

Attention to the strengths of physics interactions

Enhanced Deep Learning Event Classification for Particle Physics Experiments

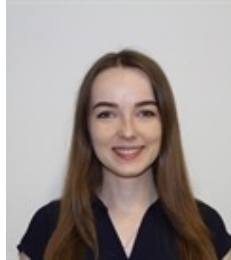
Polina Moskvitina

Sascha Caron, Clara Nellist, Roberto Ruiz de Austri, Rob Verheyen, Zhongyi Zhang

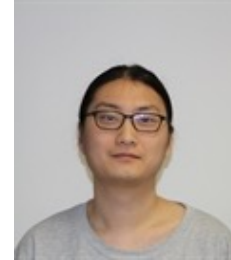
Our group



Sascha
(Supervisor,
RU/Nikhef)



Polina
(PhD,
RU/Nikhef)



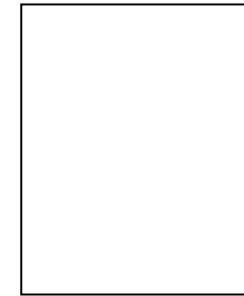
Zhongyi
(Postdoc,
RU/Nikhef)



Clara
(Co-supervisor,
RU/Nikhef)



Rob
(Postdoc,
UCL)



Roberto
(Researcher,
IFIC)

From DarkMachines :

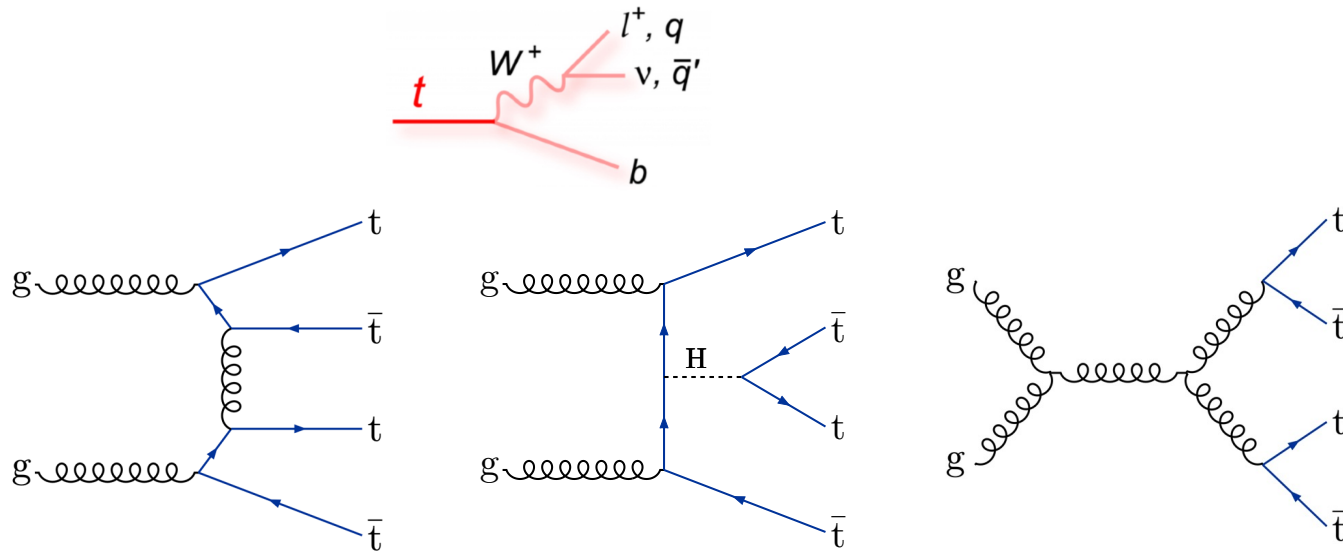
The question was: “**What is the best event classifier for the LHC?**”



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](#)]

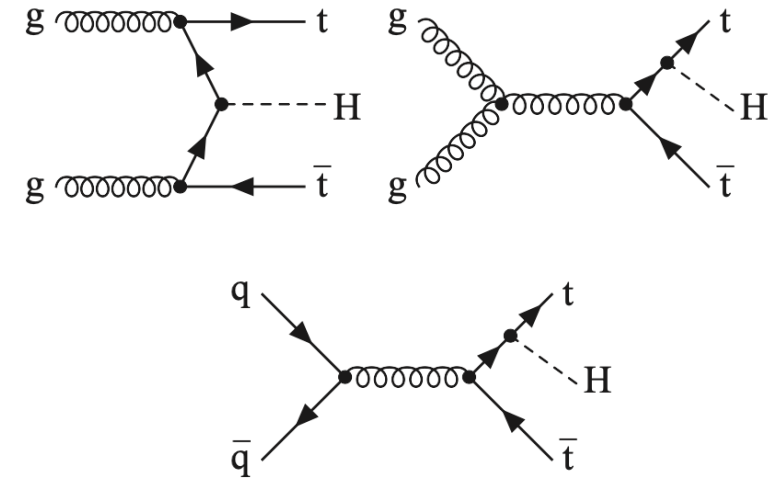


Examples of Feynman diagrams for SM $t\bar{t}t\bar{t}$ production at leading order in QCD and via an off-shell Higgs boson mediator

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)** with **BDT** by **ATLAS** [[Phys. Lett. B 784 \(2018\) 173](#)]
5.2 σ (4.2 σ) with **BDT** by **CMS** [[Phys. Rev. Lett. 120, 231801](#)]

The four-top decays and Background composition

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

Signal region:

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

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

Signal process:

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

Physical backgrounds:

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

event ID; process ID; weight; \cancel{E}_T ; $\phi_{\cancel{E}_T}$; $obj_1, E_1, p_{T_1}, \eta_1, \phi_1$; $obj_2, E_2, p_{T_2}, \eta_2, \phi_2$; ...

