

Improving ATLAS Hadronic Object Performance with ML/AI Algorithms

Lake Louise Winter Institute 2023

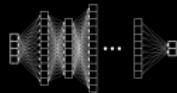
Tobias Fitschen

20 Feb 2023

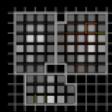
University of Manchester



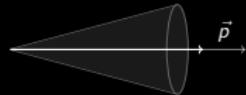
European Research Council
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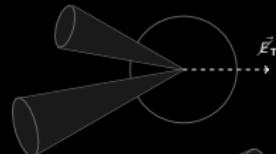
Neural Networks



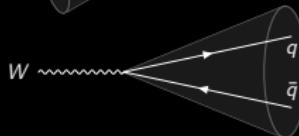
Calo Clusters



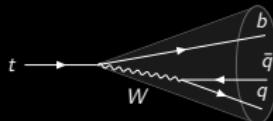
Jet Energy Scale



Missing E_T

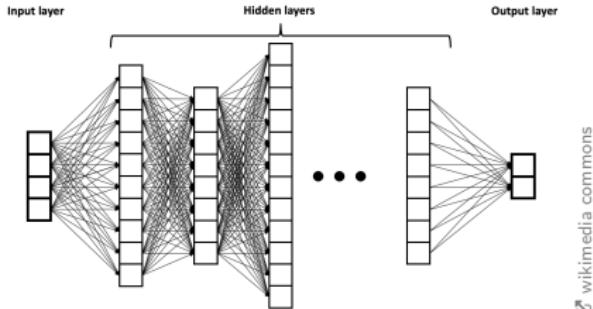


W/Z Tagging



Top Tagging

Multilayer Perceptron (MLP)

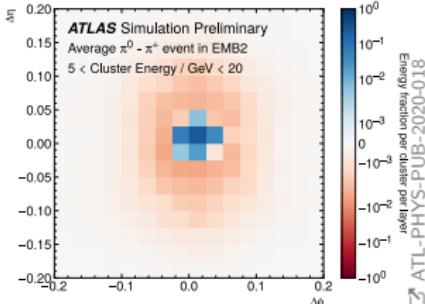


- Most simple architecture
- Fully connected layers
- Feed forward
- "Deep Neural Net" usually means this
- One or two outputs
- Binary or multi-classification

Convolutional Neural Net (CNN)

- Developed for image processing/classification
 - Input has to be projected into images (loss of information)
- Take advantage of hierarchical pattern in data
- Identifies spatially localized features

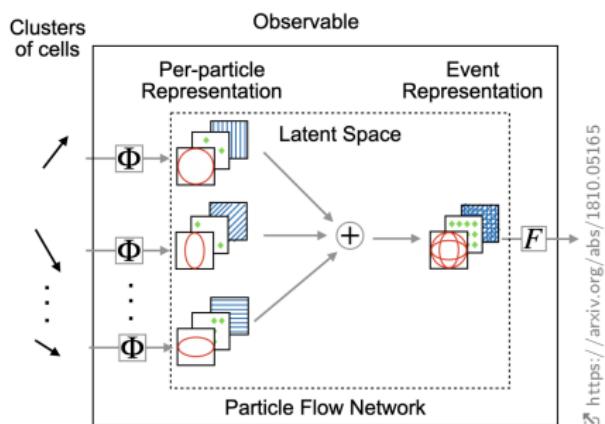
π^0/π^\pm calorimeter shower as image



Deep Sets

☒ (Energy/Particle Flow Network)

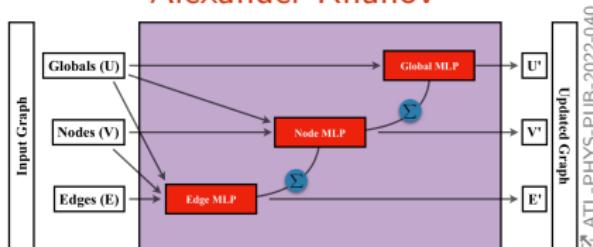
- Unorderd, variable length input
- E.g. of jet constituent momenta
- Permutation invariant



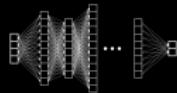
Graph Neural Net ☒ (GNN)

More info in ☒ previous talk by

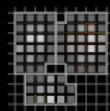
Alexander Khanov



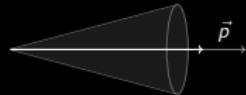
- Structured representation: nodes V , edges E
- Pairwise message passing
 - Nodes iteratively updated by exchanging information with neighbors
- Permutation invariant
- E.g. neighboring calo cells connected via edges in GNN



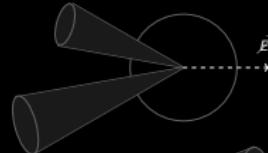
Neural Networks



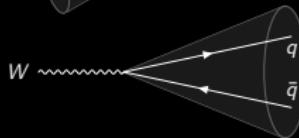
Calo Clusters



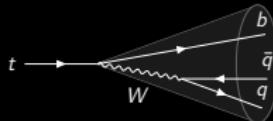
Jet Energy Scale



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W/Z Tagging



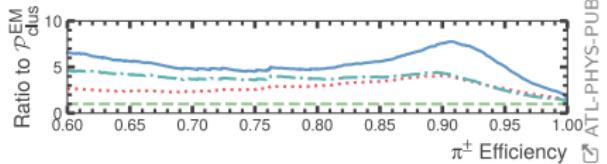
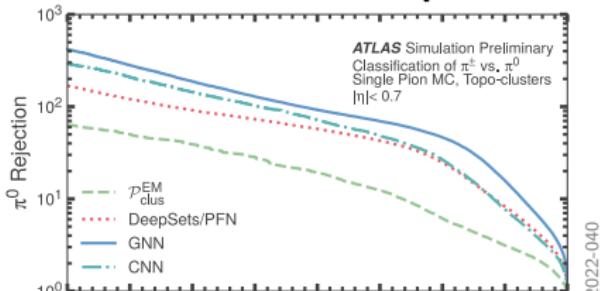
Top Tagging

π^0 vs π^\pm Shower Classification

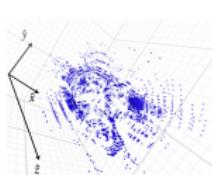
Non-compensating ATLAS calorimeter requires different calibrations for neutral/charged clusters

First step in cluster calibration: Differentiate EM from hadronic clusters

π^0 vs π^\pm classification performance

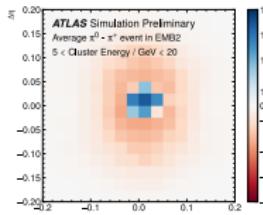


Point cloud of energy deposits in calorimeter cells



ATL-PHYS-PUB-2022-040

Image: $\pi^0 - \pi^\pm$ difference



Baseline used in LCW: $P_{\text{clus}}^{\text{EM}}$

- Binned EM-scale cluster variables
 - Total cluster energy $E_{\text{cluster}}^{\text{EM}}$
 - Pseudorapidity η
 - Longitudinal depth λ_{clus}
 - 1st cell energy density moment $\langle \rho_{\text{cell}} \rangle$
- Combined into likelihood $P_{\text{clus}}^{\text{EM}}$

