TrackOpt vertex with GNN

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Edge weights with DGL

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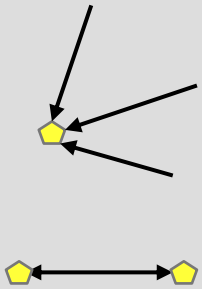
Edge weights estimation is implemented in DGL

1) Node_hidden_state = NN{Concat(Node_features, Mean(Edge_features)}

2) Edge_weight = NN{ Concat(Node_hidden_state_i, Edge_features, Node_hidden_state_j)}



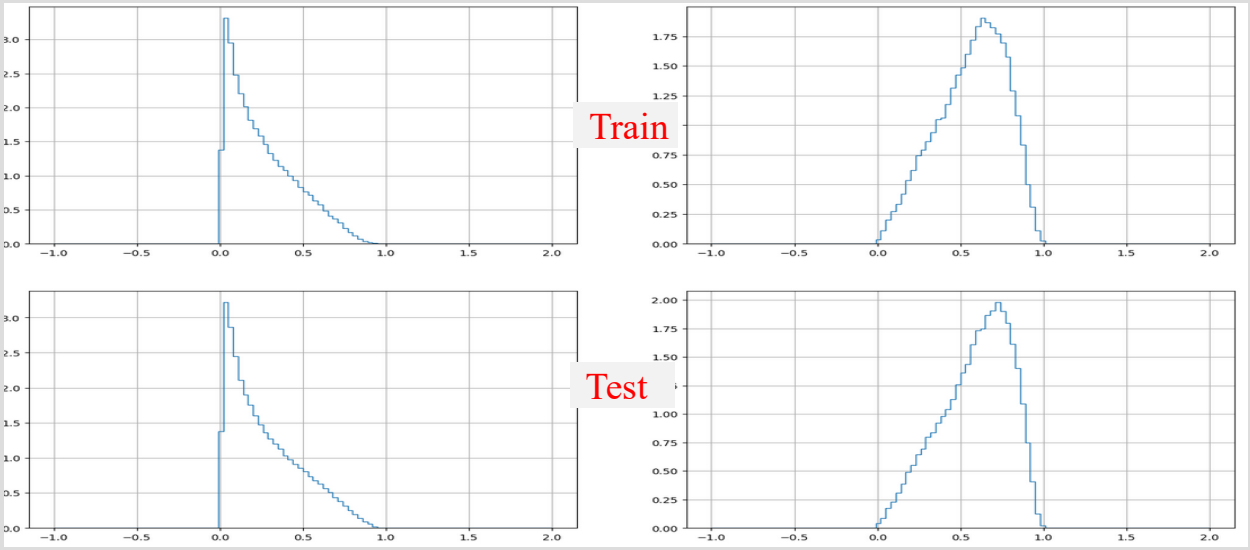
3) Node_hidden_state = NN{Concat(Node_features, Weighted_Mean(Edge_features)}
4) Upd_Edge_weight = NN{ Concat(Node_hidden_state_i, Edge_features, Node_hidden_state_j)}

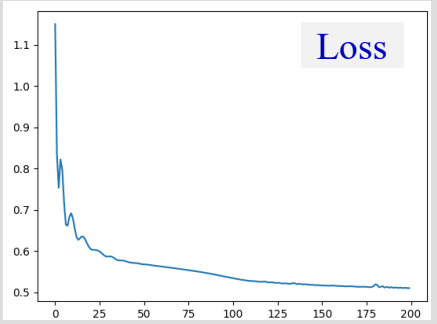
Steps (3),(4) happened to be not needed, final weights are practically the same.

Loss – binary cross-entropy (classification)
Activations – Mish + Sigmoid to get probability

DGL results (preliminary)

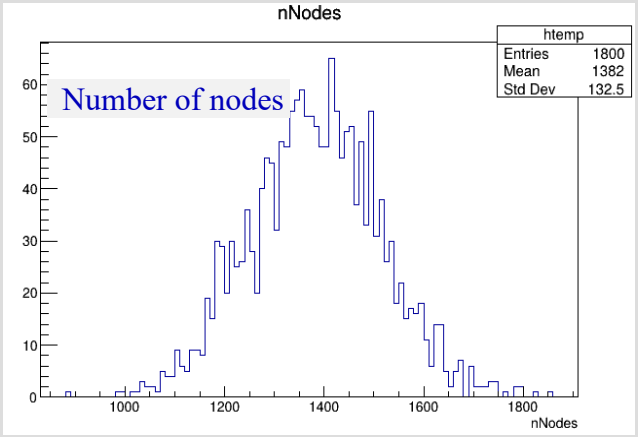
Training: 200 epoch, 100 graphs(events) batch train/test
loss= 0.5098(train), 0.5080(test) – no overtraining

