



Attention to the strengths of physics interactions

Enhanced Deep Learning Event Classification for Particle Physics Experiments

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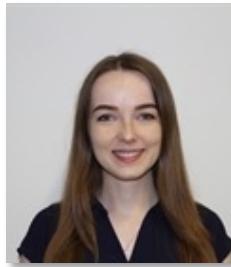
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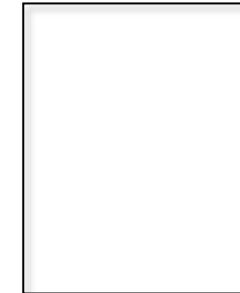
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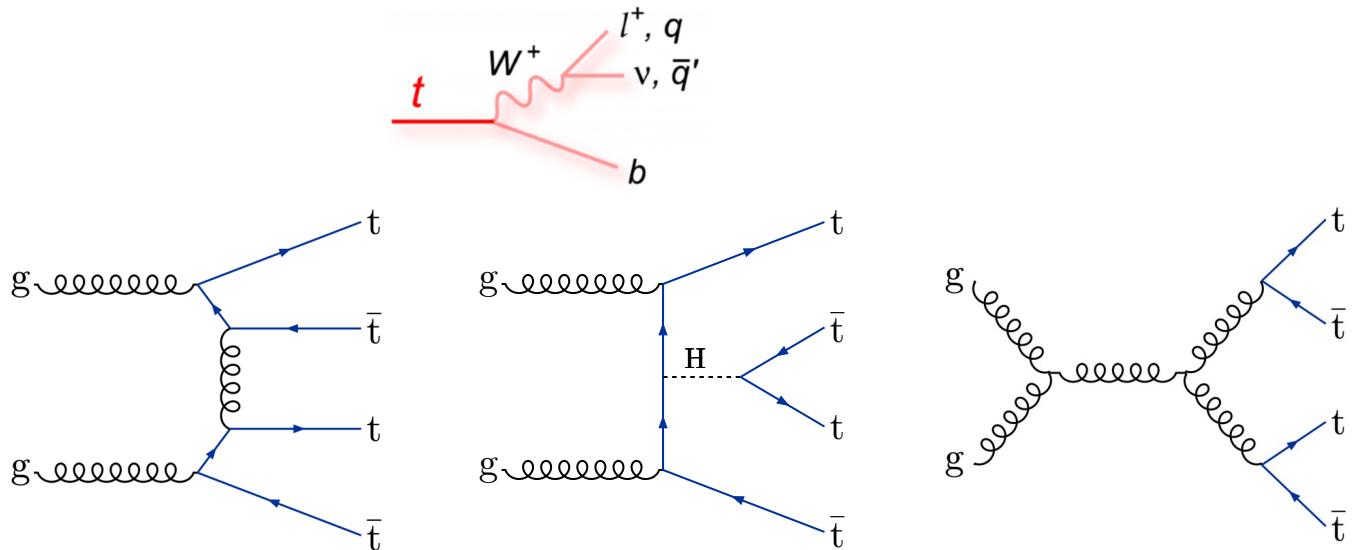
The question was: “**What is the best event classifier for the LHC?**”



The four-top-quarks and $t\bar{t}H$ production at LHC

Production of **four top quarks** is very rare

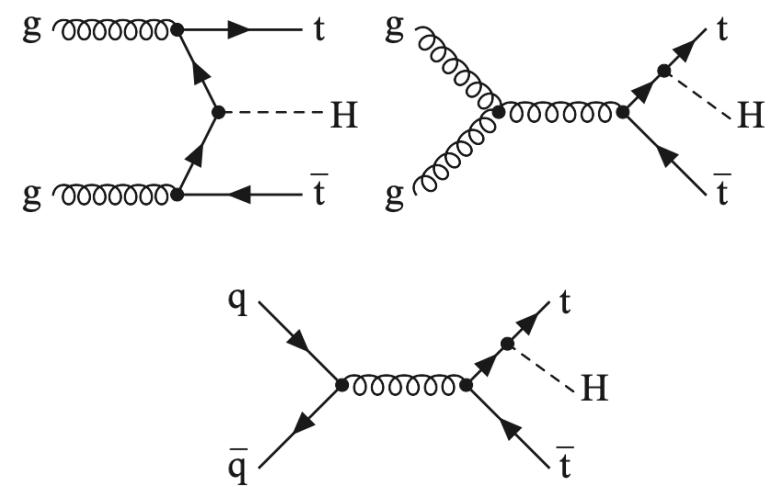
- **NLO QCD:** $\sigma(t\bar{t}t\bar{t}) = 12 \text{ fb} \pm 20\%$ [[JHEP02\(2018\)031](#)]
- **NLO+NLL:** $\sigma(t\bar{t}t\bar{t}) = 13.4 \text{ fb} \pm 11\%$ [[arXiv:2212.03259](#)]



Examples of Feynman diagrams for SM $t\bar{t}t\bar{t}$ production at leading order in QCD and via an off-shell Higgs boson mediator

First observation of $t\bar{t}t\bar{t}$ production with an observed (expected) significance of **6.1 σ (4.3 σ)** with **GNN** by **ATLAS** [[Eur. Phys. J. C 83, 496 \(2023\)](#)]
5.6 σ (4.9 σ) with **BDT** by **CMS** [[Phys. Lett. B 847 \(2023\) 138290](#)]

The **Top-top-Higgs**
has a small cross section (1/100 ggF)
 $\sigma(t\bar{t}H) \sim 0.507 \text{ pb}$



Example tree-level Feynman diagrams
for the $pp \rightarrow t\bar{t}H$

Observation of $t\bar{t}H$ production
6.3 σ (5.1 σ) by **ATLAS** [[Phys. Lett. B 784 \(2018\) 173](#)]
5.2 σ (4.2 σ) by **CMS** [[Phys. Rev. Lett. 120, 231801](#)]

The four-top decays and Background composition

Simulated pp Collisions at $\sqrt{S} = 13$ TeV

The most sensitive channel for **four-top** is:

- **Multilepton final state:**
2 Leptons Same Sign and 3 Leptons (2LSS/3L),
13% branching ration, highest sensitivity – observation

event ID; process ID; weight; \cancel{E}_T ; $\phi_{\cancel{E}_T}$; obj₁, $E_1, p_{T1}, \eta_1, \phi_1$; obj₂, $E_2, p_{T2}, \eta_2, \phi_2$; ...