Individual calorimeter cell signals

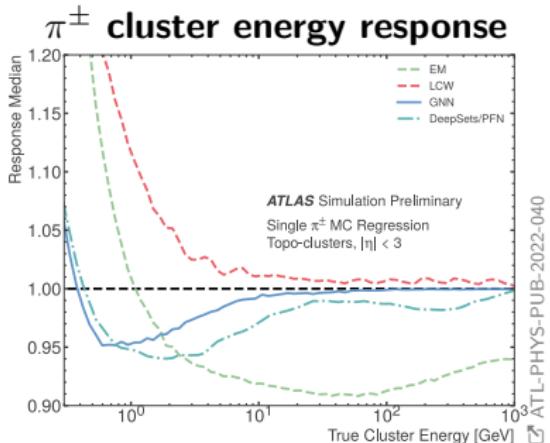
→ As point clouds (GNN, PFN)

→ Or projected on images (CNN)

Observations

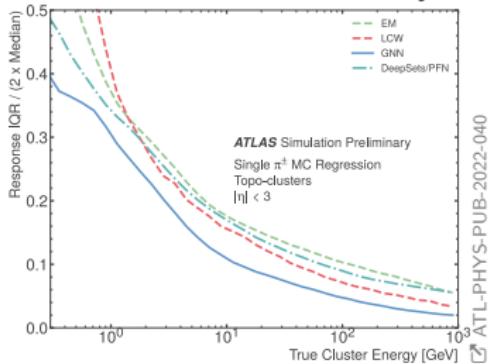
- All point cloud methods significantly outperform baseline MLP $P_{\text{clus}}^{\text{EM}}$

Energy Regression



Interquantile range IQR (measure for spread)

Calorimeter clusters only



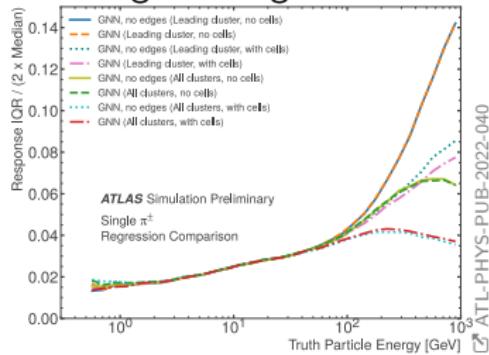
Second step: Energy Calibration

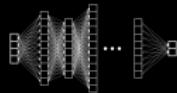
Here: charged (π^\pm) clusters

Observations

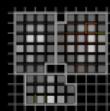
- GNN performs best wrt. response and width
- Followed by Deep Sets
- Similar for neutral π^0 clusters (see backup)

Including tracking information

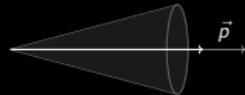




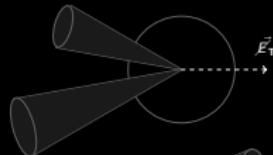
Neural Networks



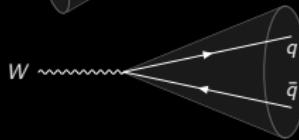
Calo Clusters



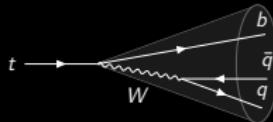
Jet Energy Scale



Missing E_T

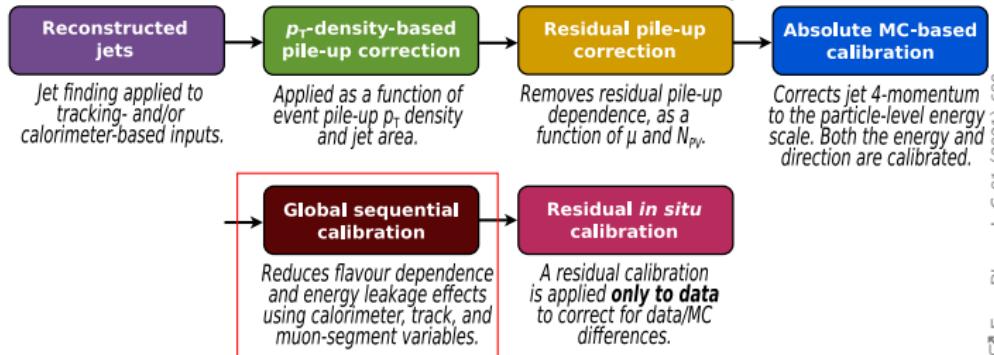


W/Z Tagging



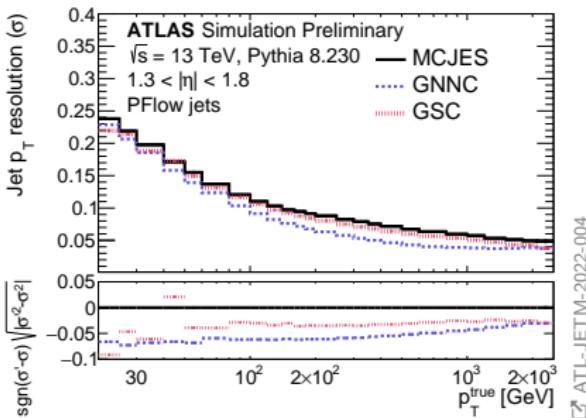
Top Tagging

ATL-JETM-2022-004: ML based Global Sequential Calibration (GSC)

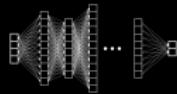


Eur. Phys. J. C 81 (2021) 689

After energy scale calibrated on average, GSC corrects for small differences for different jet flavours



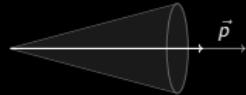
- **GSC sequentially** corrects for each variable
→ Does not exploit correlations
- New method (**GNNC**) uses MLP trained to predict p_T response
→ Improvement over full p_T range



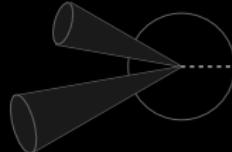
Neural Networks



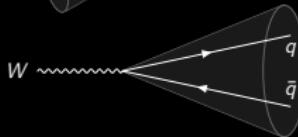
Calo Clusters



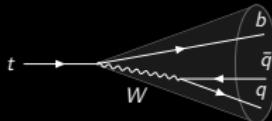
Jet Energy Scale



Missing E_T



W/Z Tagging

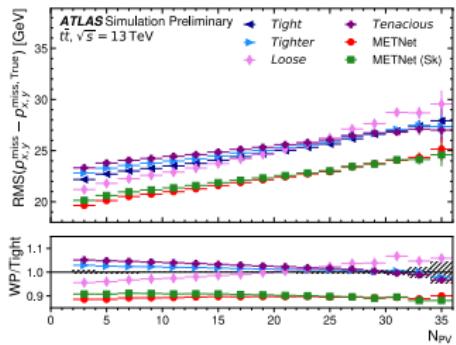


Top Tagging

ATL-PHYS-PUB-2021-025: METNet: A combined p_T^{miss} working point

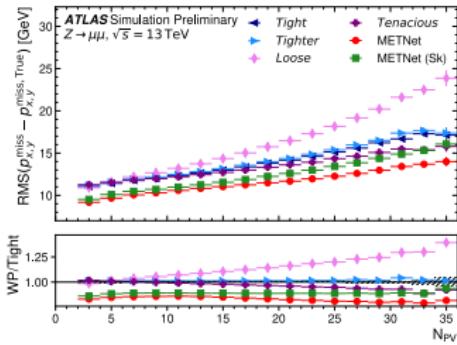
- p_T^{miss} in ATLAS: Negative sum of calibrated momenta of hard objects (e , μ , τ -jets, γ , jets)
- Plus soft term: Tracks from PV not associate to hard objects
- Different working points (WPs) defined for various pileup conditions
 - E.g. "tight": Higher p_T cuts on forward jets
- MetNet: MLP combining p_T^{miss} values from different WPs
 - Based on event kinematics and conditions
- Overall better performance than any WP alone