- **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

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

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

Summary of ML model details

arXiv:2211.05143

Variables per particle

Also receives \cancel{E}_T ; $\phi_{\cancel{E}_T}$

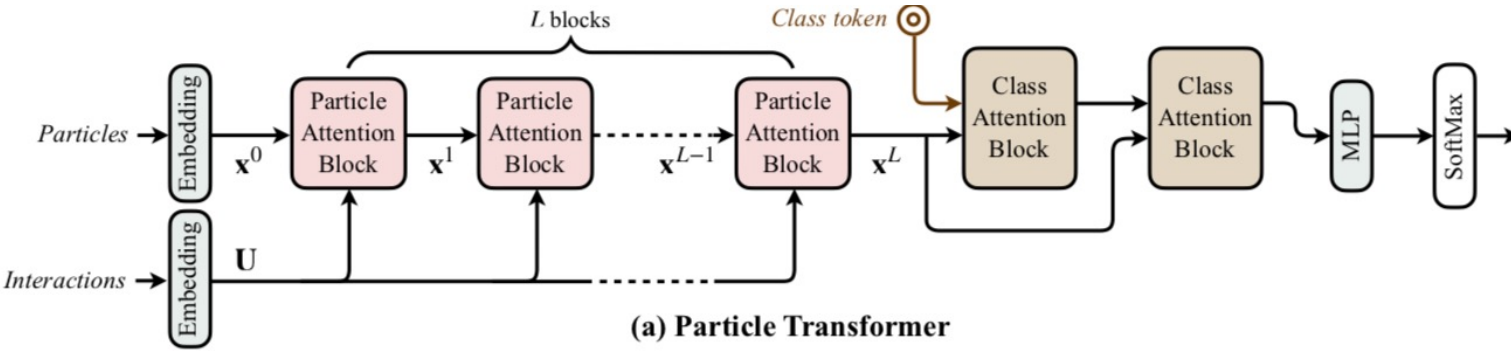
$E, p_T, \eta, \phi, \text{jet}_{\text{tag}}, \text{b-jet}_{\text{tag}}, e_{\text{tag}}^-, e_{\text{tag}}^+, \mu_{\text{tag}}^-, \mu_{\text{tag}}^+, \gamma_{\text{tag}}$

NN structure	Pairwise kinematic features	Loss function
BDT		Cross-entropy
BDT _{int.}	$m_{ij}, \Delta R_{ij}$	
FCN		
CNN		
PN		
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.}	$m_{ij}, \Delta R_{ij}$	Focal [$\alpha = 0.75, \gamma = 3$]
ParT _{int.} SM (FL)	$m_{ij}, \Delta R_{ij} + \text{SM matrix}[3]$	
ParT _{int.} SMids	$m_{ij}, \Delta R_{ij} + \text{SM matrix}[1]$	Cross-entropy
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	$m_{ij}, \Delta R_{ij} + \text{SM matrix}[3]$	

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



(a) Particle Transformer

Attention Modules

(scaled dot product attention):