- **All other kinematic variables can be calculated from four-vectors**

	jets	b-jets	e^-	e^+	μ^-	μ^+	γ	N_{\max}
FCN, BDT	4	4	1	1	1	1		12
CNN, PN, ParT			no limits					18

N_{\max} – the maximum number of objects in an event

Signal region:

≥ 6 jets ≥ 2 b-jets and $H_T \geq 500$ GeV

Signal process:

- $t\bar{t}t\bar{t}$

Physical backgrounds:

- $t\bar{t}Z$, $t\bar{t}H$, $t\bar{t}W$, $t\bar{t}WW$

Later, it is used for a second analysis as a signal (see slide 11)

Summary of ML model details

arXiv:2211.05143

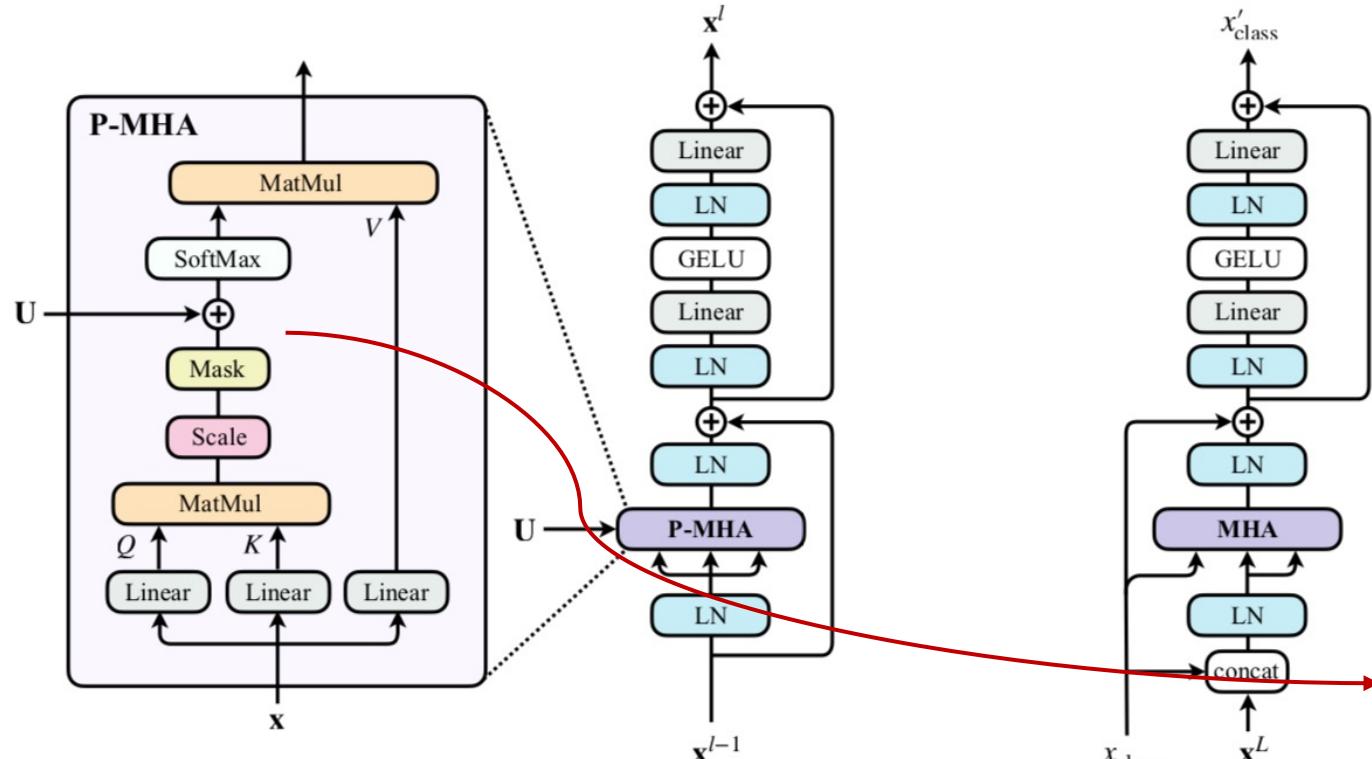
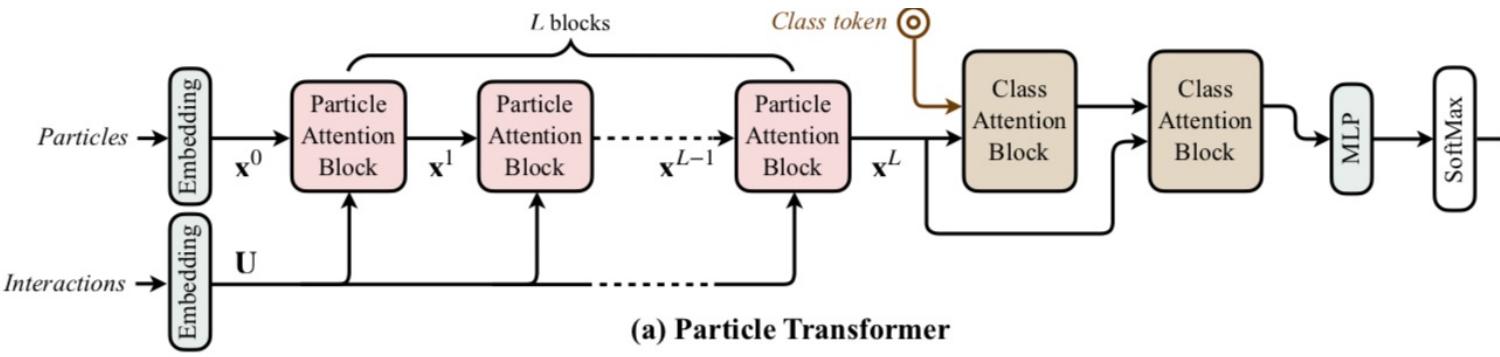
NN structure	Variables per particle		Also receives \cancel{E}_T ; $\phi_{\cancel{E}_T}$
	Pairwise kinematic features	Loss function	
BDT			
BDT _{int.}	$m_{ij}, \Delta R_{ij}$		
FCN			
CNN			
PN		Cross-entropy	
PN _{int.}	$m_{ij}, \Delta R_{ij}$		
PN _{int.} SMids	$m_{ij}, \Delta R_{ij} + \text{SM matrix}[1]$		
PN _{int.} SM const	$m_{ij}, \Delta R_{ij} + \text{SM matrix}[2]$		
PN _{int.} SM	$m_{ij}, \Delta R_{ij} + \text{SM matrix}[3]$		
ParT			
ParT _{int.}	$m_{ij}, \Delta R_{ij}$		
ParT _{int.} SM (FL)	$m_{ij}, \Delta R_{ij} + \text{SM matrix}[3]$	Focal [$\alpha = 0.75, \gamma = 3$]	
ParT _{int.} SMids	$m_{ij}, \Delta R_{ij} + \text{SM matrix}[1]$		
ParT _{int.} SM const	$m_{ij}, \Delta R_{ij} + \text{SM matrix}[2]$		
ParT _{int.} SM	$m_{ij}, \Delta R_{ij} + \text{SM matrix}[3]$		
SetT _{int.} SM	$m_{ij}, \Delta R_{ij} + \text{SM matrix}[3]$	Cross-entropy	

The **particle input variables** and **pairwise kinematic features** that were used in the **NN structures**, each with their respective **loss function**

16 MODELS IN TOTAL!

Transformers

[arXiv:2202.03772](https://arxiv.org/abs/2202.03772)



The architecture of (a) Particle Transformer (b) Particle Attention Block (c) Class Attention Block

Attention Modules

(scaled dot product attention):

- $\text{Attention}(Q, K, V) = \text{SoftMax}\left(\frac{QK^T}{\sqrt{d}} + \mathbf{U}\right)V$
- $Q = \text{queries}, K = \text{keys}, V = \text{values}$
- $\text{Self-attention} \rightarrow Q = K = V$

$$Q = Q \times W_Q$$

$$K = K \times W_K$$

$$V = V \times W_V$$

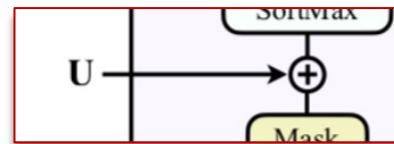
Attention is All You Need!