Trained among others on $t\bar{t}$



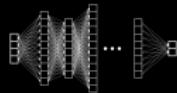
ATL-PHYS-PUB-2021-025

Extrapolates well to $Z \rightarrow \mu\mu$

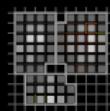


ATL-PHYS-PUB-2021-025

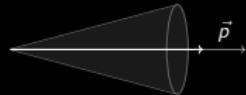
→ E_T^{miss} definition depends on process but MetNet performs best for all



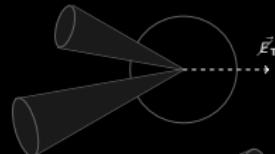
Neural Networks



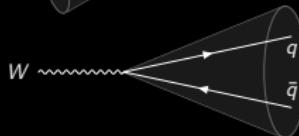
Calo Clusters



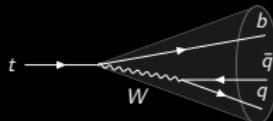
Jet Energy Scale



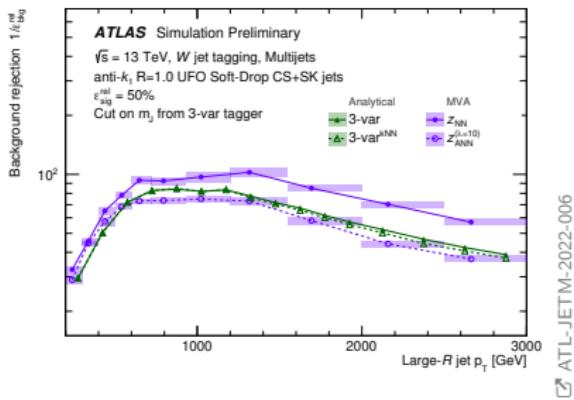
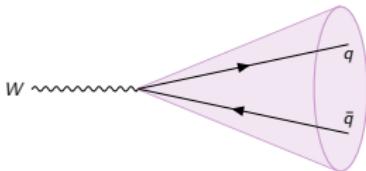
Missing E_T



W/Z Tagging



Top Tagging



3-variable cut based:

- D_2 Energy correlation ratios
- N_{trk} Number of associated tracks
- m Jet mass

Machine learning based (NN):

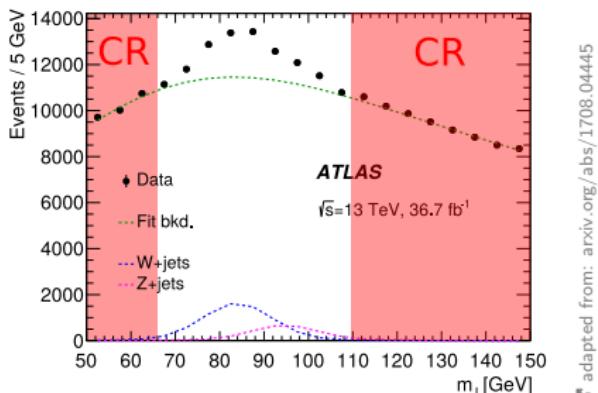
- Various substructure variables

- D_2, C_2 Energy correlation ratios
- T_{21} N -subjettiness
- R_2^{FW} Fox-Wolfram moment
- \mathcal{P} Planar flow
- a_3 Angularity
- A Aplanarity
- Z_{cut} Z -Splitting scales
- $\sqrt{d_{12}}$ d -Splitting scales
- $Kt\Delta R$ k_t -subjett ΔR
- N_{trk} Number of associated tracks
(see backup for definitions)

- **NN** tagger significantly outperformed **cut based 3-var** tagger
- Even mass-decorrelated version **ANN** shows similar performance to **cut based 3-var** using m

The Need for Mass Decorrelation

Data-driven background estimates:



adapted from: arxiv.org/abs/1708.04445

- Define mass side-bands as control regions (CR)
- Fit smooth function to data from left to right side-band
- Estimate background in signal region from fit

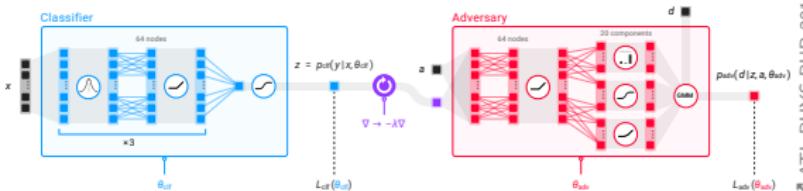
Problem: Tagger may introduce unwanted shaping of background, de-populating the sideband regions

Solution: Decorrelate tagger decision from m_j :

- Adversarial neural networks (ANN) for NN tagger

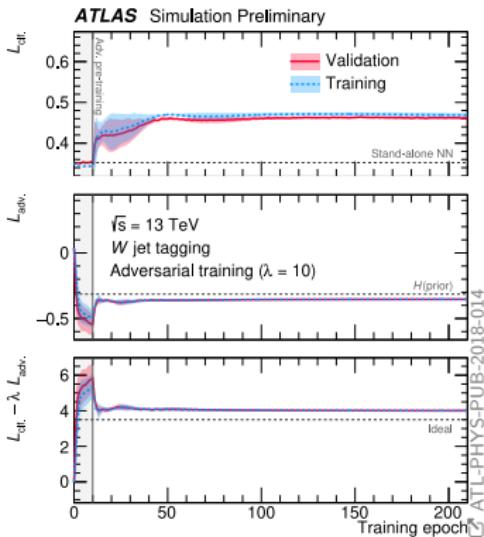
Architecture

- **Classifier** MLP for tagging task
- **Adversary** for decorrelation
(e.g. of mass)
 - Predicts mass based on classifier output (+auxiliary variables)
- **Gradient reversal layer:** During back-propagation penalise Classifier if Adversary predicts mass too well
 - Final tagger only consists of Classifier
 - Tagger decision decorrelated to mass



