Application of quantum computing techniques in particle tracking at LHC

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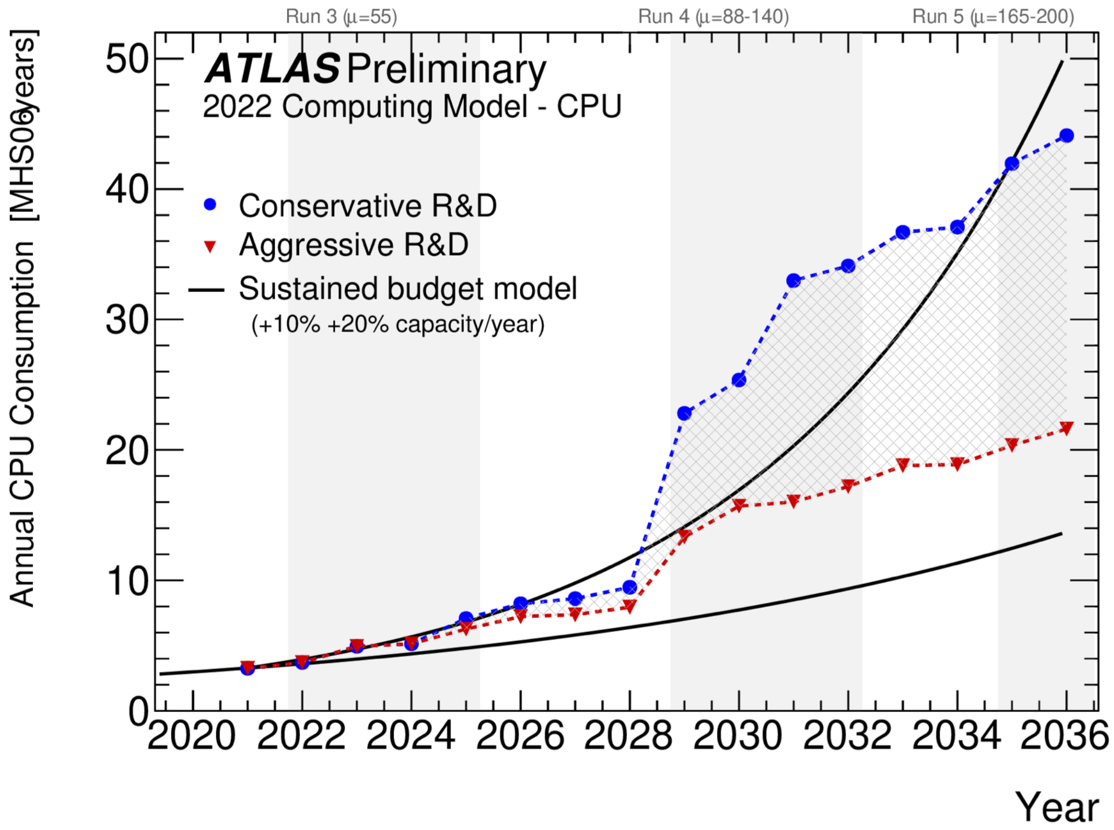
Motivation

- HL-LHC is coming (~2027).
- With larger pile-up ($\langle\mu\rangle \sim 200$) and high readout rate, CPU consumption will dramatically increase.
  - Especially track reconstruction -> New techniques are needed



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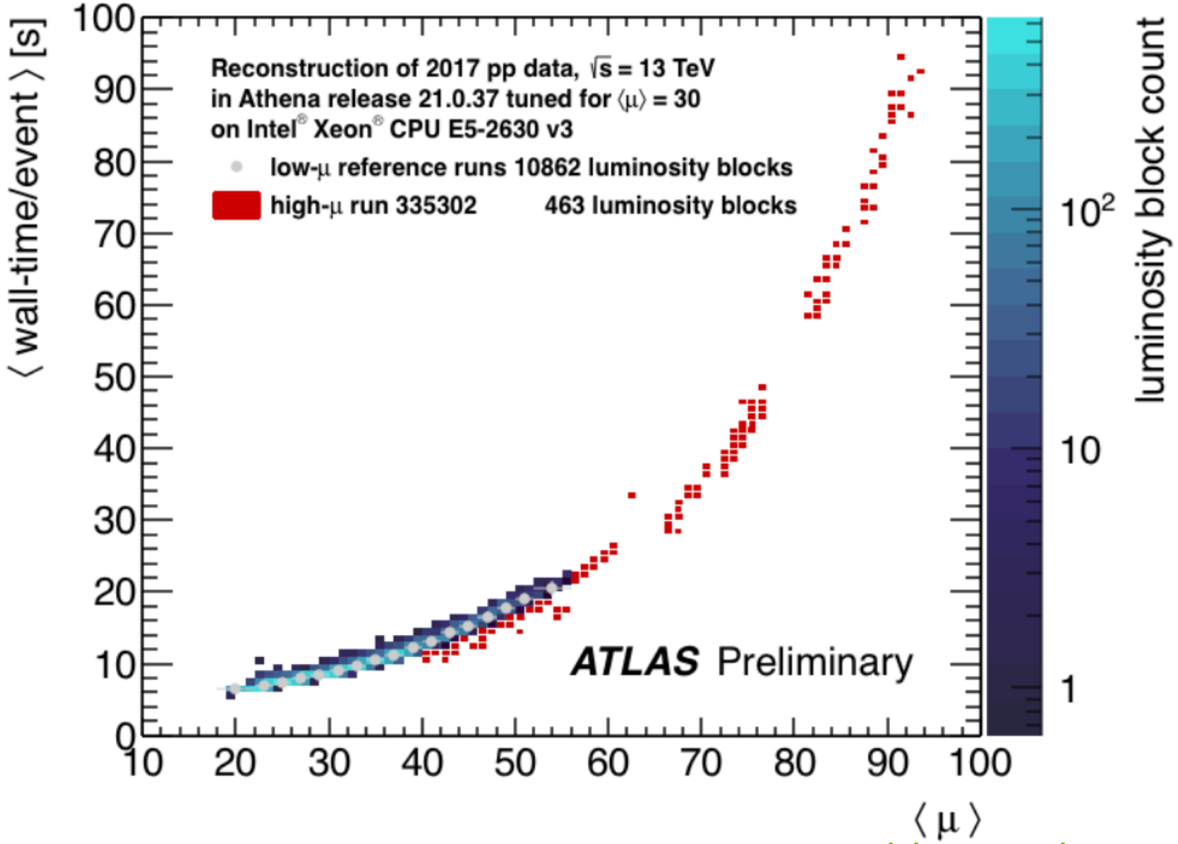
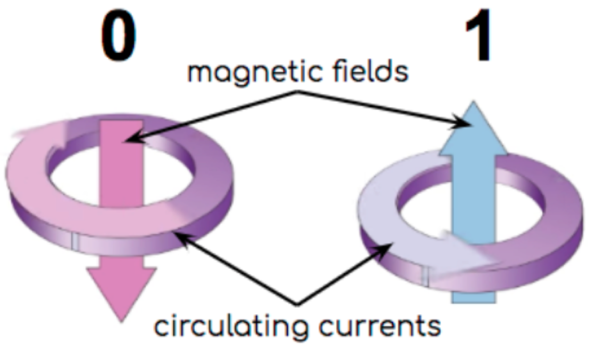


ATLAS Computing Public Result

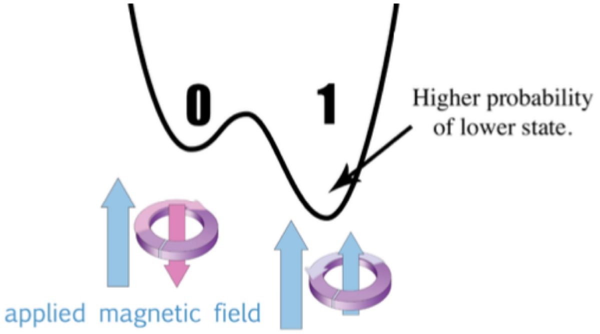
Introduction: Quantum Annealing

- Quantum Annealing:
  An optimisation process for finding the global minimum of a given function by using quantum fluctuations.

