DeepTreeGAN

Fast Generation of High Dimensional Point Clouds for Calorimeter Simulation

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The DeGeSim Project

HELMHOLTZAI
ARTIFICIAL INTELLIGENCE
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RWTH AACHEN UNIVERSITY

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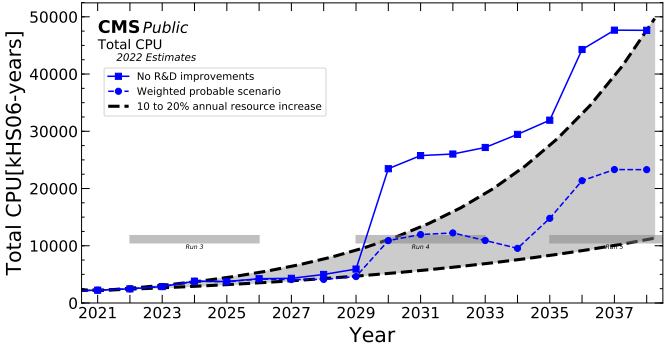
DESY.

Computing Challenge

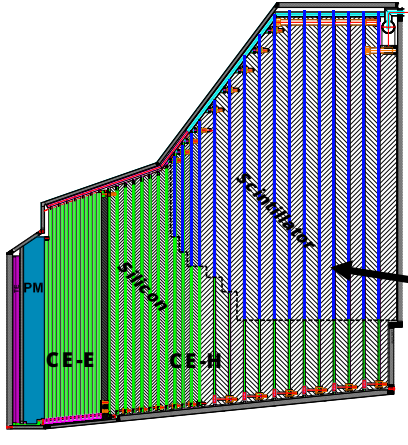


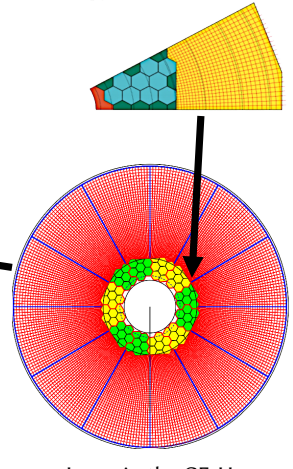
CPU time requirements [CMS-NOTE-2022-008]

- High Luminosity Phase
  - More particles to simulate
- Calorimeters w/ higher granularity – More cells
  - Complex and time-consuming simulations

⇒ Increase in computing time beyond the expected increase in resources.

The HGCAL





Interaction Point

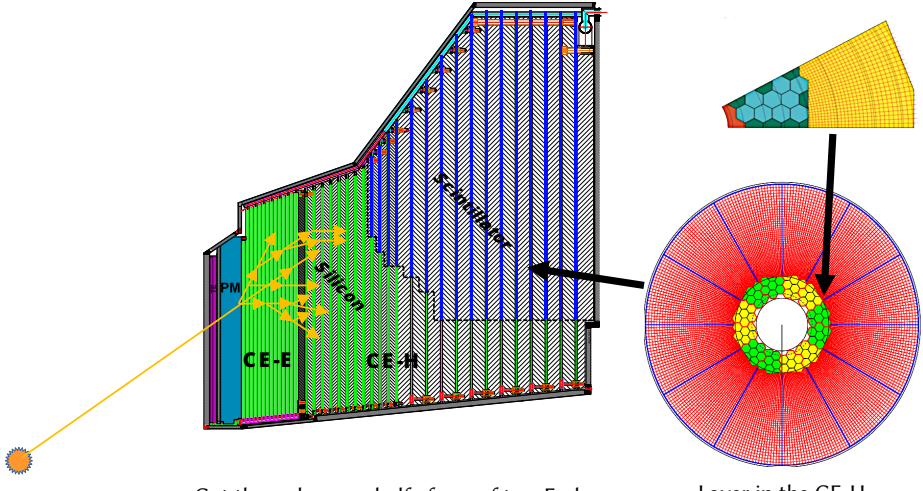
Cut through upper half of one of two Endcaps

Both endcaps: > 6M cells

Layer in the CE-H

All Pictures: CMS-TDR-019

The HGCAL



Interaction Point

Cut through upper half of one of two Endcaps

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Layer in the CE-H

All Pictures: CMS-TDR-019

Goal

»Provide a generative model for the particle showers in the CMS HGCAL«

Challenges:

- Irregular geometry
- Number of channels
- Sparsity

⇒ No ML powerful enough model yet

⇒ Data structure: Point Clouds (PCs)

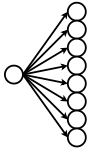
Generator

Core challenge: Upsampling Point Clouds

Same for GAN/VAE/Diffusion+UNet

Dimensionality: 1 Photon @ 300 GeV: up to ≈2k Hits× 5 [E,t,x,y,z]

Naive approach:
(with feedforward neural networks (FNNs))

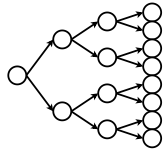


> Latent Vector ⟶ FFN ⟶ PCs

⇒ Number of parameters explodes

⇒ Not trainable

DeepTreeGAN:
(Inspired by TreeGAN `arXiv:1905.06292`)



> FFN projects one particle to multiple particles, repeat to grow a tree

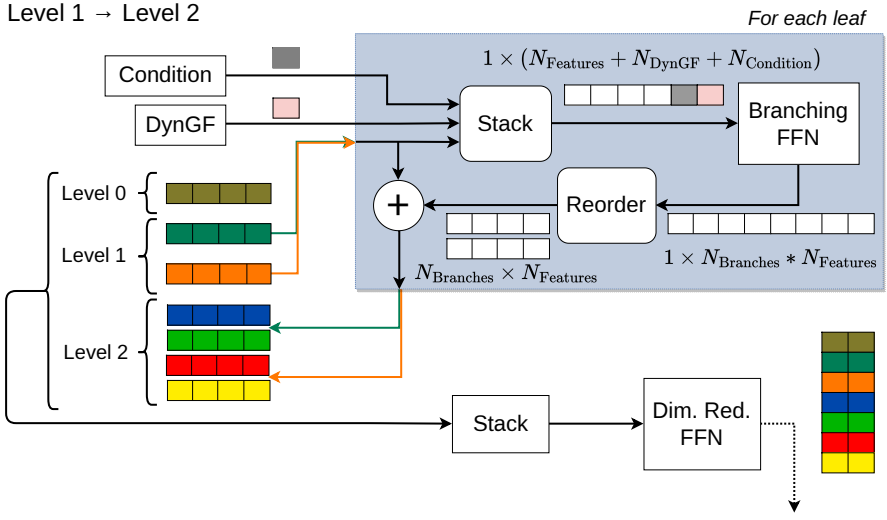
> Physics inspired

⇒ Small output space for each FFN

⇒ Small number of parameters

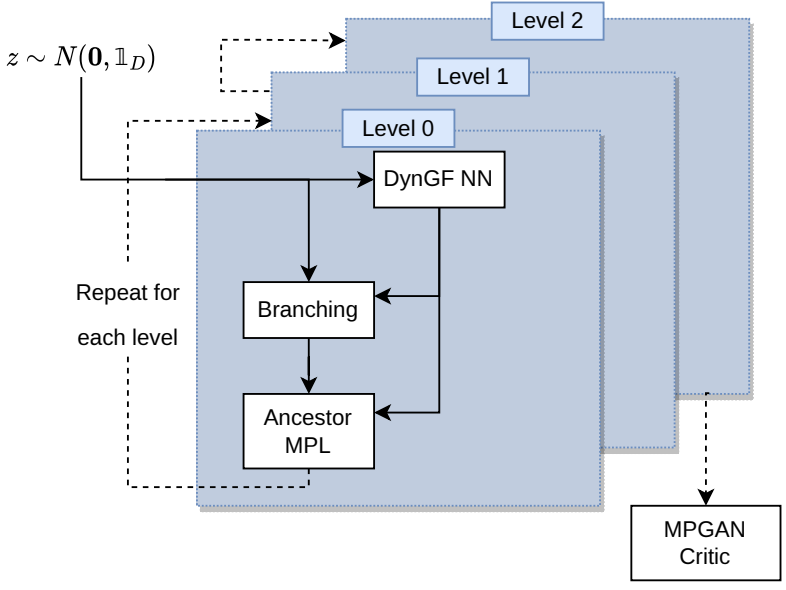
DeepTreeGAN

Branching



DeepTreeGAN

Architecture

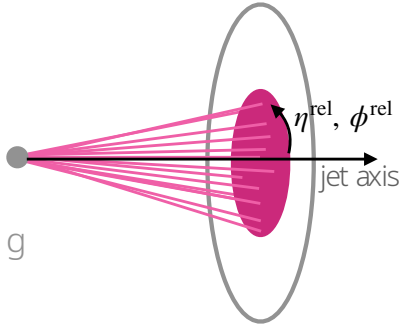


Benchmarking on JetNet-30