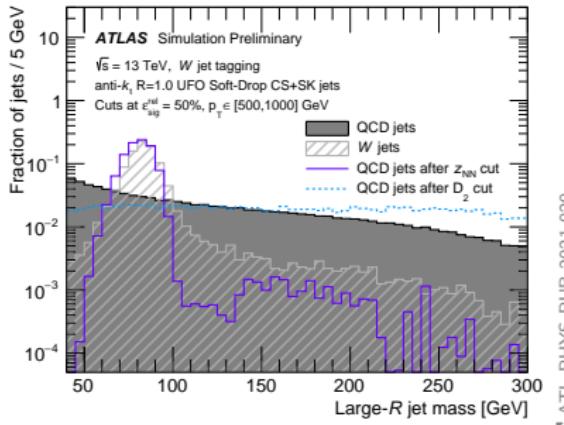
Training schedule

1. Classifier alone
2. Adversary alone
3. Both together

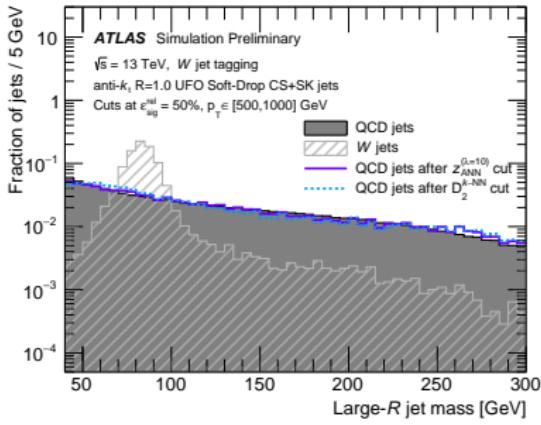


Mass Decorrelation with Adversarial Training

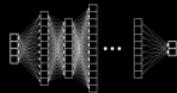
NN: Correlated to m_j



ANN: Active decorrelation



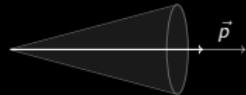
- Background mass distribution shaped according to signal by NN
- Adversarial Neural Network (ANN) successfully decorrelates



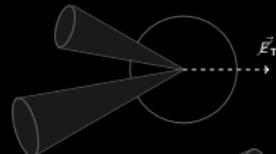
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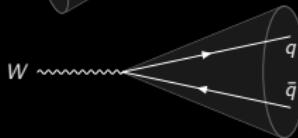
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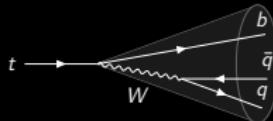
Jet Energy Scale



Missing E_T



W/Z Tagging



Top Tagging

2 taggers: Inclusive and contained

- Fixed working points: 50% and 80%
 - Defined as function of p_T
- DNN features optimised for UFO jets:

$\tau_1, \tau_2, \tau_3, \tau_4$ N -subjettiness

$\sqrt{d_{12}}, \sqrt{d_{23}}$ Splitting scales

ECF_1, ECF_2, ECF_3 Energy correlation functions

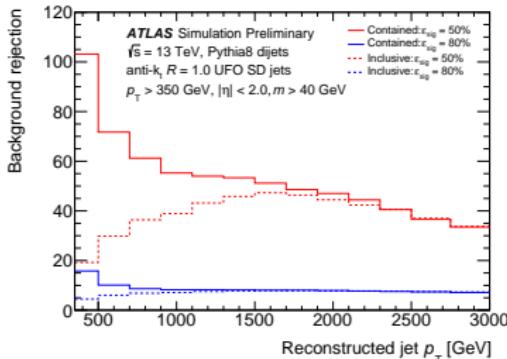
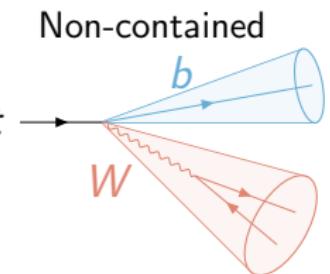
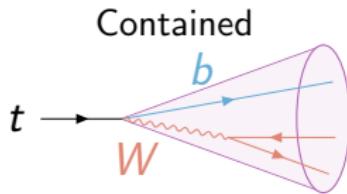
C_2, D_2 Energy correlation ratios

L_2, L_3 Generalised energy correlation ratios

Q_W Invariant mass / virtuality

T_M Thrust major

(see backup for definitions)



Constituent-Based Top Tagger

ATL-PHYS-PUB-2022-39: Constituent-Based Top-Quark Tagging

DNN top tagger (prev. slides):

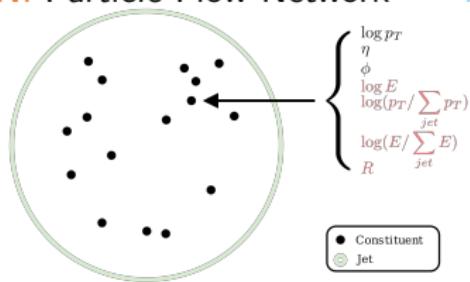
- Set of high-level features (substructure variables)
- Used as baseline (hIDNN)

Constituent-based taggers:

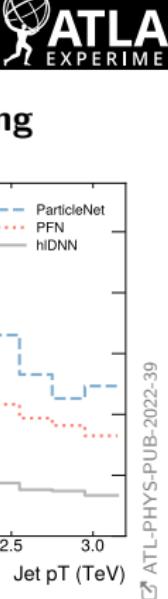
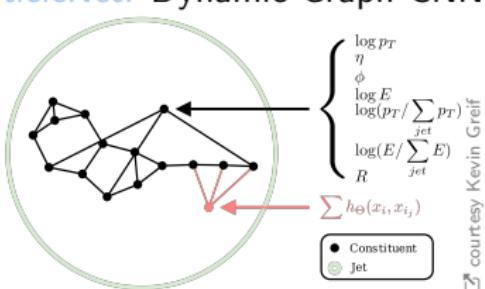
- Low-level features based on 4-vectors of jet constituents

→ Up to $\times 2$ improvement over baseline (hIDNN)!

PFN: Particle Flow Network



ParticleNet: Dynamic Graph-CNN



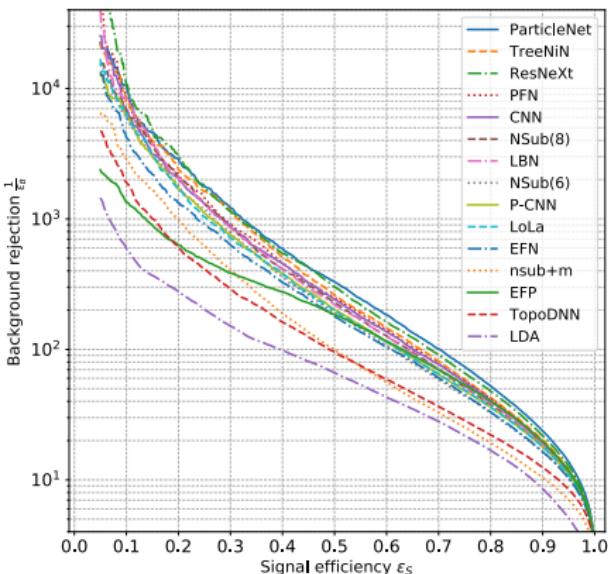
ATL-PHYS-PUB-2022-39

Constituent-Based Top Tagger

Based on: The Machine Learning landscape of top taggers

doi:10.21468/SciPostPhys.7.1.014

- Comparison of many modern ML techniques applied to the top tagging task
- Simplified detector simulation with Delphes + ATLAS card
- Calorimeter information only
→ No tracking as in UFO jets

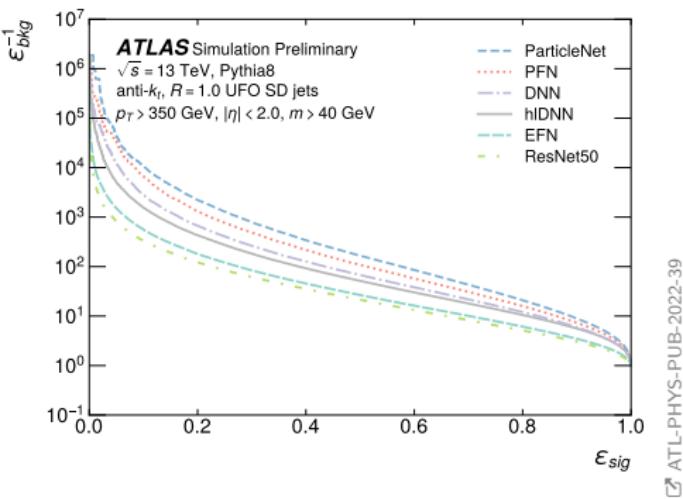


→ Best performance with **ParticleNet** and **ResNeXt**

Constituent-Based Top Tagger

ATL-PHYS-PUB-2022-39

New: How do these algorithms perform on ATLAS simulated UFO jets?