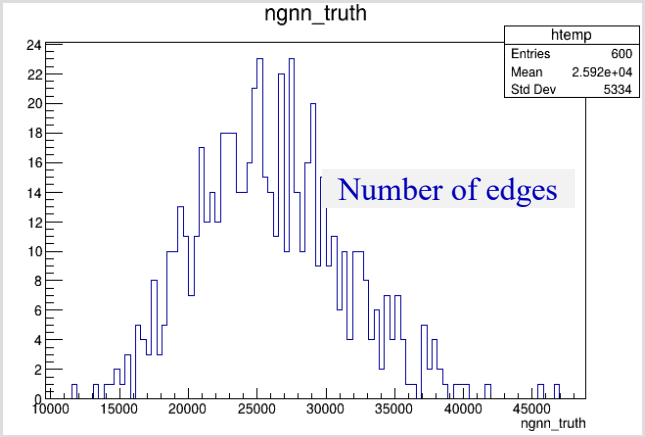




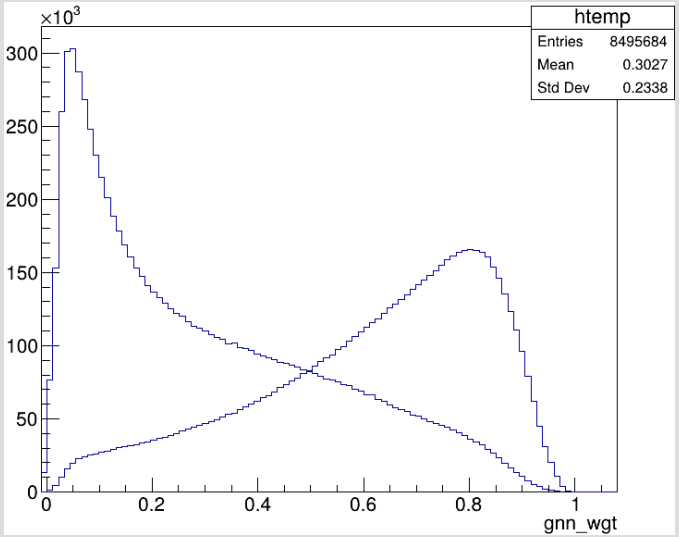
AUC(train)= 0.8265. AUC(test)= 0.8294 for primary+secondary edges. AUC(SVonly)=0.848

For comparison - XGBoost classification of edges based on the same edge features: AUC ~ 0.75



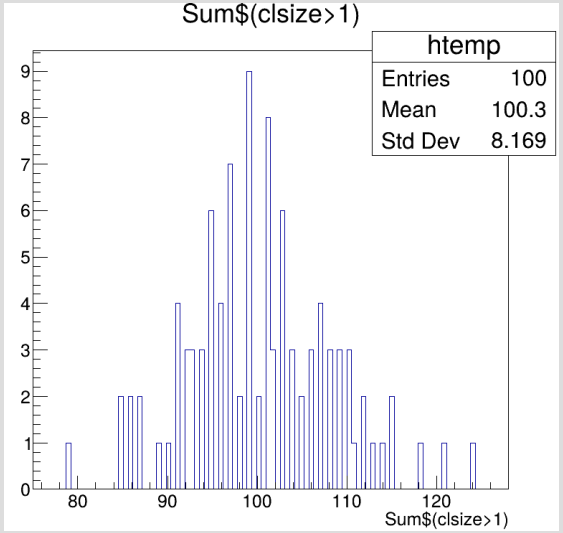


LMC after DGL

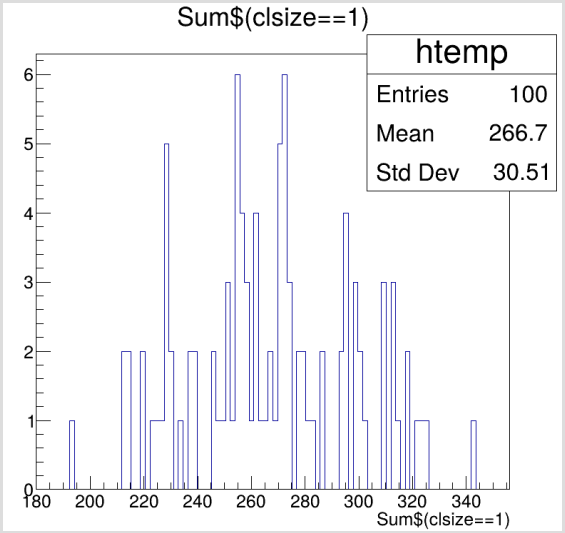


For LMC: weight=WGT_{GNN}-0.5

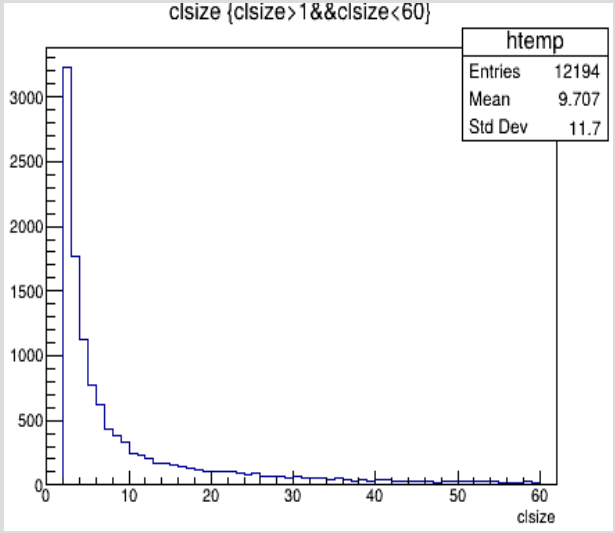
$N_{cluster}$ (size>1)



