Update of SmartBKG --
Improved Selective Background Monte Carlo Simulation at Belle II with Graph Attention Networks and Weighted Events

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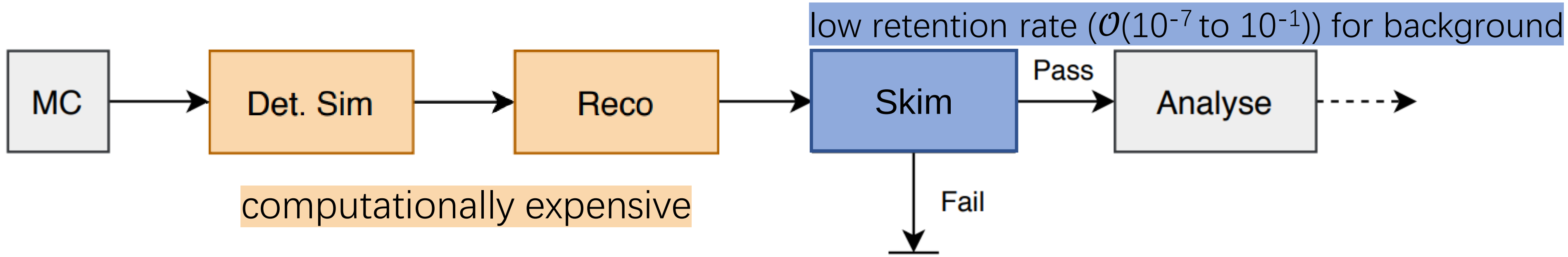
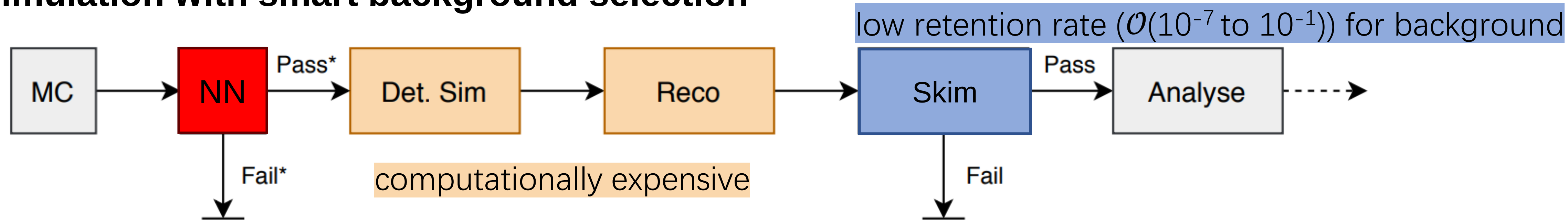
Ludwig-Maximilians-Universität München
ML4Jets, Nov. 06, 2023

Normal Monte Carlo Simulation data flow



Simulation with smart background selection

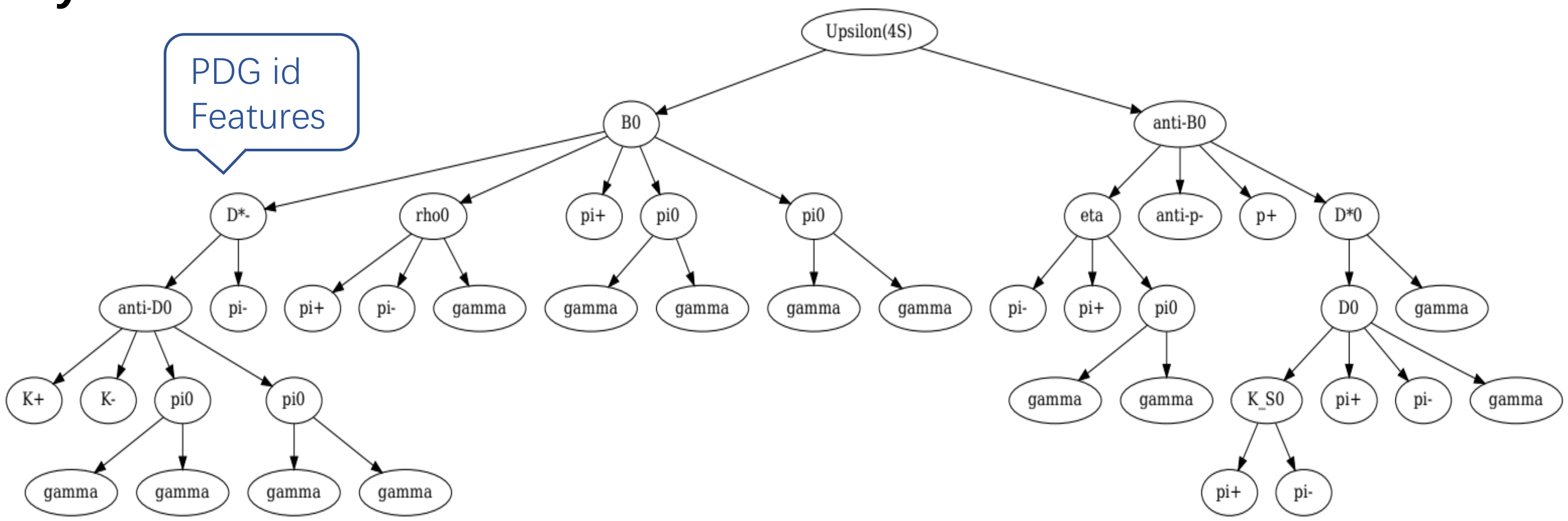


Previous Works:

- **PhD Thesis**: *Hadronic Tag Sensitivity Study of $B \to K^{(*)}\nu\bar{\nu}$ and Selective Background Monte Carlo Simulation at Belle II*, James Kahn, 2019
- **Talk**: *Selective background Monte Carlo simulation at Belle II*, James Kahn, CHEP 2019

Introduction

Tree Structures of Particle Decay
⇅
Graph Neural Network



Dataset:

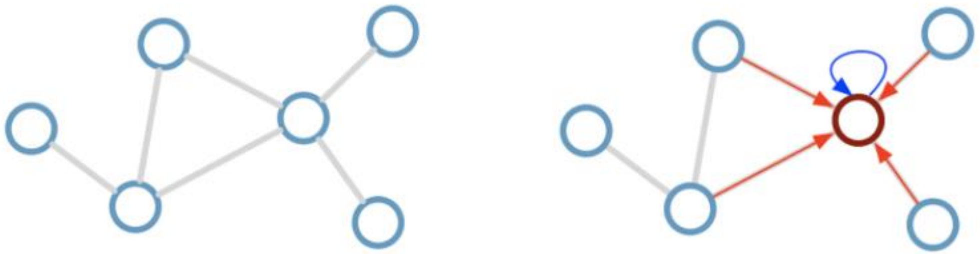
- Each event (each **Graph**):
  - Decay of $\Upsilon(4S) \rightarrow B^0\bar{B}^0$
  - Particles (**Nodes**)
  - Mother/Daughter relations (two way **Edges**) + self loops
  - Each particle (each **Node**)
    - **PDG** id
    - 8 **Features**: **Production time**, **Energy**, **Position** (3d), **Momentum** (3d)
- **Label** per event: Pass/Fail after the skims
  ⋆ FEI Hadronic B0, retention rate 4.25%
- Other event level **attributions** for further analysis: e.g. $\boldsymbol{M_{bc}}$ etc.

Previous NN

Updating node features:

Graph Convolutional Networks (GCN)

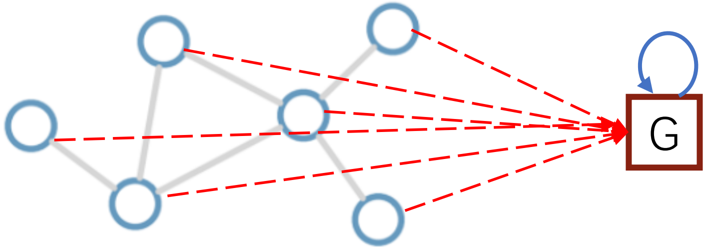
-> Graph structure remains



Updating global features:

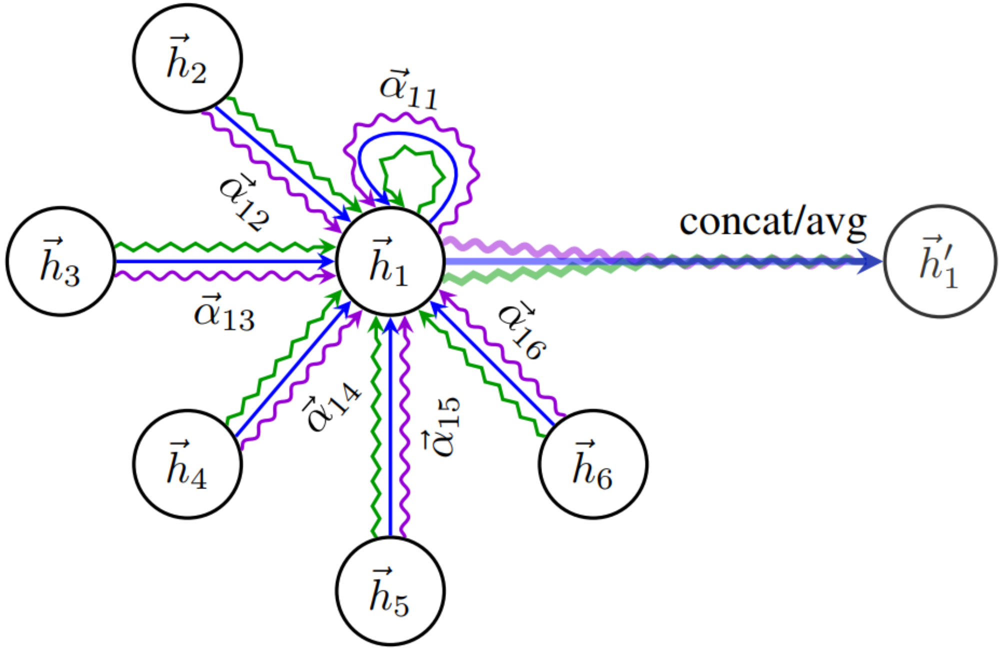
Global Average Pooling

-> Graph structure degenerated

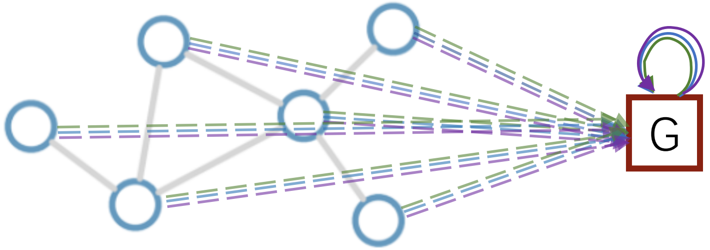


Improvement with attention mechanism

Graph Attention Networks (GAT)
-> Graph structure remains



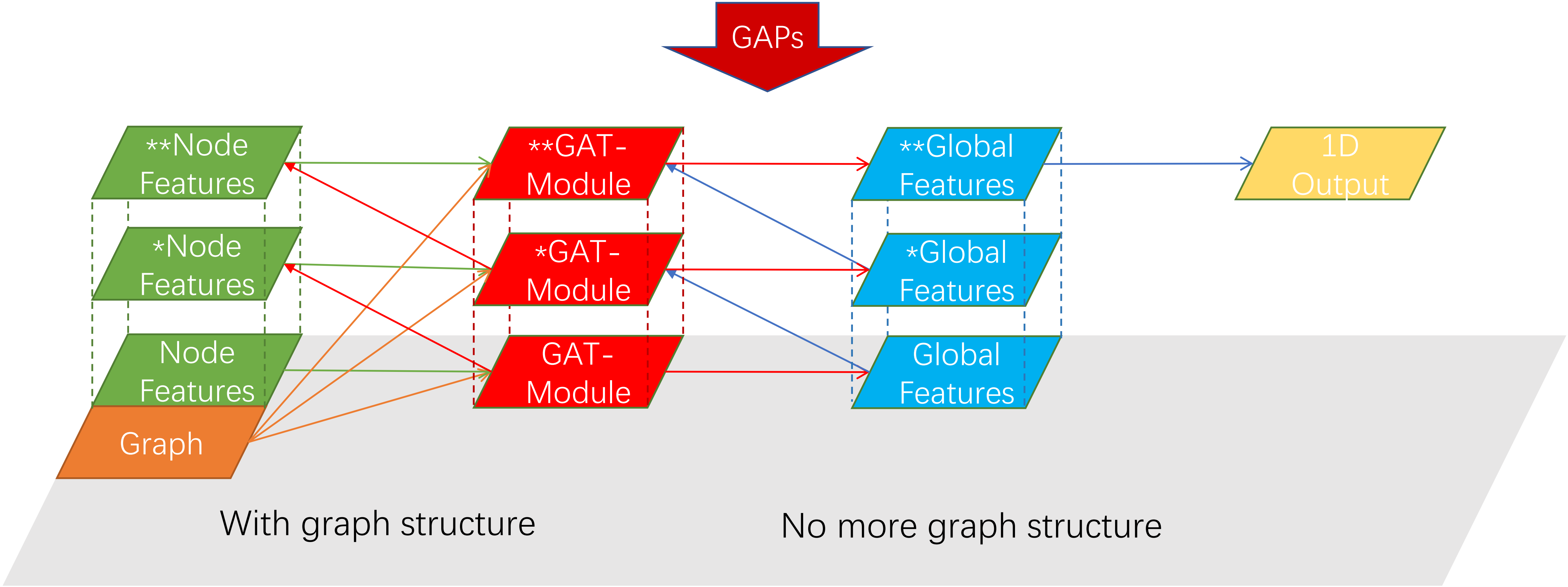
Global Attention Pooling (GAP)
-> Graph structure degenerated



Each head (color) represents a different set of attention weights

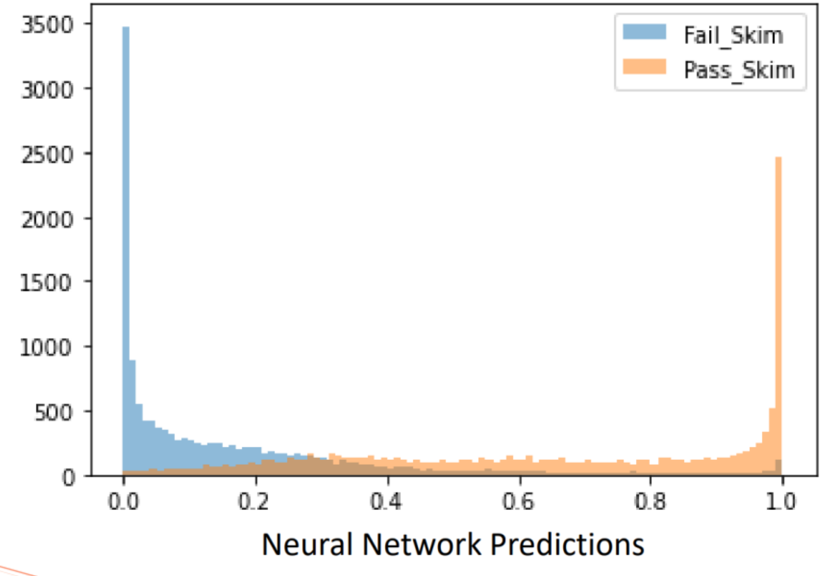
NN Structure

Final Architecture:
GAT+GAP

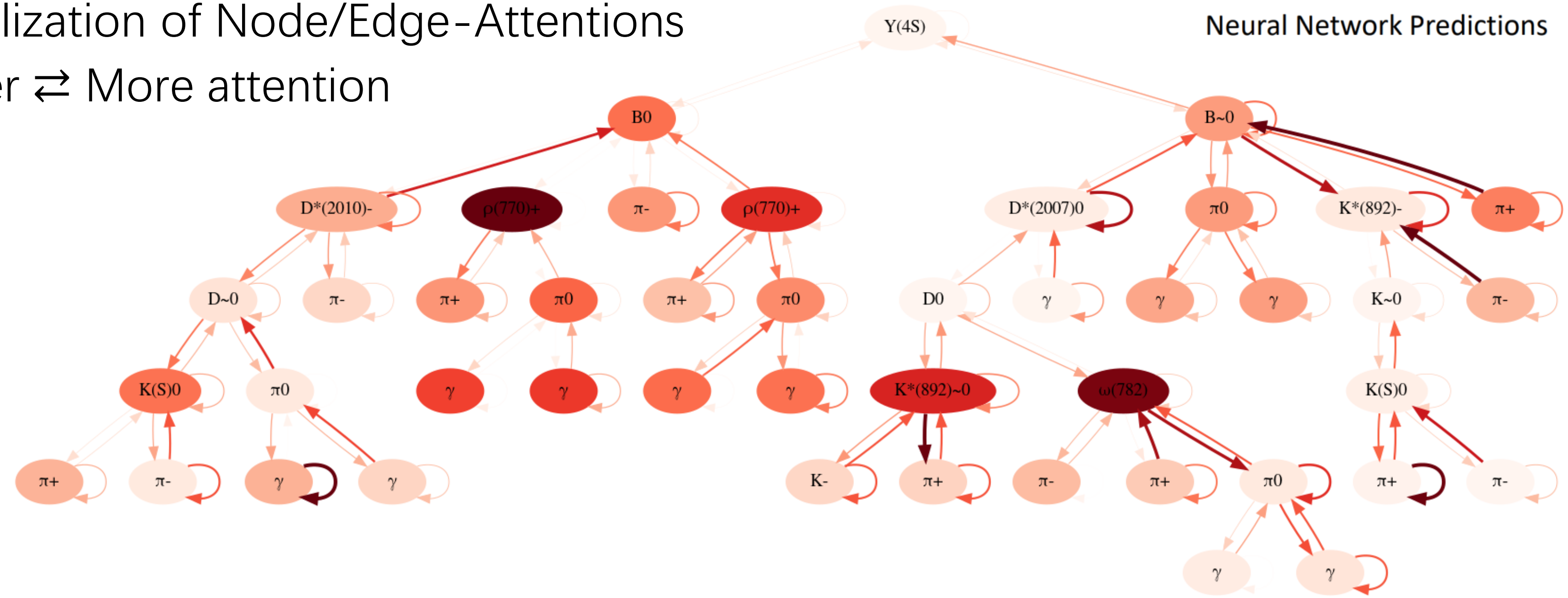


NN Performance

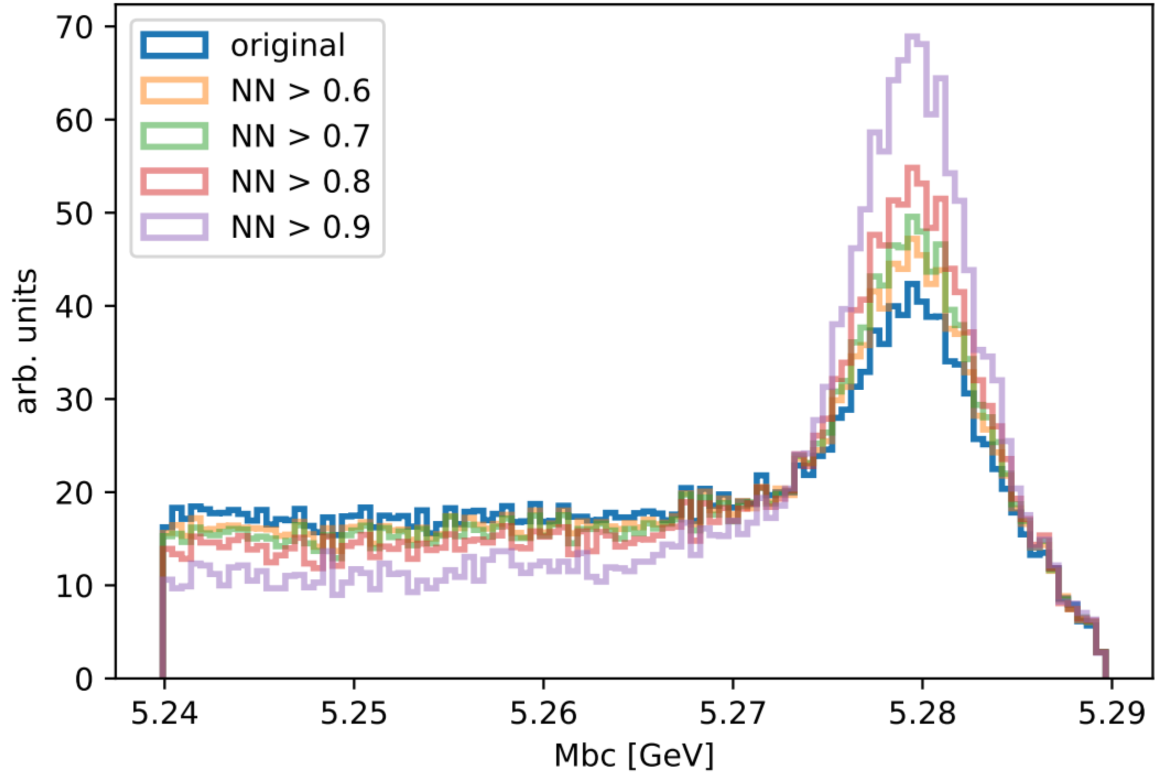
- Best AUC* improved from 0.9083 to 0.9122
  * Area under the Curve of ROC
  (The closer to 1 the better)



- Visualization of Node/Edge-Attentions
  Darker ⇄ More attention



Bias due to False-Negatives with Naive Filtering



Skim \ NN	Positive	Negative
Pass	True-Positive (TP)	**False-Negative (FN)**
Fail	False-Positive (FP)	True-Negative (TN)

Weighting

	Importance Sampling	Reweighting Method	Reject Sampling
Use of NN output	As probability to keep event randomly	As score for selection according to fix threshold	Sample in accordance with the score distribution of true positive events relative to the entire dataset.
Weight	Inverse of NN output	Decided with the help of another classifier	-
Loss to train NN	Speedup	Binary cross entropy	Binary cross entropy