[arXiv:1706.03762](https://arxiv.org/abs/1706.03762)

U → Attention matrix → correlation of “data sequence with data sequence”

U ->

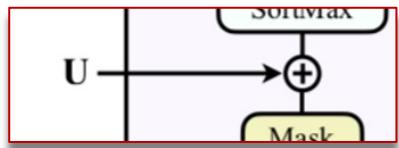
Pairwise Features + SM interaction matrix (attention matrix)



To show the interaction strength based on the SM coupling constants

Adding Pairwise features

Include pairwise features in **Particle Transformer** through a trainable embedding \mathbf{U}_{ij} for particles i and j



**Pairwise Features +
SM interaction matrix
(attention matrix)**

Attention Modules

$$\text{Attention}(Q, K, T) = \text{SoftMax} \left(\frac{QK^T}{\sqrt{d}} + \mathbf{U} \right) V$$

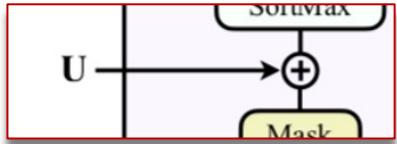
Features from the paper [\[arXiv:2202.03772\]](https://arxiv.org/abs/2202.03772)

- **ParT** uses high level features for better performance
 1. $\Delta = \sqrt{(y_a - y_b)^2 + (\phi_a + \phi_b)^2}$
 2. $k_t = \min(p_{T,a}, p_{T,b})\Delta$
 3. $z = \min(p_{T,a}, p_{T,b}) / (p_{T,a}, p_{T,b})$
 4. $m^2 = (E_a + E_b)^2 - \|p_a + p_b\|^2$
- These were also tested in **LightGBM**

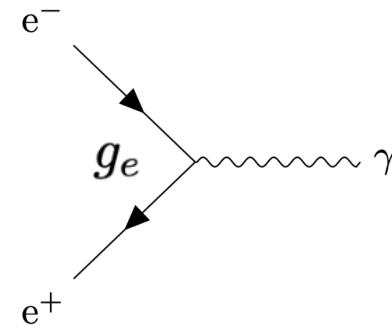
What we end up using :

\mathbf{m}_{ij} , ΔR_{ij} and dynamically calculated
coupling constants of interaction terms
(i.e. a feature that is coupling constant when
 i and j are components of a **SM** current,
and 0 otherwise)

Interaction Matrices



**Pairwise Features +
SM interaction matrix
(attention matrix)**



Matrix [1] – SM ids

```
# - j jb e- e+ m- m+ g
([[0, 0, 0, 0, 0, 0, 0, 0], # -
 [0, 1, 1, 0, 0, 0, 0, 1], # j
 [0, 1, 1, 0, 0, 0, 0, 1], # jb
 [0, 0, 0, 1, 0, 0, 0, 1], # e-
 [0, 0, 0, 1, 0, 0, 0, 1], # e+
 [0, 0, 0, 0, 0, 1, 1, 1], # m-
 [0, 0, 0, 0, 0, 1, 0, 1], # m+
 [0, 1, 1, 1, 1, 1, 1, 0]]) # g
```

Matrix [2] – SM const

#	-	j	bjet	e-	e+	m-	m+	g (photon)
[0,	0,	0,	0,	0,	0,	0,	0,	0]
[0,	g_s,	g_s,	0,	0,	0,	0,	0,	g_e/2]
[0,	g_s,	g_s,	0,	0,	0,	0,	0,	g_e/3]
[0,	0,	0,	0,	g_z,	0,	0,	0,	g_e]
[0,	0,	0,	g_z,	0,	0,	0,	0,	g_e]
[0,	0,	0,	0,	0,	0,	g_z,	g_e	g_e]
[0,	0,	0,	0,	0,	g_z,	0,	g_e	g_e]
[0,	g_e/2,	g_e/3,	g_e,	g_e,	g_e,	g_e,	0]	g]

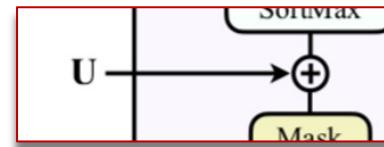
- ‘1’ indicates an interaction possible at **LO** in the SM
- ‘0’ indicates interactions that only appear at higher orders

- $g_Z = 0.758$ for the weak force for leptons
- $g_s = 1.22$ for the strong force in jet interactions
- $g_e = 0.31$ for the electromagnetic force in photon interactions

The energy dependence of the coupling constants

Matrix [3] – SM

```
# - j bjet e- e+ m- m+ g(photon)
([0, 0, 0, 0, 0, 0, 0], # -
[0, g_s, g_s, 0, 0, 0, g_e/2], # j
[0, g_s, g_s, 0, 0, 0, g_e/3], # bjet
[0, 0, 0, g_z, 0, 0, g_e], # e-
[0, 0, 0, g_z, 0, 0, g_e], # e+
[0, 0, 0, 0, 0, g_z, g_e], # m-
[0, 0, 0, 0, g_z, 0, g_e], # m+
[0, g_e/2, g_e/3, g_e, g_e, g_e, 0])]) # g
```



Pairwise Features +
SM interaction matrix
(attention matrix)

Dynamically calculated **coupling constants** of interaction terms !