N_{single_track}

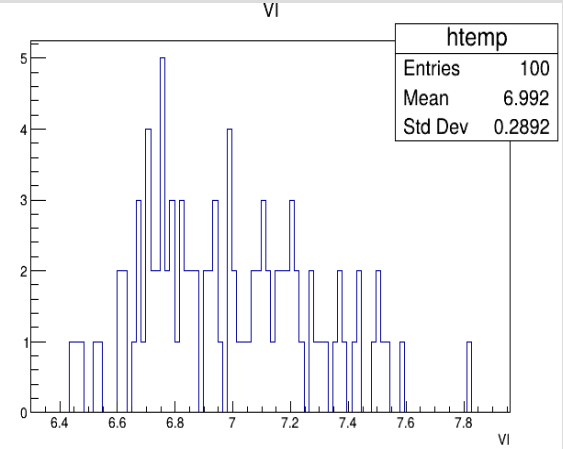


Cluster size

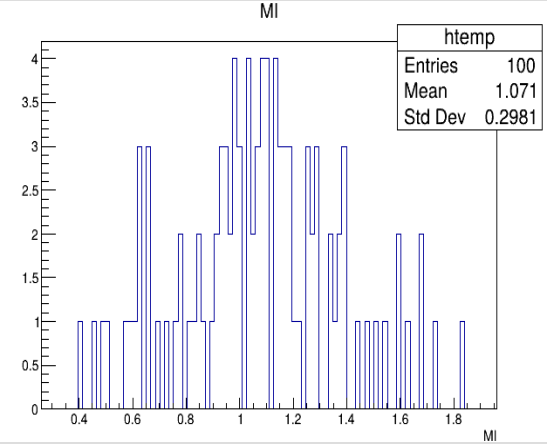


LMC metrics

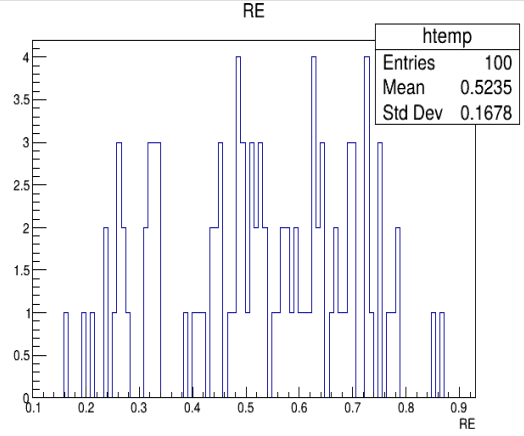
Variation of information



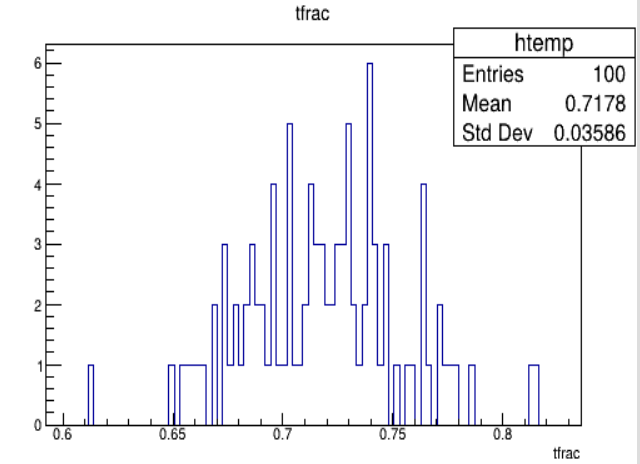
Mutual information



Rand index



Fraction of correctly resolved true edges



Conclusions and next steps

1) Basic machinery for data processing is created and works, although requires polishing/optimisation
2) R&D on GNN layer versions, LMC parameters, constraints, informative problem-dependent metrics, etc. can be started.
3) Constraints – identify fake edges connecting tracks from PV and SV.
   - ❖ First try – bad AUC=0.55. More work is needed.
4) Current technical problems(work in progress):
   a. DGL doesn't export GNN models directly (ONNX?).
      PyTorch backend/export?
   b. UPROOT buffer sizes – limit number of graphs for saving
   c. …

LMC problem

Starting energy: 2097.73

Iter	Total decrease	Pair updates	New sets	Num. of sets
1	2287.43	2286.65	0.784414	515
2	242.296	241.122	1.17428	379
3	55.2082	54.6484	0.559751	348
4	12.1379	11.8518	0.286146	347
5	11.8605	11.5254	0.33507	345
6	12.7867	12.4791	0.307552	323
7	4.79566	4.50951	0.286146	320
8	1.23263	0.94648	0.286146	320
9	2.78869	2.4156	0.373089	320
10	4.56306	4.27692	0.286146	320
11	1.23263	0.94648	0.286146	320
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