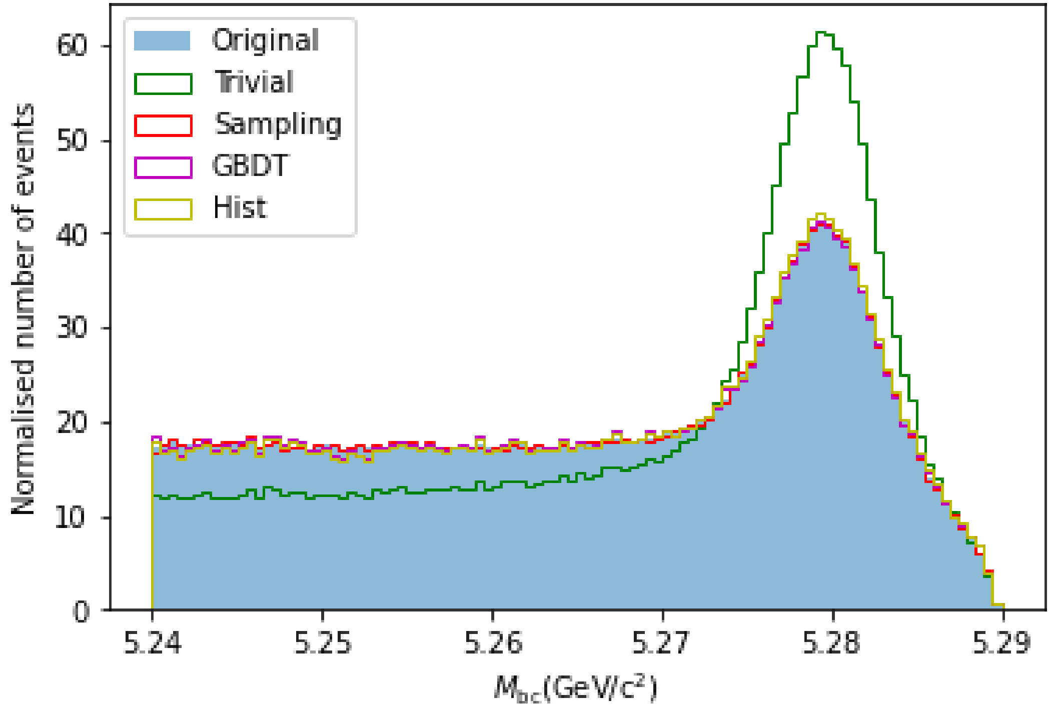
Metric: Speedup

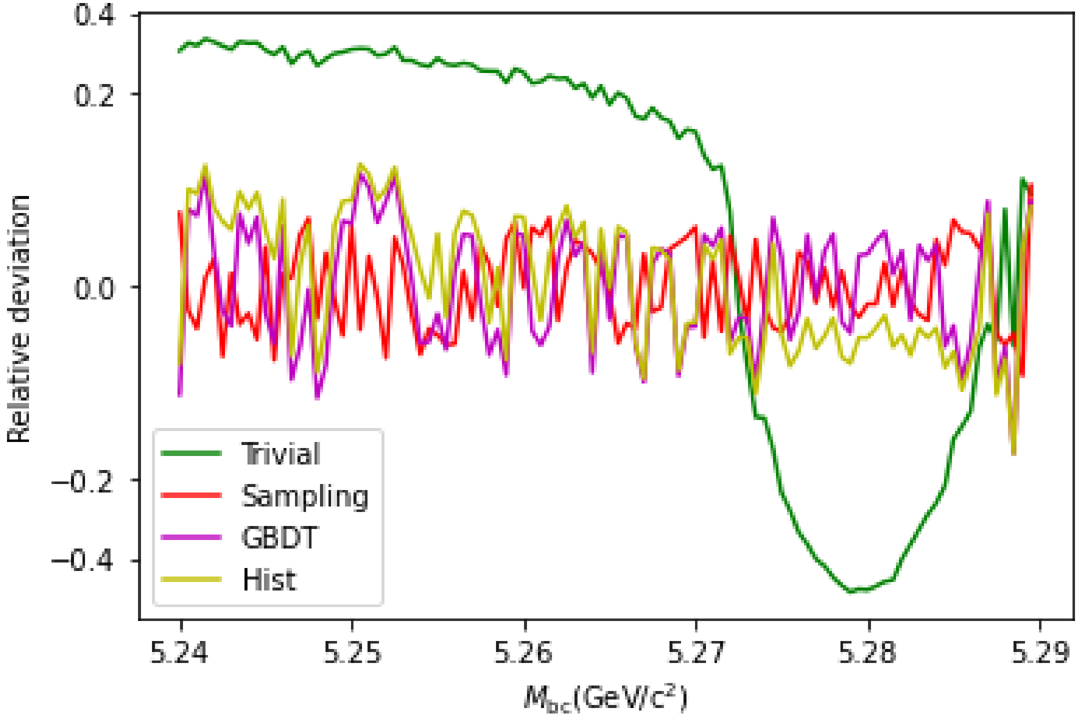
--Improvement of computation time to produce the same effective sample size with the help of NN filter:

Speedup: $s = \frac{t_{no\_filter}}{t_{filter}}$

Effective Sample Size: $N_{eff} = \frac{(\sum \omega_i)^2}{\sum \omega_i^2}$

Weighting performance

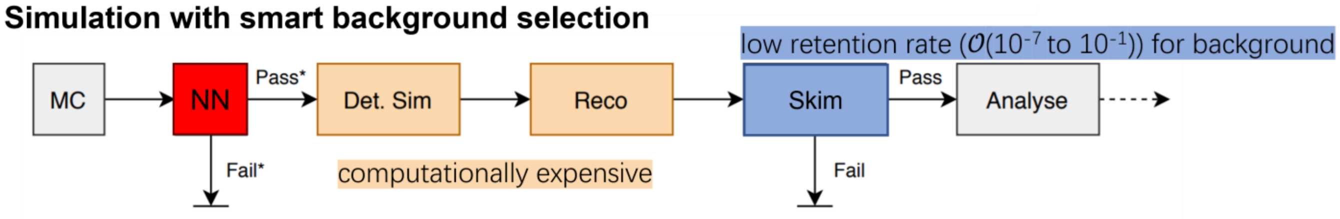




	Importance	Reweighting	Reject (ongoing)
Maximum speedup	2.0	6.5	~3.2
Bias	No bias	Small bias on some of the variables	Small bias on some of the variables

Practice

Test the module using $B^+ \to K^+\nu\nu$ inclusive reconstruction:



$B^+ \to K^+\nu\nu$ inclusive	skim.WGs.ewp	SmartBKG
Datasets	Run full chain with charged generic MC	Train: Charged generic MC14 Test: Run full chain with charged generic MC and SmartBKG
Process (Time measurement)	• DetSim & Rec • Skim • ROE • Y(4S) Reconstruction	• NN Prediction & Importance Sampling • DetSim & Rec (Test only) • Skim • ROE • Y(4S) Reconstruction
Sample sizes	0.5M	Train: 1.7M Test: 0.5M
Retention rate	3.68%	16.1% (True-Positive-Rate: 60.4%)
Speedup	-	Theoretical during training: 2.09 Measured in practice: 1.92

Summary

Conclusion:

- Attention mechanism can improve NN performance for selective background monte carlo simulation
- Bias is avoided with importance sampling method while a speedup of factor 2 can still be maintained
- Reweighting method can reach much higher speedup up to 6.5 but will still have some bias in the variables that are not used in the training of the extra classifier
- Reject sampling has a speedup around 3 and doesn’t bring any weights. But the bias and stability have to be studied

Current:

- Study of reject sampling

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Thank You for your Attention

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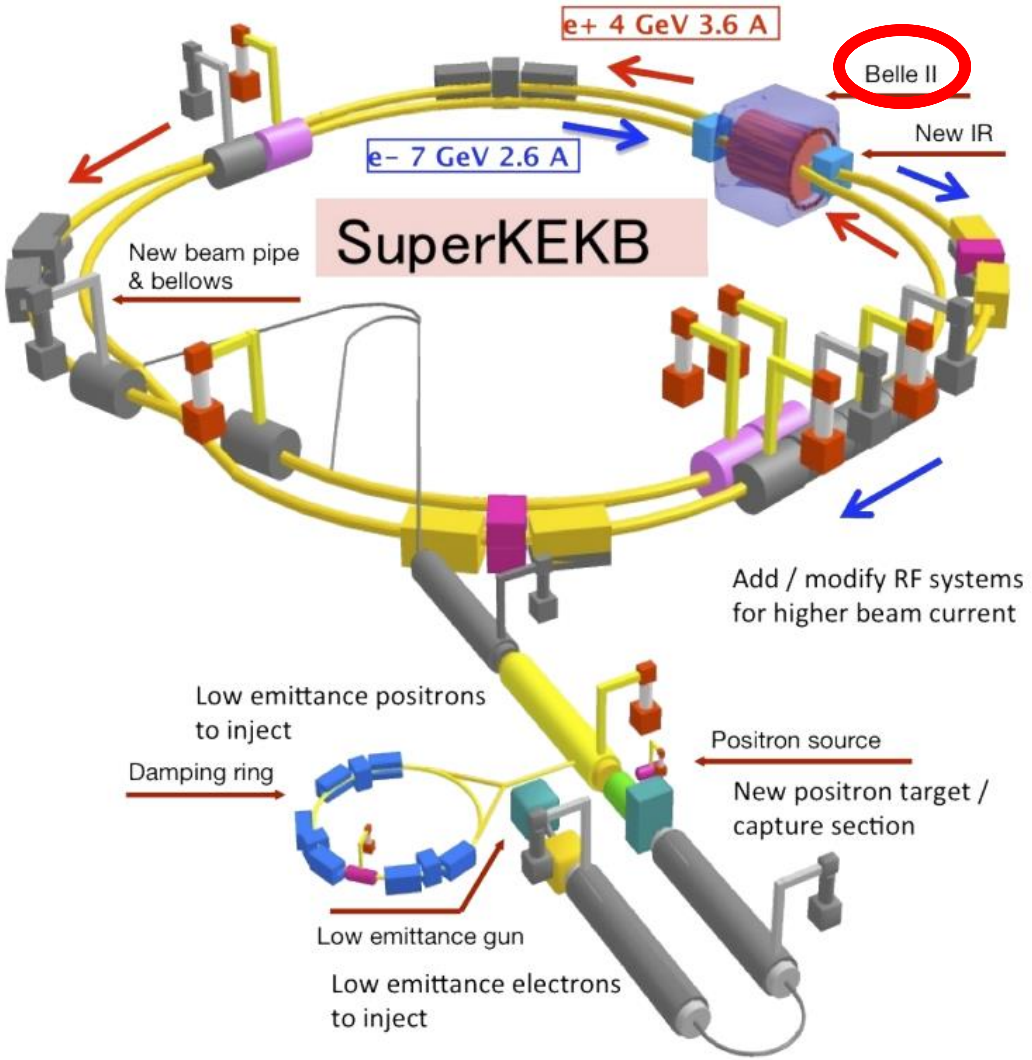
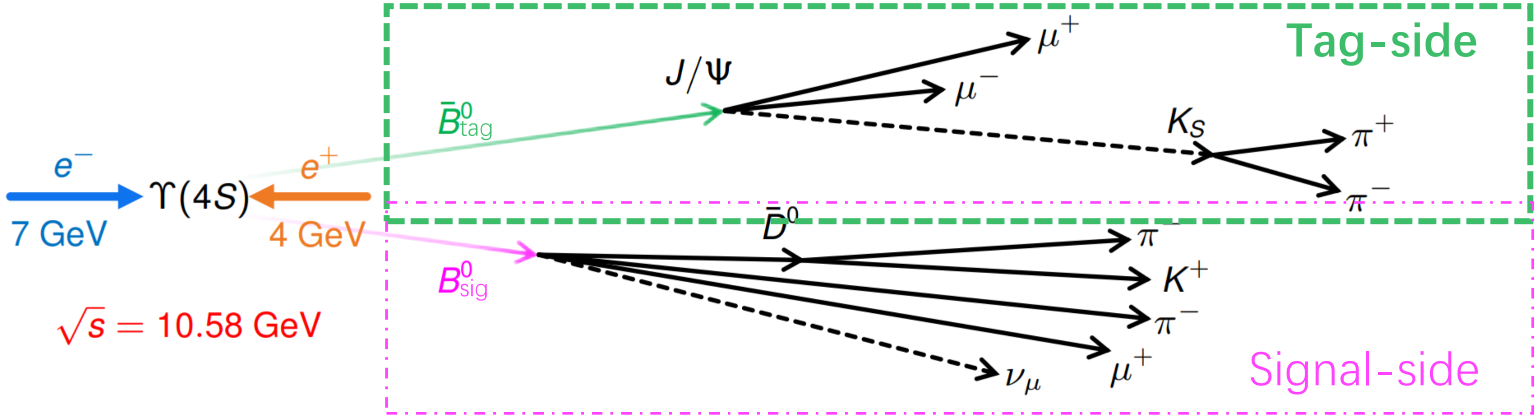
Backup

