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Application of Quantum Annealing with Graph Neural Network Preselection in Particle Tracking at LHC

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Connecting The Dots 2023

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Motivation

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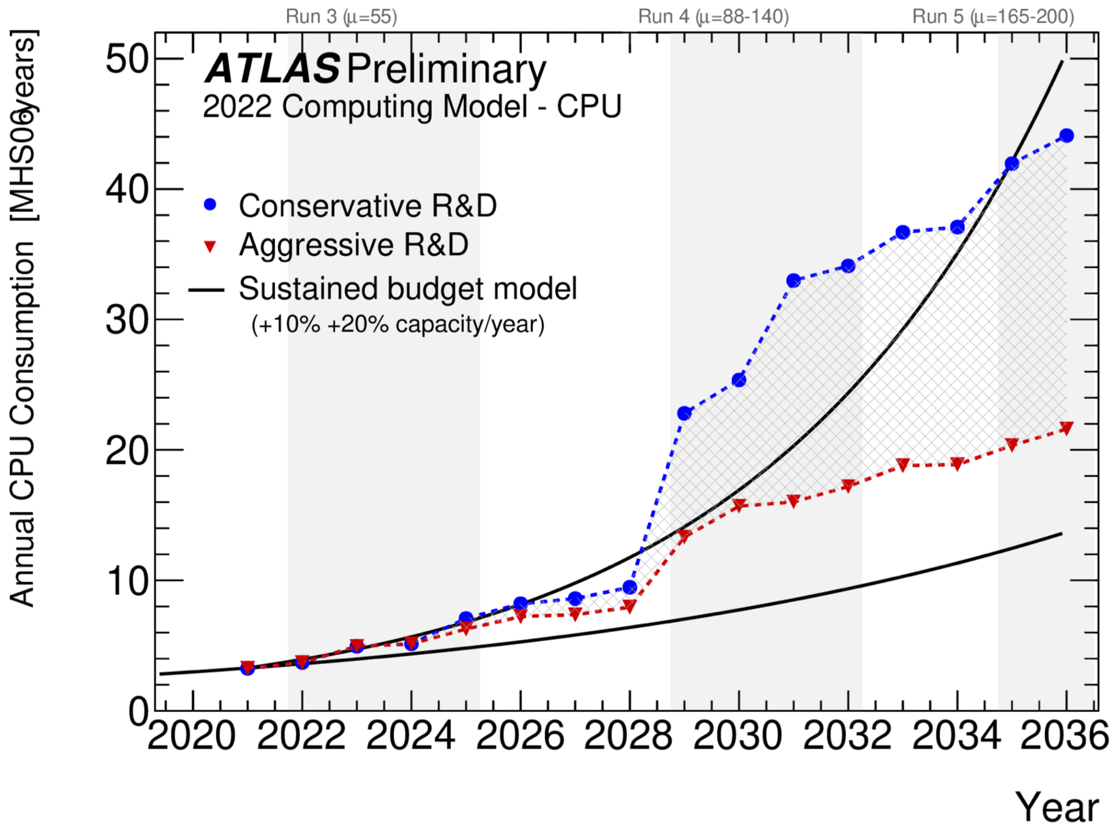
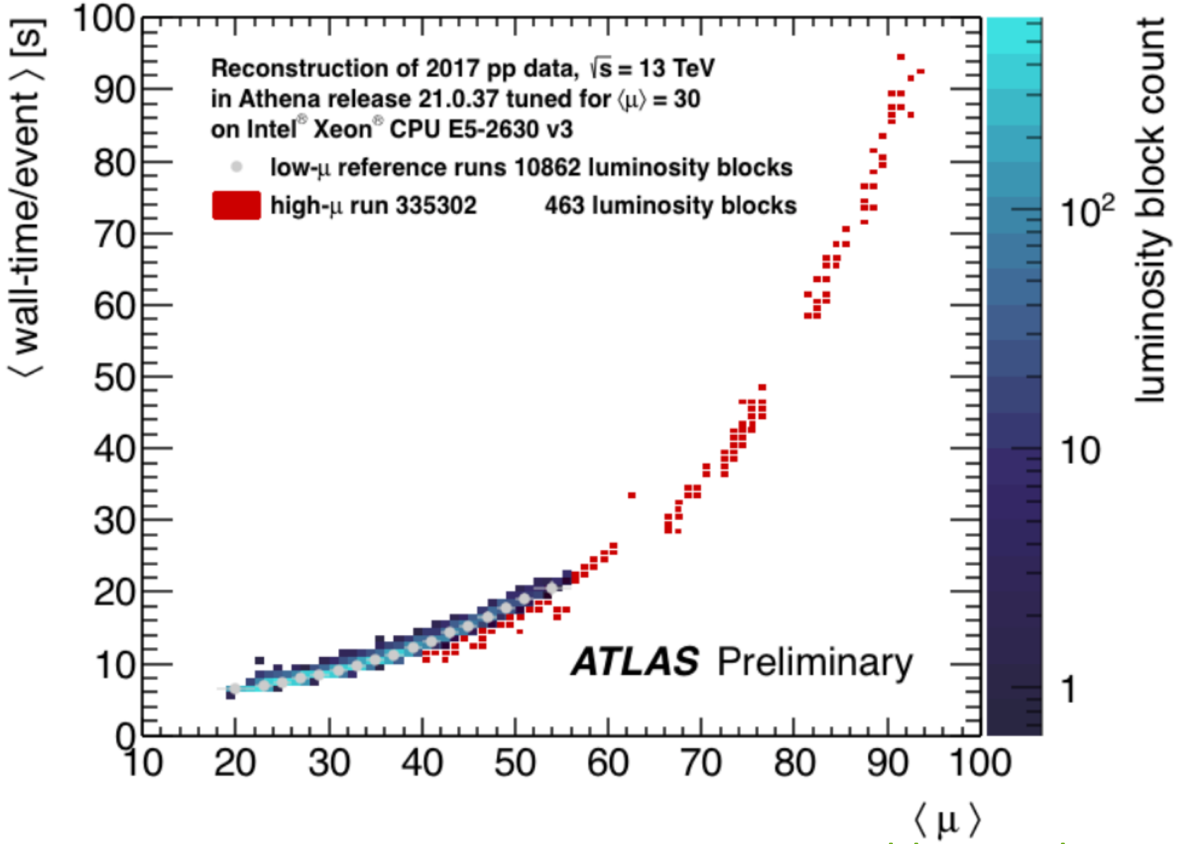
- HL-LHC is coming
- With larger pile-up ($\langle \mu \rangle \sim 200$) and high readout rate, CPU consumption will dramatically increase.
  - Especially track reconstruction -> New techniques are needed



CERN-LHCC-2022-005



ATLAS Computing Public Result

Introduction: Quantum Annealing

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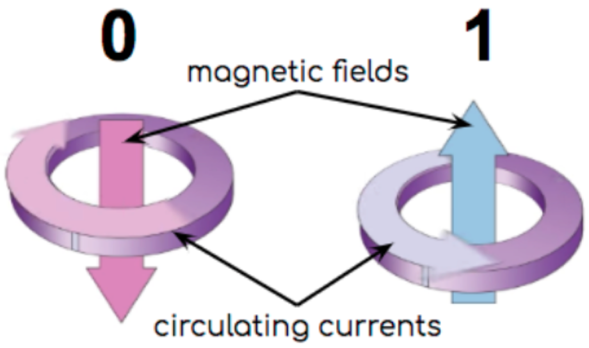
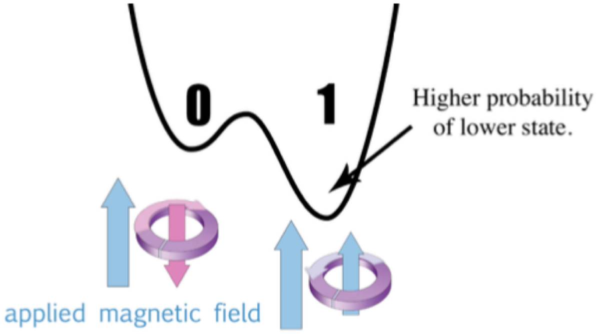
- Quantum Annealing:
  An optimisation process for finding the global minimum of a given function by using quantum fluctuations.