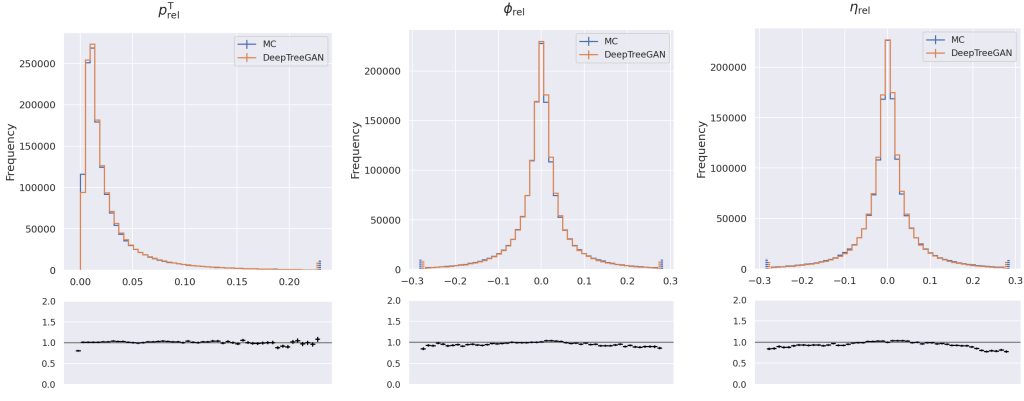
JetNet

JetNet (arXiv:2106.11535) provides :

- Dataset
  - Public dataset generated with Pythia
  - Hadronized jet from pp collisions @ 13 TeV, anti-k_T clustered (R=0.8)
  - 170k gluon jets, light quark jets and top jets (each)
  - Leading 30 constituents by p_T
  - Properties of the constituents relative to the jet

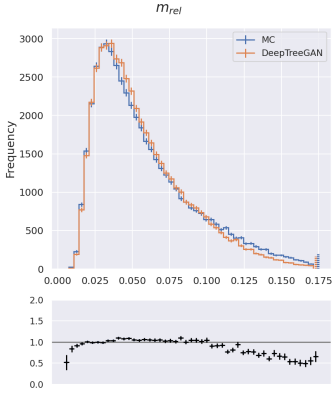


Jet Constituents – Gluon Jets

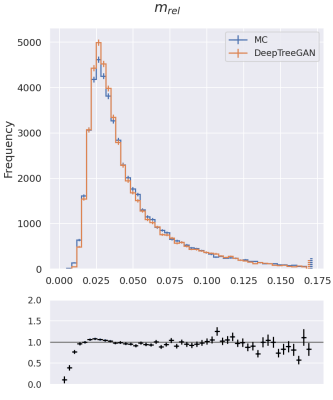


⇒ Looks good!

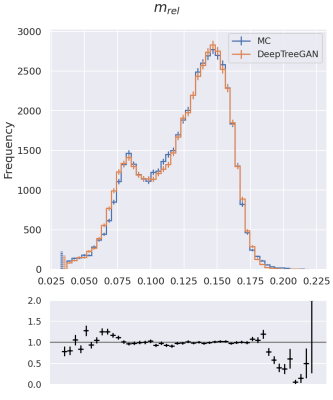
Global Features – Mass



(a) Gluon Jets



(b) Light Quark Jets



(c) Top Quark Jets

⇒ Looks good! ⇒ Metrics & Comparison to baseline in Backup

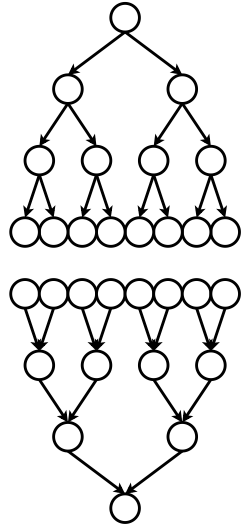
Preview: JetNet150 / DeepTree Critic

Preview: JetNet150 / DeepTree Critic

vs

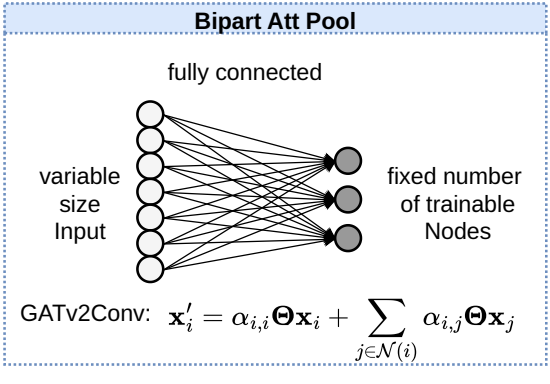
- Generator: Produce 150 points, take the first n (sampled from the dataset)