α is the running coupling constant

$$(*) \quad \alpha(Q^2) = \frac{\alpha(\mu_0^2)}{1 - \frac{n\alpha(\mu_0^2)}{3\pi} \cdot \ln\left(\frac{Q^2}{\mu_0^2}\right)},$$

$$g_e = \sqrt{4\pi\alpha}$$

$$\alpha_s(Q^2) = \frac{\alpha_s(\mu_0^2)}{1 + \frac{\alpha_s(\mu_0^2)(33-2n_f)}{12\pi} \ln\left(\frac{Q^2}{\mu_0^2}\right)},$$

$$g_s = \sqrt{4\pi\alpha_s}$$

n_f – number of quark flavors that are active

Where $\mu_0 = 91.1876$ GeV, $\alpha(\mu_0) = \frac{1}{127.5}$, $\alpha_s(\mu_0) = 0.118$, $n_f = 6$

$$Q^2 = \bar{p}_t^2 = \left(\frac{p_t^i + p_t^j}{2} \right)^2$$

energy scale

(*) Considered only leptons

$n = 3$ – approximates the contribution of the different particles in the loop

$$g_Z = 0.758$$

Results for the $t\bar{t}t\bar{t}$ signal

arXiv:2211.05143

	BDT	BDT _{int.}	FCN	CNN
$t\bar{t} + h$	AUC	0.825(0)	0.831(0)	0.821(2)
	$\epsilon_B(\epsilon_S = 0.7)$	0.206(0)	0.192(0)	0.203(1)
	$\epsilon_B(\epsilon_S = 0.3)$	0.026(1)	0.026(0)	0.026(1)
$t\bar{t} + W$	AUC	0.891(0)	0.895(0)	0.887(0)
	$\epsilon_B(\epsilon_S = 0.7)$	0.099(0)	0.092(0)	0.103(1)
	$\epsilon_B(\epsilon_S = 0.3)$	0.011(0)	0.011(0)	0.010(0)
$t\bar{t} + WW$	AUC	0.740(0)	0.746(0)	0.737(1)
	$\epsilon_B(\epsilon_S = 0.7)$	0.347(0)	0.339(0)	0.342(5)
	$\epsilon_B(\epsilon_S = 0.3)$	0.050(0)	0.051(0)	0.054(0)
$t\bar{t} + Z$	AUC	0.833(0)	0.856(0)	0.836(0)
	$\epsilon_B(\epsilon_S = 0.7)$	0.191(0)	0.163(0)	0.192(0)
	$\epsilon_B(\epsilon_S = 0.3)$	0.026(0)	0.019(0)	0.023(0)
	PN	PN _{int.}	PN _{int. SM}	ParT _{int. SM (FL)}
$t\bar{t} + h$	AUC	0.824(0)	0.842(1)	0.846(1)
	$\epsilon_B(\epsilon_S = 0.7)$	0.199(0)	0.176(3)	0.171(2)
	$\epsilon_B(\epsilon_S = 0.3)$	0.025(0)	0.019(1)	0.020(1)
$t\bar{t} + W$	AUC	0.887(0)	0.895(2)	0.900(1)
	$\epsilon_B(\epsilon_S = 0.7)$	0.102(1)	0.097(1)	0.091(1)
	$\epsilon_B(\epsilon_S = 0.3)$	0.011(0)	0.011(0)	0.010(0)
$t\bar{t} + WW$	AUC	0.742(0)	0.760(1)	0.765(0)
	$\epsilon_B(\epsilon_S = 0.7)$	0.335(2)	0.311(1)	0.297(2)
	$\epsilon_B(\epsilon_S = 0.3)$	0.051(0)	0.044(1)	0.044(1)
$t\bar{t} + Z$	AUC	0.851(0)	0.879(1)	0.887(1)
	$\epsilon_B(\epsilon_S = 0.7)$	0.168(4)	0.136(1)	0.126(2)
	$\epsilon_B(\epsilon_S = 0.3)$	0.020(0)	0.016(1)	0.016(0)
	ParT	ParT _{int.}	ParT _{int. SM}	SetT _{int. SM}
$t\bar{t} + h$	AUC	0.824(0)	0.837(2)	0.846(1)
	$\epsilon_B(\epsilon_S = 0.7)$	0.197(3)	0.179(6)	0.174(1)
	$\epsilon_B(\epsilon_S = 0.3)$	0.023(0)	0.020(0)	0.020(0)
$t\bar{t} + W$	AUC	0.896(1)	0.899(1)	0.905(2)
	$\epsilon_B(\epsilon_S = 0.7)$	0.097(2)	0.090(1)	0.089(3)
	$\epsilon_B(\epsilon_S = 0.3)$	0.010(0)	0.010(0)	0.009(0)
$t\bar{t} + WW$	AUC	0.737(0)	0.767(1)	0.769(0)
	$\epsilon_B(\epsilon_S = 0.7)$	0.354(3)	0.295(5)	0.288(2)
	$\epsilon_B(\epsilon_S = 0.3)$	0.050(1)	0.040(0)	0.042(0)
$t\bar{t} + Z$	AUC	0.839(1)	0.885(0)	0.891(1)
	$\epsilon_B(\epsilon_S = 0.7)$	0.182(2)	0.130(1)	0.119(3)
	$\epsilon_B(\epsilon_S = 0.3)$	0.021(1)	0.016(0)	0.014(0)

The areas under the ROC curve
and the background efficiencies, at
signal efficiencies of 70% and 30%
respectively

- Quoted uncertainties are extracted from three independent runs for each network architecture
- Numbers in bold indicate the best performance

Let's zoom in →

Results for the $t\bar{t}t\bar{t}$ and $t\bar{t}H$ signals

arXiv:2211.05143

The **AUC** for both **4 top and top-top-Higgs** signal detection

	PN	PN _{int.}	PN _{int. SMids}	PN _{int. SM const}	PN _{int. SM}
$t\bar{t}t\bar{t}$	AUC	0.8471(1)	0.8729(0)	0.8725(0)	0.8727(0)
	$\epsilon_B(\epsilon_S = 0.7)$	0.1758(3)	0.1387(1)	0.1377(0)	0.1369(1)
	$\epsilon_B(\epsilon_S = 0.3)$	0.0207(0)	0.0182(0)	0.0178(0)	0.0176(0)
$t\bar{t}t\bar{t}$	ParT	ParT _{int.}	ParT _{int. SMids}	ParT _{int. SM const}	ParT _{int. SM}
	AUC	0.8404(0)	0.8708(0)	0.8715(0)	0.8732(0)
	$\epsilon_B(\epsilon_S = 0.7)$	0.1842(3)	0.1394(0)	0.1389(2)	0.1366(0)
	$\epsilon_B(\epsilon_S = 0.3)$	0.0230(0)	0.0172(0)	0.0180(0)	0.0167(0)

The models containing both the **pairwise features** and the **SM interaction matrix** performs **best**

	PN	PN _{int.}	PN _{int. SMids}	PN _{int. SM const}	PN _{int. SM}
$t\bar{t} + h$	AUC	0.8146(2)	0.8505(0)	0.8489(1)	0.8505(0)
	$\epsilon_B(\epsilon_S = 0.7)$	0.2292(1)	0.1787(0)	0.1785(1)	0.1733(1)
	$\epsilon_B(\epsilon_S = 0.3)$	0.0471(1)	0.0345(0)	0.0343(1)	0.0340(0)
$t\bar{t} + h$	ParT	ParT _{int.}	ParT _{int. SMids}	ParT _{int. SM const}	ParT _{int. SM}
	AUC	0.8058(1)	0.8507(0)	0.8473(0)	0.8497(0)
	$\epsilon_B(\epsilon_S = 0.7)$	0.2399(2)	0.1794(1)	0.1836(3)	0.1748(1)
	$\epsilon_B(\epsilon_S = 0.3)$	0.0502(0)	0.0357(0)	0.0355(1)	0.0351(0)