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

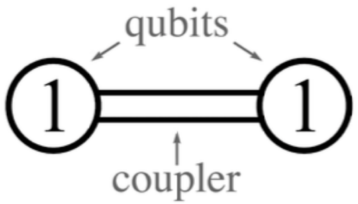


qubits ⇒ q_i



bias weights ⇒ a_i

degree to which a qubit tends to a particular state



coupling strength ⇒ b_{ij}

degree to which two qubits tend to the same state

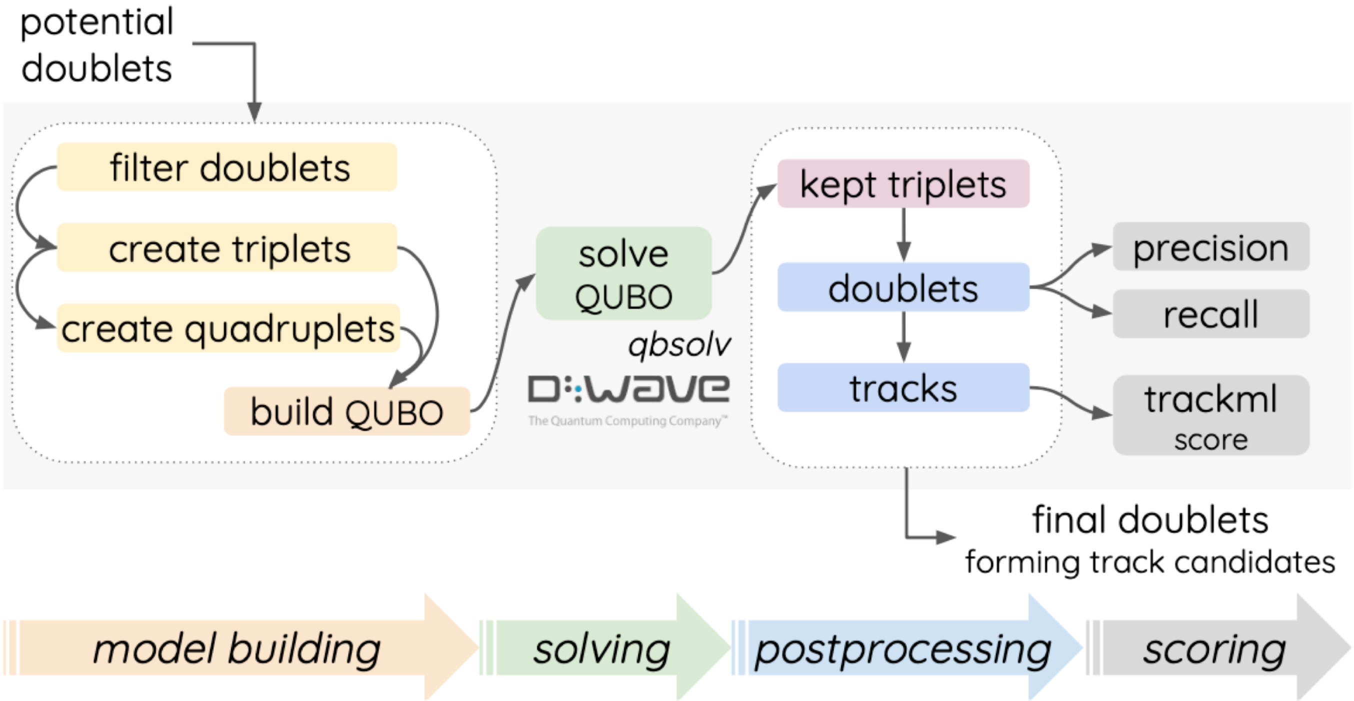
$$O(a;b;q) = \sum_{i=1}^{N} a_i q_i + \sum_{i}^{N}\sum_{j}^{N} b_{ij} q_i q_j \quad q_i \in \{0,1\}$$

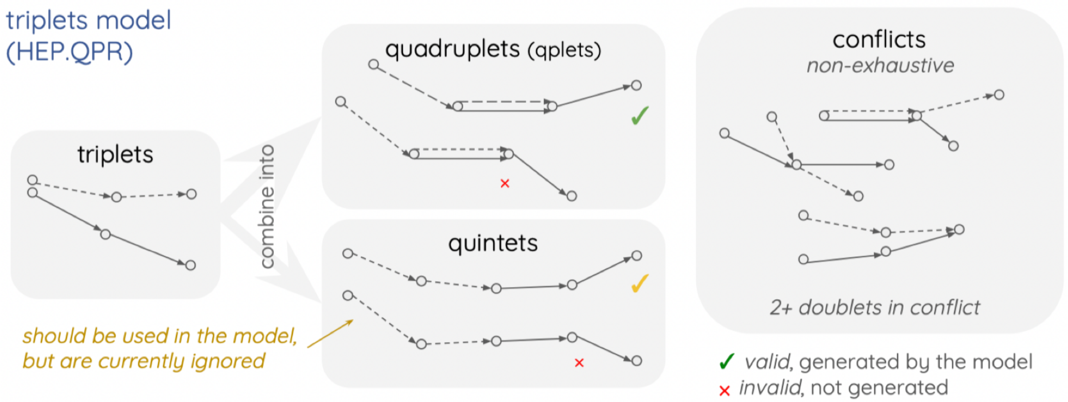
QUBO

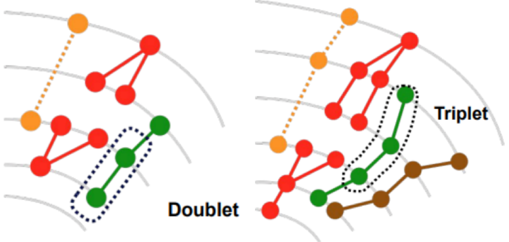
Quadratic
Unconstrained
Binary
Optimisation

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

- 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





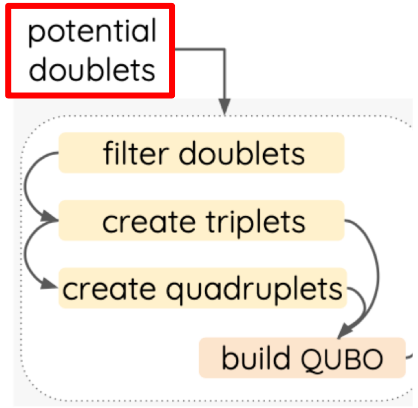


$$O(a,b,T) = \sum_{i}^{N} a_i T_i + \sum_{i}^{N} \sum_{j<i}^{N} b_{ij} T_i T_j$$

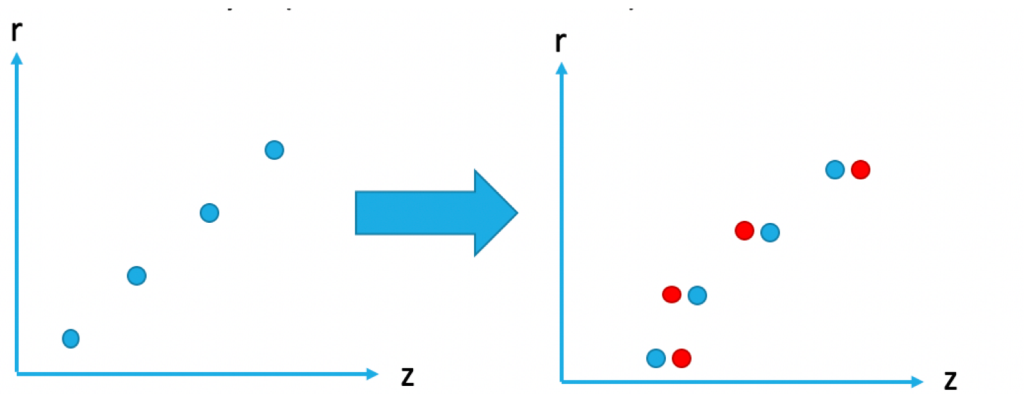
- T_i : potential triplet
- a_i : Bias weight which has been set to 0.
- b_i : The coupling strength, depending on the relation between T_i & T_j

GNN doublet selection: Phase I

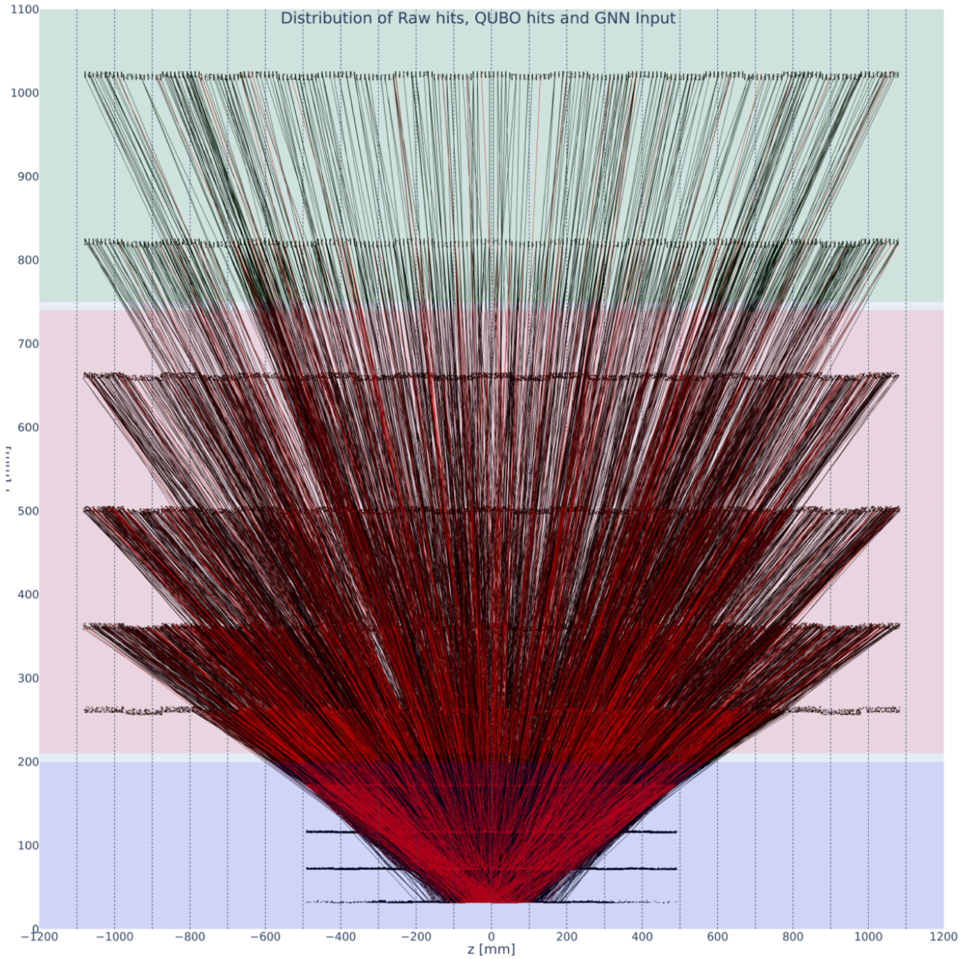
We wonder can we improve the tracking performance by implement the GNN technique in the doublet building section



- A test has been carried out by considering a graph which contain 1 track with 4 hits.



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



In single event:
- T_iT_j from the QA solved QUBO (Hit ID)
- "Raw input" from TrackML challenge datasets: (HitID, x,y,z, detector layers etc.)