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

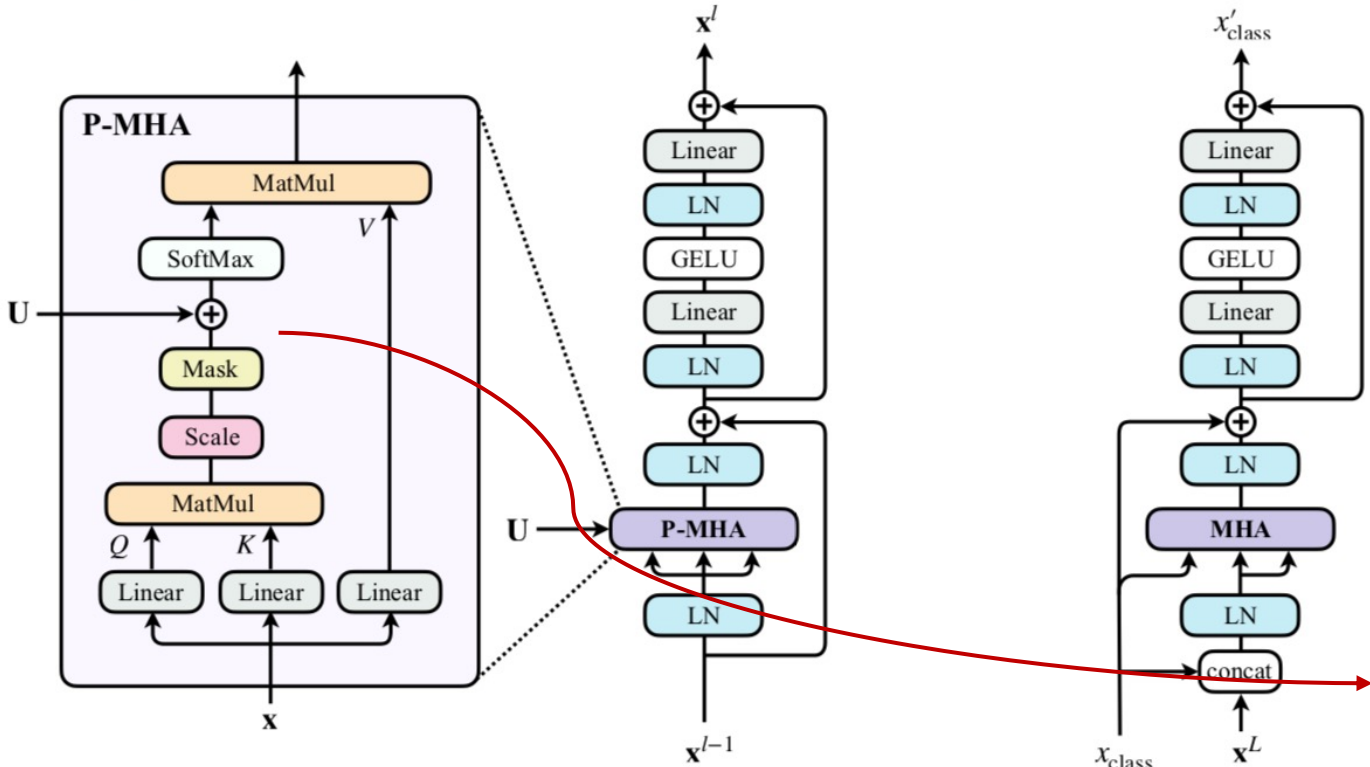
$$Q = q \times W_Q$$

Attention is All You Need!

$$K = k \times W_K$$

$$V = v \times W_V$$

U \rightarrow **Attention matrix** \rightarrow correlation of “data sequence with data sequence”



(b) Particle Attention Block

(c) Class Attention Block

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

U \rightarrow

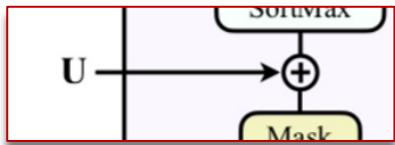
Pairwise Features + SM interaction matrix
(attention matrix)



To show the interaction strength based on the SM coupling constants

Adding Pairwise features

Include pairwise features in **Particle Transformer** through a trainable embedding U_{ij} for particles i and j



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

Attention Modules

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

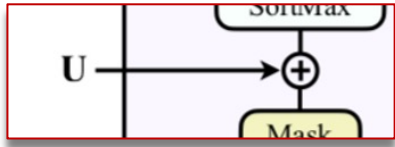
Features from the paper [\[arXiv:2202.03772\]](https://arxiv.org/abs/2202.03772)

- **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**

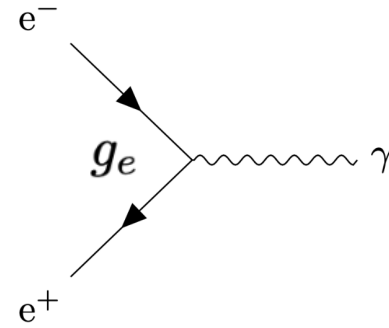
What we end up using :