The **background** can be significantly **reduced** by about **30%** compared to a **PN (GNN)**

Significance

arXiv:2211.05143

Highlights the **enhanced performance**
of **ParT int. SM** models over baseline
PN (GNN) (neglecting sys err) for 4top signal

$$\sigma = \frac{s}{\sqrt{b}} \quad \sigma_{\delta_{sys}=0.2} = \frac{s}{\sqrt{b_{sys}}} \\ b_{sys} = b + (b \cdot \delta_{sys})^2$$

- At $\epsilon_S = 0.7$: significance boost from **2.21** to **2.98 σ**
with **ParT int. SM** => **PN** requires **82% more luminosity !**
- At $\epsilon_S = 0.3$: significance boost from **8.29** to **9.88 σ**
with **ParT int. SM** => **PN** needs **42% more luminosity !**
- At $\epsilon_S = 0.3$: significance boost from **8.29** to **10.48 σ**
with **ParT int. SM (FL)** => **PN** needs **60% more luminosity !**

Significance table (calculations assume $L = 100 fb^{-1}$)

		σ	$\sigma_{\delta_{sys}=0.2}$
BDT	$\epsilon_S = 0.3$	20.77	6.79
	$\epsilon_S = 0.7$	16.82	2.01
$BDT_{int.}$	$\epsilon_S = 0.3$	21.93	7.53
	$\epsilon_S = 0.7$	17.51	2.17
FCN	$\epsilon_S = 0.3$	20.31	6.51
	$\epsilon_S = 0.7$	16.67	1.97
CNN	$\epsilon_S = 0.3$	20.88	6.86
	$\epsilon_S = 0.7$	16.73	1.98
PN	$\epsilon_S = 0.3$	23.09	8.29
	$\epsilon_S = 0.7$	17.68	2.21
$PN_{int.}$	$\epsilon_S = 0.3$	25.30	9.83
	$\epsilon_S = 0.7$	20.51	2.97
$PN_{int. SM}$	$\epsilon_S = 0.3$	25.65	10.09
	$\epsilon_S = 0.7$	20.50	2.97
ParT	$\epsilon_S = 0.3$	22.37	7.82
	$\epsilon_S = 0.7$	17.72	2.23
$ParT_{int.}$	$\epsilon_S = 0.3$	24.54	9.29
	$\epsilon_S = 0.7$	20.21	2.89
$ParT_{int. SM}$	$\epsilon_S = 0.3$	25.36	9.88
	$\epsilon_S = 0.7$	20.53	2.98
$ParT_{int. SM (FL)}$	$\epsilon_S = 0.3$	26.19	10.48
	$\epsilon_S = 0.7$	20.28	2.91
SetT _{int. SM}	$\epsilon_S = 0.3$	25.58	10.03
	$\epsilon_S = 0.7$	20.18	2.88

Results

arXiv:2211.05143

We asked the question: → “**Do the models saturate?**”

PN and ParT Models (with the pairwise features + the SM coupling constants)

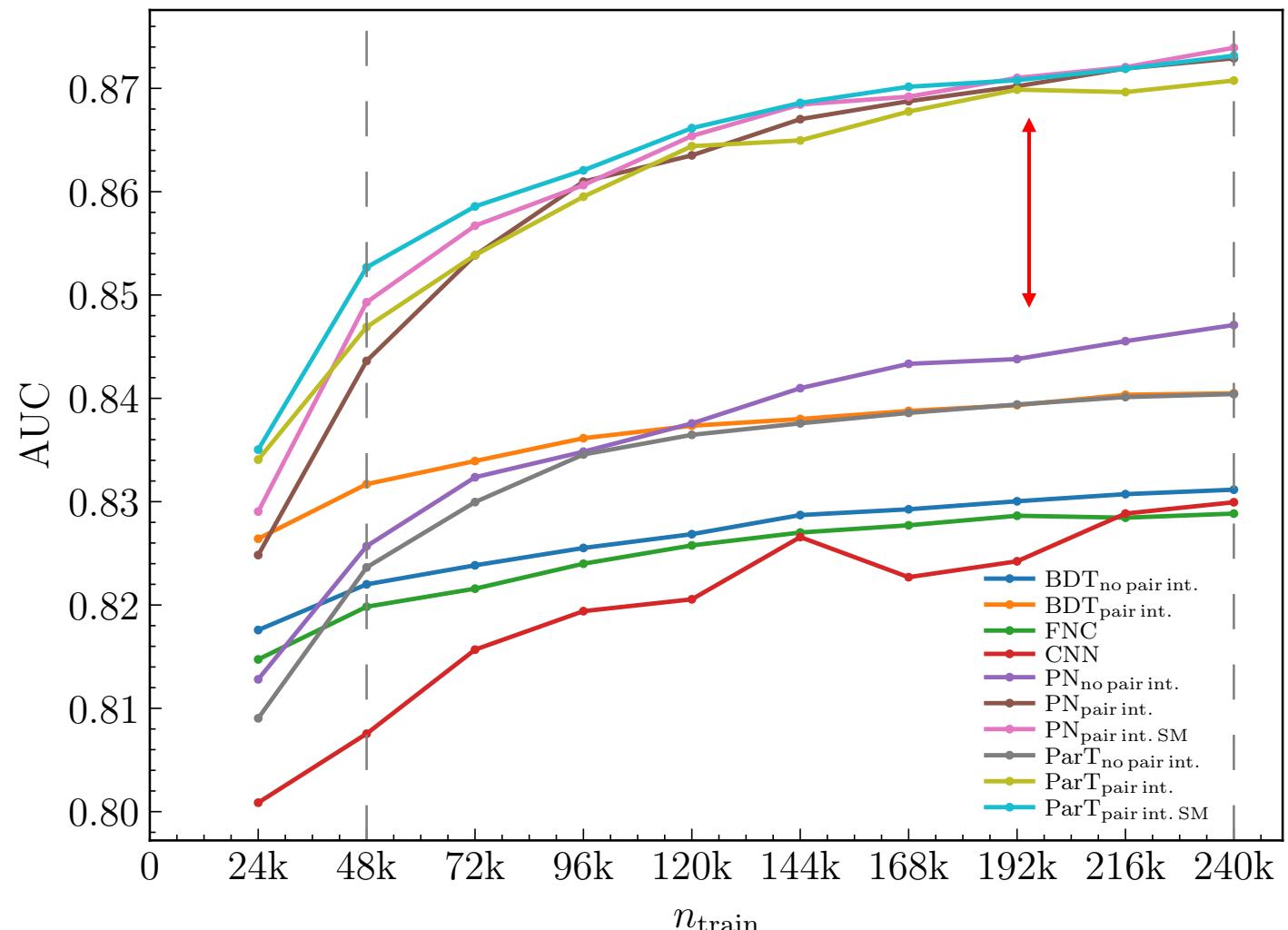
- Shows a steeper increase in **AUC** with fewer data
- Indicate higher data efficiency → less data needed for strong performance