- **hIDNN:** Baseline similar to DNN top tagger
→ [ATL-PHYS-PUB-2021-028](#)
- **DNN:** Using constituent 4-momenta
→ [arxiv.org/abs/1704.02124](#)
- **EFN/PFN:** Energy/Particle-flow networks
→ [arxiv.org/abs/1810.05165](#)
- **ResNet50:** CNN using jet images
→ [arxiv.org/abs/1512.03385](#)
- **ParticleNet:** Dynamic Graph-CNN
→ [arxiv.org/abs/1902.08570](#)

- ParticleNet and PFN show best performance
- ResNet50 & EFN underperform → Do not translate well from Delphes study

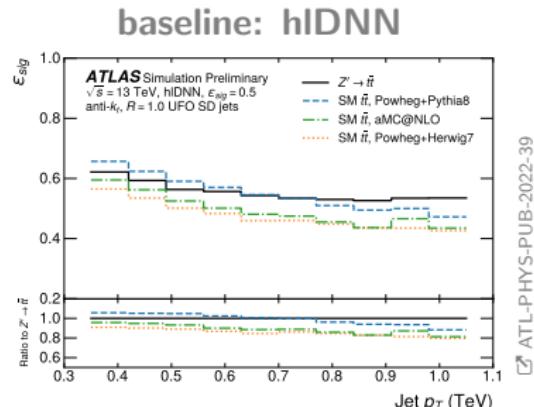
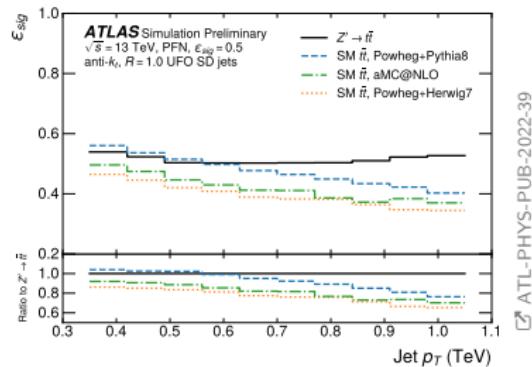
Simulated data made public for ML experts along with PUB-note!

Constituent-Based Top Tagger

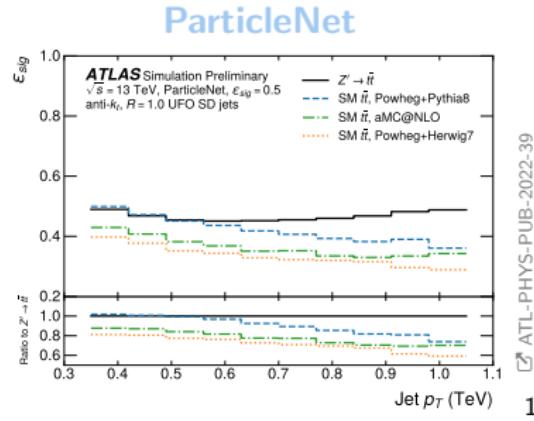
Model dependence

- Different parton shower and hadronisation models
- ϵ^{sig} measured at threshold for $\epsilon^{\text{sig}} = 50\%$ in nominal sample
- PFN and ParticleNet: Slightly more model dependent than baseline hIDNN

PFN (Particle Flow Network)



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Summary

Many ML applications for hadronic objects in ATLAS

- Calorimeter cluster classification and energy regression
- Jet energy scale calibration
- MET calibration
- W/Z and top tagging with and without mass decorrelation
- Many more...

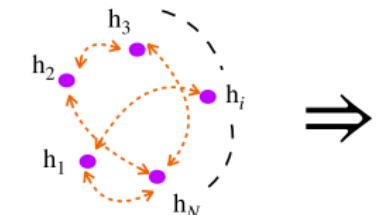
Constituent based methods perform best in all domains

- In most cases: GNN > Deep Sets > CNN > MLP > BDT > cuts
- **Important:** Better ROC curves are great, but data/MC agreement & model independence should not be neglected!

Appendix

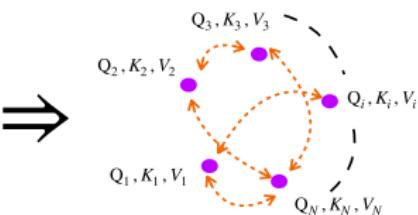
ML for Calo Clusters

Transformer for Graph Updates

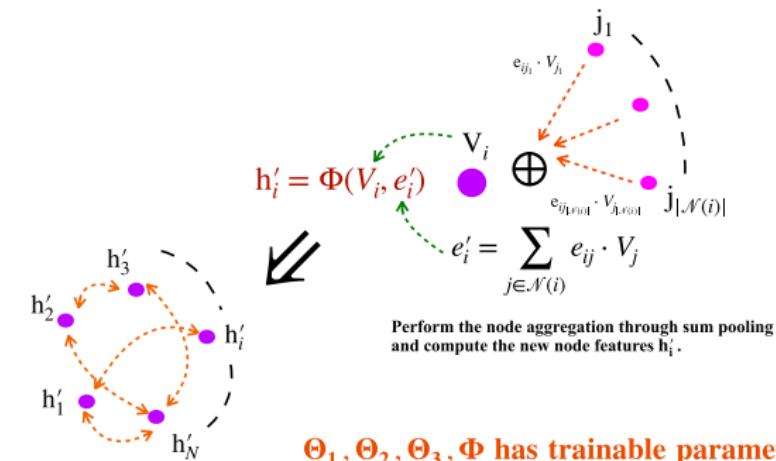


Start with a graph G having N nodes with node-features h_i on the i -th node.

$$\begin{aligned} Q_i &= \Theta_1(h_i) \\ K_i &= \Theta_2(h_i) \\ V_i &= \Theta_3(h_i) \end{aligned}$$



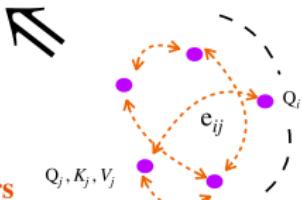
Form the query, key and value features using three MLP.



Perform the node aggregation through sum pooling and compute the new node features h'_i .