$m_{ij}, \Delta R_{ij}$ 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, 0, 1, 0, 0, 1], # e-
  [0, 0, 0, 1, 0, 0, 0, 1], # e+
  [0, 0, 0, 0, 0, 0, 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, g_s, g_s, 0, 0, 0, 0, g_e/2], # j
  [0, g_s, g_s, 0, 0, 0, 0, g_e/3], # bjet
  [0, 0, 0, 0, g_z, 0, 0, g_e ], # e-
  [0, 0, 0, g_z, 0, 0, 0, g_e ], # e+
  [0, 0, 0, 0, 0, 0, g_z, g_e ], # m-
  [0, 0, 0, 0, 0, g_z, 0, g_e ], # m+
  [0, g_e/2, g_e/3, g_e, g_e, g_e, g_e, 0] ] ) # g
```

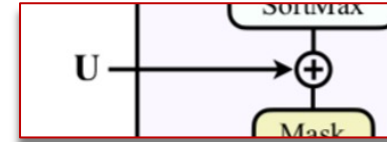
- '1' indicates an interaction possible at **LO** in the **SM**
- '0' indicates interactions that only appear at higher orders

- $g_z = 0.758$ 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], # -
  [0, g_s, g_s, 0, 0, 0, 0, g_e/2], # j
  [0, g_s, g_s, 0, 0, 0, 0, g_e/3], # bjet
  [0, 0, 0, 0, g_z, 0, 0, g_e ], # e-
  [0, 0, 0, g_z, 0, 0, 0, g_e ], # e+
  [0, 0, 0, 0, 0, 0, g_z, g_e ], # m-
  [0, 0, 0, 0, 0, g_z, 0, g_e ], # m+
  [0, g_e/2, g_e/3, g_e, 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

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

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

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

$$g_s = \sqrt{4\pi\alpha_s} \quad n_f - \text{number of quark flavors that are active}$$

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

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

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

		BDT	BDT _{int.}	FCN	CNN
$t\bar{t} + h$	AUC	0.825(0)	0.831(0)	0.821(2)	0.778(6)