Other Models

- **AUC** scores improve more gradually
- Suggest a requirement for larger datasets to match **PN** and **ParT** performance

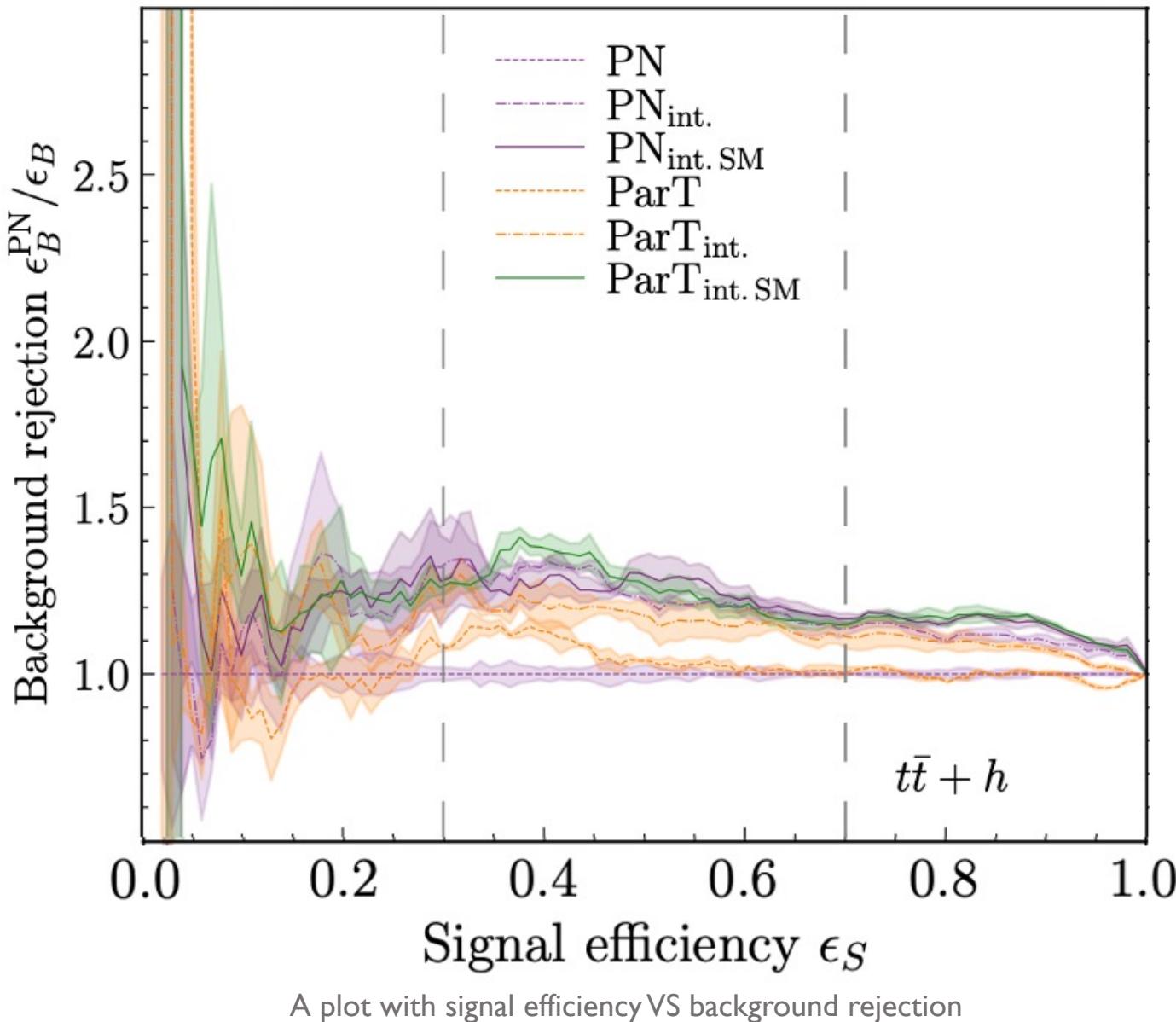
PN and ParT models could be preferable in data-scarce cases

The **AUC** scores as a function of training size



Results

arXiv:2211.05143



*compared to the **ParticleNet (GNN)**

Models with integrated **pairwise features + SM interactions** exhibit up to a **40% higher background rejection**

Demonstrates the strength of **SM interaction matrix** as a powerful inductive bias in learning

X-axis – the signal efficiency
Y-axis – the background rejection

Summary

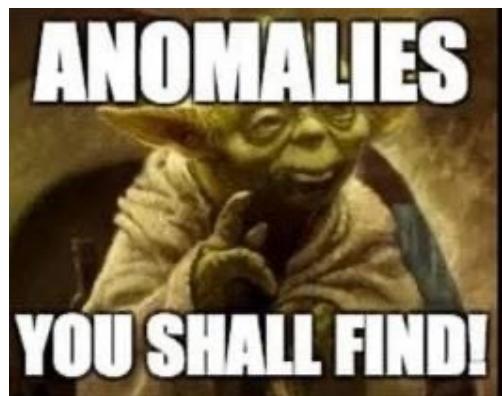


Integration of energy-dependent SM interactions into ML models

- Embedding pairwise features and energy-dependent **SM** interactions into **ML** architectures significantly boosts event classification accuracy and efficiency:
 - Enhanced background suppression by **10-40%** compared to baseline **PN (GNN)** models
 - Approximately **10%** of this improvement is due to the **SM interaction matrix**
 - ML models show up to **30%** increase in significance vs. baseline
 - Achieving similar significance via increased luminosity would require **~70%** more data (compare to the baseline model)

Transformers, when supplemented with **pairwise features** and **SM couplings**, show potential as a **powerful tool** for collider physics challenges!

CAN WE TURN CLASSIFIERS INTO ANOMALY DETECTORS ?



★ It has been observed that, **on average**,
the top-performing classifiers serve as best anomaly detectors
(with the SM interactions)

For further details, refer to Adrian's [talk](#)

Thank you for your attention!

Back up

Math Behind the Attention Mechanism

Attention Modules

(scaled dot product attention):

- $\text{Attention}(Q, K, V) = \text{SoftMax} \left(\frac{QK^T}{\sqrt{d}} + \mathbf{U} \right) V$
- $Q = \text{queries}, K = \text{keys}, V = \text{values}$
- $\text{Self-attention} \rightarrow Q = K = V$

How Particles Inform Each Other ?