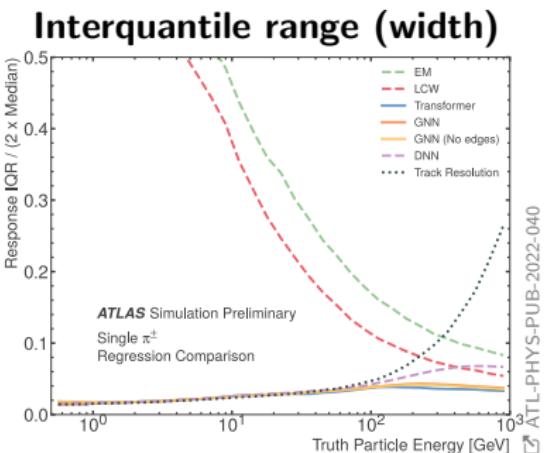
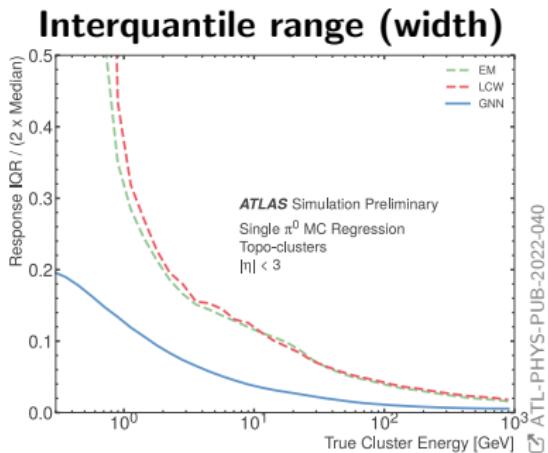
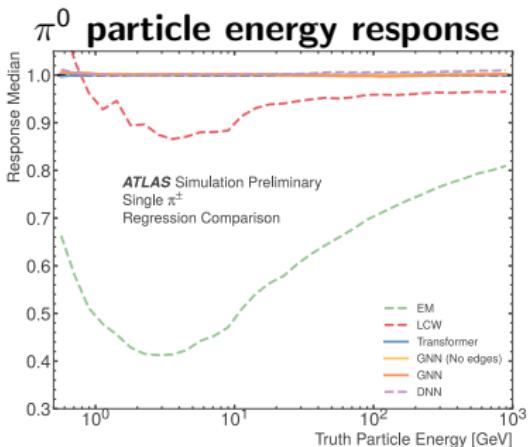
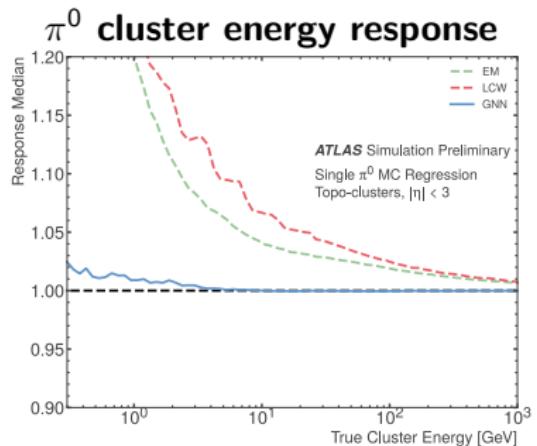
$$e_{ij} = \sigma\left(\frac{Q_i \cdot K_j^T}{\sqrt{d}}\right)$$

Create edge data using attention mechanism



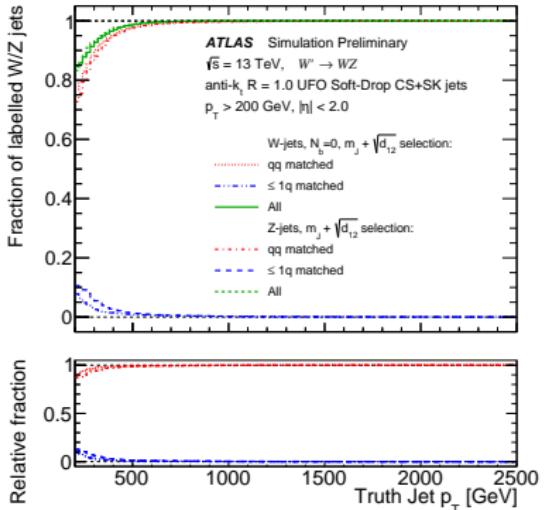
$\Theta_1, \Theta_2, \Theta_3, \Phi$ has trainable parameters

Performance



W/Z Taggers

Truth Labelling



Truth jet definition:

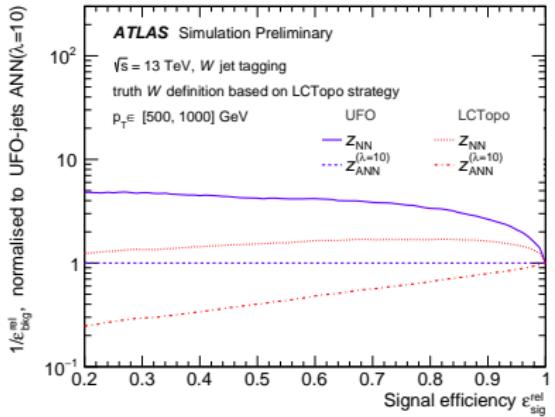
- Parton level MC to label jets as:
 - Signal: Containing full $W \rightarrow q\bar{q}$
 - Background: From single q/g
- Truth jets: Reconstructed from stable particles, anti- k_T $R = 1.0$
 - No grooming applied to ensure independence of grooming algorithm
- Requirements for truth signal jets:
 - Truth W/Z within $\Delta R < 0.75$
 - $m_J > 50$ GeV
 - $\sqrt{d_{12}} > 55.25 + e^{-2.35 \frac{p_T}{\text{GeV}}} \text{ GeV}$
 - $N_B = 0$ for W jets to reduce top contamination
- Matched to UFO jets with $\Delta R < 0.75$
- Optimised for $\epsilon_{\text{sig}} = 85\%$ at $p_T = 200$ GeV, 100% at $p_T = 300$ GeV

Matching to daughter quarks q, q' :

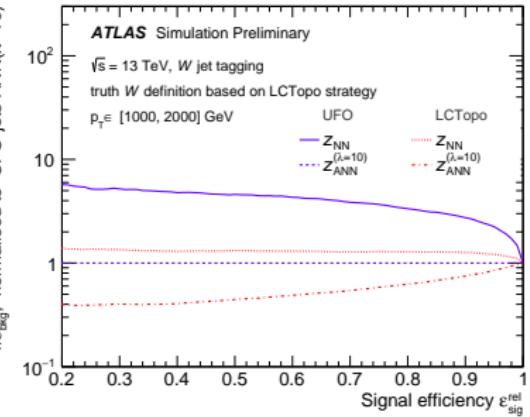
- Fraction of W (Z) containing both q, q' within $\Delta R < 0.75$:
 $> 98\% (96\%)$ at $p_T > 300$ GeV
 (previously: 90%)

Tagger Performance: UFO vs LCTopo

Low p_T



High p_T



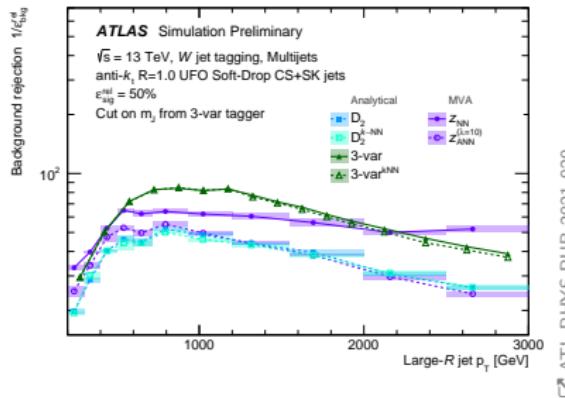
- Bkg rejection with **UFO** improved by a factor of 2-3 w.r.t. **LCTopo**!
- Mass decorrelation (ANN) comes with tradeoff of reduced efficiency
 - But may be better option for data-driven background estimates on m_J distribution