	$\epsilon_B(\epsilon_S = 0.7)$	0.206(0)	0.192(0)	0.203(1)	0.272(11)
	$\epsilon_B(\epsilon_S = 0.3)$	0.026(1)	0.026(0)	0.026(1)	0.037(1)
$t\bar{t} + W$	AUC	0.891(0)	0.895(0)	0.887(0)	0.867(5)
	$\epsilon_B(\epsilon_S = 0.7)$	0.099(0)	0.092(0)	0.103(1)	0.125(8)
	$\epsilon_B(\epsilon_S = 0.3)$	0.011(0)	0.011(0)	0.010(0)	0.011(1)
$t\bar{t} + WW$	AUC	0.740(0)	0.746(0)	0.737(1)	0.745(2)
	$\epsilon_B(\epsilon_S = 0.7)$	0.347(0)	0.339(0)	0.342(5)	0.335(3)
	$\epsilon_B(\epsilon_S = 0.3)$	0.050(0)	0.051(0)	0.054(0)	0.051(0)
$t\bar{t} + Z$	AUC	0.833(0)	0.856(0)	0.836(0)	0.839(1)
	$\epsilon_B(\epsilon_S = 0.7)$	0.191(0)	0.163(0)	0.192(0)	0.190(4)
	$\epsilon_B(\epsilon_S = 0.3)$	0.026(0)	0.019(0)	0.023(0)	0.021(1)
		PN	PN _{int.}	PN _{int. SM}	ParT _{int. SM (FL)}
$t\bar{t} + h$	AUC	0.824(0)	0.842(1)	0.846(1)	0.844(1)
	$\epsilon_B(\epsilon_S = 0.7)$	0.199(0)	0.176(3)	0.171(2)	0.176(2)
	$\epsilon_B(\epsilon_S = 0.3)$	0.025(0)	0.019(1)	0.020(1)	0.020(1)
$t\bar{t} + W$	AUC	0.887(0)	0.895(2)	0.900(1)	0.902(4)
	$\epsilon_B(\epsilon_S = 0.7)$	0.102(1)	0.097(1)	0.091(1)	0.091(5)
	$\epsilon_B(\epsilon_S = 0.3)$	0.011(0)	0.011(0)	0.010(0)	0.011(0)
$t\bar{t} + WW$	AUC	0.742(0)	0.760(1)	0.765(0)	0.768(3)
	$\epsilon_B(\epsilon_S = 0.7)$	0.335(2)	0.311(1)	0.297(2)	0.294(7)
	$\epsilon_B(\epsilon_S = 0.3)$	0.051(0)	0.044(1)	0.044(1)	0.044(1)
$t\bar{t} + Z$	AUC	0.851(0)	0.879(1)	0.887(1)	0.892(0)
	$\epsilon_B(\epsilon_S = 0.7)$	0.168(4)	0.136(1)	0.126(2)	0.119(4)
	$\epsilon_B(\epsilon_S = 0.3)$	0.020(0)	0.016(1)	0.016(0)	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)	0.845(1)