Belle II Experiment:

- At SuperKEKB
  - Electron-positron collider
  - Centre-of-momentum energy close to the mass of $Y(4S)$ resonance to mainly produce B mesons
  - Located in Tsukuba, Japan
- Detector for reconstruction and identification of charged and neutral particles
- Search for new physics
- World's highest luminosity
- Huge MC dataset for analysis



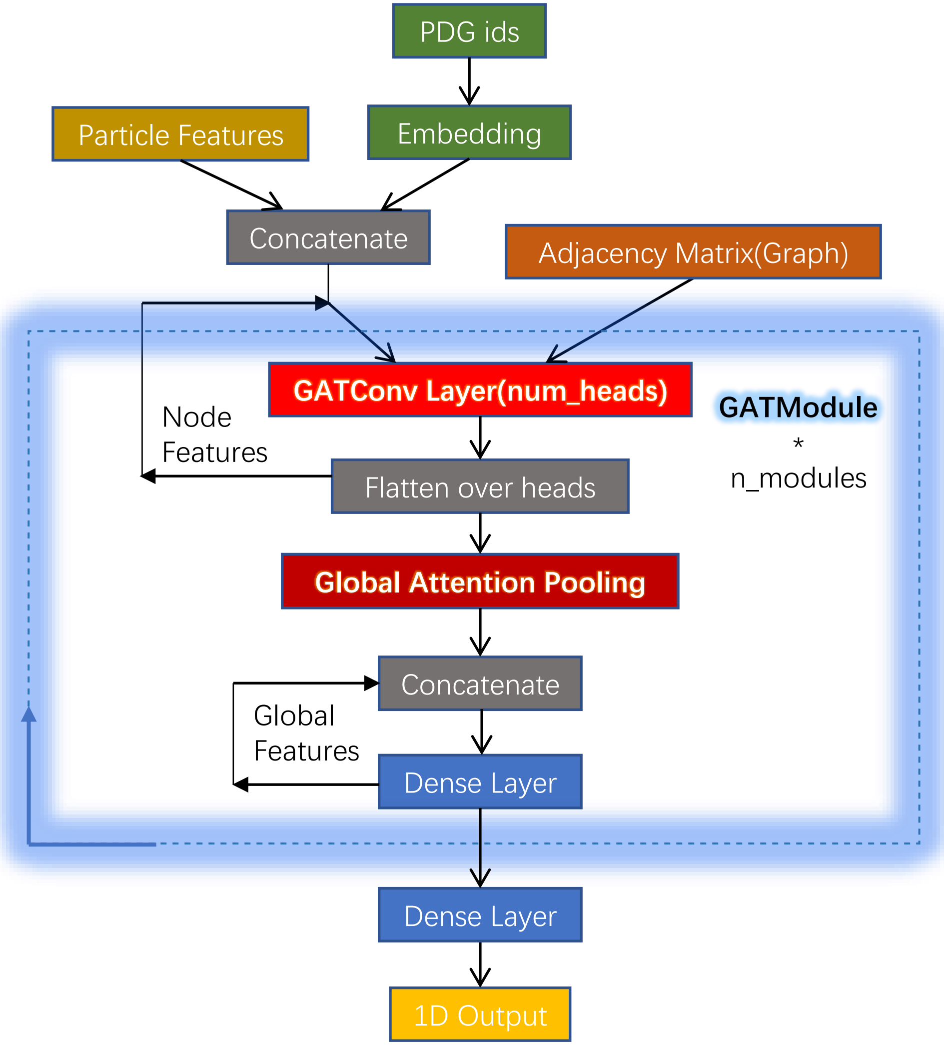
Tagging method:

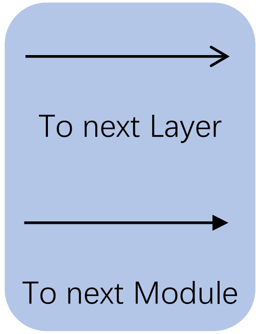


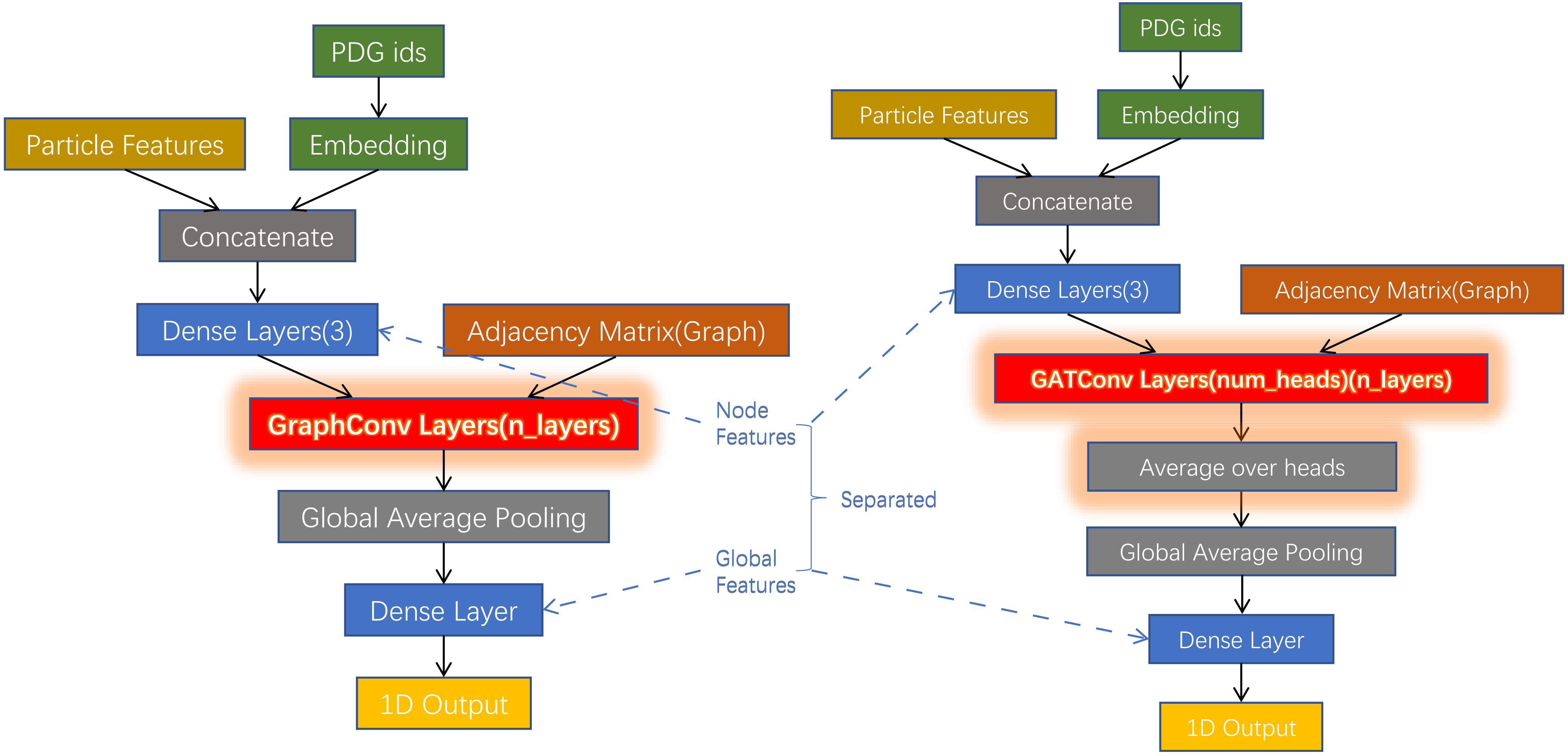
Retention rate after reconstruction and selection of tag-side B candidate:

FEI Skim	Hadronic B^+	Hadronic B^0
Mixed ($\Upsilon(4s) \to B^0\bar{B}^0$)	5.62%	4.25%