- MPGAN critic becomes slow ⇒ develop critic
  - Idea: Iteratively reduce the number of points
  - Pooling requirements:
    - Differentiable
    - Arbitrary input size
    - Adjustable output size
    - Permutation invariant



Bipartite Attention Pool

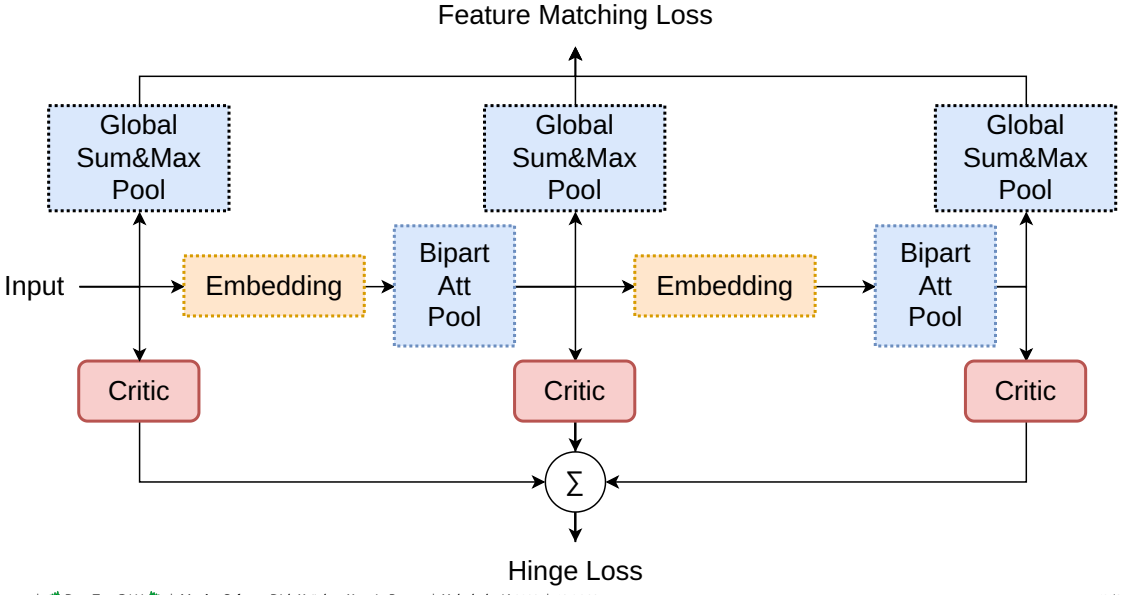
Architecture



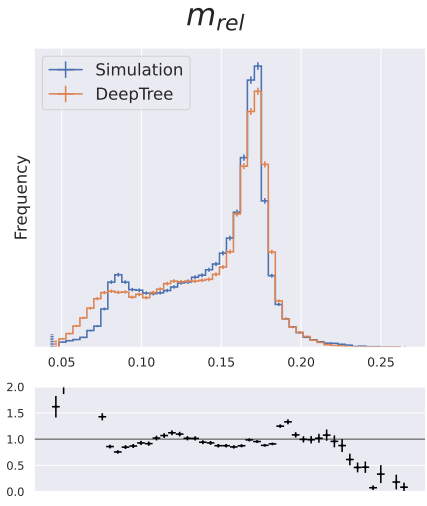
$$\alpha_{i,j} = \underset{j \in \mathcal{N}(i) \cup \{i\}}{\text{softmax}} \left(\mathbf{a}^\top \text{LeakyReLU} \left(\Theta[\mathbf{x}_i + \mathbf{x}_j] \right) \right)$$

DeepTree Critic

Top Quark Jets



First Results



⇒ Not perfect, but promising!

Conclusion

- New, differentiable up/downprojection method for PCs
- Excellent modeling for JetNet30
- JetNet150 work in progress
- Promising approach for scaling to even larger PCs (e.g. HGCAL)
- Paper in preparation

Thank you!