	$\epsilon_B(\epsilon_S = 0.7)$	0.197(3)	0.179(6)	0.174(1)	0.176(3)
	$\epsilon_B(\epsilon_S = 0.3)$	0.023(0)	0.020(0)	0.020(0)	0.020(0)
$t\bar{t} + W$	AUC	0.896(1)	0.899(1)	0.905(2)	0.898(1)
	$\epsilon_B(\epsilon_S = 0.7)$	0.097(2)	0.090(1)	0.089(3)	0.094(2)
	$\epsilon_B(\epsilon_S = 0.3)$	0.010(0)	0.010(0)	0.009(0)	0.011(0)
$t\bar{t} + WW$	AUC	0.737(0)	0.767(1)	0.769(0)	0.763(1)
	$\epsilon_B(\epsilon_S = 0.7)$	0.354(3)	0.295(5)	0.288(2)	0.301(5)
	$\epsilon_B(\epsilon_S = 0.3)$	0.050(1)	0.040(0)	0.042(0)	0.047(1)
$t\bar{t} + Z$	AUC	0.839(1)	0.885(0)	0.891(1)	0.886(2)
	$\epsilon_B(\epsilon_S = 0.7)$	0.182(2)	0.130(1)	0.119(3)	0.129(4)
	$\epsilon_B(\epsilon_S = 0.3)$	0.021(1)	0.016(0)	0.015(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)	0.8739(0)
	$\epsilon_B(\epsilon_S = 0.7)$	0.1758(3)	0.1387(1)	0.1377(0)	0.1384(0)	0.1369(1)
	$\epsilon_B(\epsilon_S = 0.3)$	0.0207(0)	0.0182(0)	0.0178(0)	0.0178(0)	0.0176(0)
	ParT	ParT _{int.}	ParT _{int. SMids}	ParT _{int. SM const}	ParT _{int. SM}	
$t\bar{t}t\bar{t}$	AUC	0.8404(0)	0.8708(0)	0.8715(0)	0.8717(0)	0.8732(0)
	$\epsilon_B(\epsilon_S = 0.7)$	0.1842(3)	0.1394(0)	0.1389(2)	0.1372(1)	0.1366(0)
	$\epsilon_B(\epsilon_S = 0.3)$	0.0230(0)	0.0172(0)	0.0180(0)	0.0167(0)	0.0169(0)

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

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

	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)	0.8523(0)
	$\epsilon_B(\epsilon_S = 0.7)$	0.2292(1)	0.1787(0)	0.1785(1)	0.1764(3)	0.1733(1)