Final Architecture:
GAT+GAP

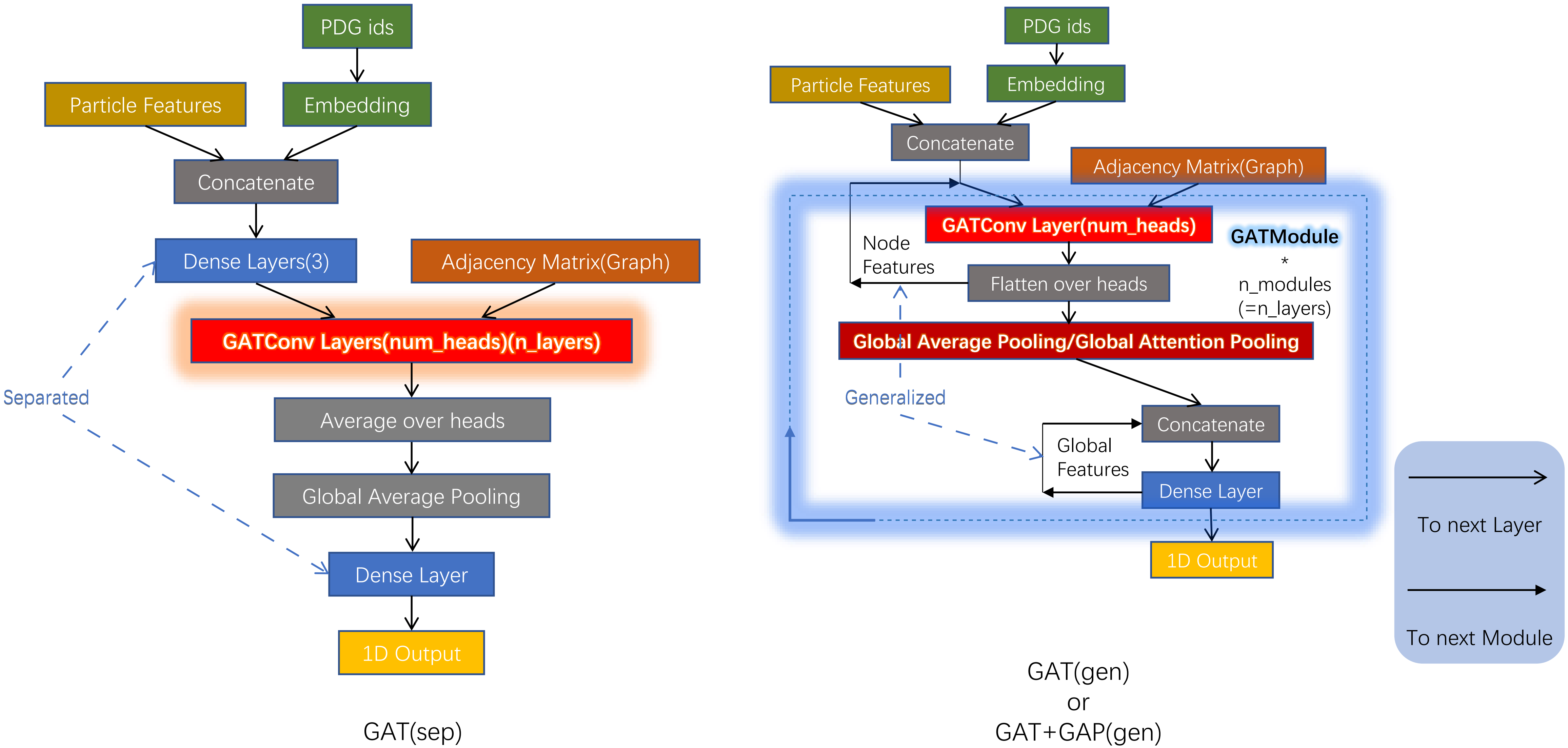




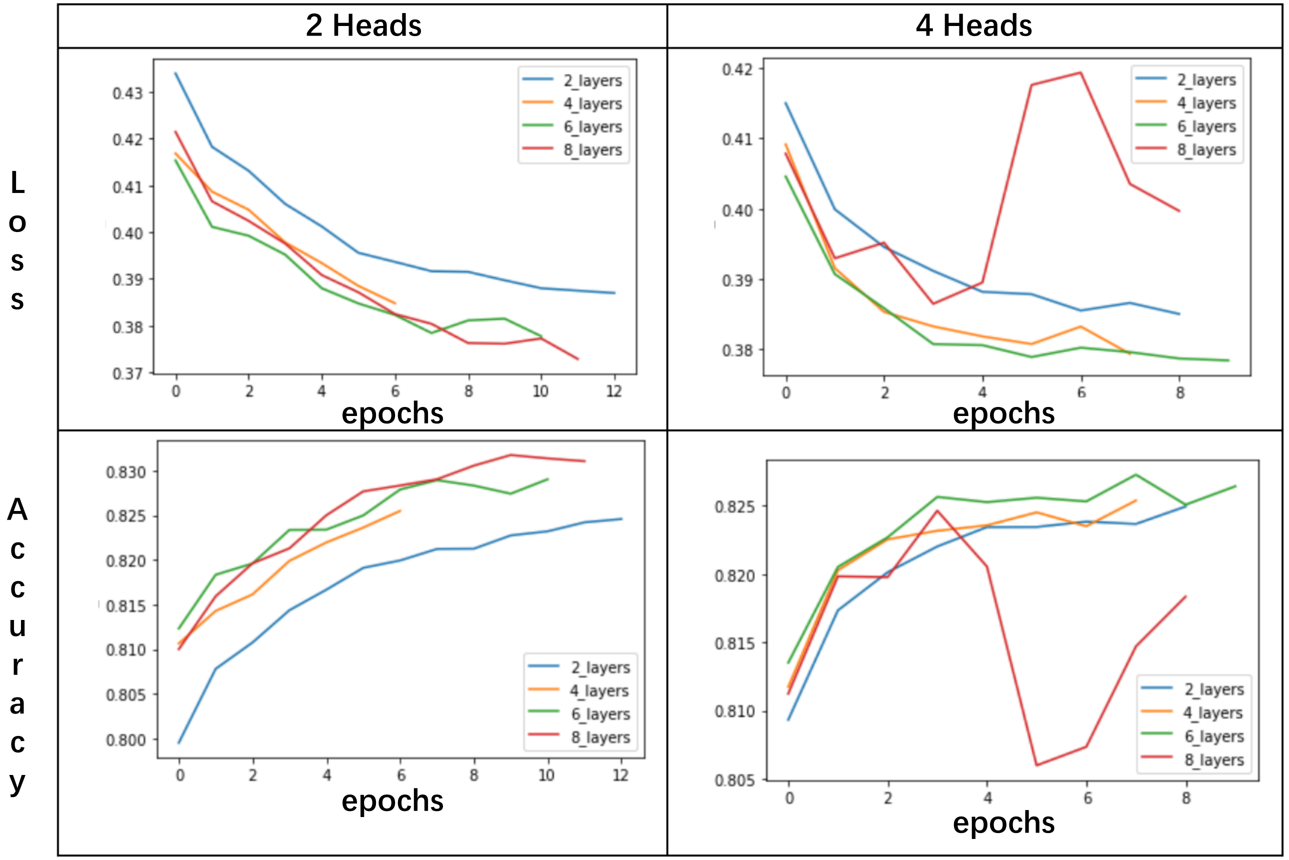


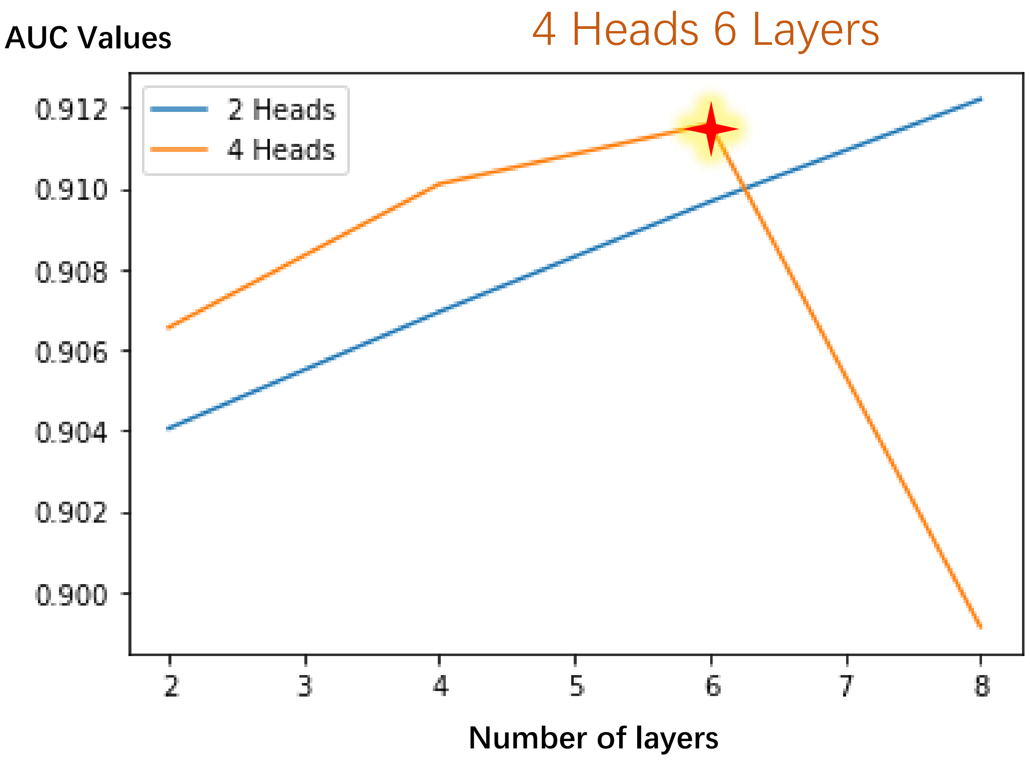
GCN(sep)

GAT(sep)


PDG ids
Particle Features
Embedding
Concatenate
Dense Layers(3)
Adjacency Matrix(Graph)
GATConv Layers(num_heads)(n_layers)
Separated
Average over heads
Global Average Pooling
Dense Layer
1D Output
GAT(sep)
PDG ids
Particle Features
Embedding
Concatenate
Adjacency Matrix(Graph)
GATConv Layer(num_heads)
GATModule
*
n_modules
(=n_layers)
Node
Features
Flatten over heads
Global Average Pooling/Global Attention Pooling
Generalized
Concatenate
Global
Features
Dense Layer
1D Output
To next Layer
To next Module
GAT(gen)
or
GAT+GAP(gen)

Quantitative Studies





Comparison

Parameters:

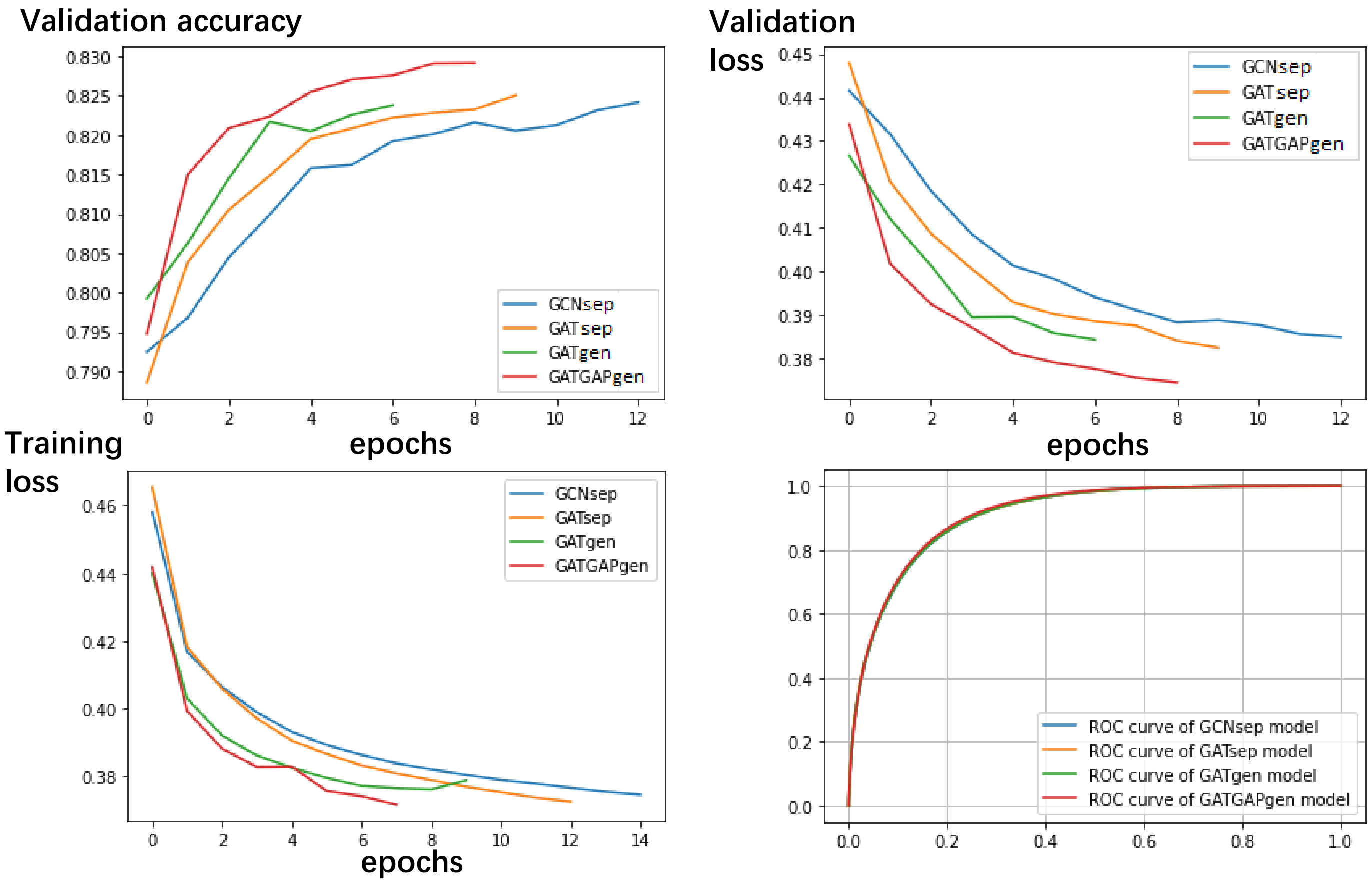
- n_heads = 4
- n_layers = 6
- n_units = 128
- batch_size = 128
- n_train = 0.9M
- n_val = 0.1M
- n_test = 0.5M