- **Calculating Interaction Scores:**

➤ **Attention Score** $(Q, K) = \frac{QK^T}{\sqrt{d}}$

where \sqrt{d} is the dimensionality of the key vector, used to scale the dot product

- **Normalizing Scores to Probabilities:**

➤ **Attention Weights** = $\text{SoftMax}(\text{Attention Score})$
normalizes the scores to ensure they sum up to 1, acting as probabilities

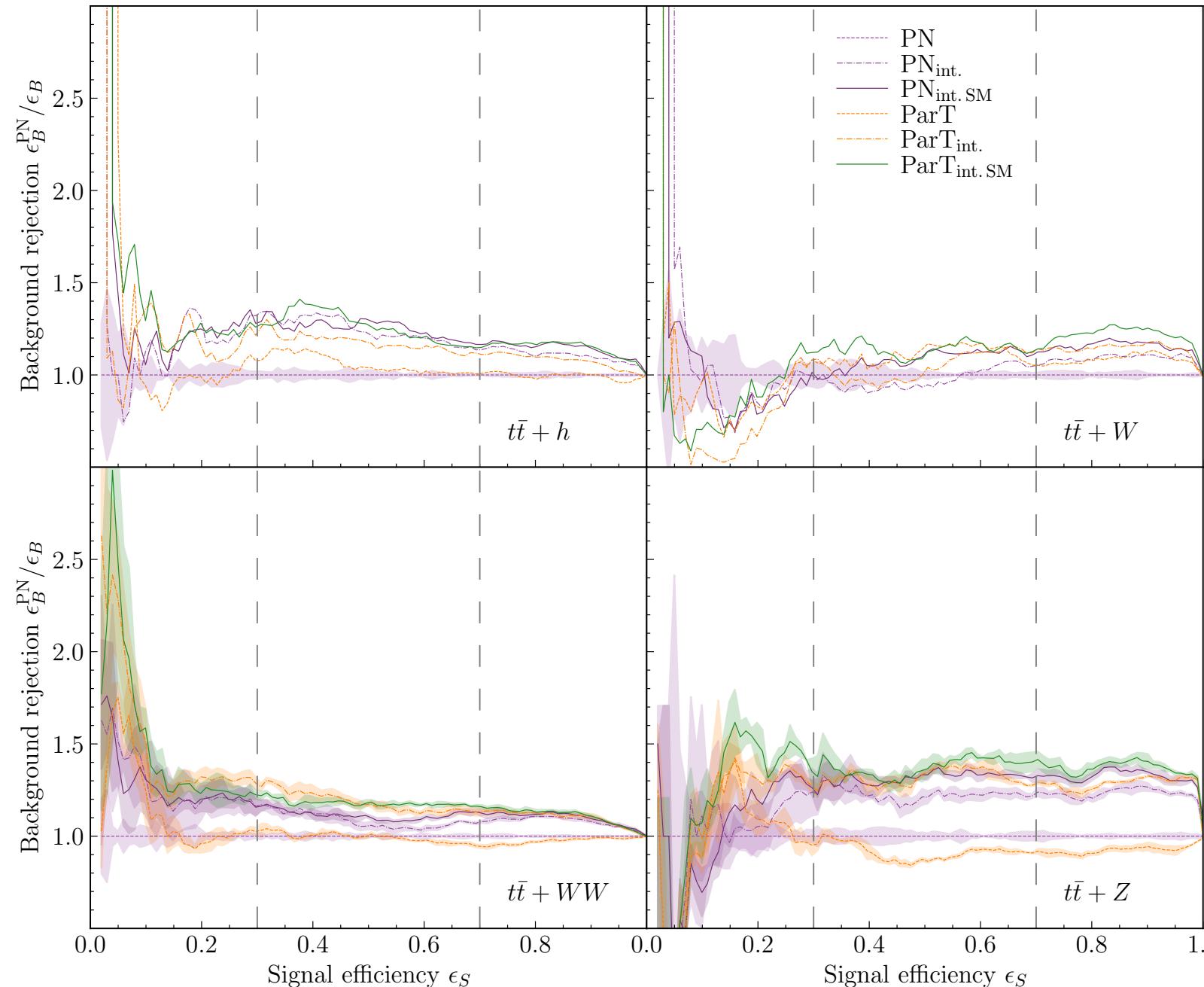
- **Particle Representation:**

➤ **Output** = **Attention Weights** * V
each particle's output is a combination of all particles' information, weighted by their computed relevance

Result: captures the dynamic interactions between particles

A plot with signal efficiency VS background rejection

[arXiv:2211.05143](https://arxiv.org/abs/2211.05143)