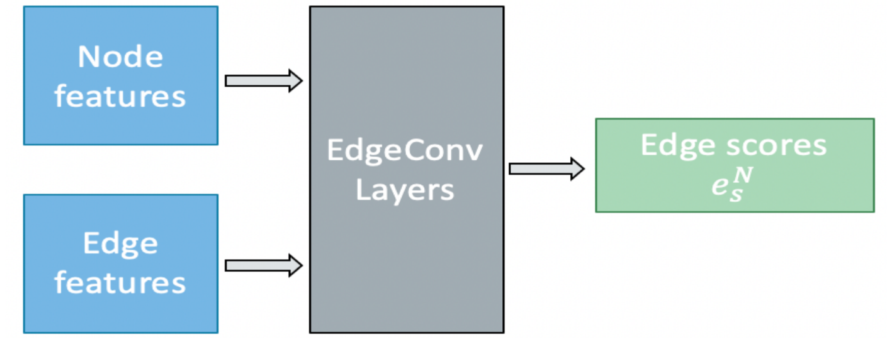
→

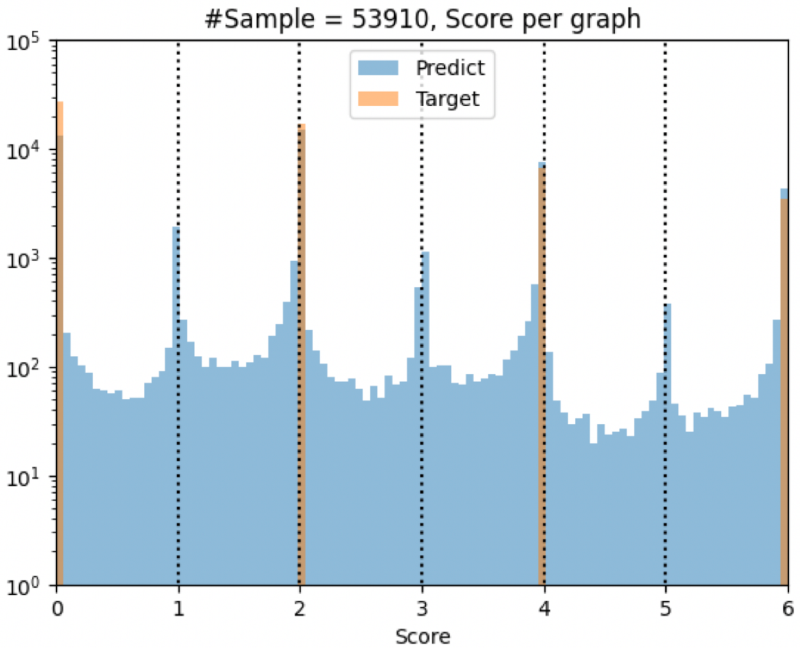
For each T_iT_j:
- Doublet list (3 pair of HitID) →
- Hit list (HitID, x,y,z, detector layers etc.) →

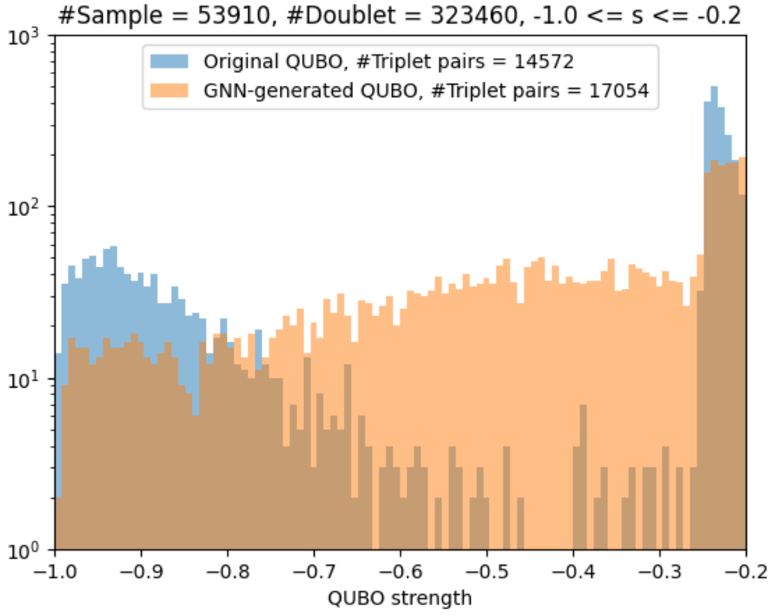
In 1 GNN sample:
- GNN Target
- Trainable parameters

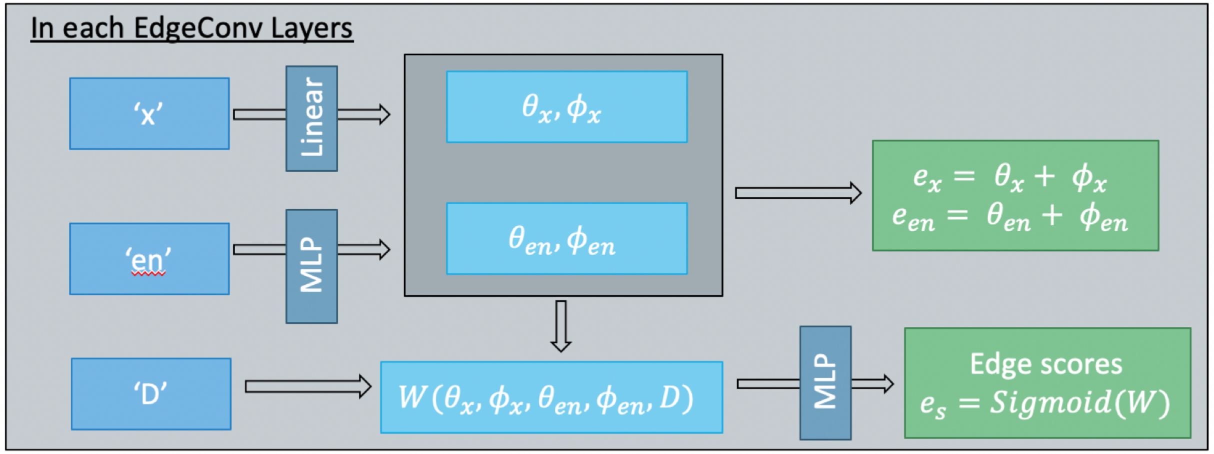
GNN doublet selection: Phase I

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	







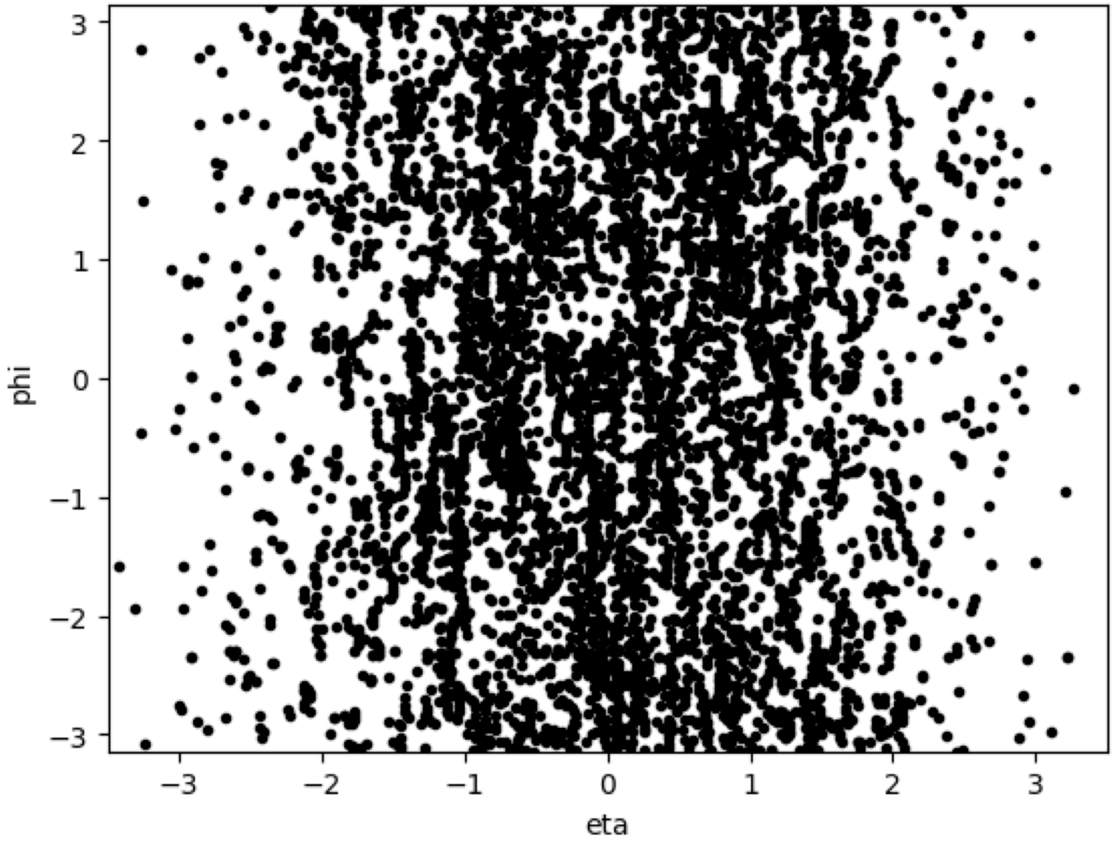


Conclusion of Phase I

- Graph: 4 hits only, nearby hits = BKGs
- Edge classification
- Result: The network didn’t recognise that $e_{ij} = e_{ji}$ in this bi-directed graph
- QUBO strength doesn’t looks like the target at all.
- Talk @ CHEP2023