- Quantum Annealer: The machine which is designed to perform the quantum annealing process.
  e.g. D-Wave computers

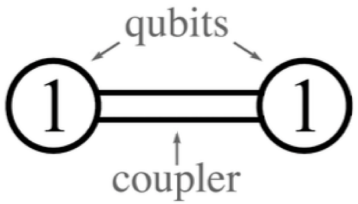


qubits $\Rightarrow q_i$



bias weights $\Rightarrow a_i$

degree to which a qubit tends to a particular state



coupling strength $\Rightarrow b_{ij}$

degree to which two qubits tend to the same state

$$O(a;b;q) = \sum_{i=1}^{N} a_i q_i + \sum_{i}^{N}\sum_{j}^{N} b_{ij} q_i q_j \quad q_i \in \{0,1\}$$

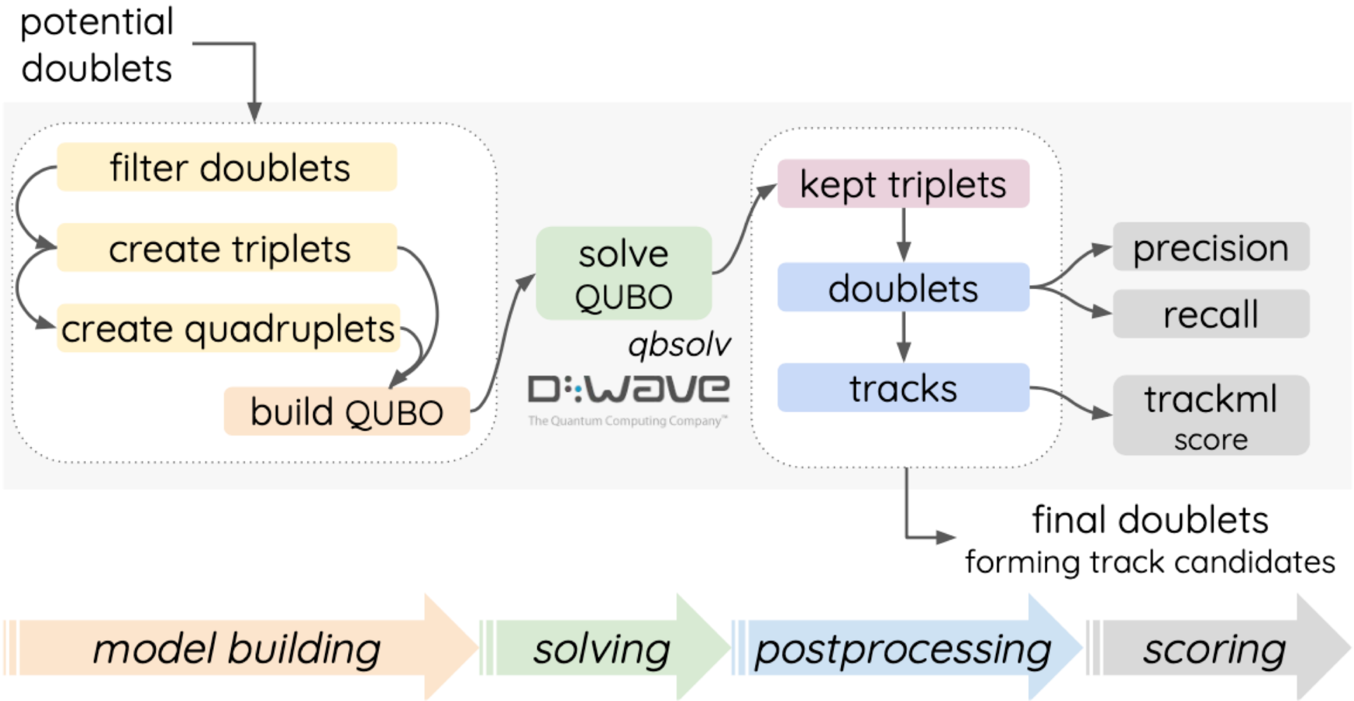
QUBO

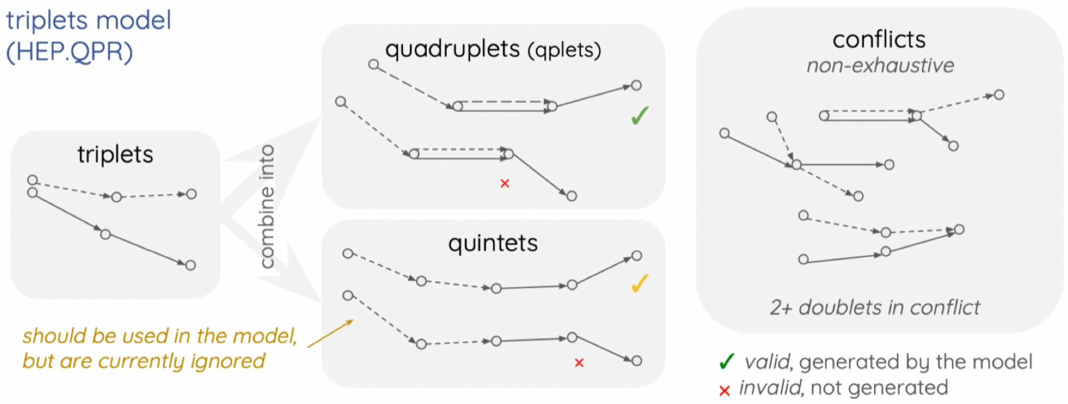
Quadratic
Unconstrained
Binary
Optimisation

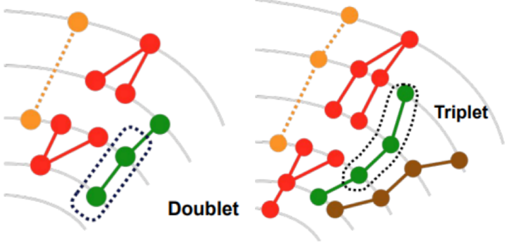
- Quantum Annealer can only deal with the problem which can be transform to a ”QUBO” or “Ising” function.

Quantum Pattern Recognition: Algorithm Overview

- We found the Quantum Annealing could improve the speed of pattern recognition and provide another way to perform the particle tracking. Result published on: arXiv: 1902.08324







$$O(a,b,T) = \sum_{i}^{N} a_i T_i + \sum_{i}^{N} \sum_{j<i}^{N} b_{ij} T_i T_j$$

- T_i : potential triplet
- a_i : Bias weight which has been set to 0.
- b_i : The coupling strength, depending on the relation between T_i & T_j

GNN application in Quantum Pattern Recognition

Data preparation (I)

- Motivation: Replace QUBO formation by ML techniques.
- Graph neural network (GNN) is a suitable choice to deal with it.

$$O(a,b,T) = \sum_{i}^{N} a_i T_i + \sum_{i}^{N} \sum_{j<i}^{N} b_{ij} T_i T_j$$

In single event:

- $T_i T_j$ from the QA solved QUBO (Hit ID)
- "Raw input" from TrackML challenge datasets: (HitID, x,y,z, detector layers etc.)

→

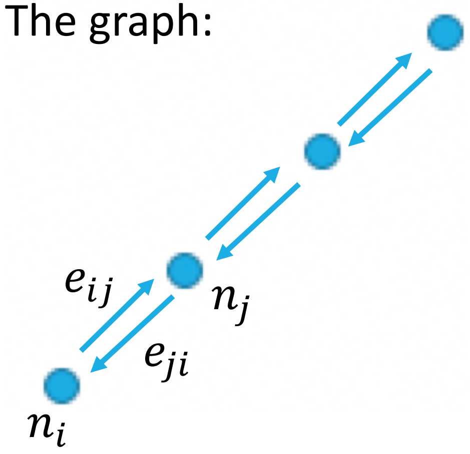
For each $T_i T_j$:

- Doublet list (3 pair of HitID) → GNN Target
- Hit list (HitID, x,y,z, detector layers etc.) → Trainable parameters

In 1 GNN sample:

- GNN Target
- Trainable parameters

The graph:

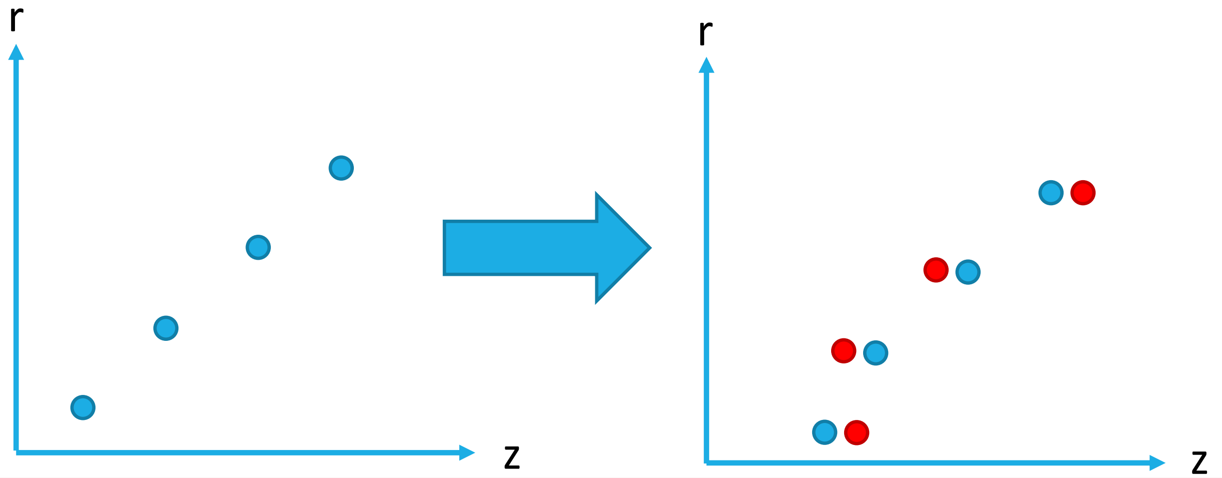


n_i: node i
e_{ij}: edge for n_i to n_j

- The parameter "Hit ID" parameter is the key for the data extraction.
  - Hits in each Triplet T contained Hit ID.
  - These IDs are used to form the doublet list and the hit list.
    - The GNN Target, is given by matching the Hit ID from the Hit list per $T_i T_j$
    - If the Hit ID from a pair of hits (n_i, n_j) in the is equal to Hit ID in the doublet list: Target (edge score) = 1
    - If it's not, then Target (edge score) = 0
    - We want to train the GNN to predict the correction combination of edge scores.
- We would like to preform a edge classification in order to form the $T_i T_j$ from raw hits.
  - To do that we need to consider all the combinations of edges scores per graph.

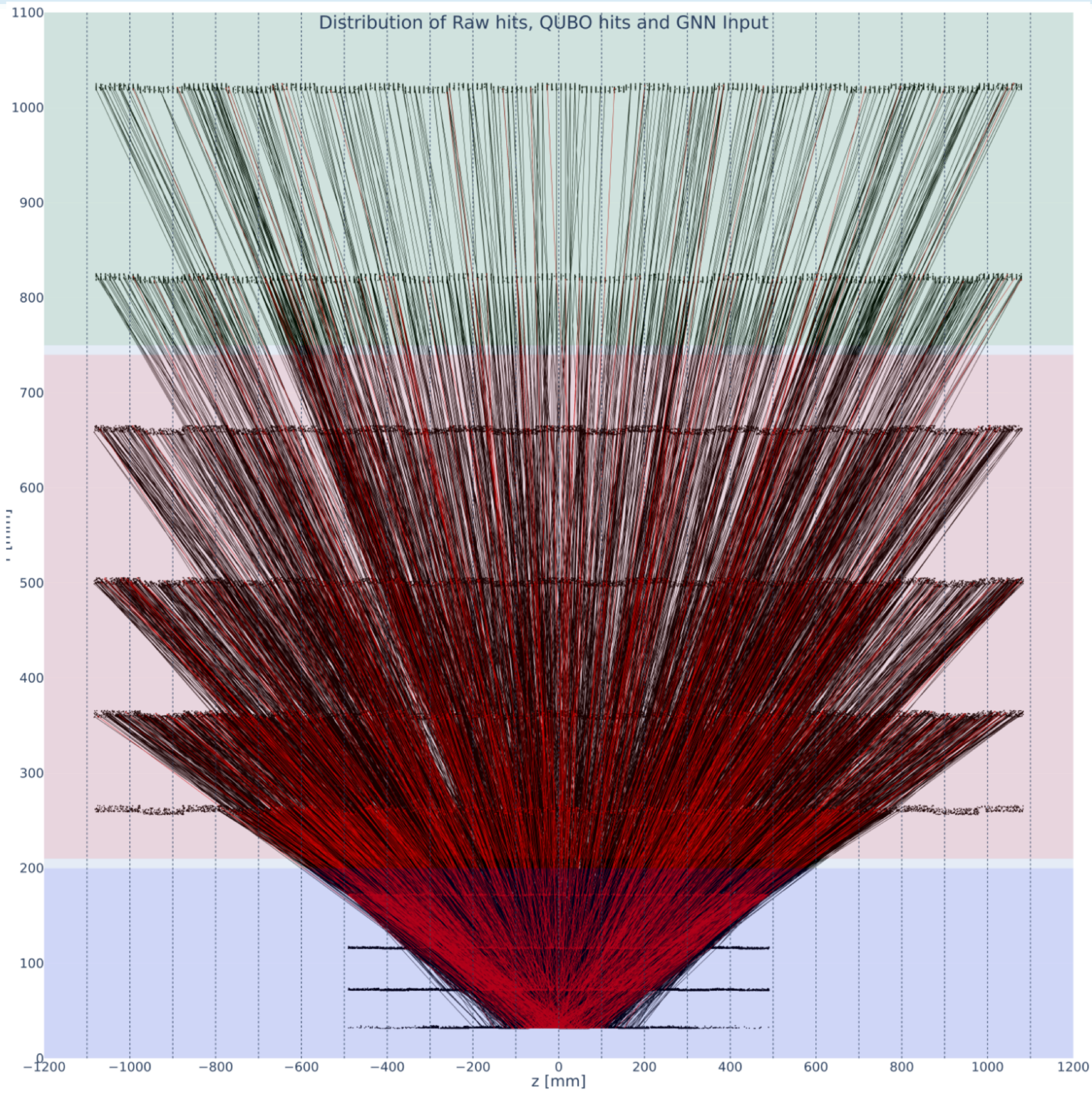
Nearby Hits Searching (II)

- In order to get all the combinations, we need to search for nearby hits which is close to the original hits in the same detector layer (i.e. same r-coordinate).