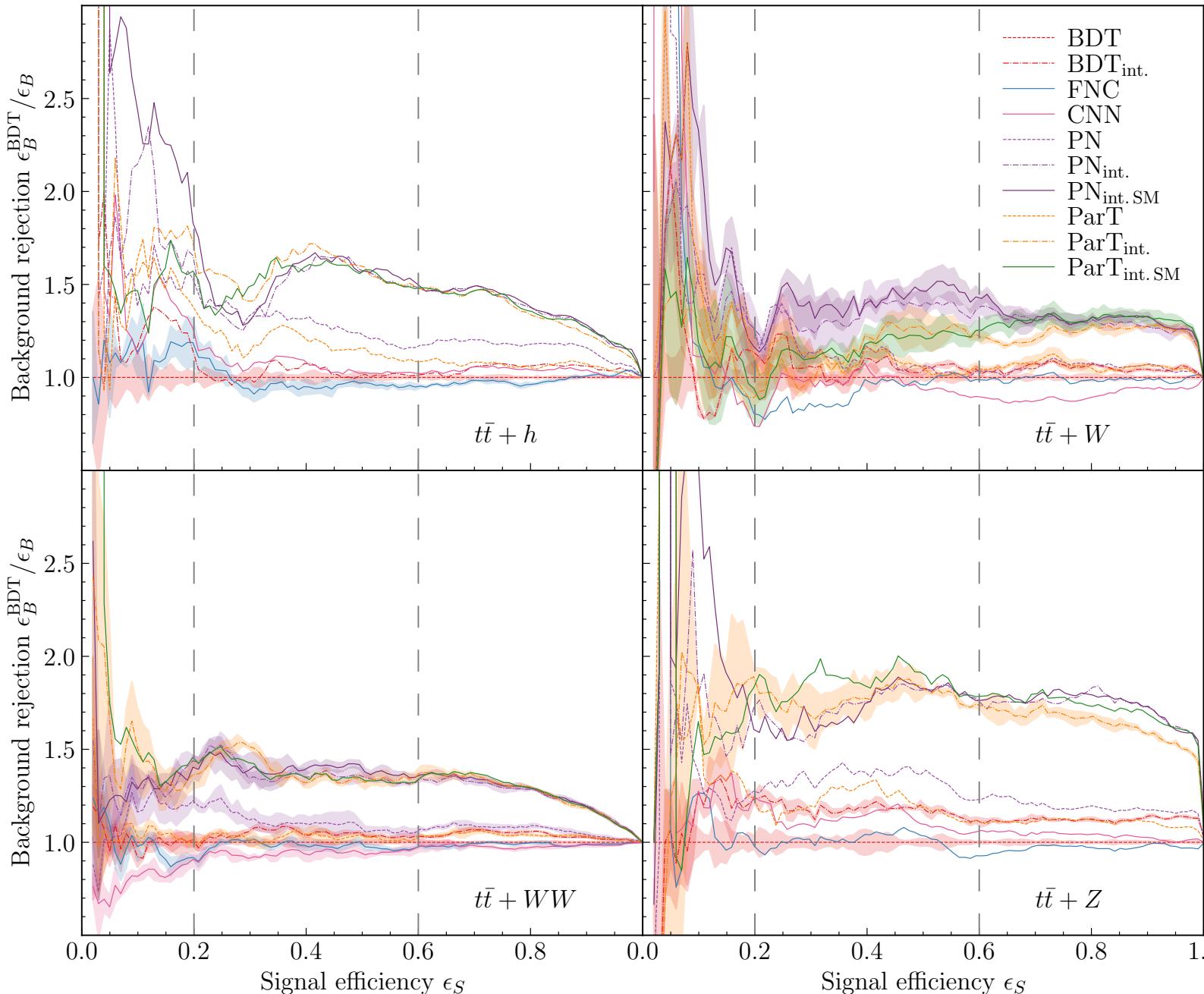
compared to the **ParticleNet (GNN)**

We can achieve a **10-40% higher background rejection** for signal efficiencies between 30-90% by switching from **GNN** to **models with the pairwise features + the SM coupling constants**

X-axis – the signal efficiency
Y-axis – the background rejection

A plot with signal efficiency VS background rejection

[arXiv:2211.05143](https://arxiv.org/abs/2211.05143)

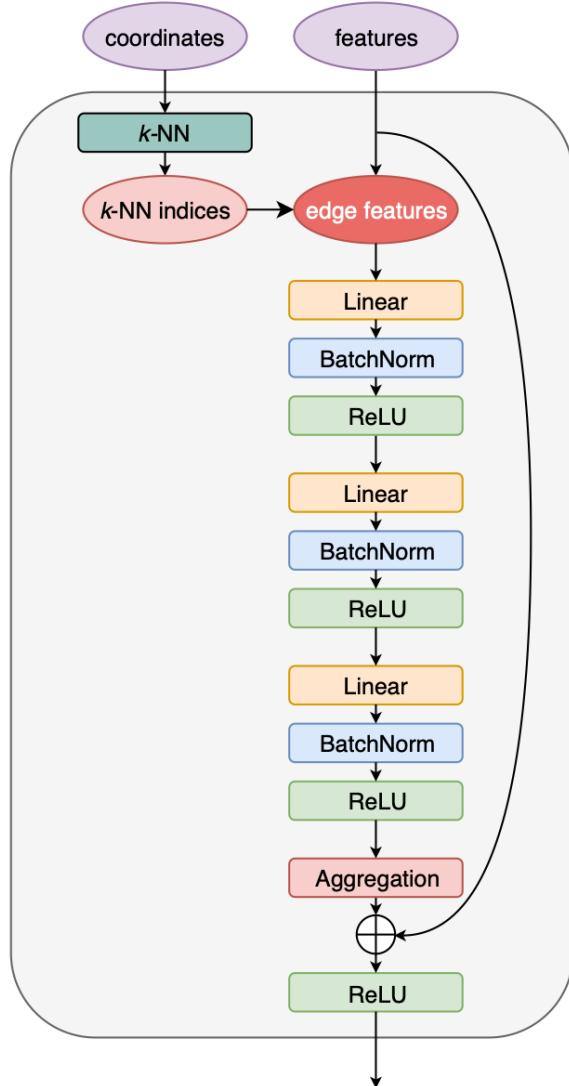


Compared to the **BDT**
for full size of the dataset

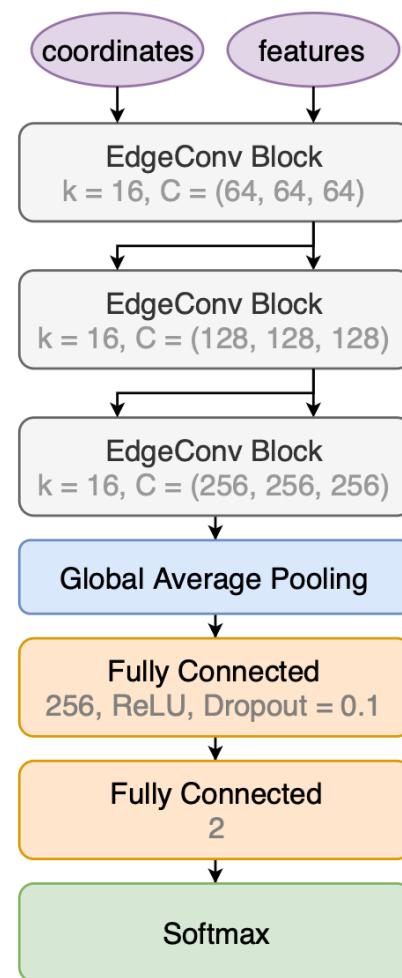
X-axis – the signal efficiency
Y-axis – the background rejection

EdgeConv and ParticleNet

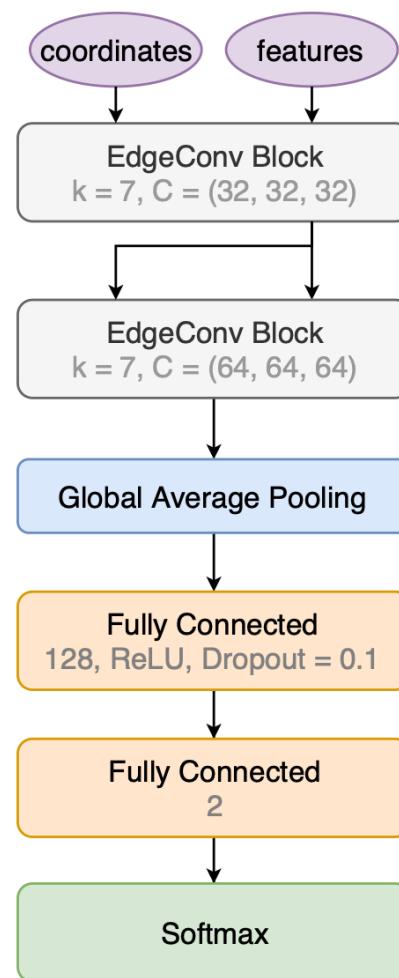
arXiv:1902.08570



The structure of the EdgeConv block



(a) ParticleNet



(b) ParticleNet-Lite

The architectures of the ParticleNet and
the ParticleNet-Lite networks

1D CNN

[arXiv:2011.13466](https://arxiv.org/abs/2011.13466)

- Input is a **Particle List**
- **LRP** is a backpropagation method