GNN doublet selection: Phase II

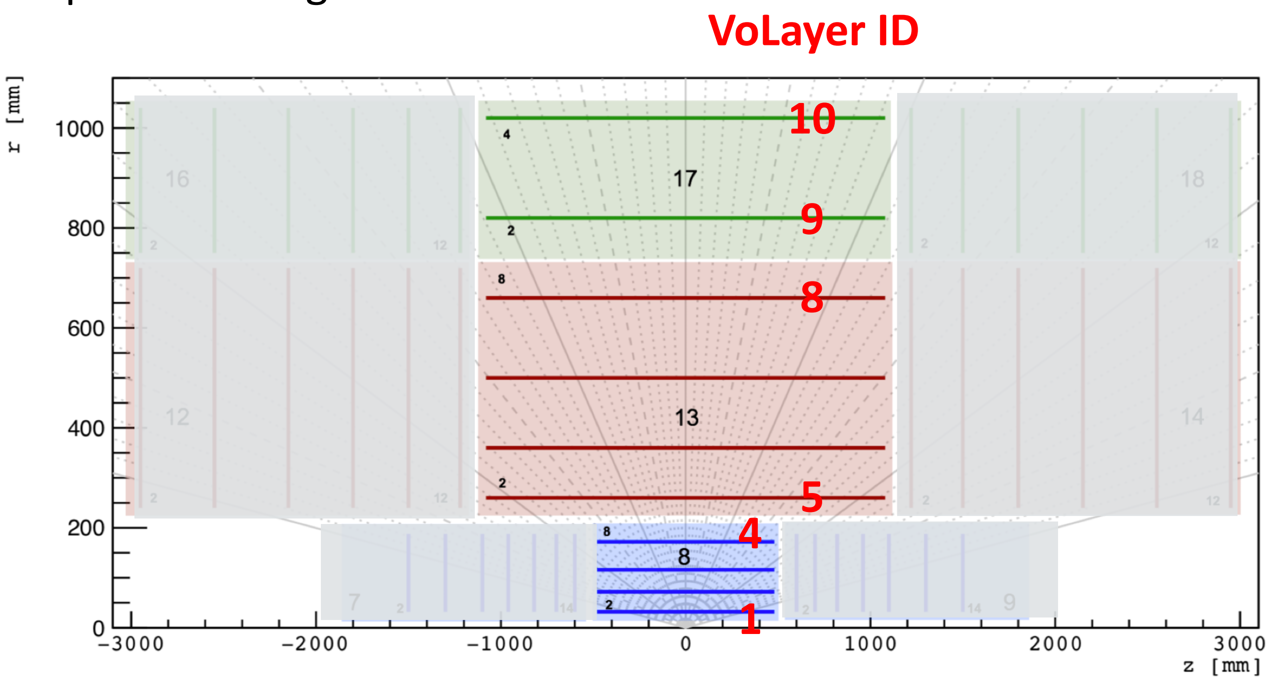
Main goal in phase II:
- Classify doublet that can be form the QUBO from the "nature" geometry.
- Make a usable QUBO based on GNN results.



A bi-directed graph is formed with the following node features:

Node features 'x'	Node features 'h'
r	eta
phi	VoLayer ID
z	

- Hit ID also pass through the network but not being use in the pattern recognition.

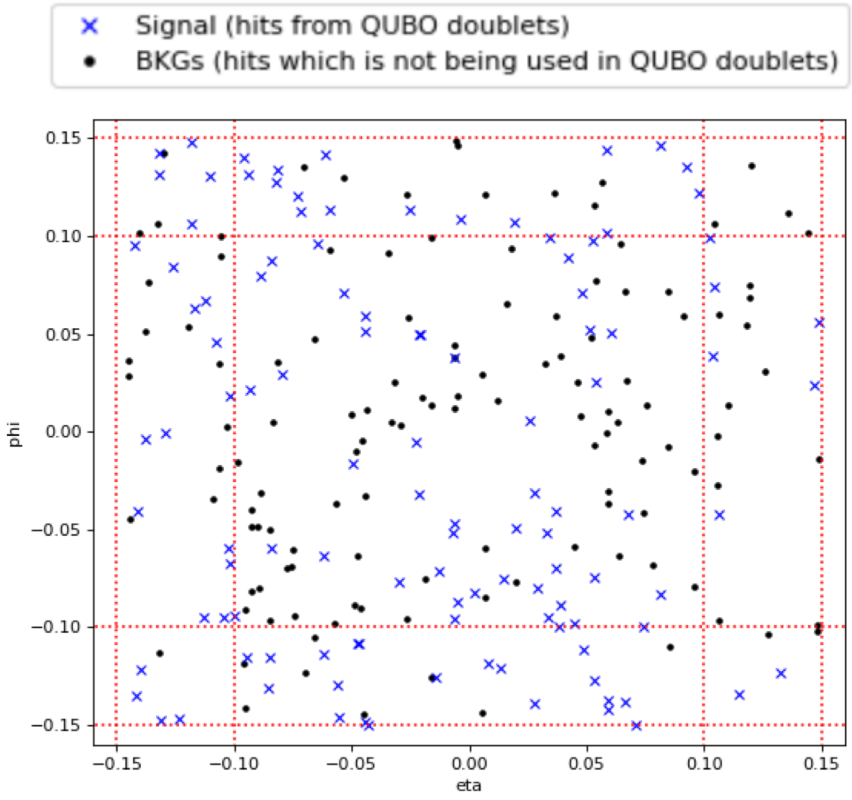


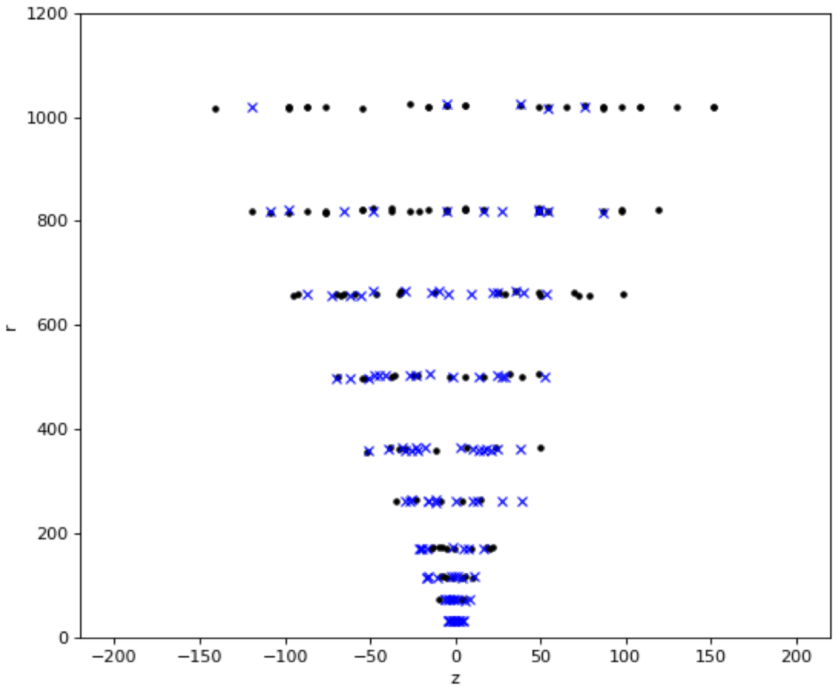
Sample pre-selection

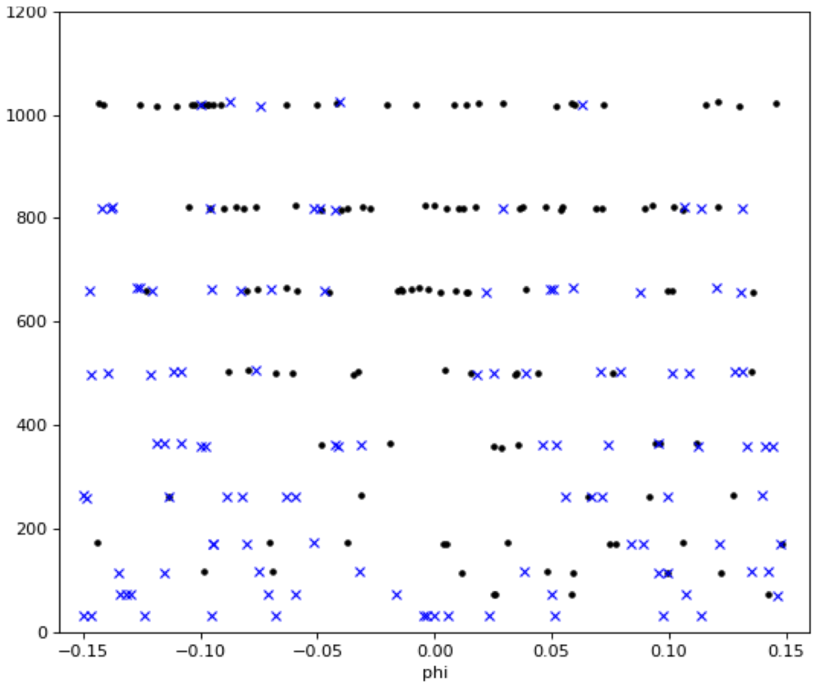
A small sample is used to train the network. We focus on |eta| <= 1 region.