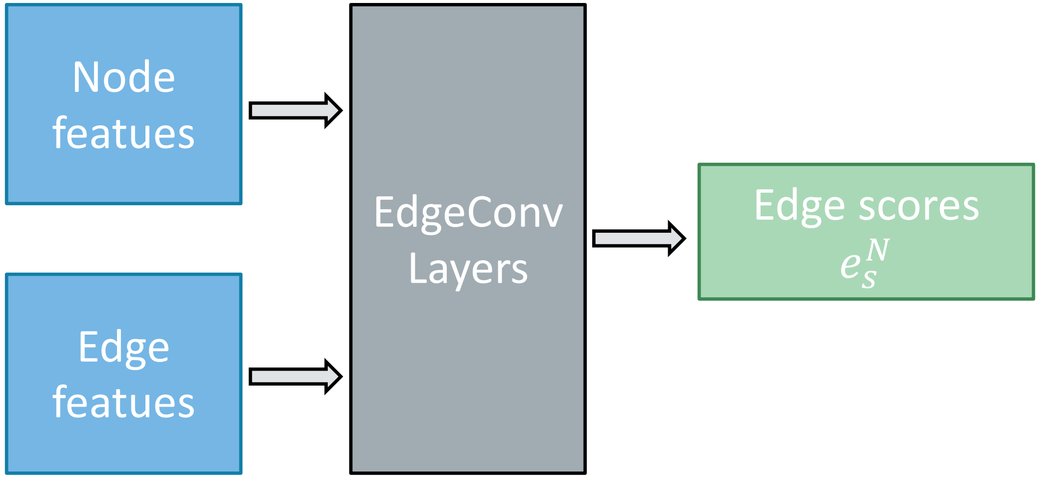


1 Fully connected graph	Signal	1 Fully connected graph
	BKGs	1 Fully disconnected graph 6 partially connected graphs

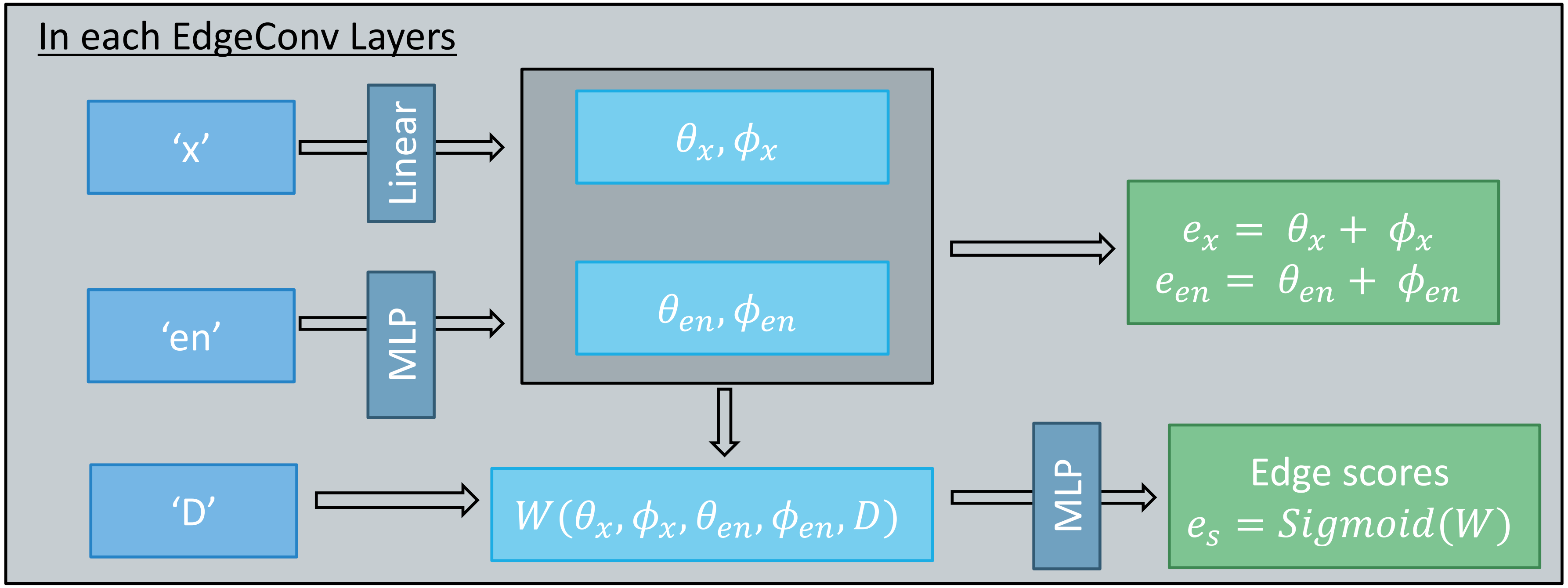
- Our dataset have 269550 samples, only 6% of them are Signal samples.
- 40% are used for training; 40% are used for validation; 20% are used for test.



Network architecture



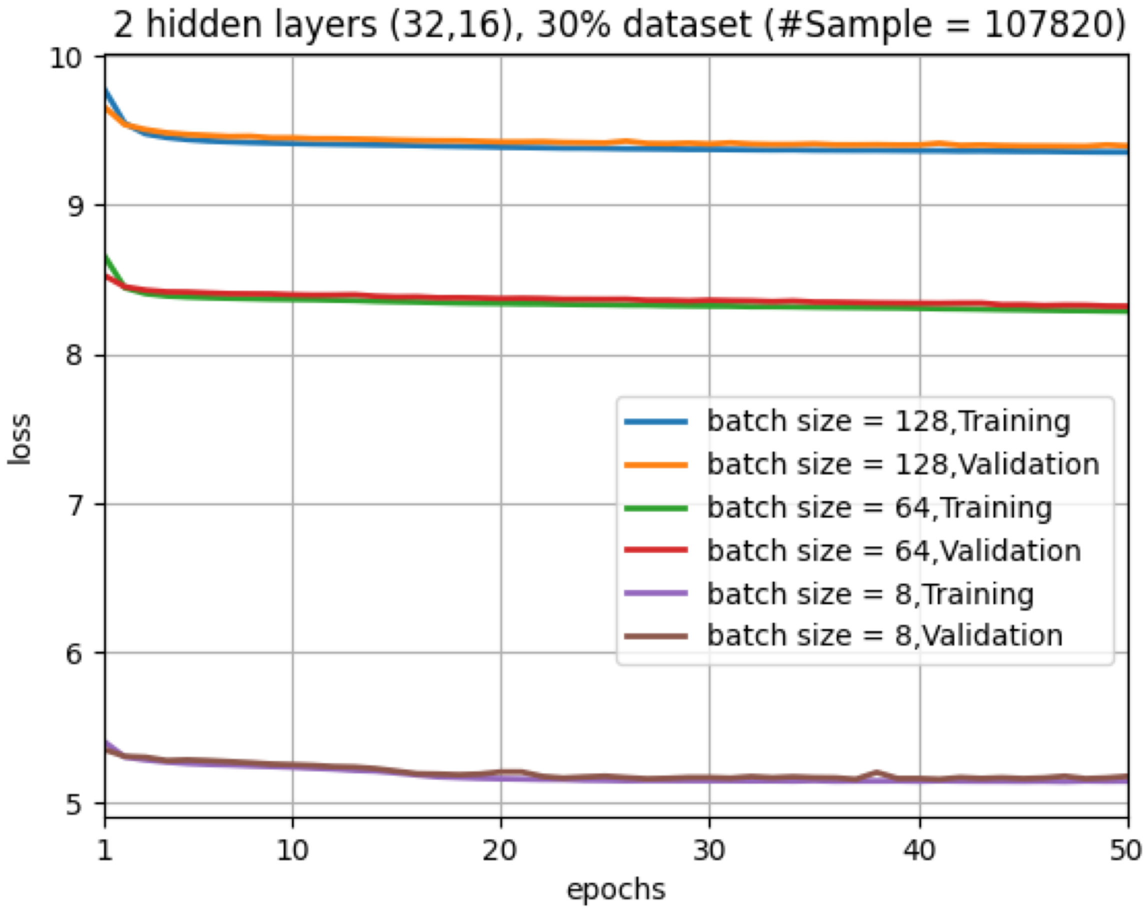
Node features ‘x’	Node features ‘en’	Edge features ‘D’
x	r	Δr
y	Detector layer ID	Δz
z	Detector volume ID	Curturve $atan2(\Delta r, \Delta z)$
	Detector module ID	

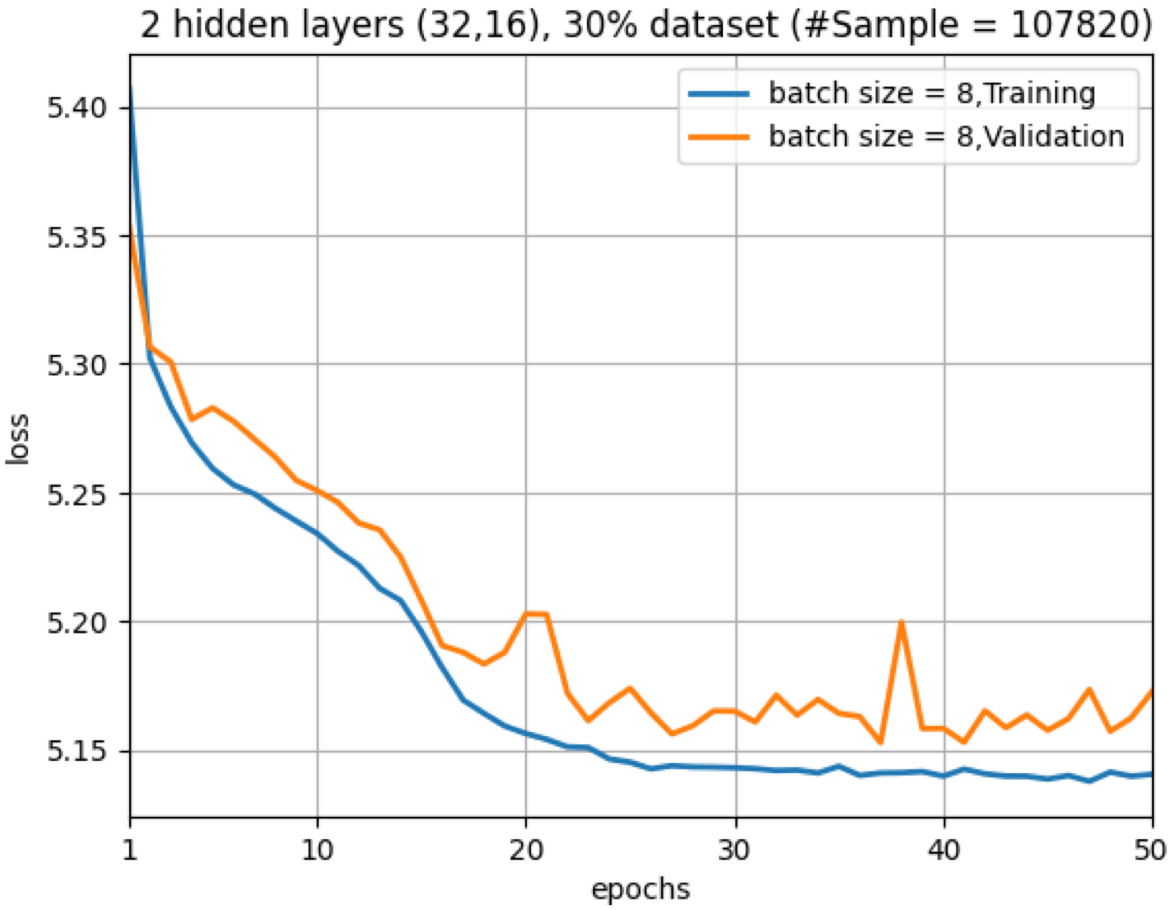


- From each layer, the EdgeConv parameters e_x, e_{en} are passing to the next layer.
- Final output, e_s^N is the edge score coming from the last EdgeConv layer.