Loss:

- Entropy

EarlyStopping:

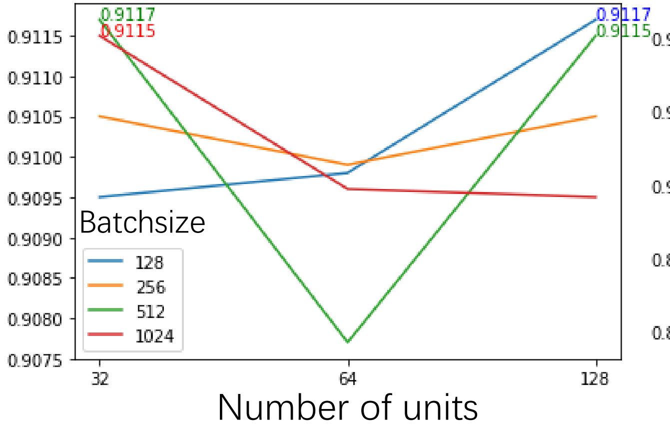
- patience = 3
- delta = 1e-5



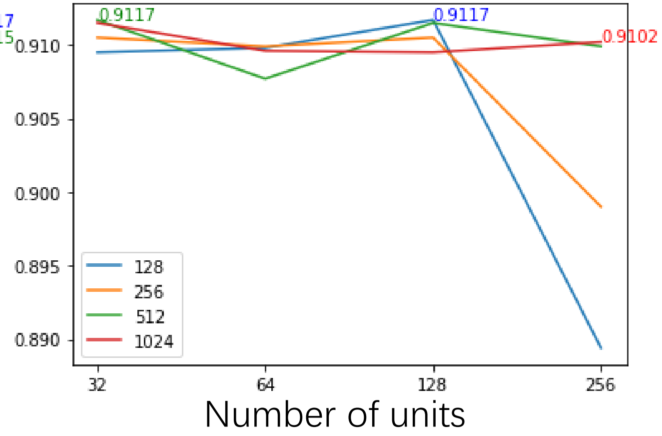
	GCN(sep)	GAT(sep)	GAT(gen)	GAT+GAP(gen)
TrainingTime	3619.46s	4047.47s	3471.48s	5049.81s
AUCValues	0.90831	0.90937	0.90891	0.91216

Grid Search

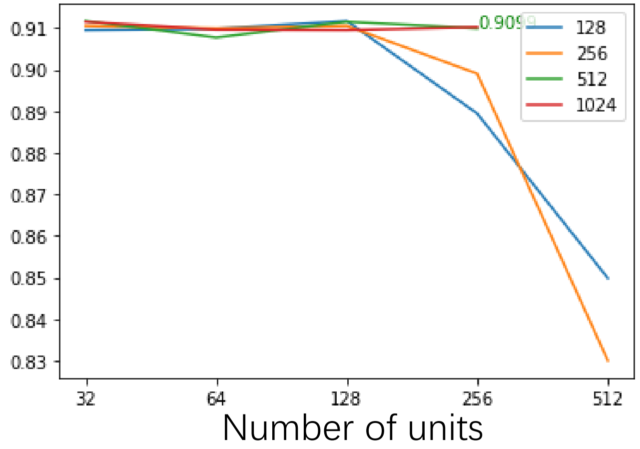
AUC



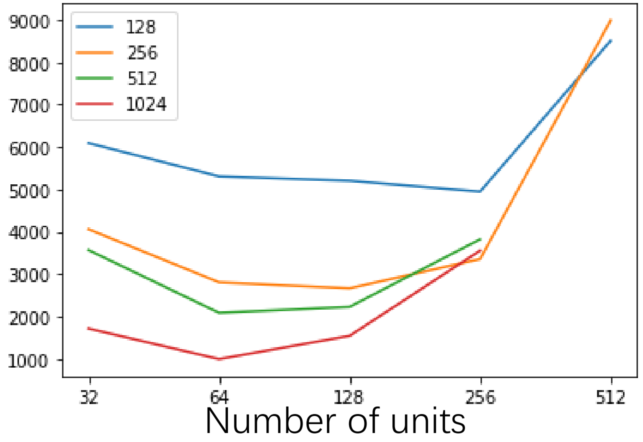
AUC



AUC



Training Time



Best Combinations

Batch-size	Number of units	AUC	Training Time
128	128	0.9117	5205
256	32	0.9105	4061
256	128	0.9105	2666
512	32	0.9117	3568
512	128	0.9115	2228
1024	32	0.9115	1716
1024	256	0.9102	3556

Network Sizes

# Units	# Parameters
32	120,527
64	459,951
128	1,808,495
256	7,184,367
512	28,651,247

Hyperparameter Optimization

Model	AUC
GCN(sep)	0.908
GAT(sep)	0.909
GAT(gen)	0.909
GATGAP(gen)	0.912

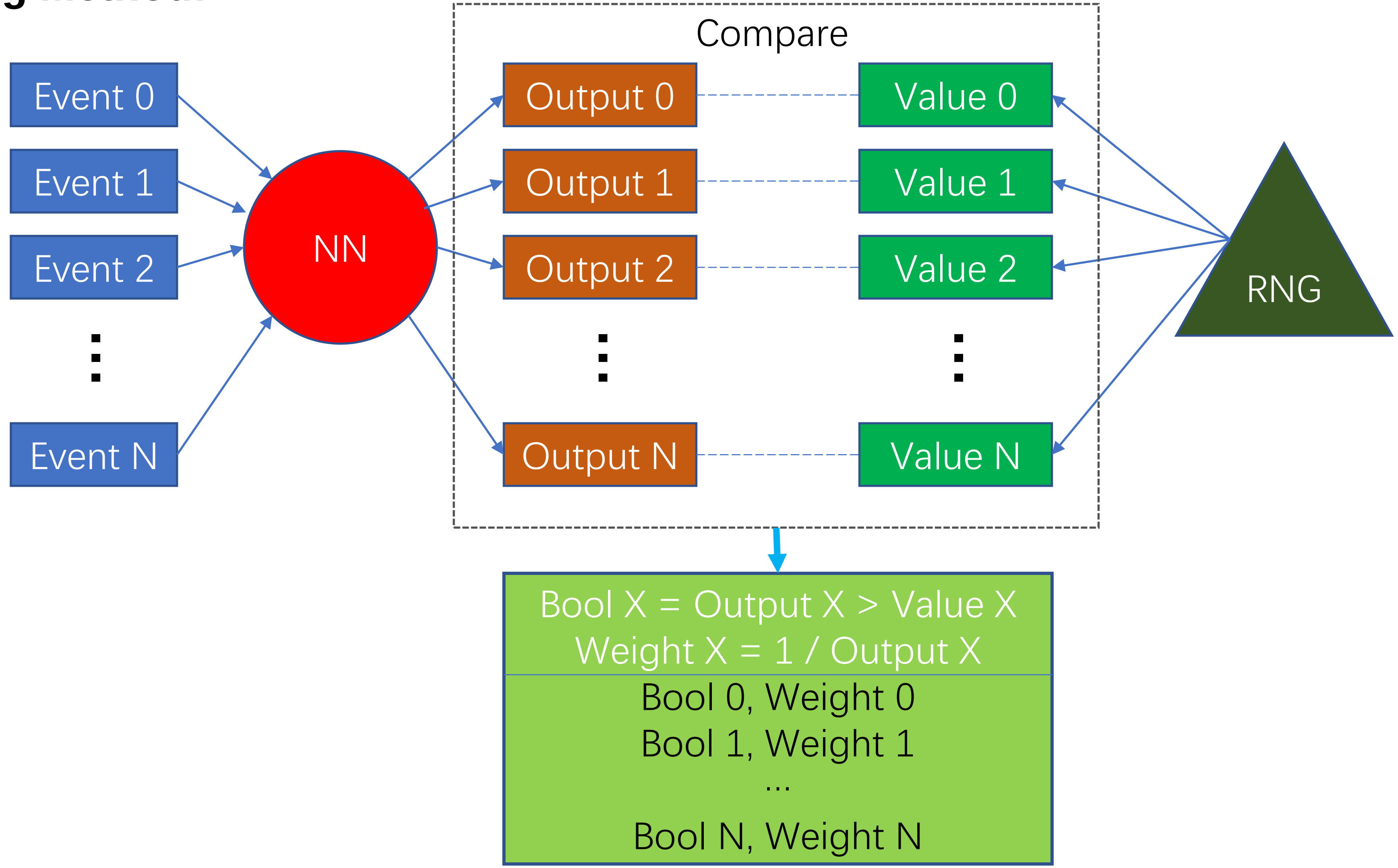
Batch Size	Number of Units	AUC	Training Time in s
128	16	0.9131	10940
512	32	0.9117	3568
128	128	0.9117	5205
1024	32	0.9115	1716
512	128	0.9115	2228
256	128	0.9115	2666
256	32	0.9115	4061

Number of Units	Number of Parameters
16	34,911
32	120,527
64	459,951
128	1,808,495

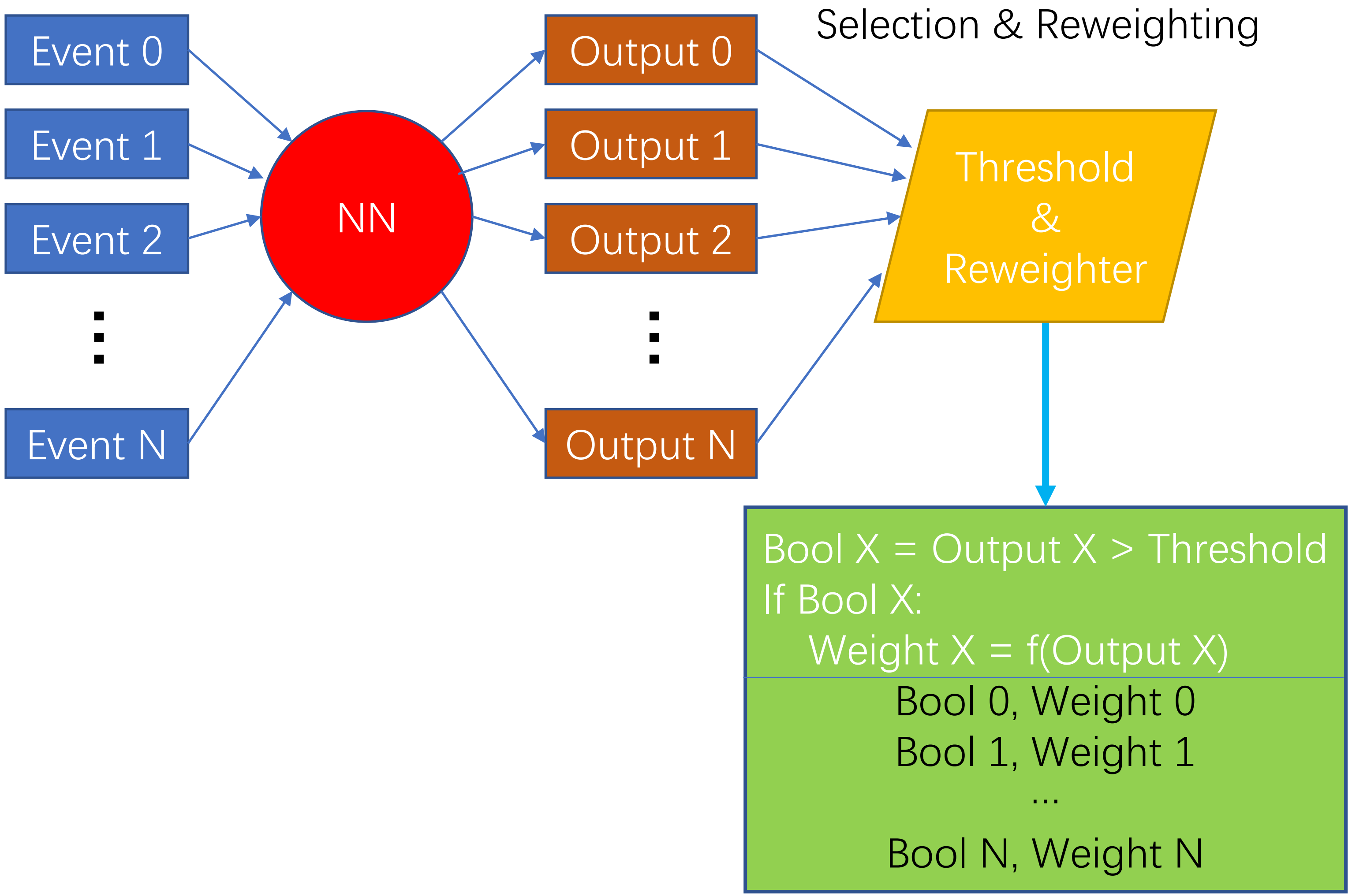
Final Configuration:

- GATGAP Model using PyTorch + Deep Graph Library (DGL)
- 6 layers with 4 attention heads each and 32 units for GAT output & global features
  -> ≈ 120k parameters
- Batch size 1024 (GPU training)

Sampling Method:



Reweighting Method:



Studied reweighters:

- GBDT Reweighting
- Histogram Reweighting

Reweighting Method:

- Train a Gradient Boosting Decision Tree (GBDT) classifier with some event level variables to distinguish between True-Positve events and False-Negative events
- GBDT Reweighting: use the outputs of the classifier directly:

$$w = \frac{1}{p_{clf}} = \frac{1}{p_{TP}/p_{TP+FN}} = \frac{p_{pass\_skim}}{p_{TP}}$$

- Histogram Reweighting: compare the score histogram of all the events that can pass the skim (True-Positive + False-Negative) with the score histogram of True-Positives to give each bin of score a scaling factor:

$$w = w_{bin_i}|_{p_{clf} \in bin_i} = \frac{H_{pass\_skim,i}}{H_{TP,i}}|_{p_{clf} \in bin_i}$$

Skim \ NN	Positive	Negative
Pass	True-Positive (TP)	False-Negative (FN)
Fail	False-Positive (FP)	True-Negative (TN)

Relative statistical uncertainty and effective sample size

Variable	Formula	Remark
NN outputs / Probabilities to pass	$\{p_i\}$	‘i‘ refers to each event in the whole sample (batch)
Weights	$\{\omega_i\} = \left\{\frac{1}{p_i}\right\}$	Infinities (at $p_i = 0$) are excluded and set to 0 Avoid the bias by construction
Relative statistical uncertainty	$S = \frac{\sqrt{\sum \omega_i^2 p_i}}{\sum \omega_i p_i}$	$\sum \omega_i^2 p_i = \sum \omega_i$ $\sum \omega_i p_i = N$ Here consider only passed events (label = 1)
Effective sample size	$N_{eff} = \frac{1}{S^2}$	Number of events needed to reach **the same statistical uncertainty without sampling**

Speedup rate

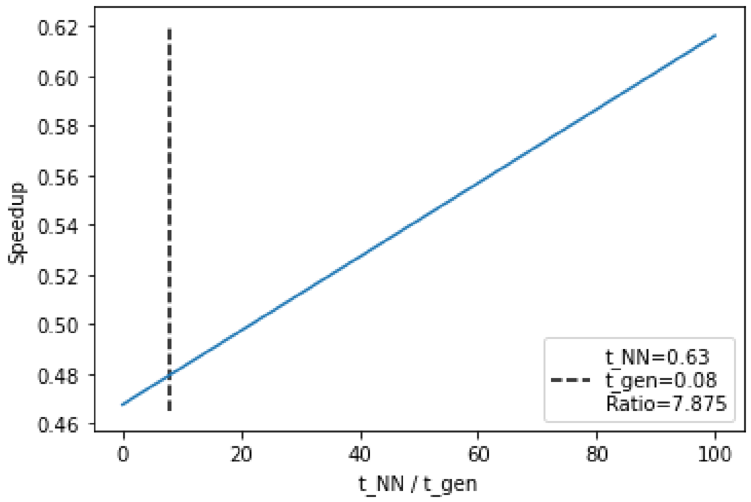
Variable	Formula	Remark
Skim retention rate	$r = 0.05$	Probability to pass the skim process
Times of different phases in ms	$t_{gen} = 0.08$ $t_{NN} = 0.63$ $t_{SR} = 97.04$	Taken from previous studies
Effective number of events after sampling	$n_+ = \sum p_i$ $n_- = \sum (1 - p_i)$	$\{p_i\}$ will be devided into two subsets where the events will/won't pass the skim process
Time consuming with NN filter	$t_+ = [n_{TP} r + n_{FP}(1-r)]\left(t_{gen} + t_{NN} + t_{SR}\right)$ $t_- = [n_{FN} r + n_{TN}(1-r)]\left(t_{gen} + t_{NN}\right)$	Positive/Negative: Result of sampling True/False: Result of sampling == skim process
Time consuming without NN	$t_0 = N_{eff}\left(t_{gen} + t_{NN}\right)$	To reach the same statistical uncertainty
(Inverse) Speedup rate	$R = \frac{t_+ + t_-}{t_0}$	The lower the better

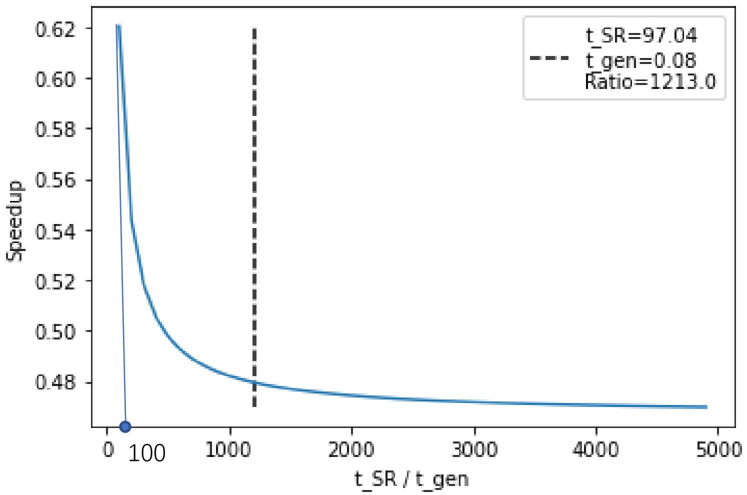
Robustness:

Weak dependency of **Speedup** on $\boldsymbol{t_{NN}}$ and $\boldsymbol{t_{SR}}$