- To further simplify the graph (mainly number of edges) we only consider |phi|,|eta| < 0.15 in the training
- Also edges can only being formed under these conditions:
  - |dz| < 50
  - |dphi| < 0.2

Event 1001	#Nodes	#Edges	Edges/node
|eta| < 1.0	51	398	7.8
|eta| < 1.5	141	1866	13.2
|eta| < 2.0	267	4806	18







Network architecture

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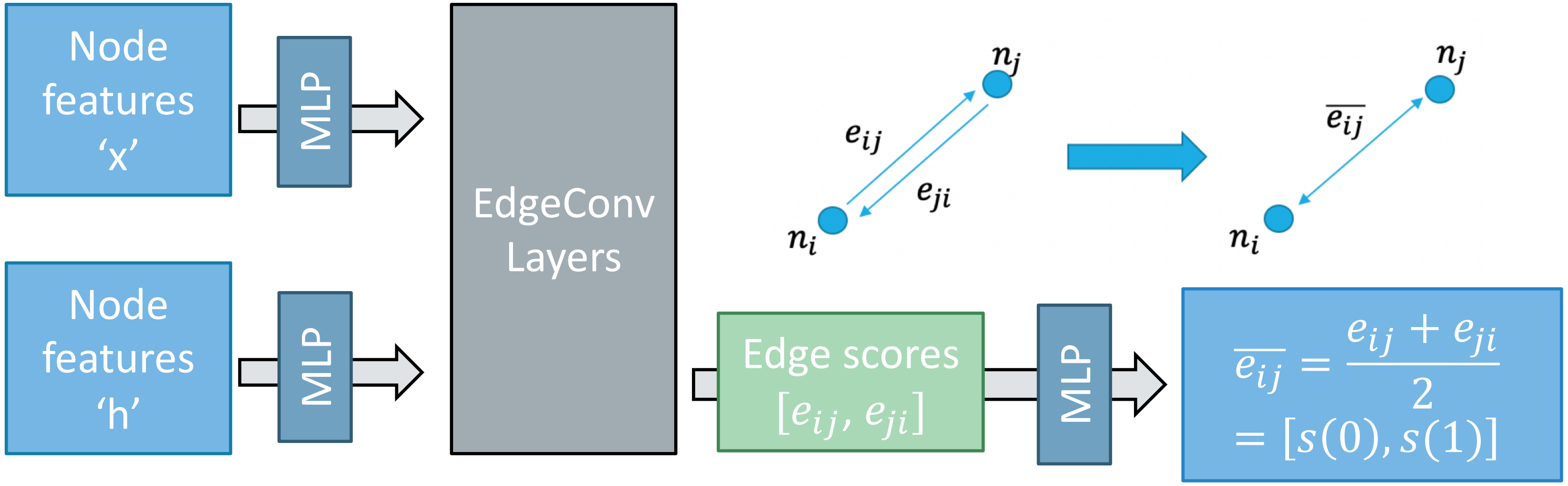

- Our training target, is to match the doublet which being use in the QUBO in the same |eta|,|phi| region.
- By comparing the Hit ID from the nodes which formed the edges, one can calculate the confusion matrix for each graph.

<u>In each EdgeConv Layers</u>

$$x_i^{l+1} = mean\left[\theta_{x,m}\left(x_j^l - x_j^l\right) + \phi_{x,m}\left(x_i^l\right)\right]_j$$
$$h_i^{l+1} = mean\left[\theta_{x,m}\left(h_j^l - h_j^l\right) + \phi_{x,m}\left(h_i^l\right)\right]_j$$

$$e_{ij}^1 = W(\theta_x, \phi_x, \theta_{en}, \phi_{en})$$
$$e_{ij}^{l+1} = e_{ij}^l + W(\theta_x, \phi_x, \theta_{en}, \phi_{en})$$

- Since we are constructing a bi-directed graph, a doublet is represented by 2 edges, and we have 2 classes for each edges.
- By taking average score between e_{ij} and e_{ji} , we ensure that both edges going into opposite directions reserve the symmetry.
- The score, $\overline{e_{ij}}$ contain 2 values: $s(0)$ and $s(1)$, which is the score for the edges belongs to class 0 (BKG-like), and belongs to class 1 (Signal-like), respectively.

Performances with 1 event

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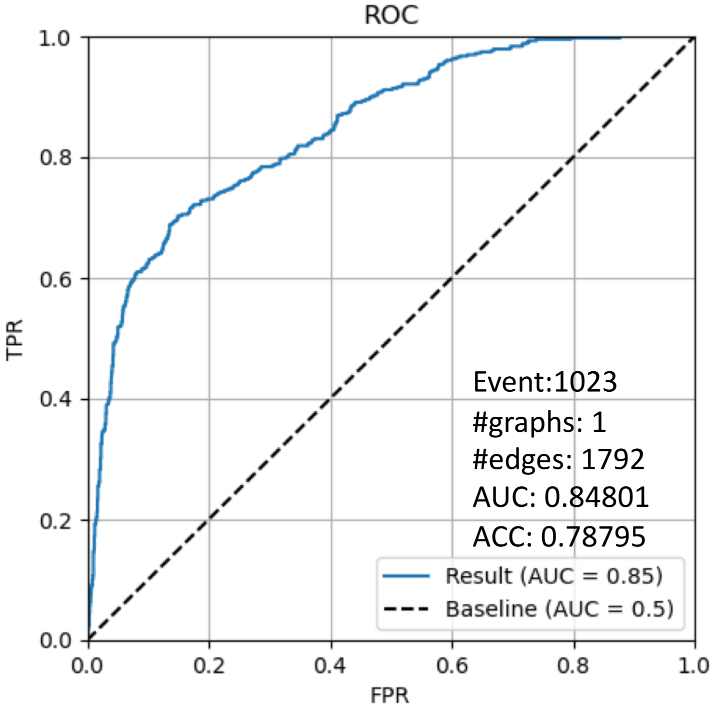
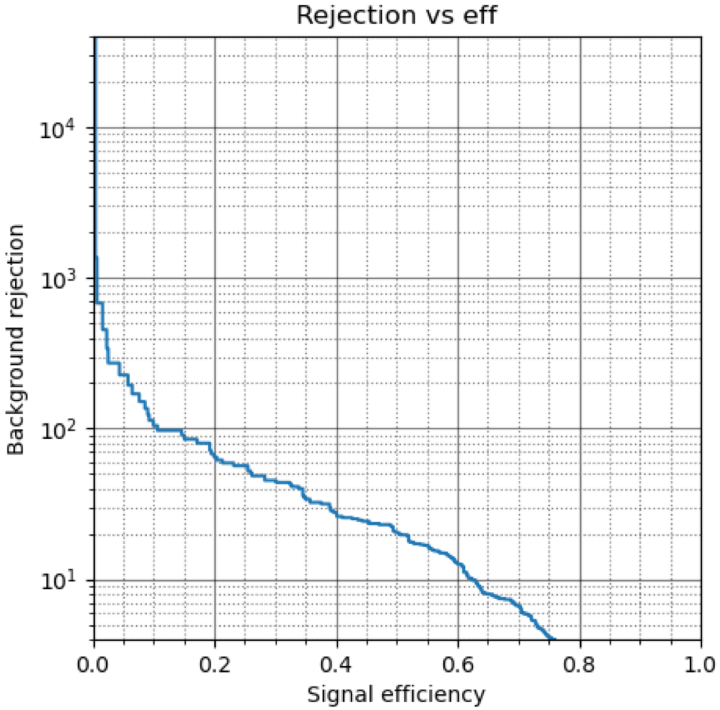
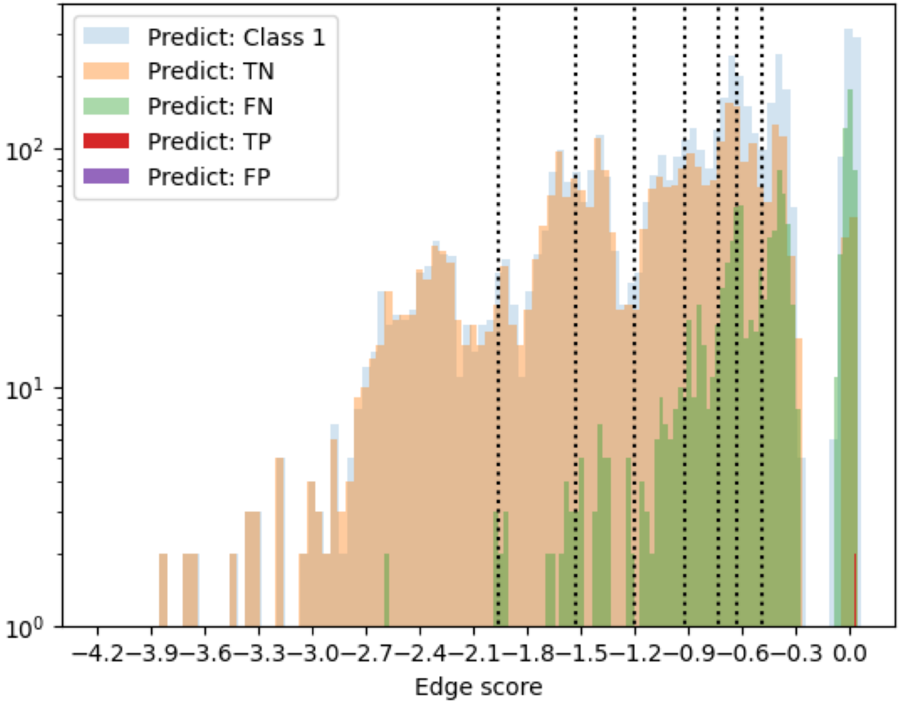
After training the model, we use one of the events to generate the QUBO, as QUBO is an event-based object.