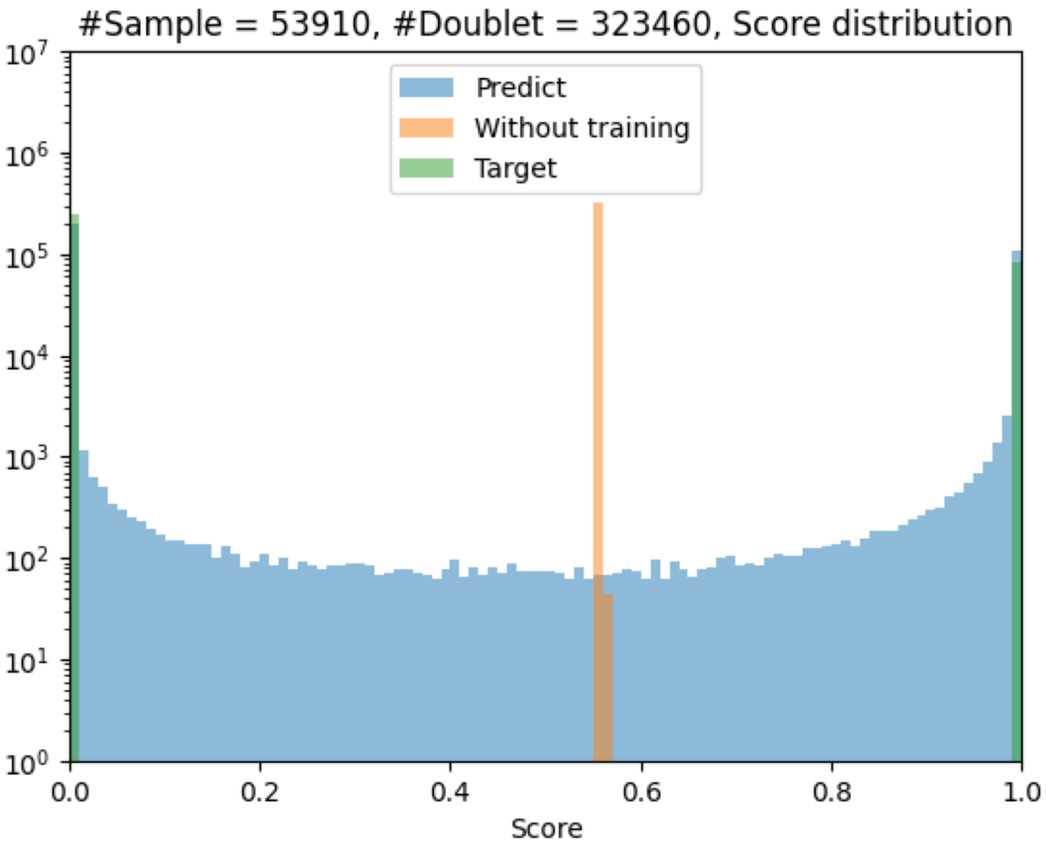
Loss function and score distribution

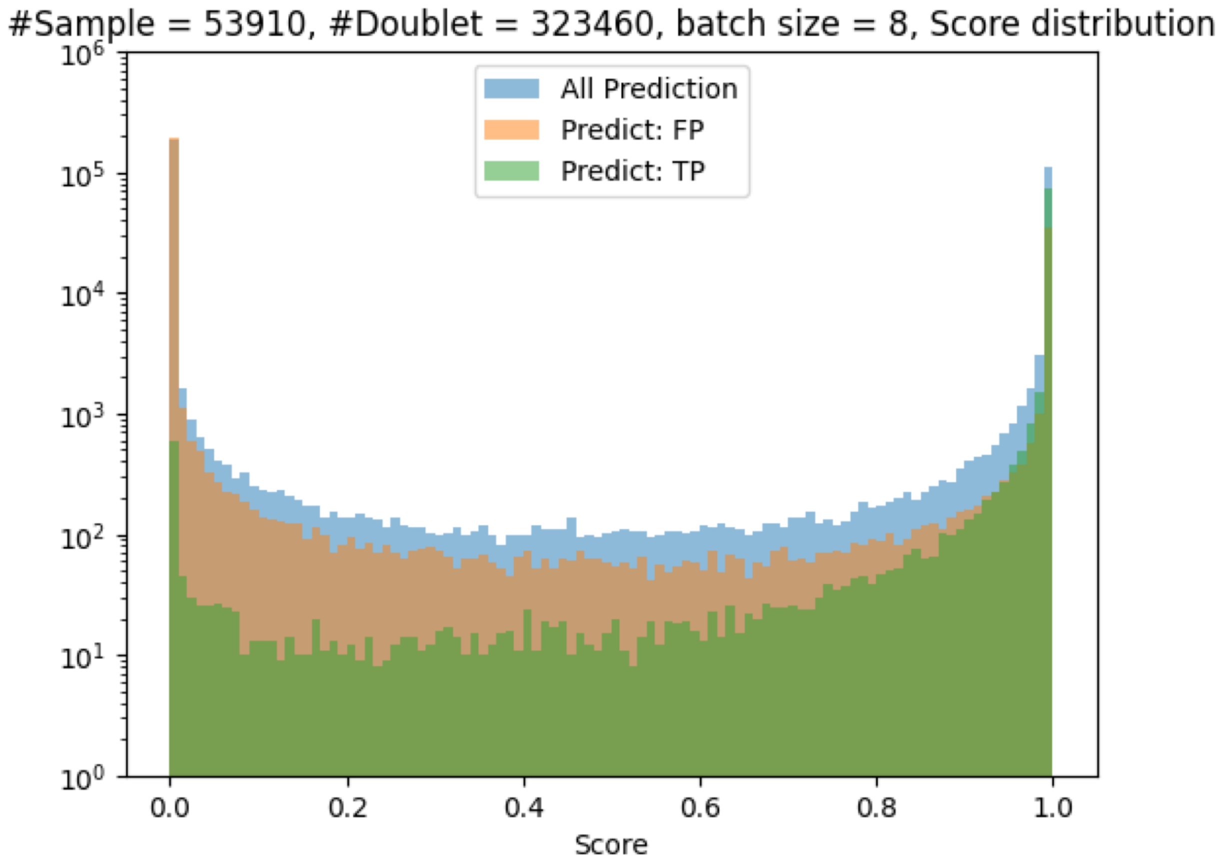
- We use Cross Entropy Loss as our Loss function.
- The impact of batch size is studies and batch size = 8 has been used.
- Underfitting observed.