NN/ANN Tagger with n_{trk}



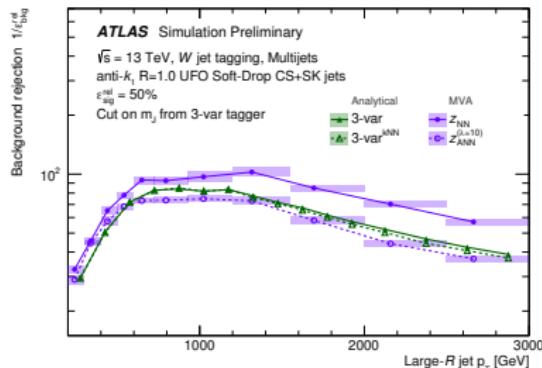
Previously:

ATL-PHYS-PUB-2021-029



Follow up publication:

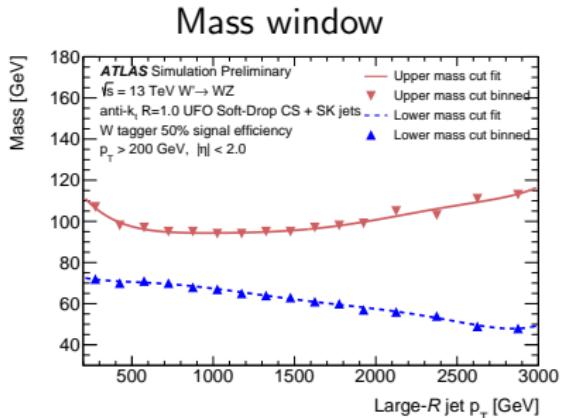
With n_{trk} as additional feature



ATL-JETM-2022-006

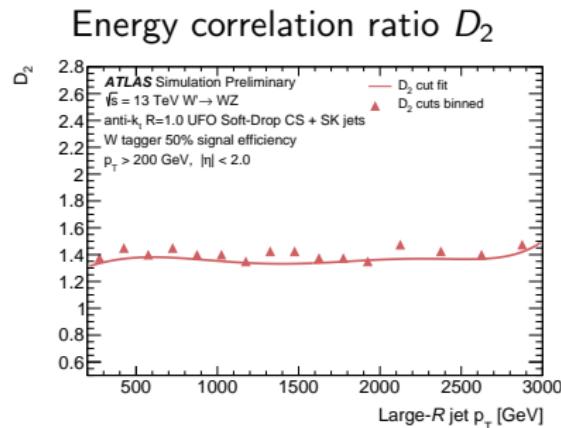
- Previously: 3-variable tagger showed better performance than NN
- Now: NN much better after including n_{trk} as additional feature!
 - ANN comparable with 3-variable tagger, but with decorrelation!
- Reason for such strong improvement:
 - Most other features exploit 2-prongedness of W/Z decay
 - n_{trk} is good quark/gluon discriminator

3-Variable Tagger

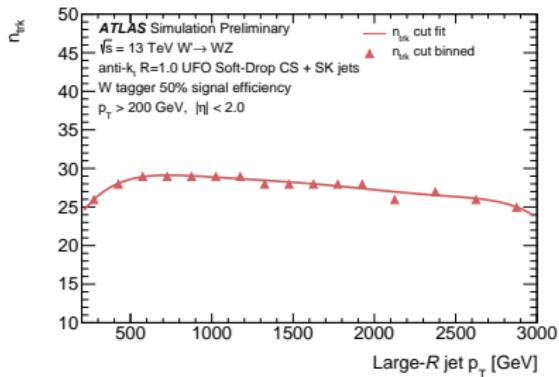


3-variable tagger: W

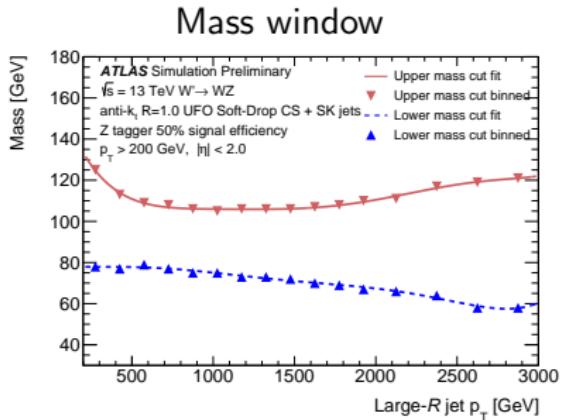
- p_T -dependent cuts on 3 features
- Maximise background rejection while keeping 50% signal efficiency per bin
- D_2 nearly flat in p_T
 - Thanks to angular resolution of UFO constituents
 - Fixed D_2 cut possible



Number of tracks n_{trk}

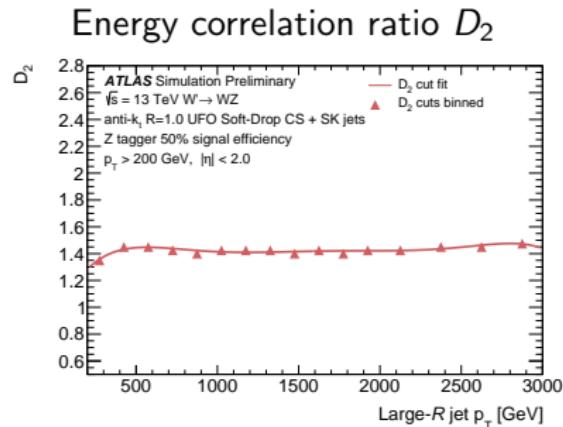


3-Variable Tagger

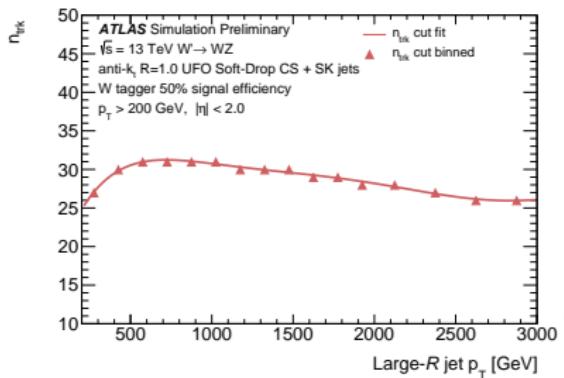


3-variable tagger: Z

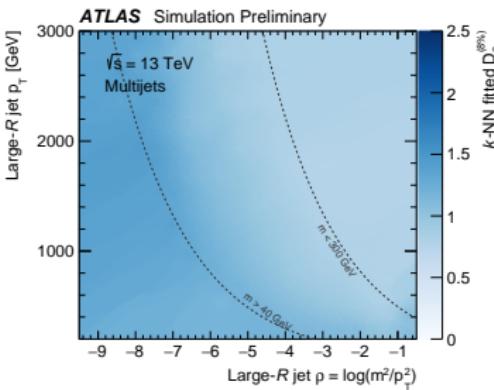
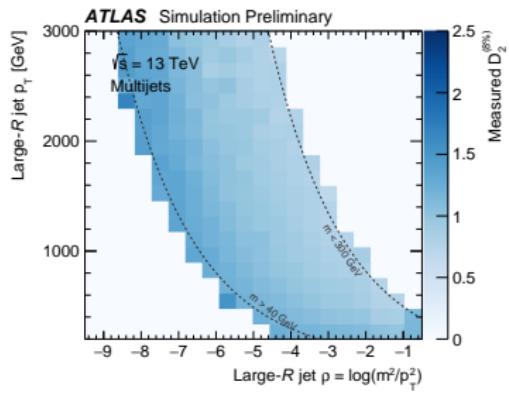
- p_T -dependent cuts on 3 features
- Maximise background rejection while keeping 50% signal efficiency per bin
- D_2 nearly flat in p_T
 - Thanks to angular resolution of UFO constituents
 - Fixed D_2 cut possible