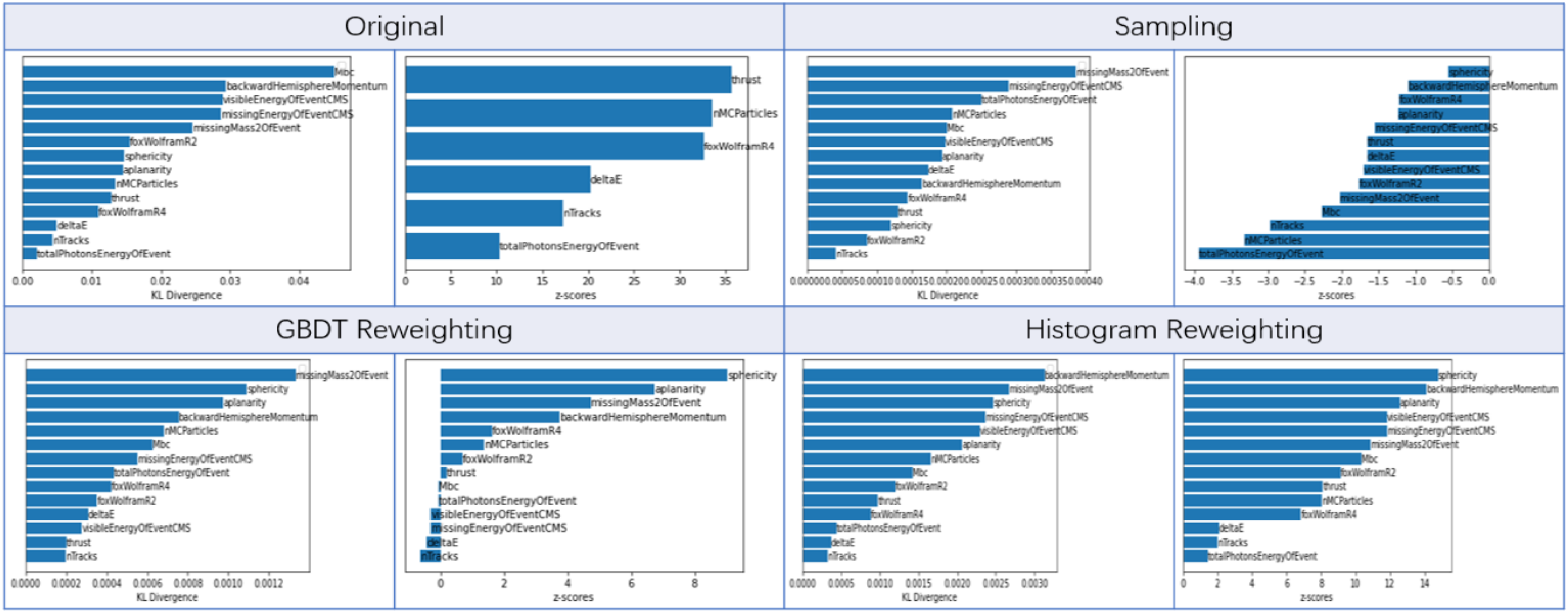
↓

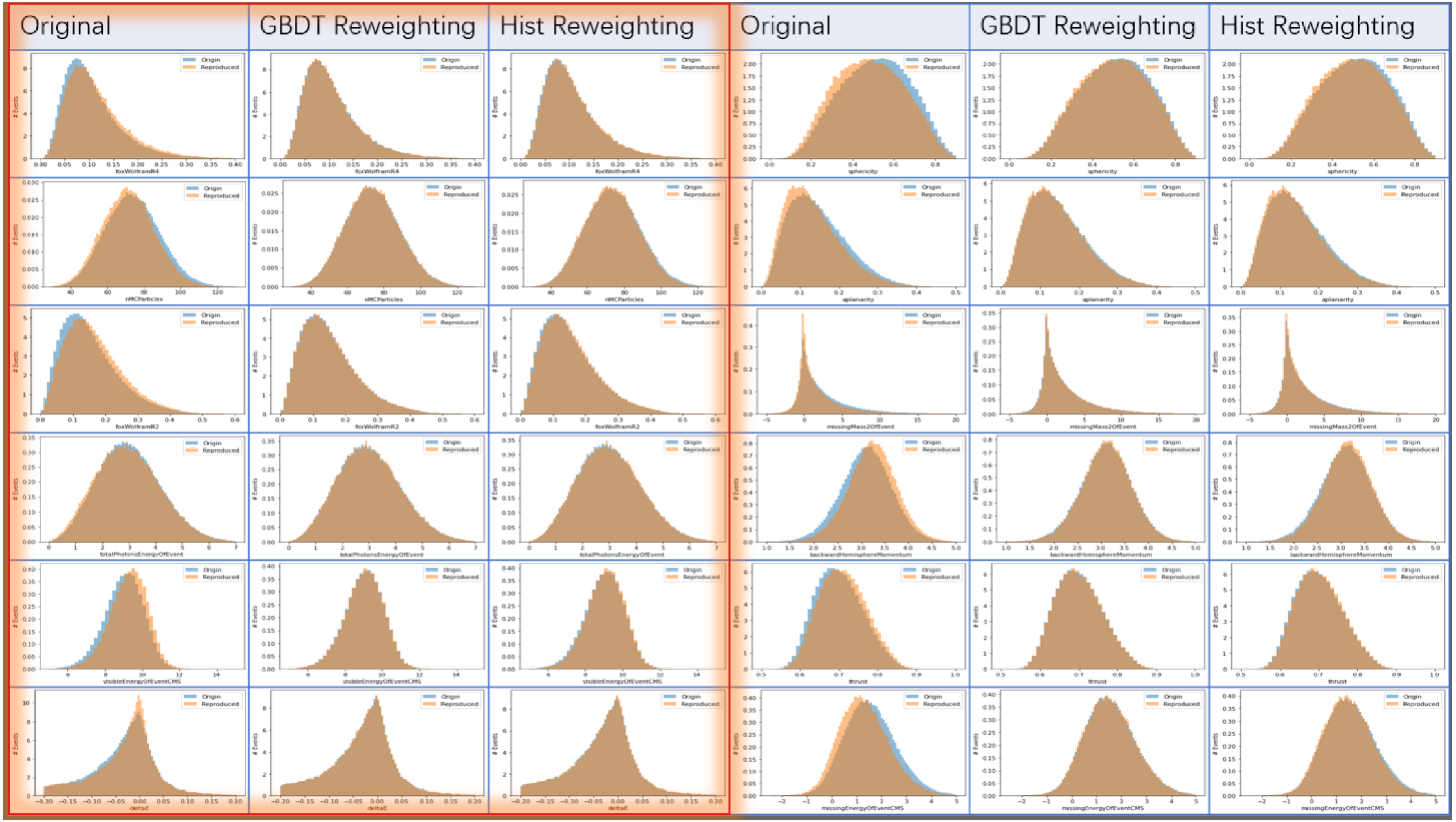
Safe to generalize



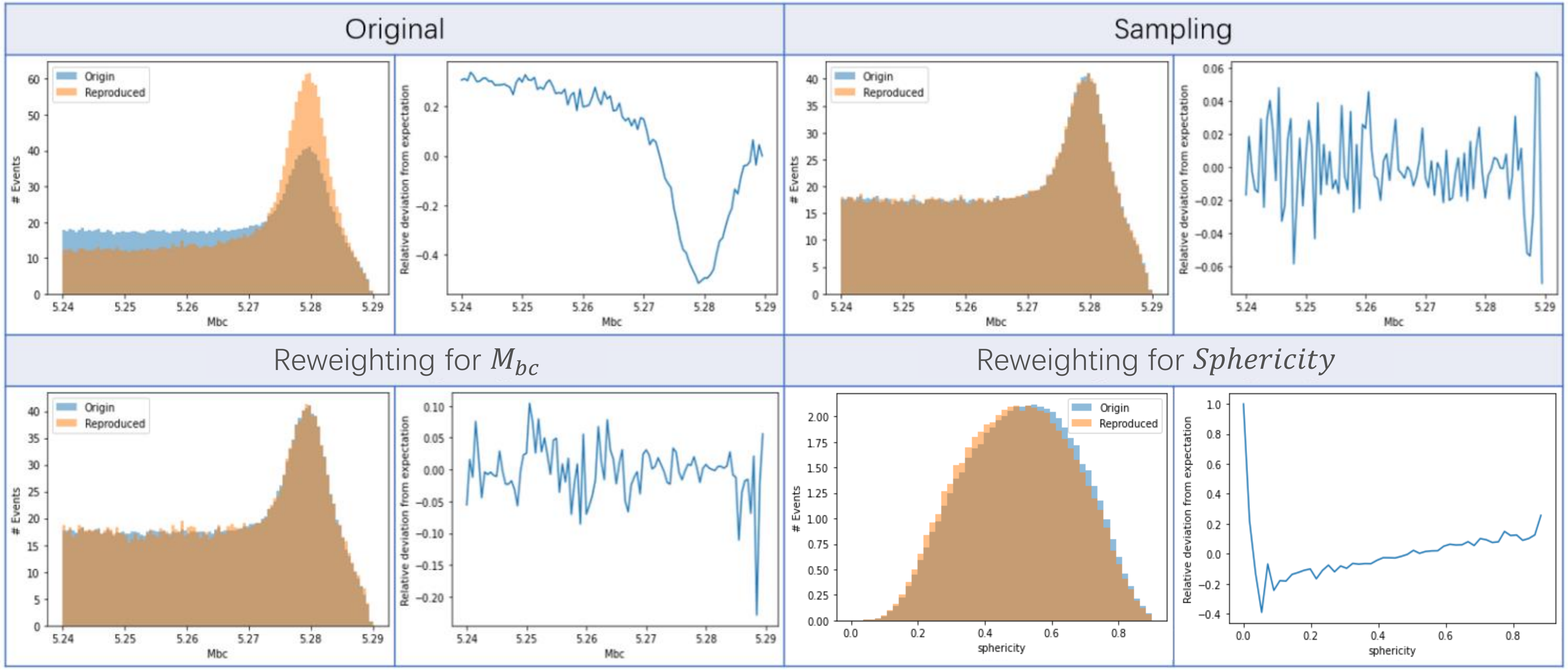


KS-Test

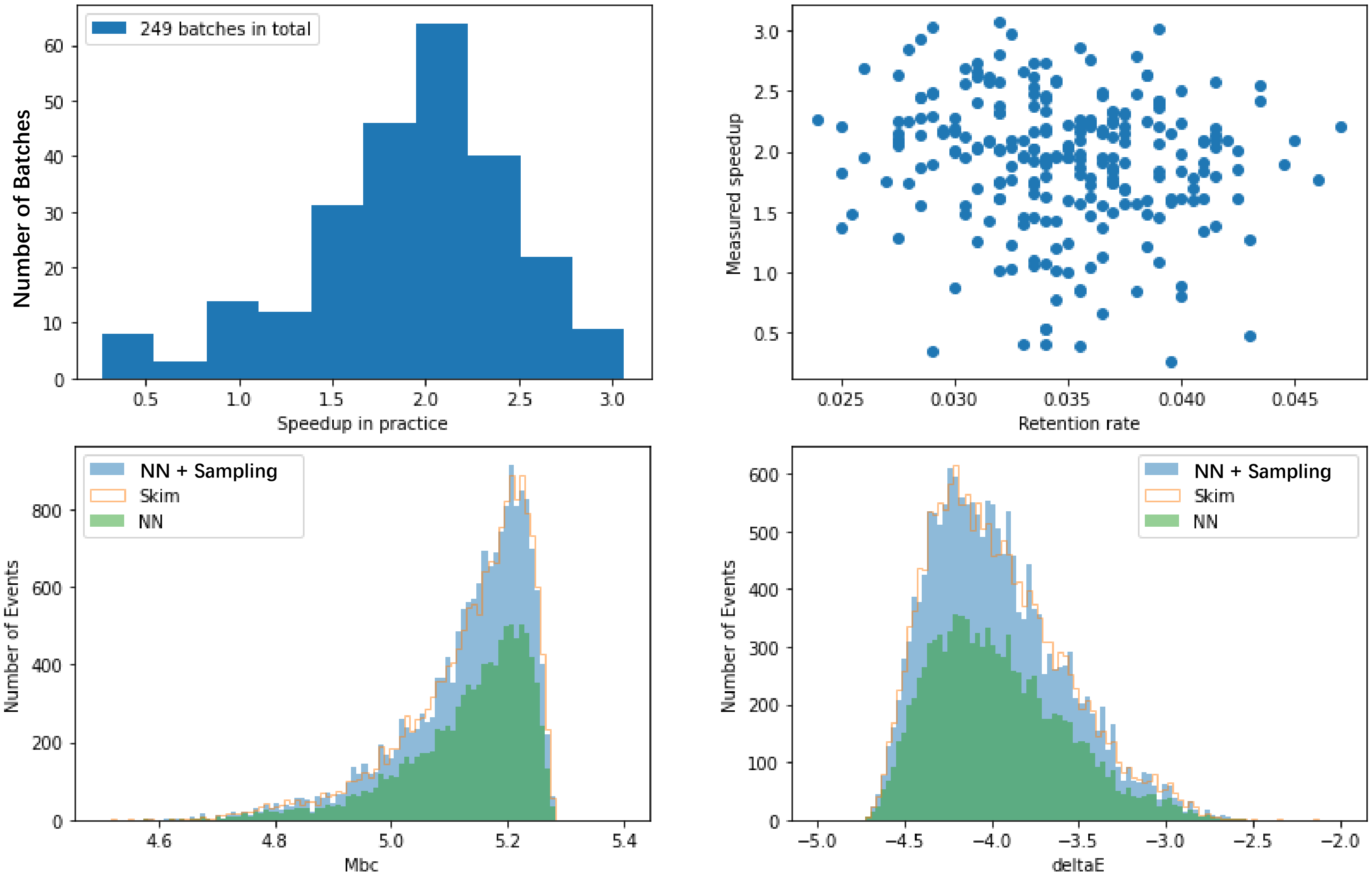

Original
Sampling
GBDT Reweighting
Histogram Reweighting
KL Divergence
z-scores
KL Divergence
z-scores
KL Divergence
z-scores
KL Divergence
z-scores



Original
GBDT Reweighting
Hist Reweighting
Original
GBDT Reweighting
Hist Reweighting
Origin
Reproduced
Events
foxWolframR4
nMCParticles
foxWolframR2
totalPhotonsEnergyOfEvent
visibleEnergyOfEventCMS
deltaE
sphericity
aplanarity
missingMass2OfEvent
backwardHemisphereMomentum
thrust
missingEnergyOfEventCMS


Original
Sampling
Reweighting for M_{bc}
Reweighting for $Sphericity$
Origin
Reproduced
Events
Relative deviation from expectation
Mbc
sphericity

Test the module using $B^+ \to K^+\nu\nu$ inclusive reconstruction



skim.WGs.ewp.inclusiveBplusToKplusNuNu

- Track cleanup:
  - p_t > 0.1
  - thetaInCDCAcceptance
  - dr<0.5 and abs(dz)<3.0
- Event cleanup:
  - 3 < nCleanedTracks < 11
- Kaon pre-cuts:
  - track cleanup + event cleanup + nPXDHits > 0
- **K+ reconstruction**
- Kaon cuts:
  - p_t rank=1
  - kaonID>0.01
- **B+ reconstruction**
- B+ cut:
  - mva_identifier: MVAFastBDT_InclusiveBplusToKplusNuNu_Skim > 0.5