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Backup

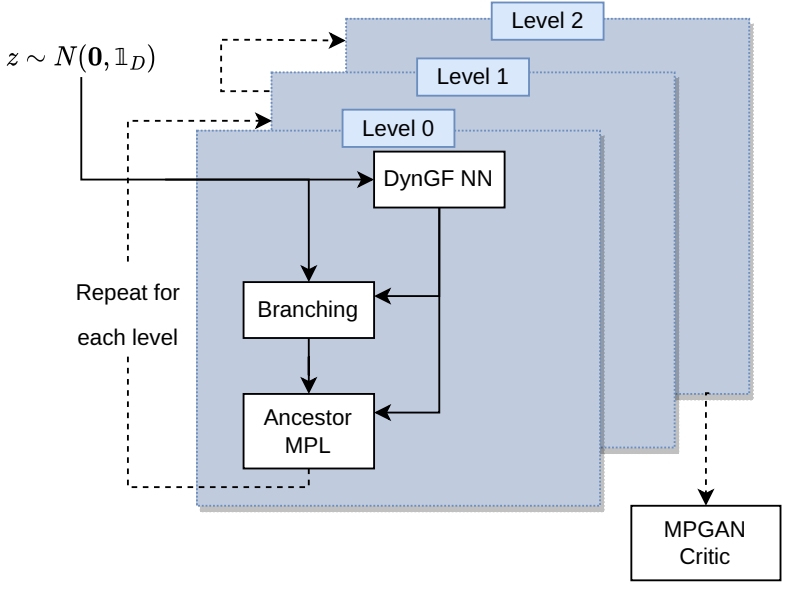
Metrics on JetNet-30

Dataset	Model	$W_1^{\mathrm{M}} \times 10^3$	$W_1^{\mathrm{P}} \times 10^3$	$W_1^{\mathrm{EFP}} \times 10^5$	FPND
Gluon	Limit	0.7±0.2	0.44±0.09	0.63±0.07	?
	MPGAN	**0.7±0.2**	**0.9±0.3**	**0.7±0.2**	**0.12**
	DeepTree	2.5±0.3	1.7±0.3	2.6±0.5	0.35
Light Quarks	Limit	0.5±0.1	0.5±0.1	0.46±0.04	?
	MPGAN	**0.7±0.2**	4.9±0.5	0.7±0.4	0.35
	DeepTree	1.0±0.5	**1.7**±0.6	0.8±0.5	**0.15**
Top	Limit	0.51±0.07	0.55±0.07	1.1±0.1	?
	MPGAN	0.6±0.2	2.3±0.3	2±1	0.37
	DeepTree	0.7±0.2	**0.9±0.4**	2±1	**0.09**

- Always generate 30 points
- Without conditioning
- MPGAN evaluated on validation set, optimized for W_1^M