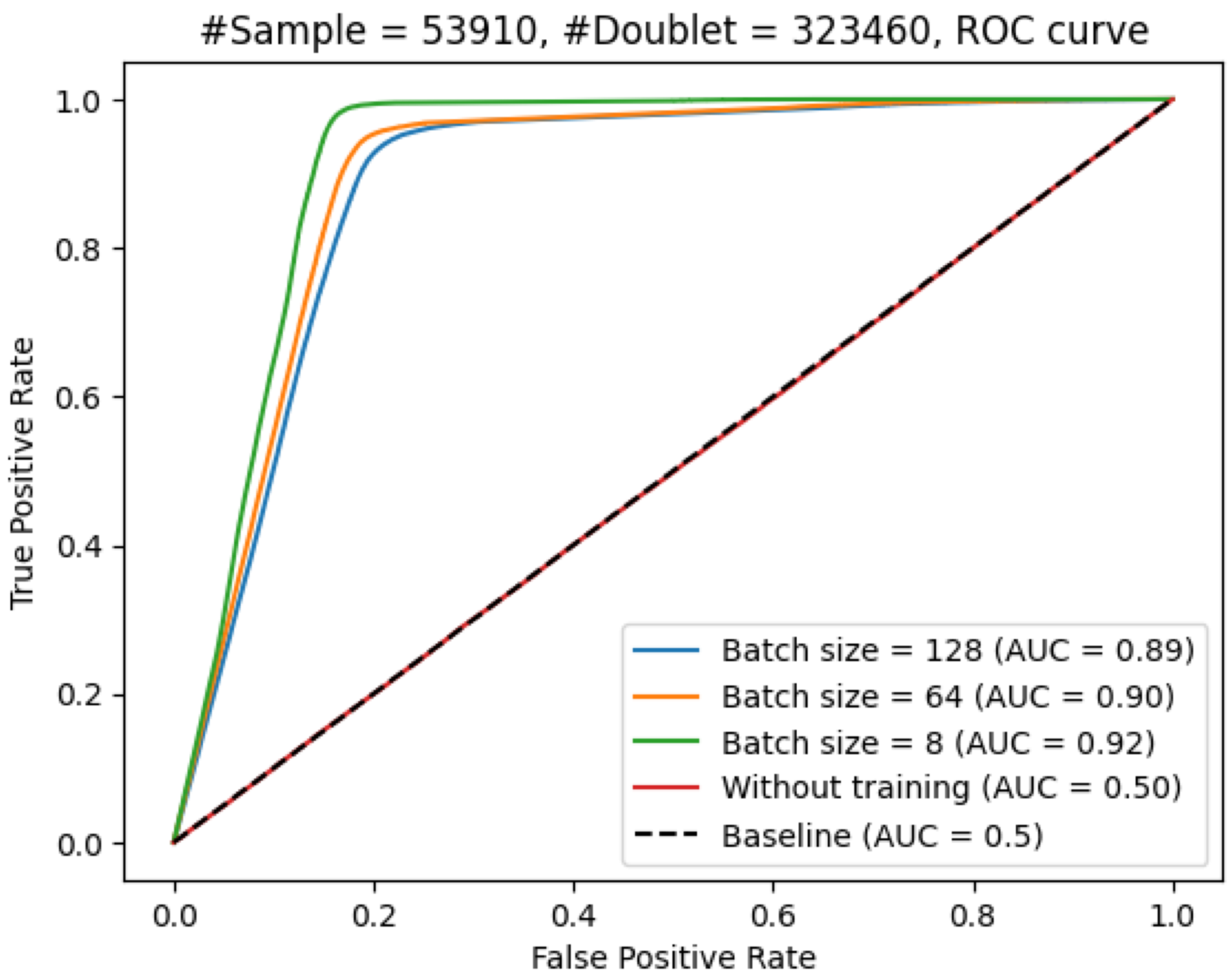
Edge score distributions





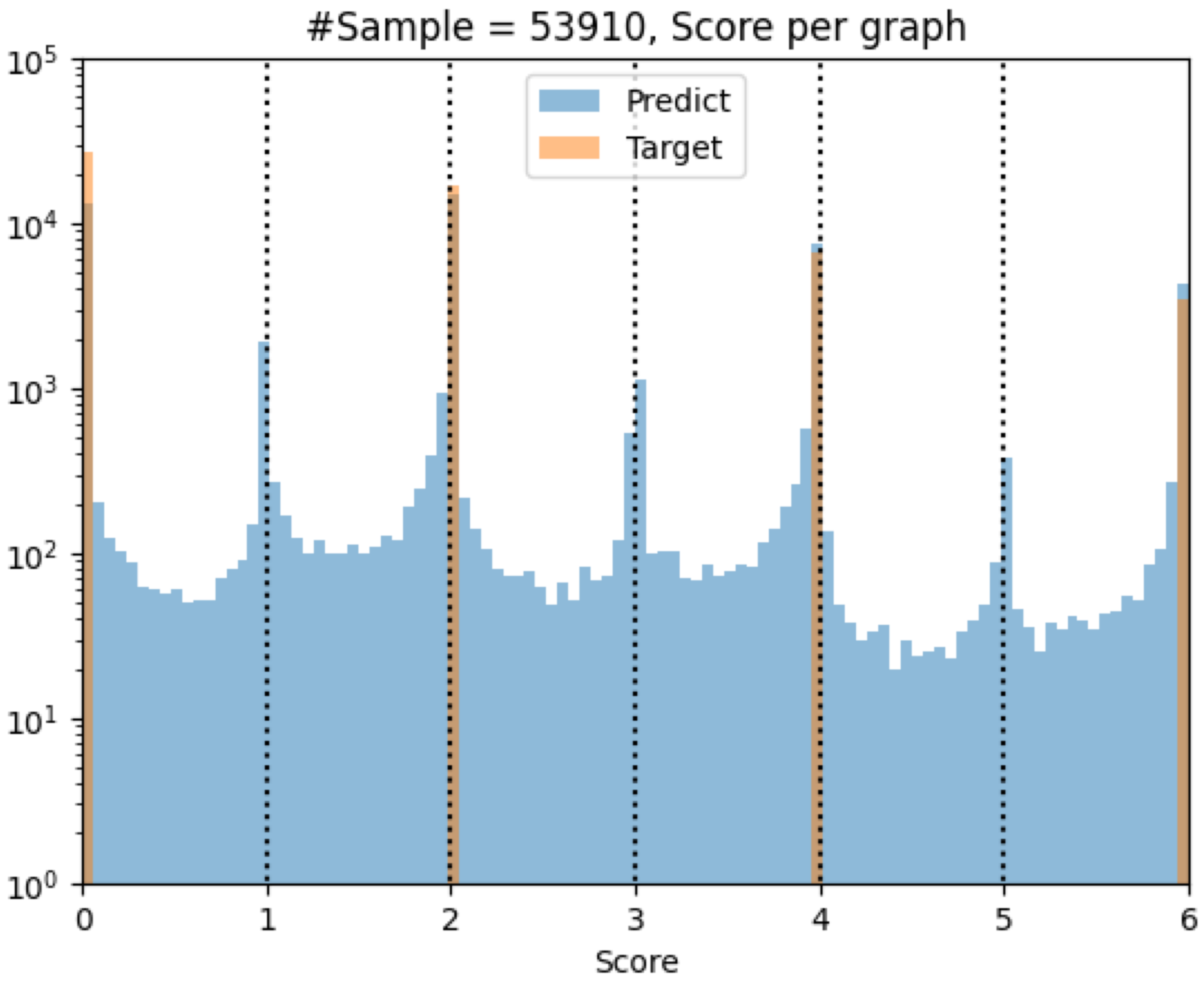
- "Predict: TP" : edges have target edge score = 1
- "Predict: FP" : edges have target edge score = 0

ROC curve



- ROC curves are shown with different batch size.
- Smaller batch size gives higher AUC.
- The best cases here is given by batch size = 8, with AUC = 0.92