	$\epsilon_B(\epsilon_S = 0.3)$	0.0471(1)	0.0345(0)	0.0343(1)	0.0350(0)	0.0340(0)
	ParT	ParT _{int.}	ParT _{int. SMids}	ParT _{int. SM const}	ParT _{int. SM}	
$t\bar{t} + h$	AUC	0.8058(1)	0.8507(0)	0.8473(0)	0.8497(0)	0.8532(0)
	$\epsilon_B(\epsilon_S = 0.7)$	0.2399(2)	0.1794(1)	0.1836(3)	0.1801(1)	0.1748(1)
	$\epsilon_B(\epsilon_S = 0.3)$	0.0502(0)	0.0357(0)	0.0355(1)	0.0367(0)	0.0351(0)

Significance

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

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

- 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 $L = 100 \text{ fb}^{-1}$)

		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	<u>8.29</u>
	$\epsilon_S = 0.7$	17.68	<u>2.21</u>
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	<u>9.88</u>
	$\epsilon_S = 0.7$	20.53	2.98
ParT _{int. SM (FL)}	$\epsilon_S = 0.3$	26.19	<u>10.48</u>
	$\epsilon_S = 0.7$	20.28	2.91
SetT _{int. SM}	$\epsilon_S = 0.3$	25.58	10.03
	$\epsilon_S = 0.7$	20.18	2.88

Results

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

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

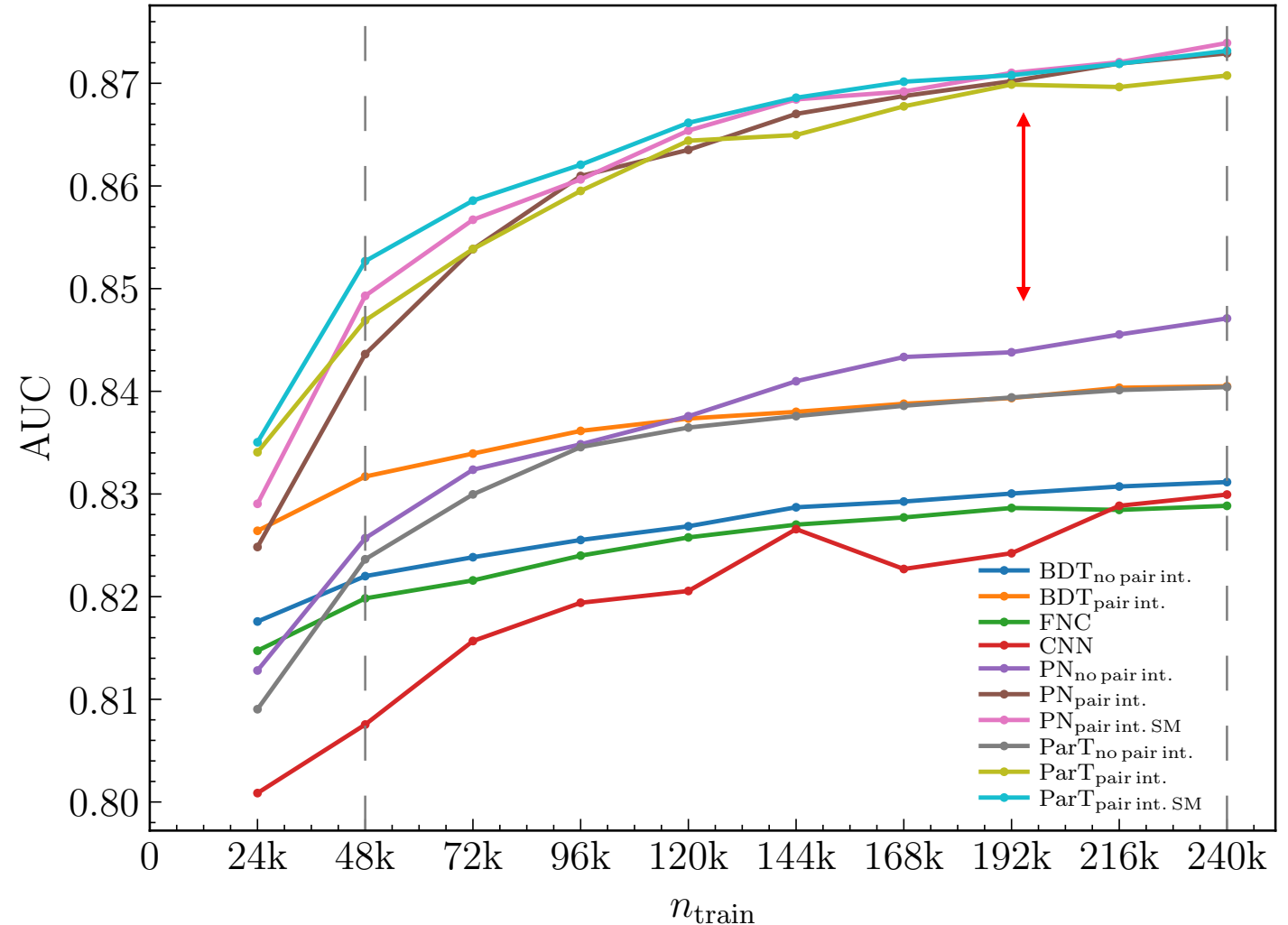
- Shows a steeper increase in **AUC** with fewer data
- Indicate higher data efficiency → less data needed for strong performance

Other Models

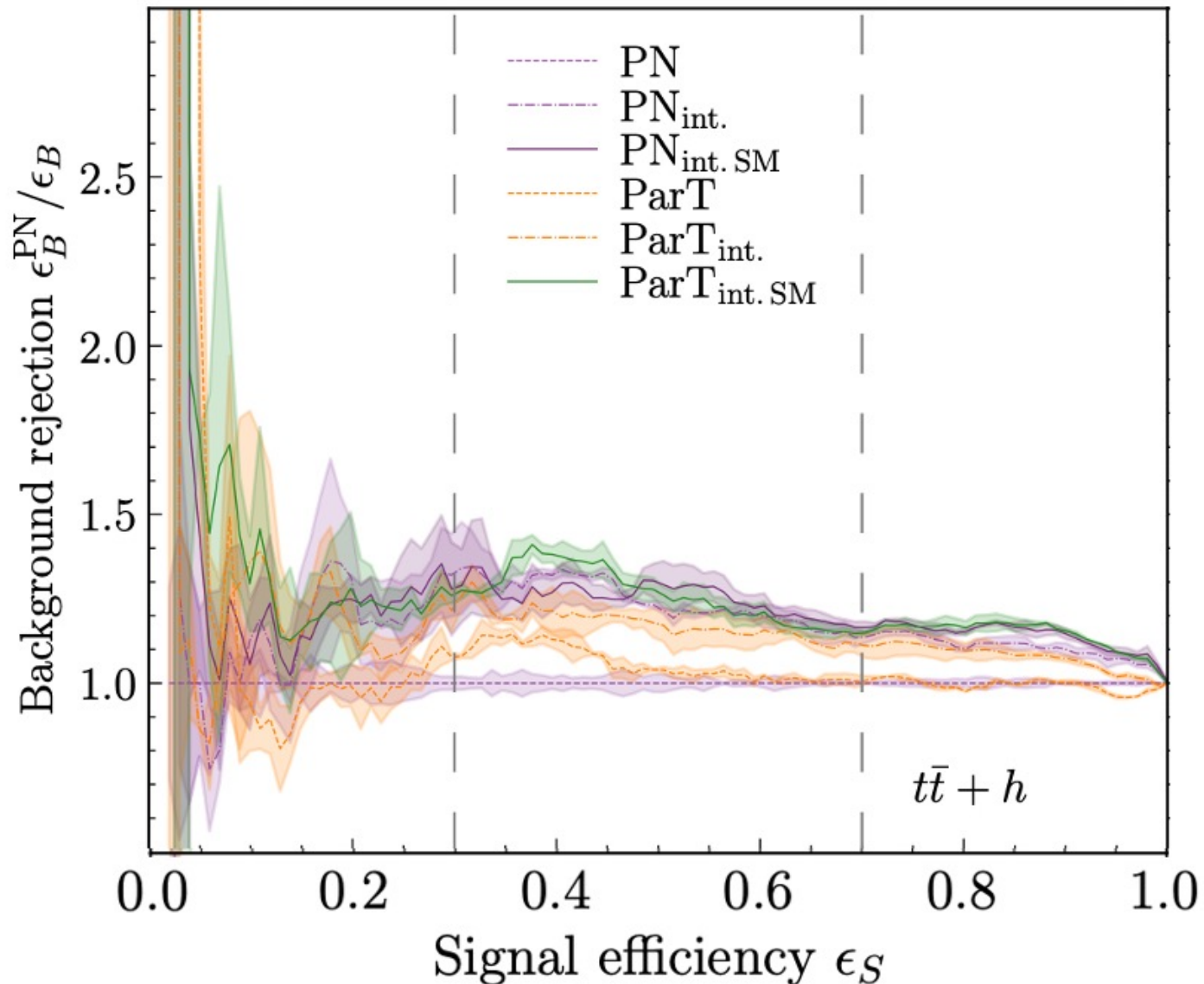
- **AUC** scores improve more gradually
- Suggest a requirement for larger datasets to match **PN** and **ParT** performance

PN and ParT models
(including the pairwise interactions)
could be preferable in data-scarce cases