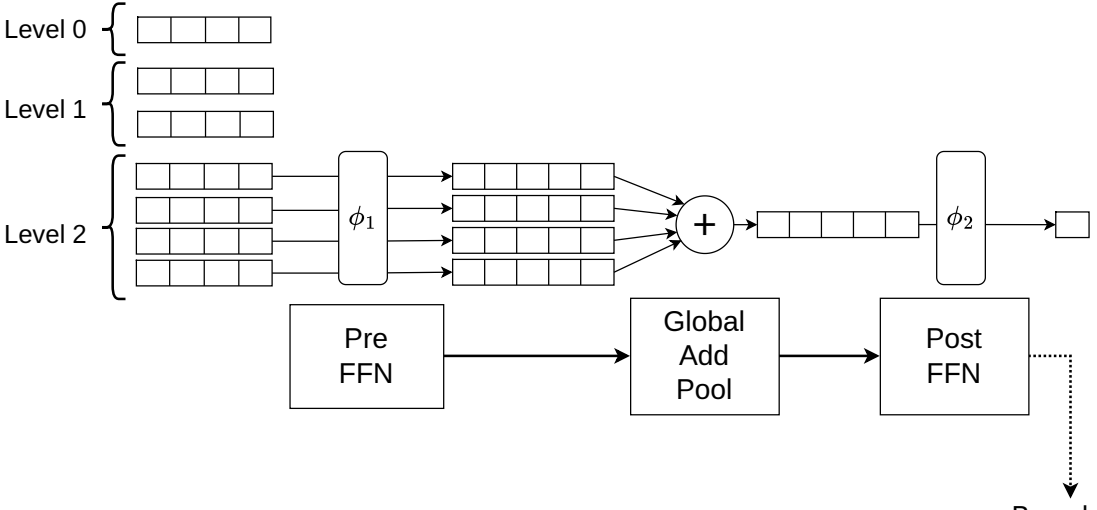
DeepTreeGAN

Architecture

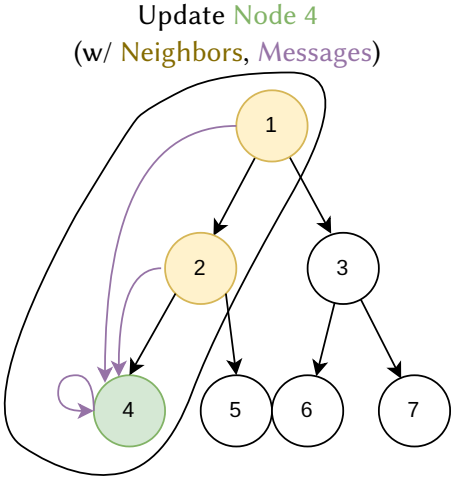


Dynamic Global Features

Idea: Provide the network with self-constructed global features



Ancestor Convolution



Used here: GINConv `arXiv:1810.00826`

1. Message:

$$\mathbf{Msg}_{j\to i} = \mathbf{x}_j$$

2. Aggregate:

$$\mathbf{Aggr}_i = \sum_{j\in\mathcal{N}(i)} \mathbf{Msg}_{j\to i}$$

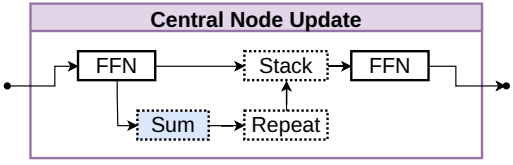
3. Update:

~~$$\mathbf{x}_i \leftarrow \mathrm{NN}\left((1+\epsilon)\mathbf{x}_i + \mathbf{Aggr}_i\right)$$~~

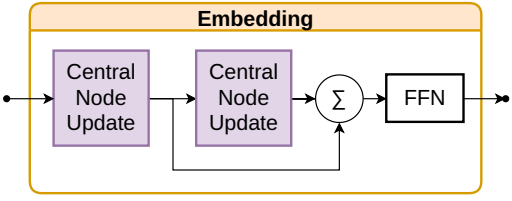
$$\mathbf{x}'_i = \mathrm{NN}\left((1+\epsilon)\cdot \mathbf{x}_i + \textstyle\sum_{j\in\mathcal{N}(i)} \mathbf{x}_j\right) + \mathbf{x}_i$$

(Residual connection)

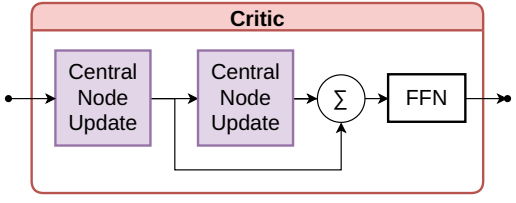
Components



(a) Updates the points with global information



(b) Embed points in higher dimension



(c) Map “real” to 1, “fake” to -1

Details

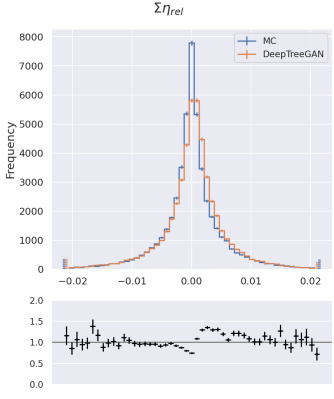
- Scaling:
  - $p_{\mathrm{T}}^{\mathrm{rel}}$: PowerTransformer (Box-Cox)
  - η^{rel}, Φ^{rel}: StandardScalar
- Training
  - LSGAN
  - Batch Size: 200
  - 6000 epochs
  - CyclicLR scheduler for Generator
    - $10^{-5} \rightarrow 10^{-3}$ over 2000 steps