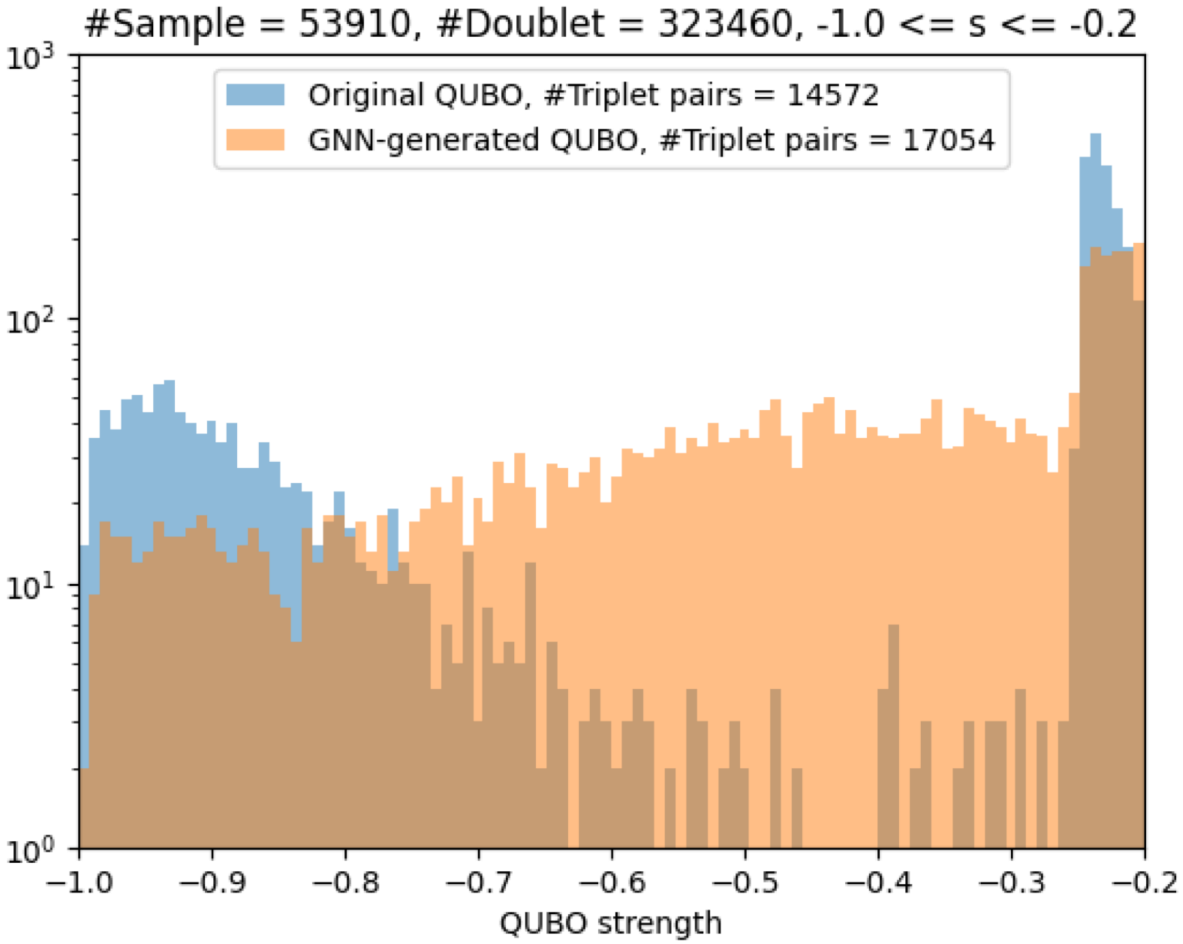
Score distribution per graph



- Sum of edge scores per graph is shown.
- In target, only score = 0,2,4,6 are allowed since $e_{ij} = e_{ji}$ is always true.
- The predicted score, on the other hand, have also score = 1,3,5; this is because in some cases, score of $e_{ij} \neq e_{ji}$. This is possible as we didn't add $e_{ij} = e_{ji}$ as one of the input features of our network.
- However, this is a non-physical result. Since the edges, $e_{ij} = e_{ji}$ have to be always true as this is a physical doublet.

QUBO comparision

$$O(a,b,T) = \sum_{i}^{N} a_i T_i + \sum_{i}^{N}\sum_{j<i}^{N} b_{ij} T_i T_j$$



- Graphs with scores > 3 are selected
- $-1 \leq b_{ij} \leq -0.2$ is given by the pervious study.
- We are expecting similar distribution to the original QUBO.
- More investigation is needed for the distribution for GNN-generated QUBO in -0.85 to -0.25.

Application for the ATLAS dataset

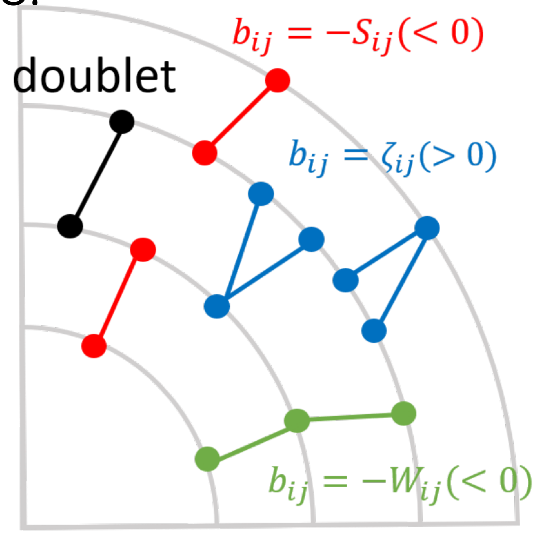
Application for the ATLAS dataset

- We verified if track finding by annealing machines works in a realistic environment with the ATLAS dataset.
- Detector-hit information is taken from the dataset processed by the ATLAS software (https://cds.cern.ch/record/2767187), while the annealing tracking is done by other standalone software.
- This study has been performed independently from the previous GNN study.

- We used Fixstars Amplify Annealing Engine(AE) which was an annealing machine developed by Fixstars.
  - Perform simulated annealing using GPU(NVIDIA A100)
  - 262k bits, fully connected

- This time, we used ***"doublets"*** for bits.
  - When two doublets have close curvature in X-Y plane or close angle in R-Z plane, we give them low energy.
  - Doublets and double-pairs were selected before a QUBO building to reduce the size of QUBO.

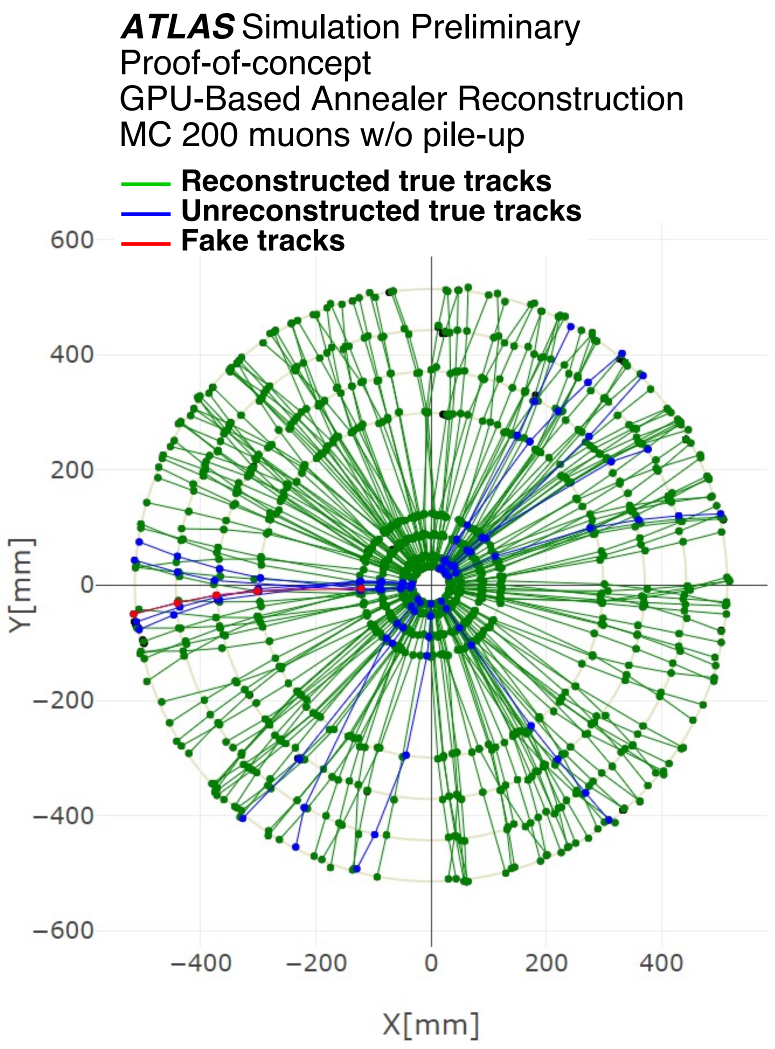
$$H(a,b,D) = \sum_{i}^{N} a_i D_i - \underbrace{\sum_{i}^{N}\sum_{j<i}^{N} S_{ij} D_i D_j} - \underbrace{\sum_{i}^{N}\sum_{j<i}^{N} W_{ij} D_i D_j} + \underbrace{\sum_{i}^{N}\sum_{j<i}^{N} \zeta_{ij} D_i D_j}$$