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



Results



A plot with signal efficiency VS background rejection

**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)

Embedding **SM interactions** as physical information in **NN structures** is an important avenue in this field that could lead to more accurate and efficient event classification in particle physics!

Thank you for your attention!

Back up

Math Behind the Attention Mechanism

Attention Modules

(scaled dot product attention):

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

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** = $SoftMax(Attention\ Score)$

normalizes the scores to ensure they sum up to 1, acting as probabilities

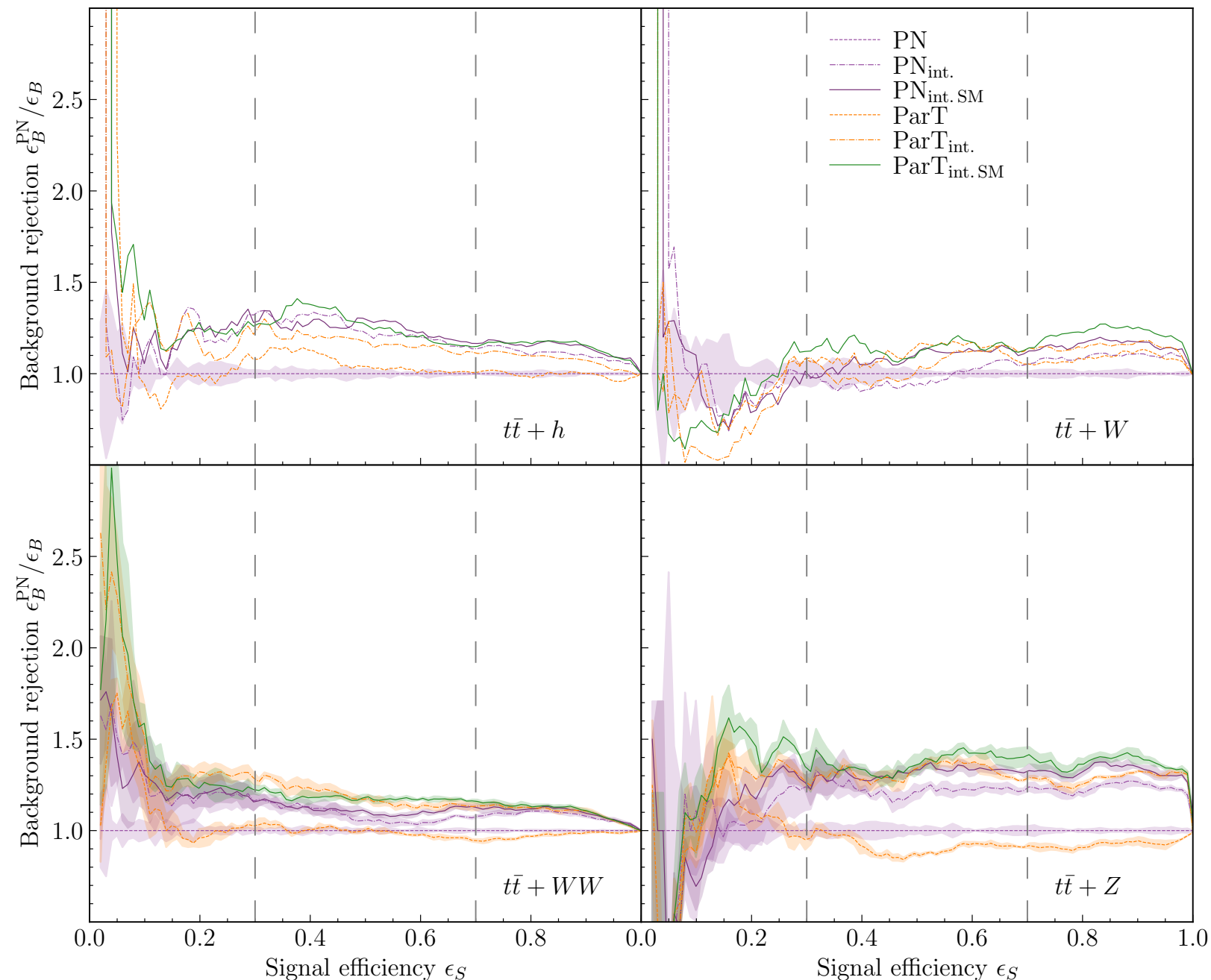
• Particle Representation:

➤ **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



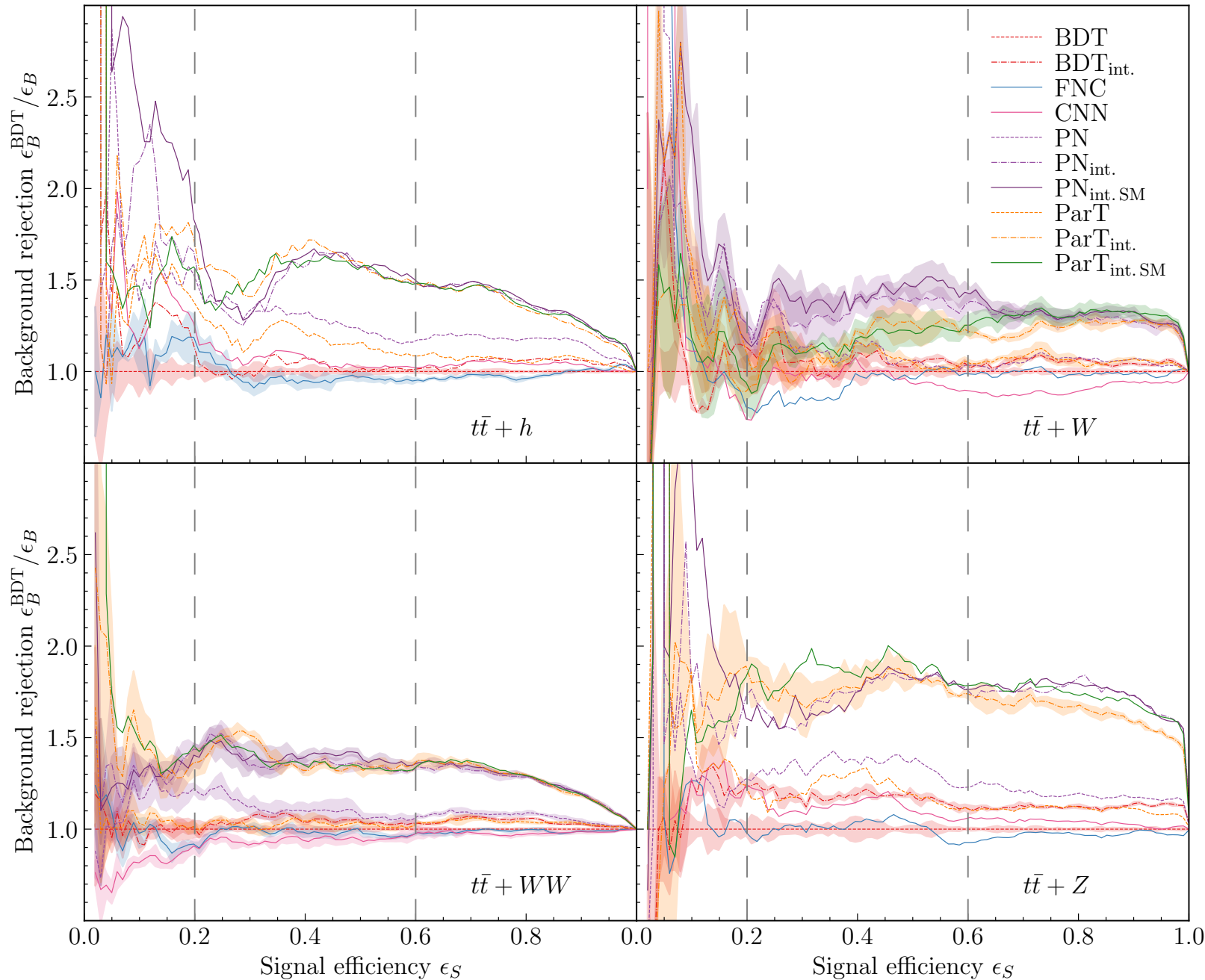
compared to the **ParticleNet (GNN)**

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

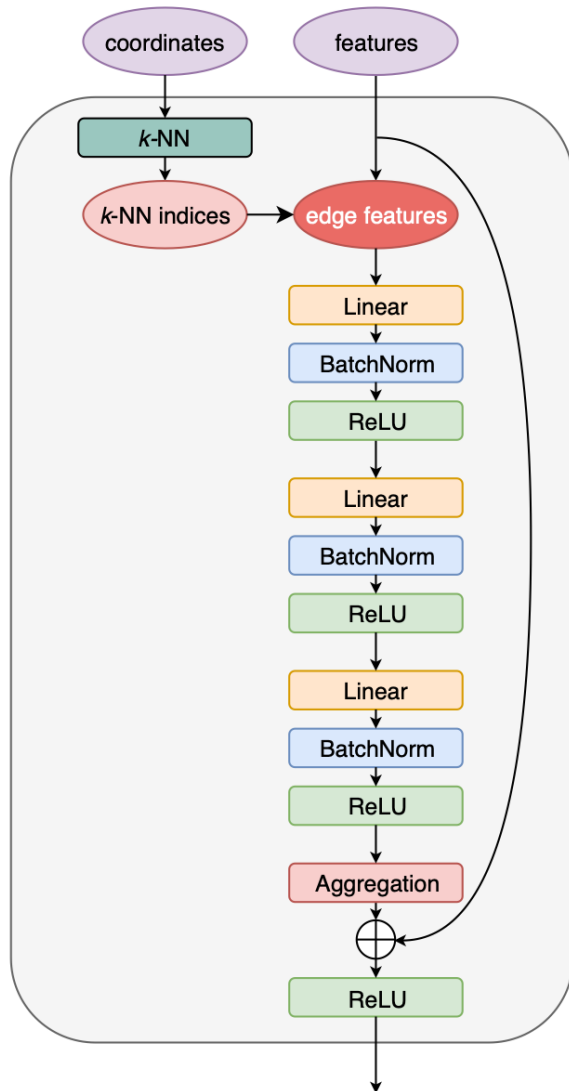
A plot with signal efficiency VS background rejection



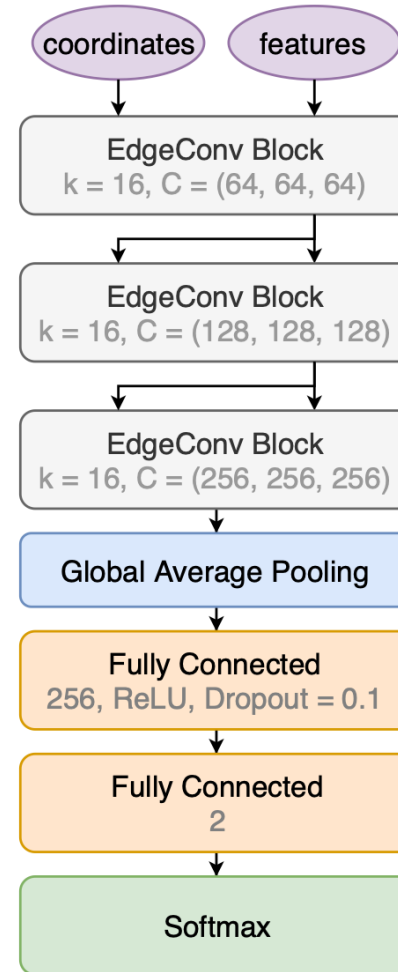
Compared to the **BDT**
for full size of the dataset

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

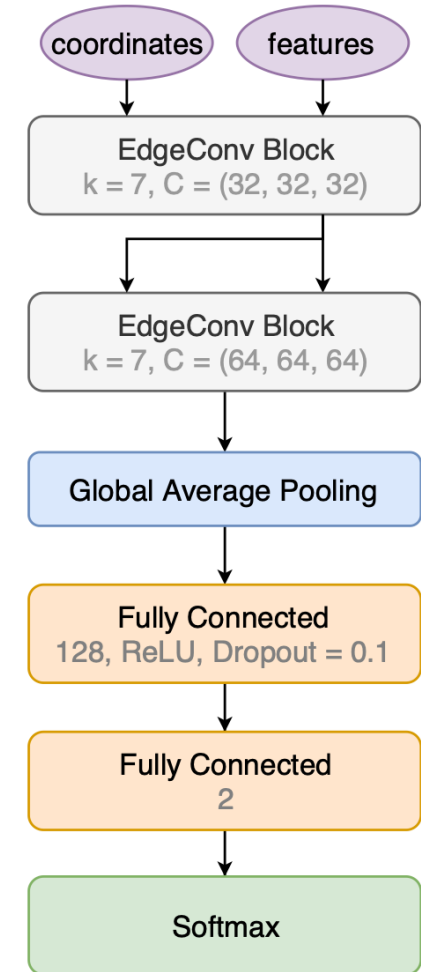
EdgeConv and ParticleNet



The structure of the EdgeConv block



(a) ParticleNet



(b) ParticleNet-Lite

The architectures of the ParticleNet and the ParticleNet-Lite networks

1D CNN

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