Details

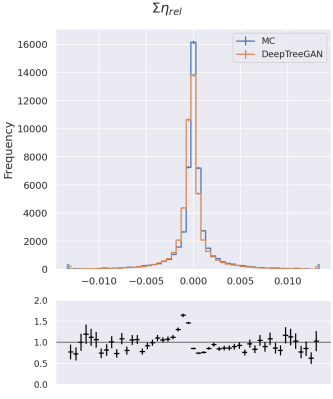
Architecture

- Size of the global features: 10
- Tree:
  - Branches: [1,2,3,5] (2*3*5 = 30 particles)
  - Features: [64,32,16,3]
- Feed Forward Networks
  - 100 hidden nodes
  - 3 layers
    - Linear → Batch Norm → LeakyReLU(0.1)
  - No Bias

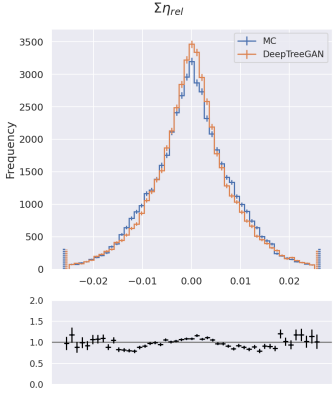
Global Features – $\sum \eta^{\text{rel}}$



(a) Gluon Jets



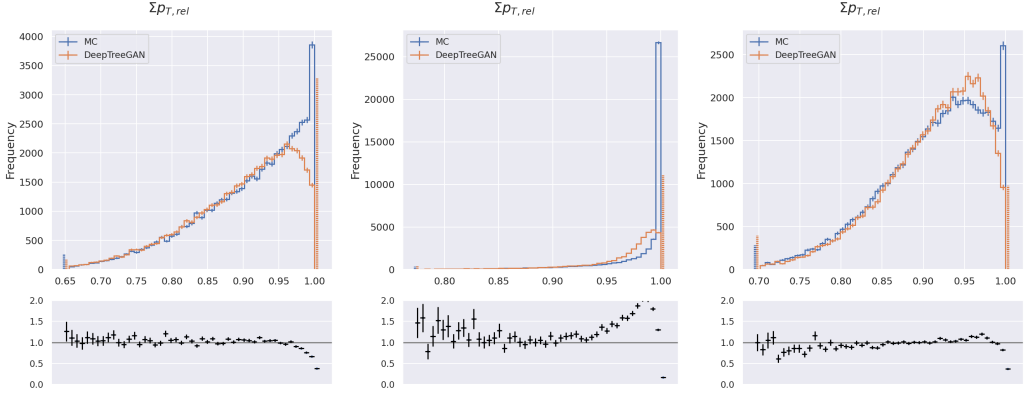
(b) Light Quark Jets



(c) Top Quark Jets

⇒ Looks good!

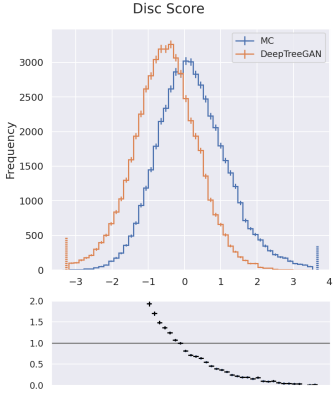
Jet Features – $\sum p_{\mathrm{T}}^{\mathrm{rel}}$



(a) Gluon Jets **(b)** Light Quark Jets **(c)** Top Quark Jets

$\Rightarrow$ Not able to model the artificial $\sum p_{\mathrm{T}}^{\mathrm{rel}}$ cut-off well, problematic for light quark jets

Discriminator



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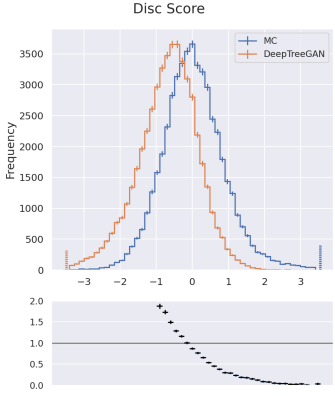
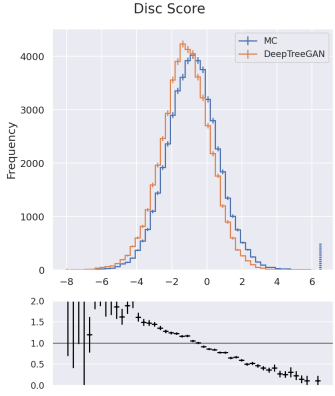


(b) Light Quark Jets



(c) Top Quark Jets