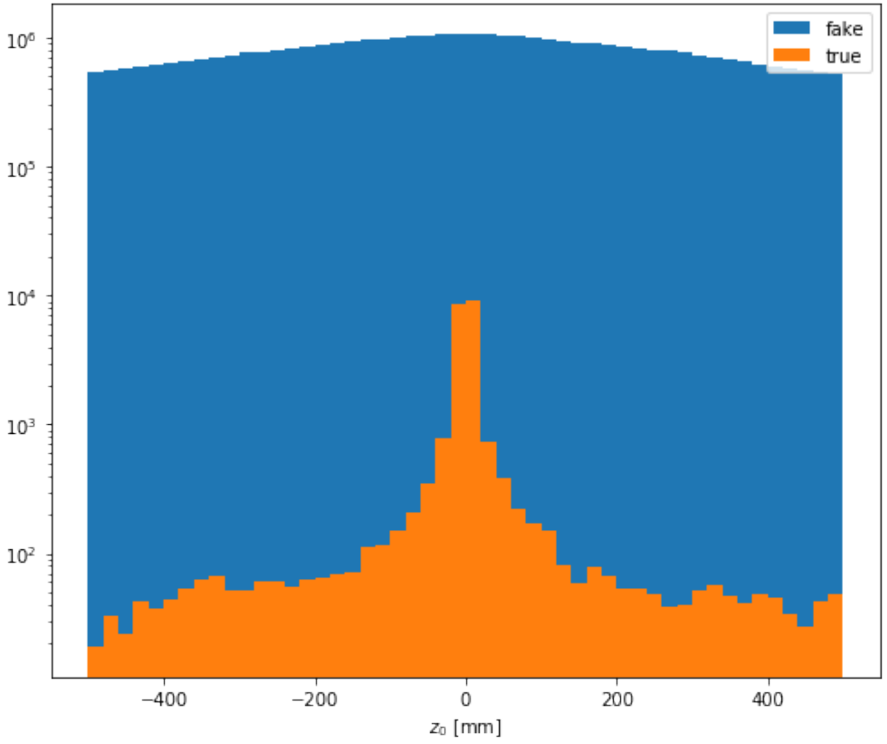
Backup Slides

Preprocessing

Following cuts are applied to the TrackML data:

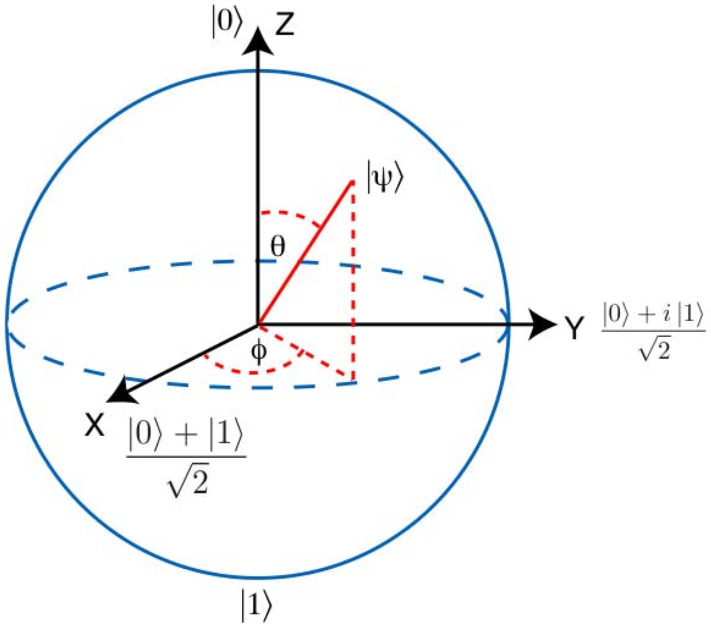
- P_t > 1.0 GeV
- $\Delta\phi/\Delta r < 0.006$
- $z_o <$ 100
- $-5 > \eta > 5$





Plot from: https://github.com/HEPTrkX/heptrkx-gnn-tracking

Quantum Gates



Bloch sphere courtesy of
http://www.laborsciencenetwork.com

Simple Gates :

single parameter, rotation on a plane

$$|0\rangle = \begin{bmatrix}1\\0\end{bmatrix} \rightarrow \text{Apply } R_y(\theta) \rightarrow \begin{bmatrix}\cos(\frac{\theta}{2})\\ \sin(\frac{\theta}{2})\end{bmatrix}$$

General Gates:

multiple parameters, rotation on the whole bloch sphere

$$|0\rangle = \begin{bmatrix}1\\0\end{bmatrix} \rightarrow \text{Apply } U_3(\theta, \emptyset, \lambda) \rightarrow \begin{bmatrix}\cos(\frac{\theta}{2})\\ e^{i\emptyset}\sin(\frac{\theta}{2})\end{bmatrix}$$