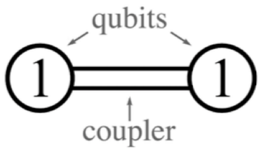




TP = 68	FP = 17
FN = 363	TN= 1344

Threshold	100%	90%	80%	70%	60%	50%	40%	30%
score	-4.3	-1.96	-1.53	-1.2	-0.923	-0.73	-0.631	-0.49
#Doublets	4648	4188	3719	3256	2789	2326	1860	1396

QUBO strength distribution: explanation



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

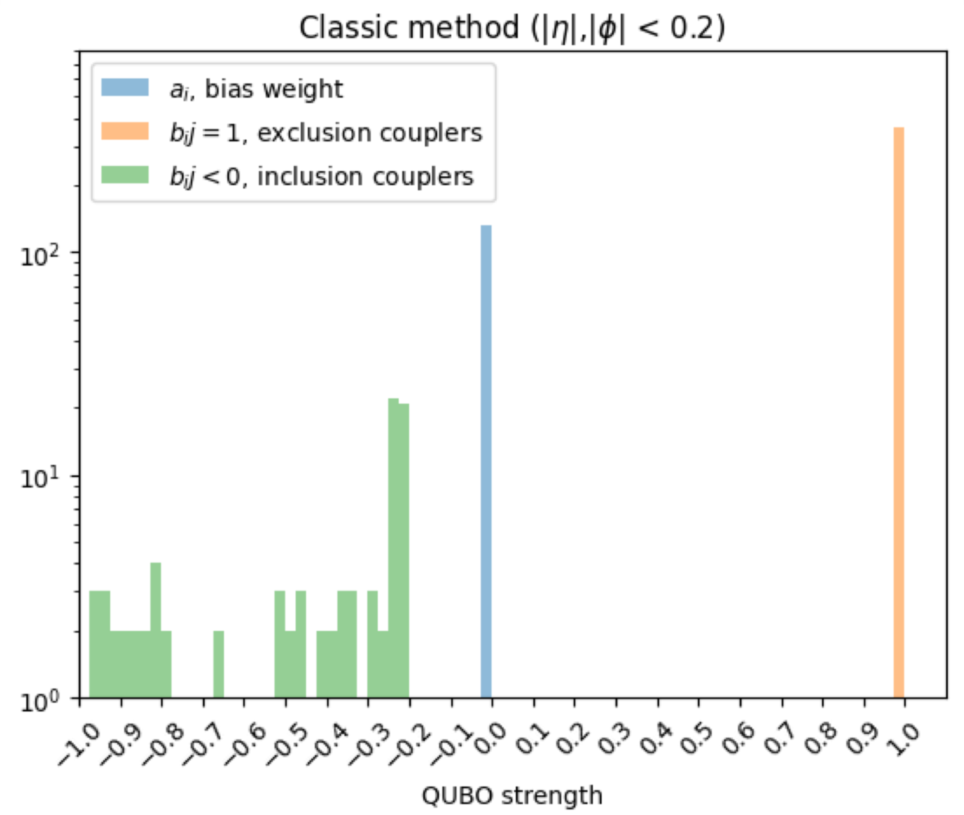
bias weight a_i	influences one qubit q_i	-1	q_i tends to collapse into 0.
		1	q_i tends to collapse into 1.
coupling strength b_{ij}	influences two qubits q_i and q_j	-2	both q_i and q_j tend to collapse into 1.
		2	at least one of q_i and q_j tends to collapse into 0.

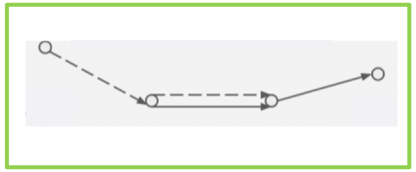
In the code, 3 steps to create a QUBO:

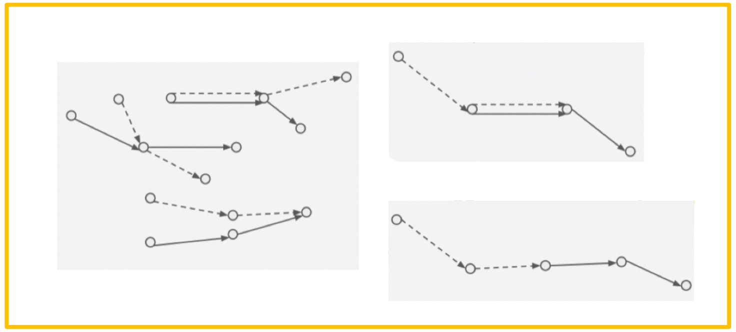
1: Set Qbits with their weight (doublets with a common weight)
e.g. ('23472_31455_38557', '23472_31455_38557'): 0

2: exclusion couplers
Add more entries to QUBO, e.g.:
('83840_90726_96873', '76774_83829_96873'): 1

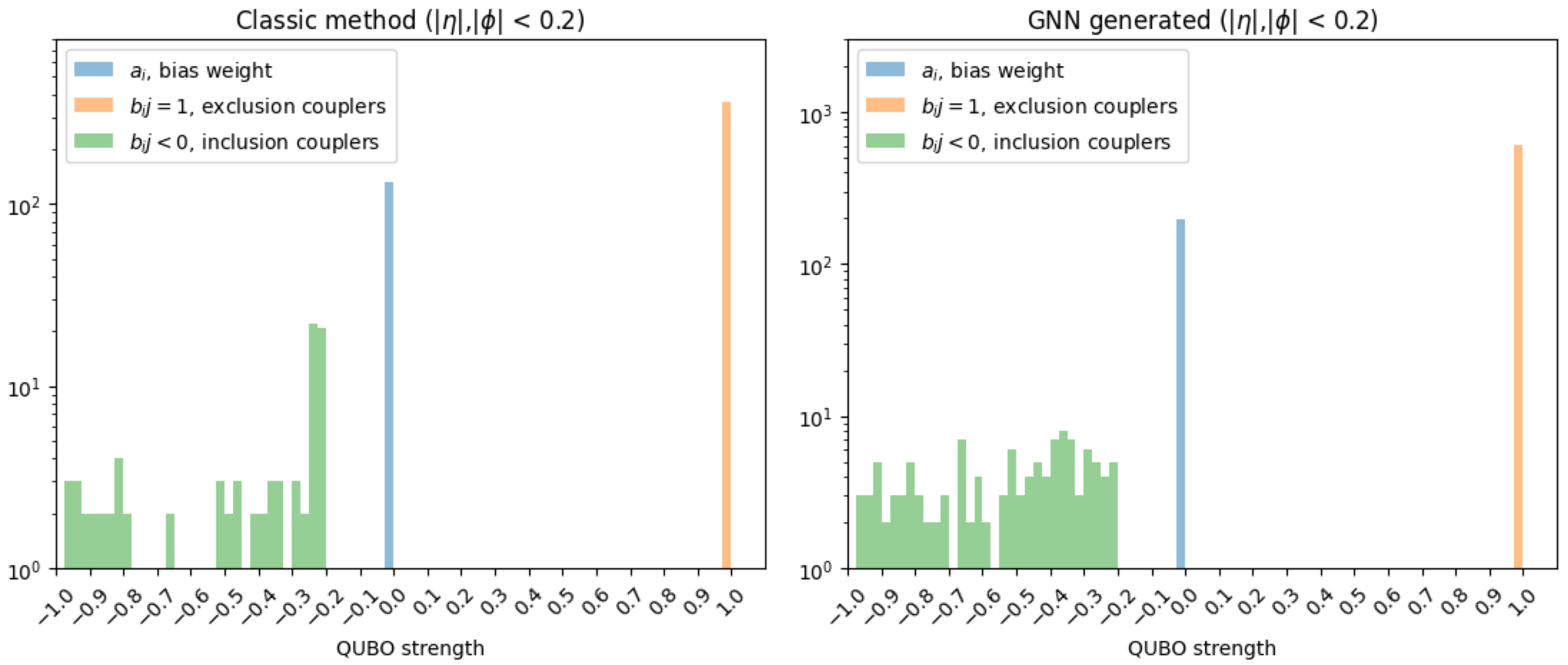
3: inclusion couplers
Add more entries to QUBO, e.g.:
('18380_27166_34273', '27166_34273_40293'): -0.6423072319215068