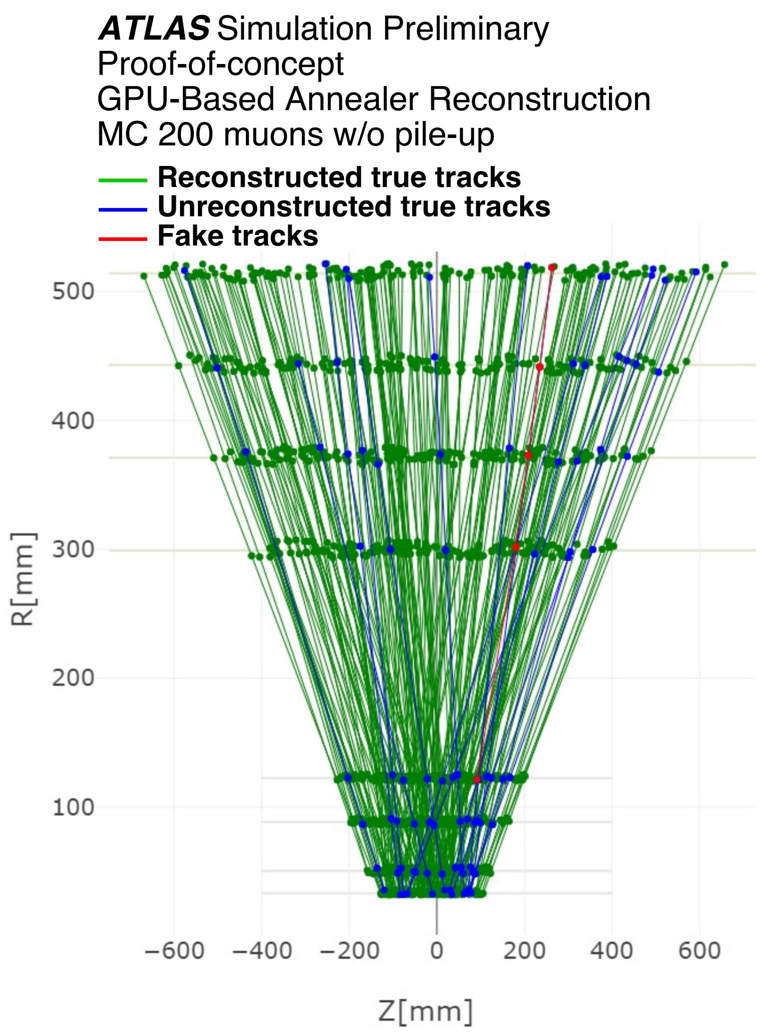


- D_i : Potential doublet
- a_i : Bias weight which is depending on N_{holes} in a doublet.
- S_{ij}, W_{ij} : The coupling strength, depending on the $\Delta\left(\frac{1}{R}\right), \Delta\theta$ between D_i and D_j.
- ζ_{ij} : The coupling strength, we give constant (ζ_{ij}=5).

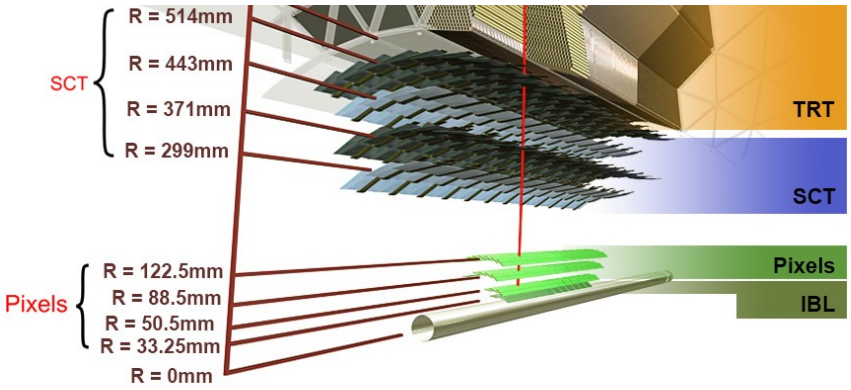
Event display

- Reconstructed results with 200 muons/event MC sample generated with the ATLAS software.
  - 0.5 GeV < p_T < 10 GeV in $1/p_T$ flat distribution, $|\eta| < 1.0$





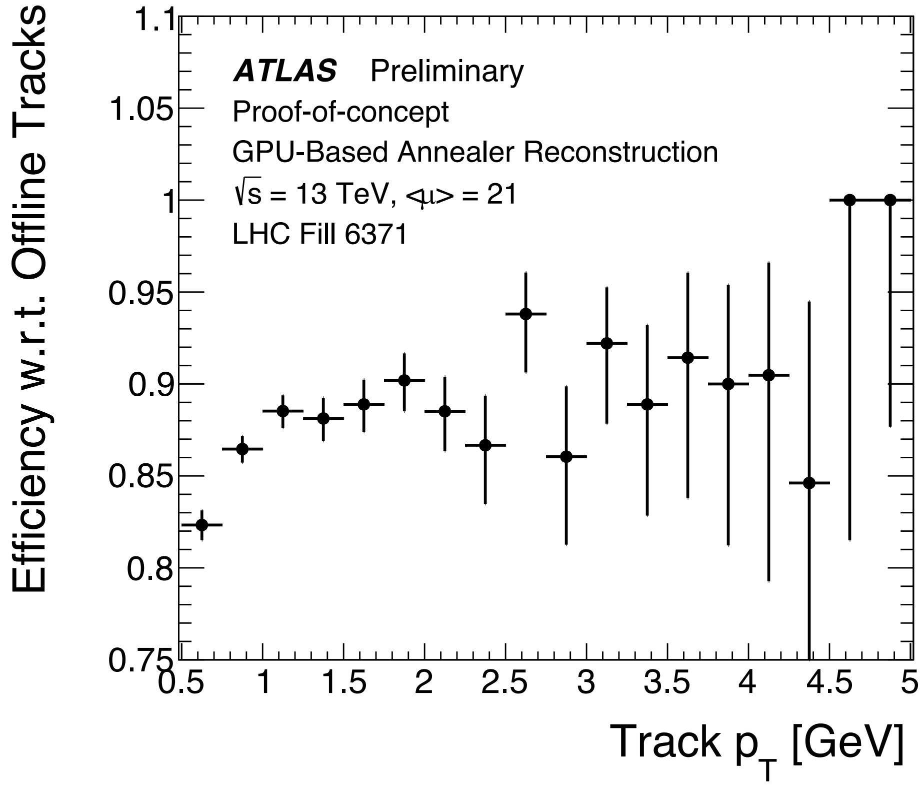
- Layout of the ATLAS inner tracker

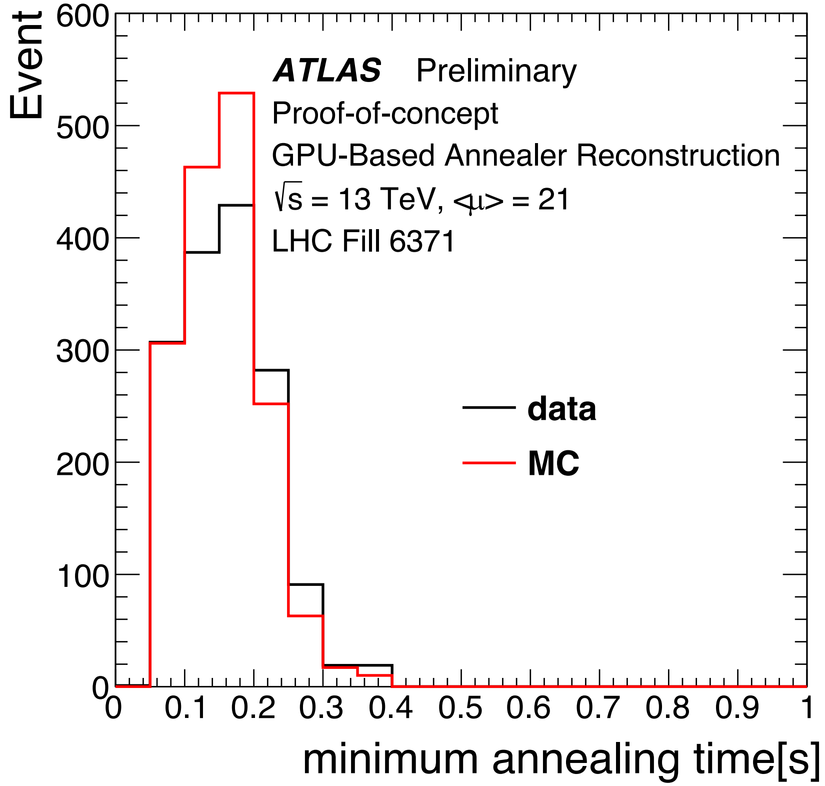


Track findings by annealing machines work successfully in a realistic environment.

Results with real data

- We applied this algorithm to real ATLAS data taken by non-physics random triggers.
- The efficiency is calculated w.r.t. the ATLAS offline tracks. The matching to the offline tracks is performed if reconstructed tracks with annealing machines share more than 50% of hits with the offline tracks.
- The annealing time was compared with MC sample(10 pions/event with pile-up 20).





Average pre-processing time for data is ~0.6 sec. (single core, 11th Gen Intel(R) Core(TM) i9-11900K @ 3.50GHz)

- Our algorithm also works successfully with real ATLAS data.
- It is a good starting point to further explore the method.

Conclusions

- 2 type of studies are performed with the annealing tracking algorithm:
  - GNN application in Quantum Pattern Recognition
    - In order to make use of the GNN in the pre-processing stage of this algorithm, we performed an edge-classification using a bi-directional graph made by simplified sample which only contain 4 hits.
    - The result indicated that it is possible but there are rooms to improve.
  - Application for the ATLAS dataset
    - Another study shows that the algorithm can also deal with real data collected from the ATLAS detector using low pileup (and no pileup) samples, in both MC and data.
    - Result looks promising and further development is under consideration.