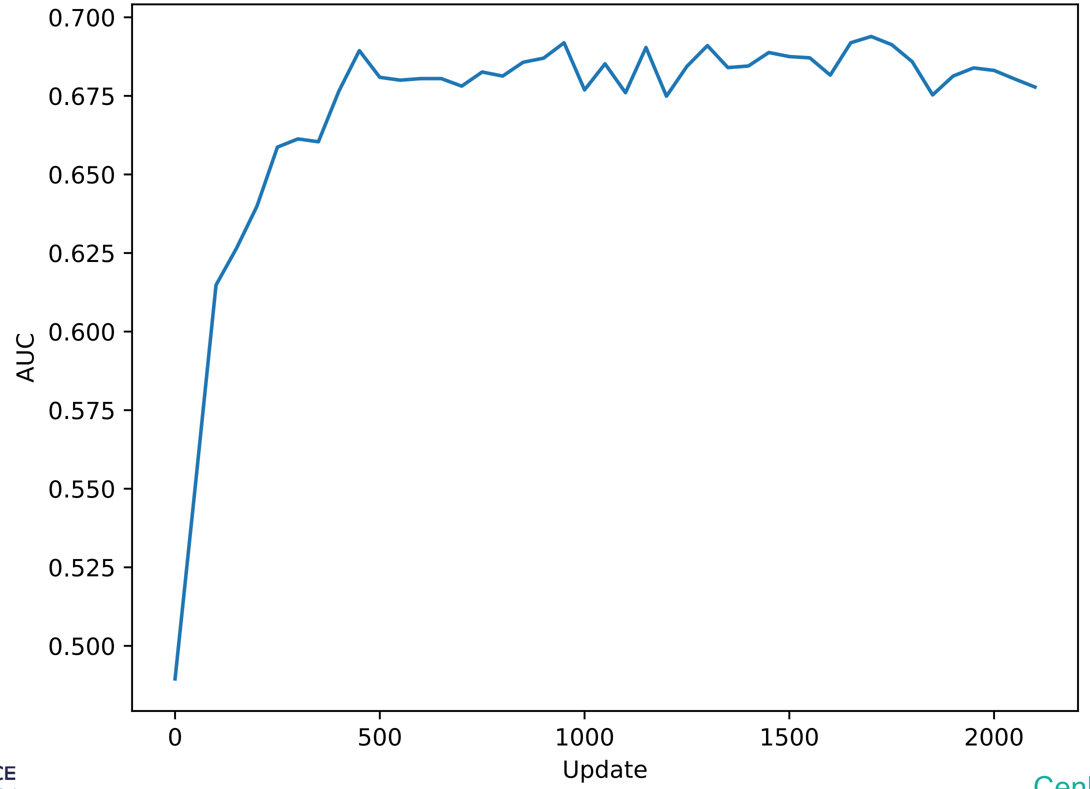
AUC

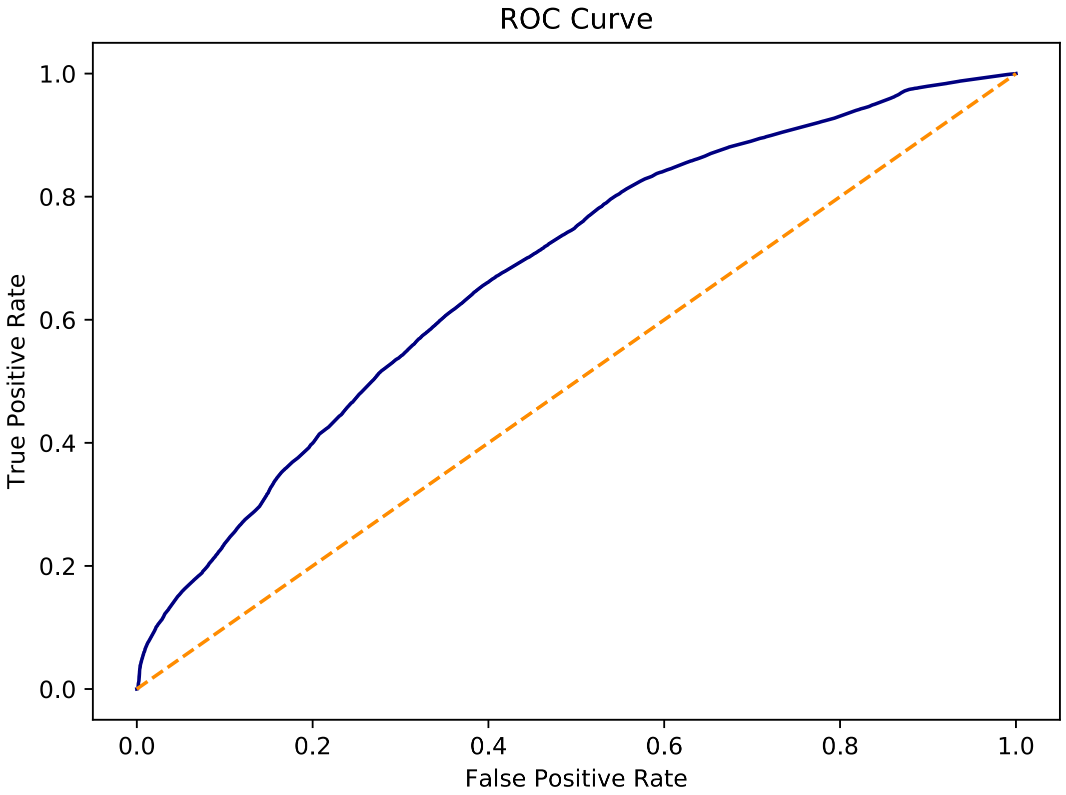
True Positive Rate (**TPR**) is a synonym for recall and is therefore defined as follows:

$$TPR = \frac{TP}{TP + FN}$$

False Positive Rate (**FPR**) is defined as follows:

$$FPR = \frac{FP}{FP + TN}$$





AUC cont'd

True Positive (TP):	False Positive (FP):
• Reality: A wolf threatened. • Shepherd said: "Wolf." • Outcome: Shepherd is a hero.	• Reality: No wolf threatened. • Shepherd said: "Wolf." • Outcome: Villagers are angry at shepherd for waking them up.
False Negative (FN):	**True Negative (TN):**
• Reality: A wolf threatened. • Shepherd said: "No wolf." • Outcome: The wolf ate all the sheep.	• Reality: No wolf threatened. • Shepherd said: "No wolf." • Outcome: Everyone is fine.