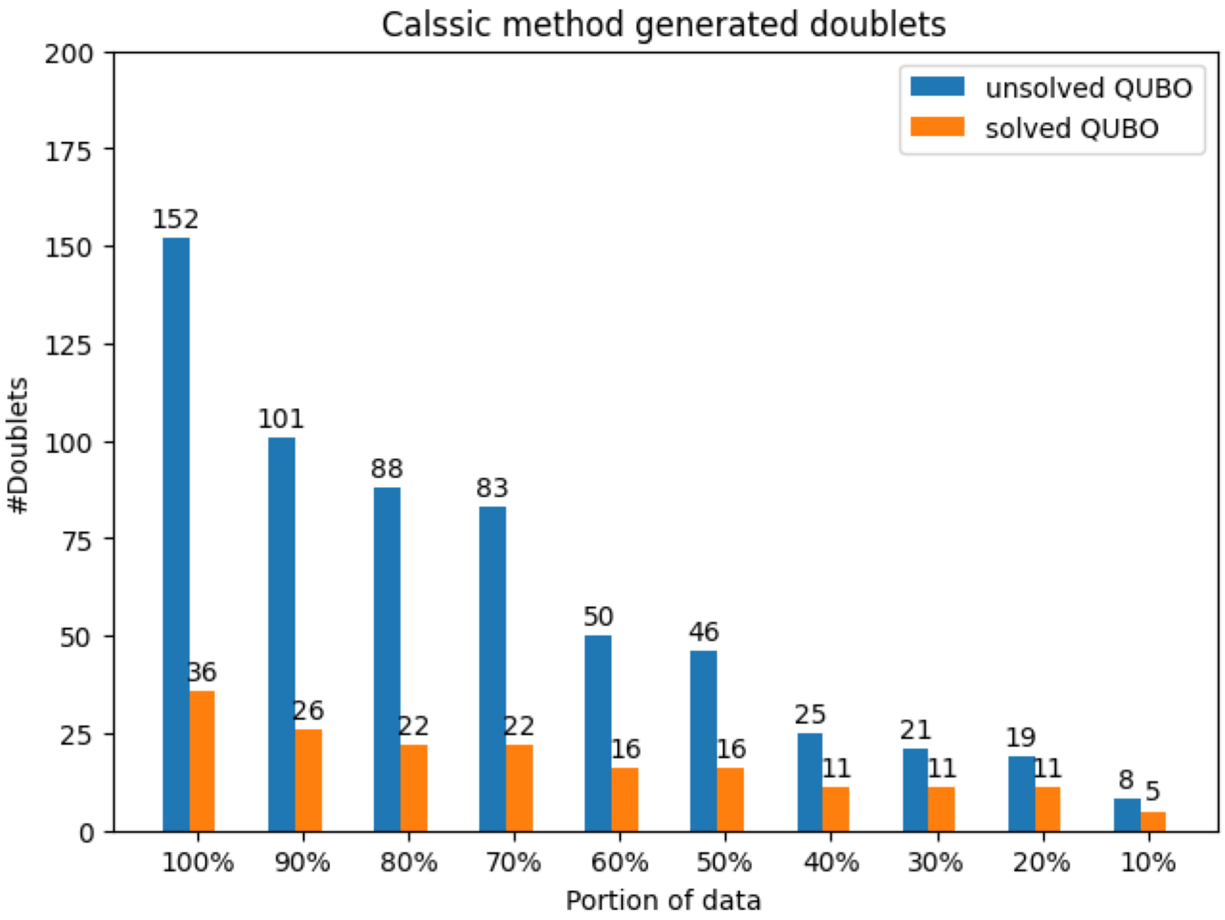


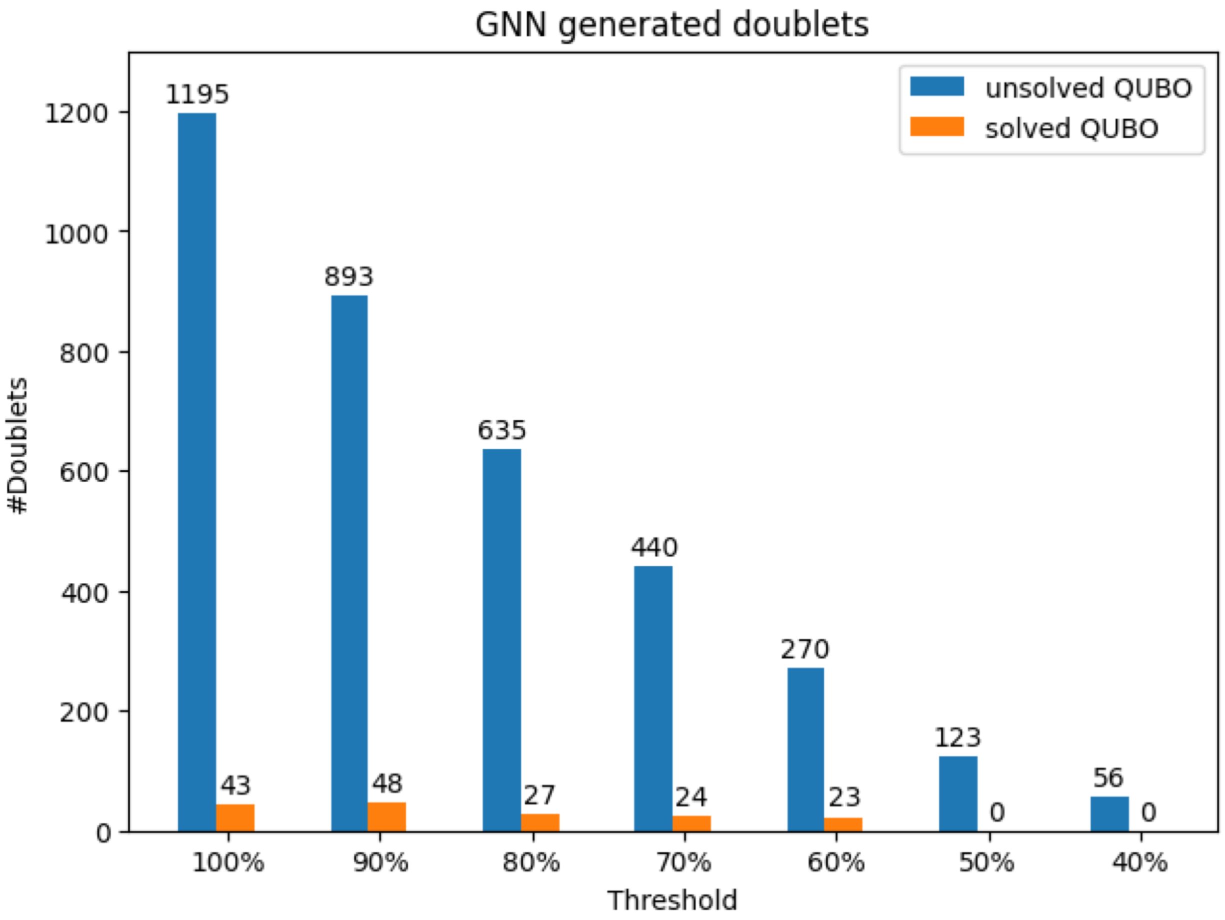
Compare to classic method: QUBO strength



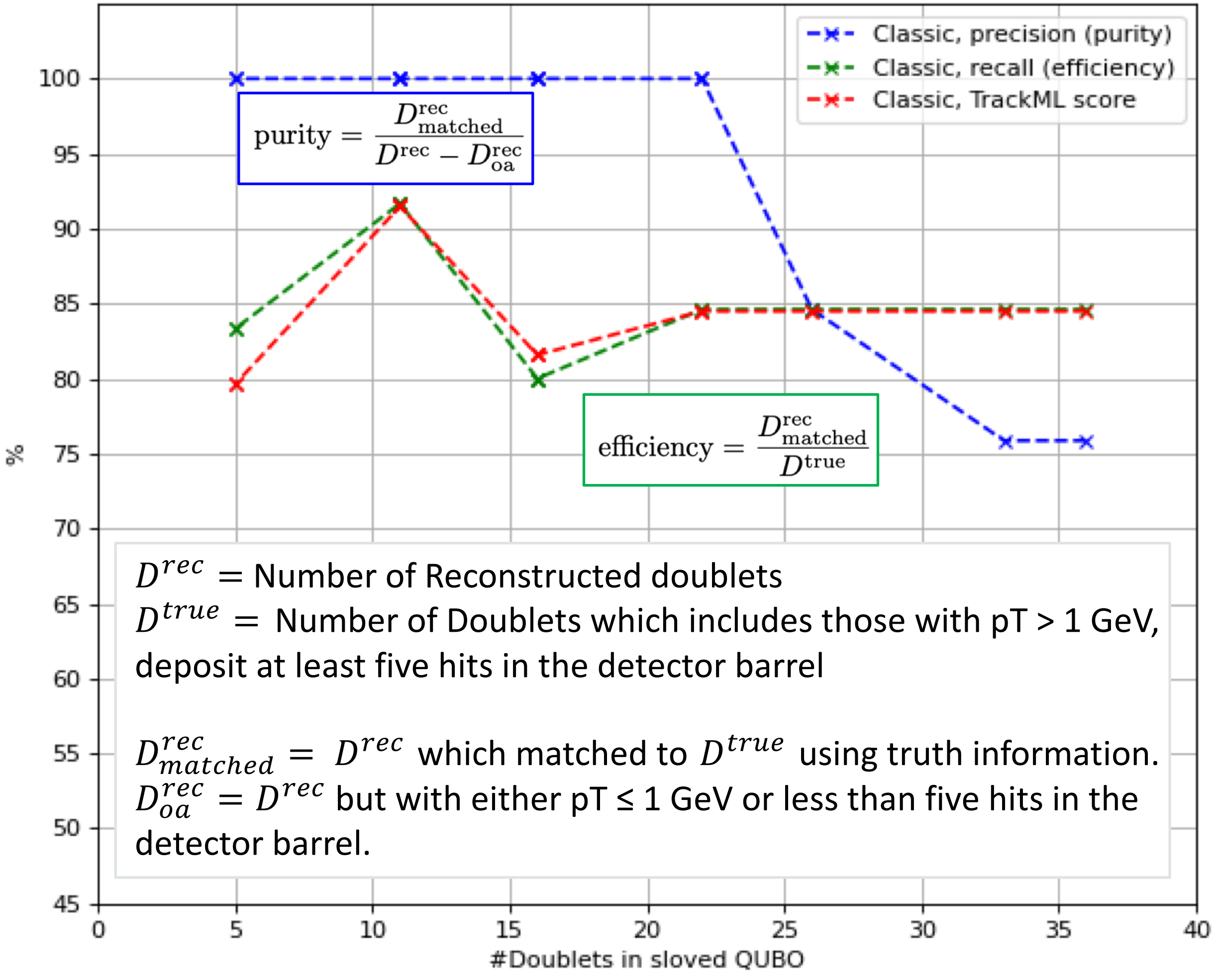
Compare to classic method: #Doublets

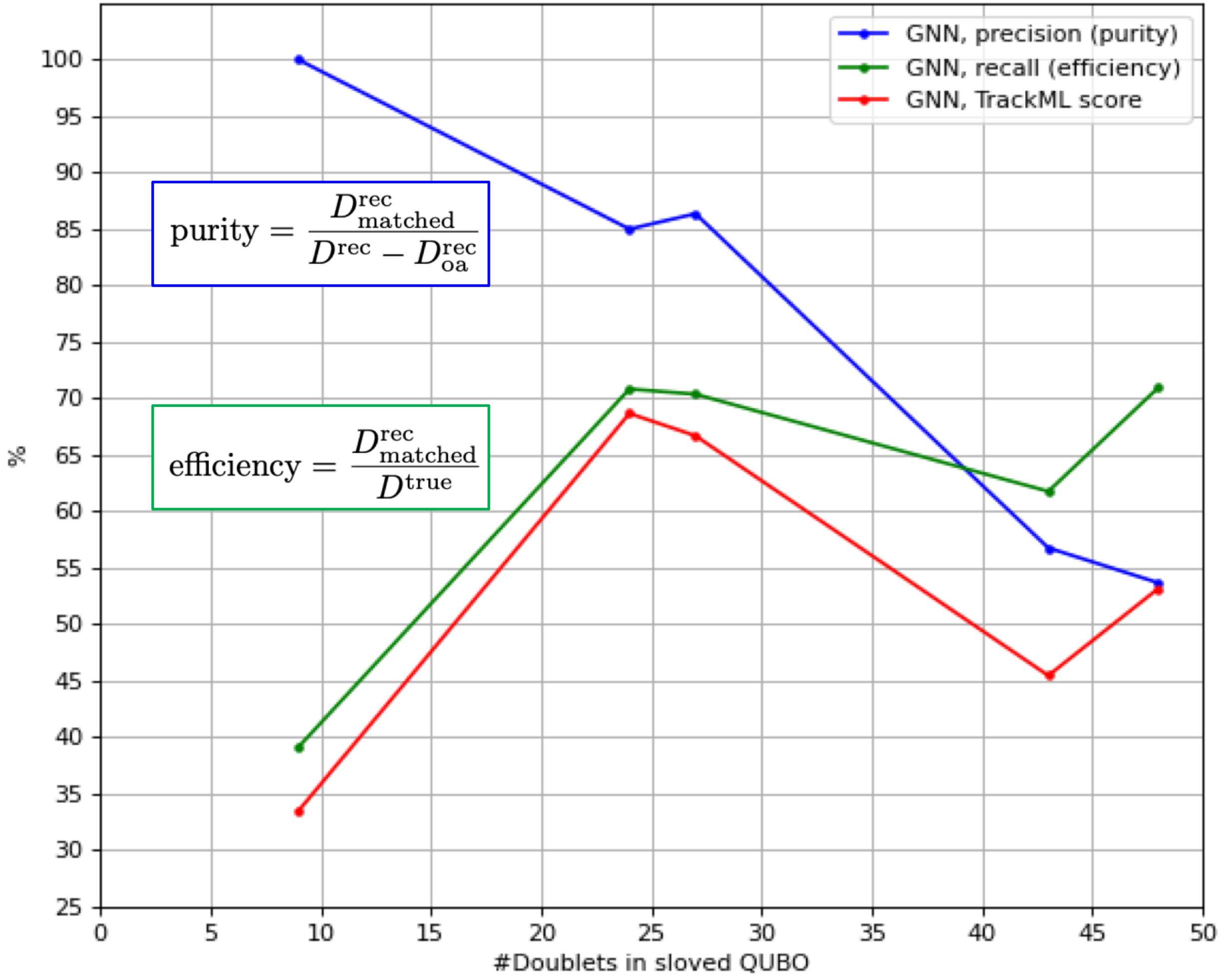
- Simulated Annealing Sampler has been used to solve the QUBO
- Simulated Annealing Sampler: An annealing process performed with CPU rather than QPU



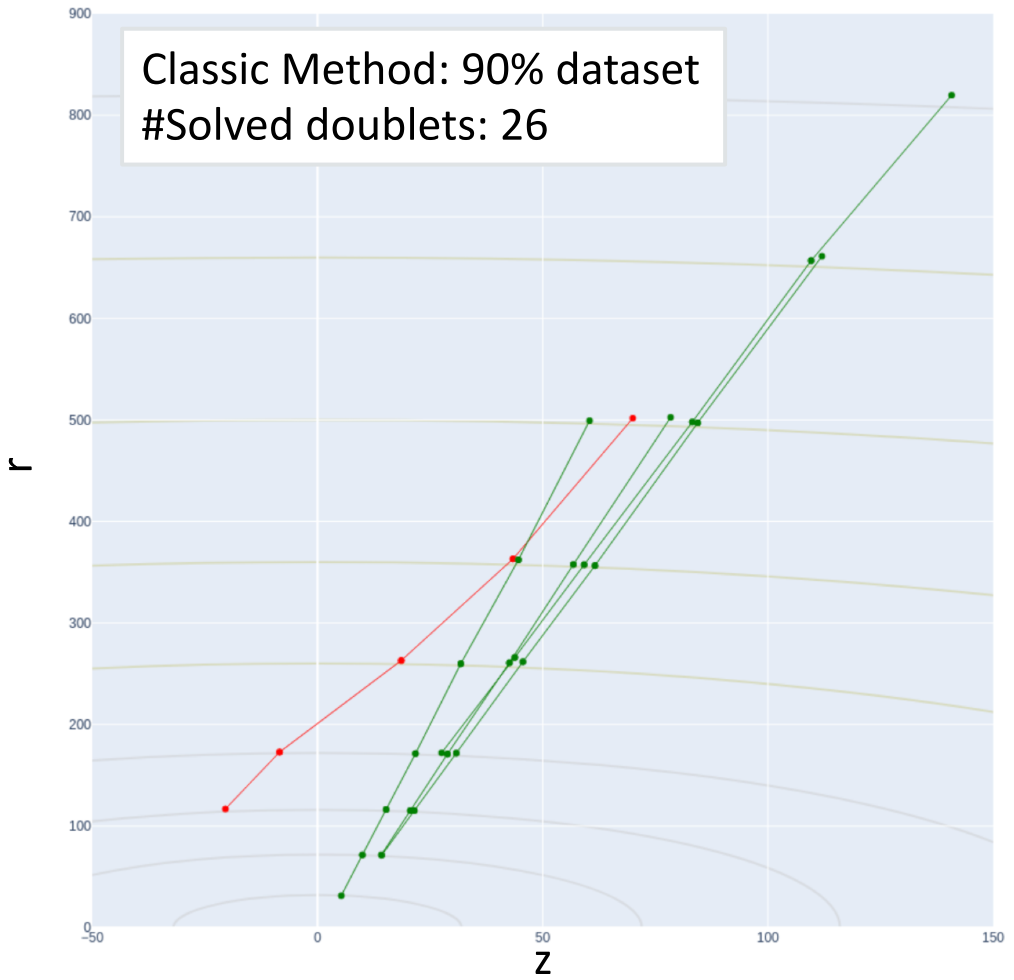


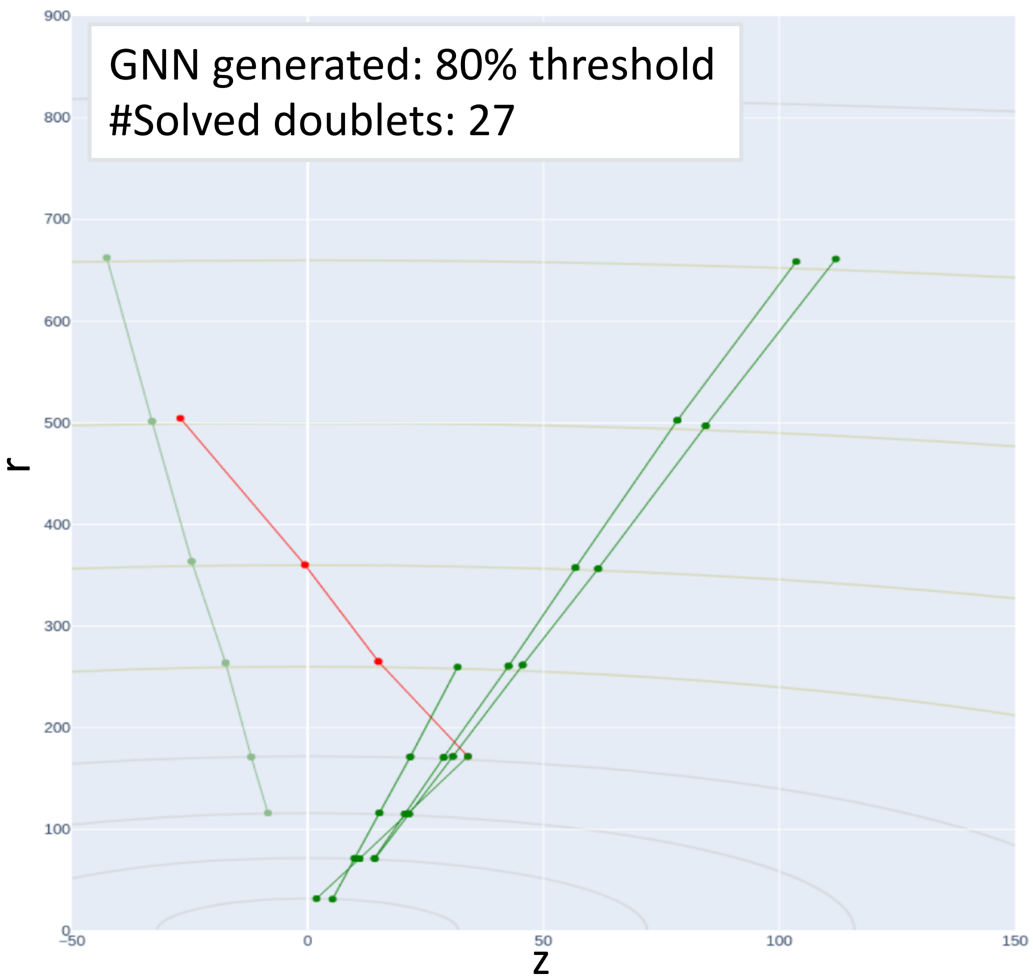
The track reconstruction performance of an event can be judged by TrackML score, efficiency (recall) and purity(precision).





Compare to classic method: Reconstructed tracks display (r-z plane)





- Fake doublets
- Reconstructed doublets (without the momentum acceptance)
- Reconstructed doublets (within the momentum acceptance)

Conclusion & Outlook

Conclusion

- A GNN has been implemented into the Quantum annealing-based tracking algorithm.
- In phase I, the network didn’t recognise the opposite edges between 2 nodes should form a single doublet.
- In Phase II, the following improvement has been made:
    - A more general graph has been used.
    - The network architecture has been improved, and the average edge score between opposite edges are considered.
    - Instead of calculating the probability, the target matching is preformed.
    - The GNN generated doublets are being used to construct QUBO, and the strength looks different to the original QUBO.
    - The QUBO generated based on the GNN model, have much more doublets.
    - However, the tracking performance of the solved QUBO is worse.

Outlook

- Phase II model looks ok, but still have more room to improve.
- In Phase III, we are aiming to:
    - Improve the ROC
    - Redefine the task: matching doublets -> purely edge classification
    - Try to use k-nn graph / graph clustering instead of bi-directed graph.
    - Steady with a larger dataset.
    - Construct triplet / triplet pair objects from GNN.