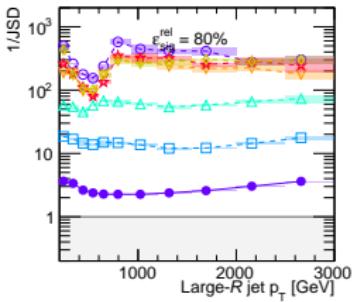
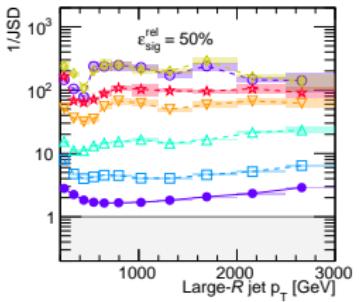
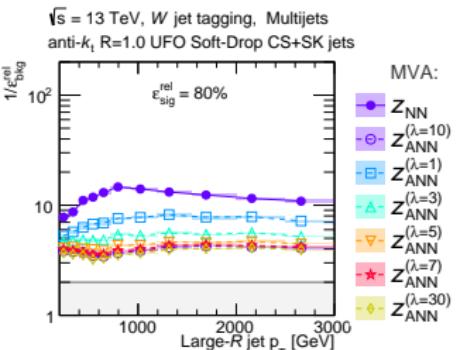
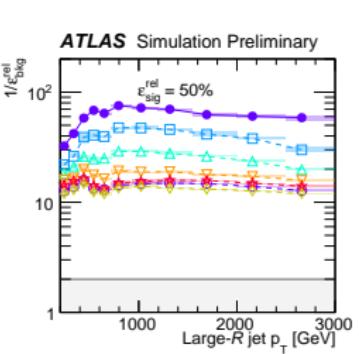
Number of tracks n_{trk}



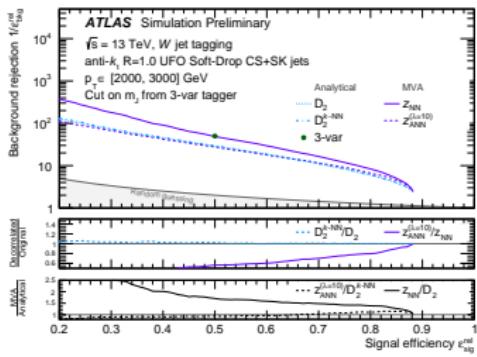
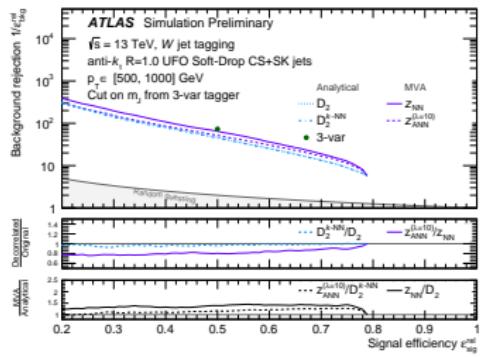
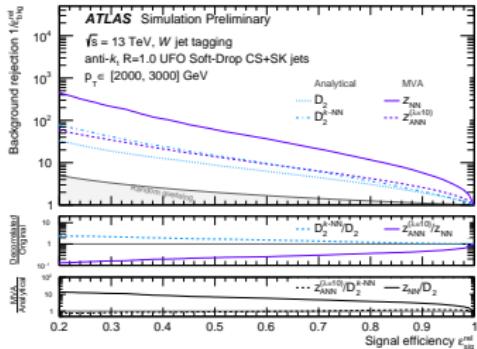
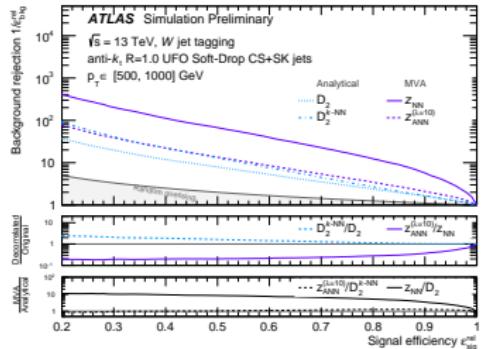
W/Z Tagger: k-NN Method



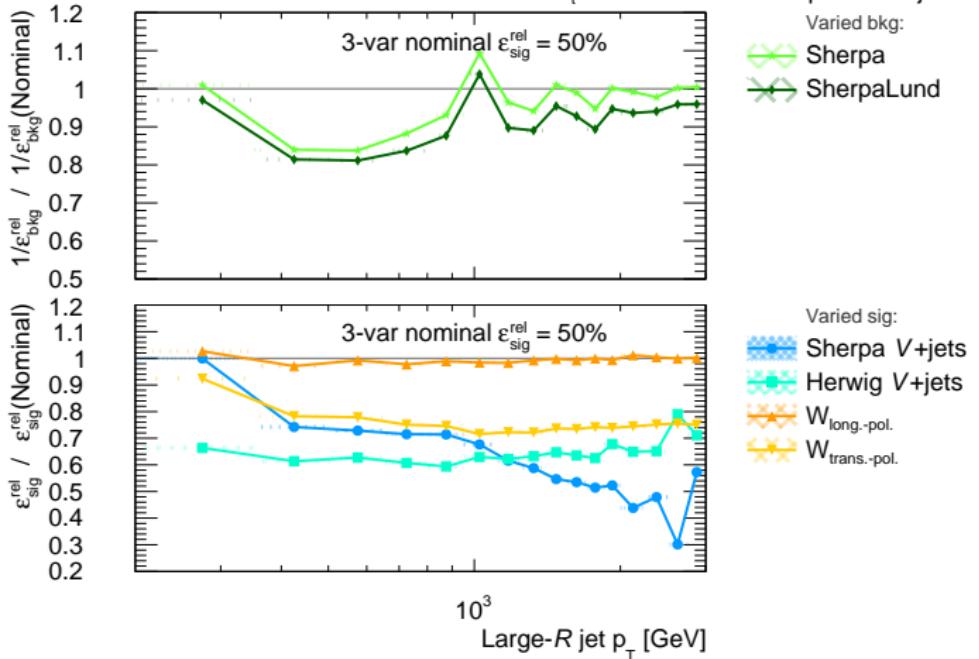
W/Z Tagger: Effect of λ



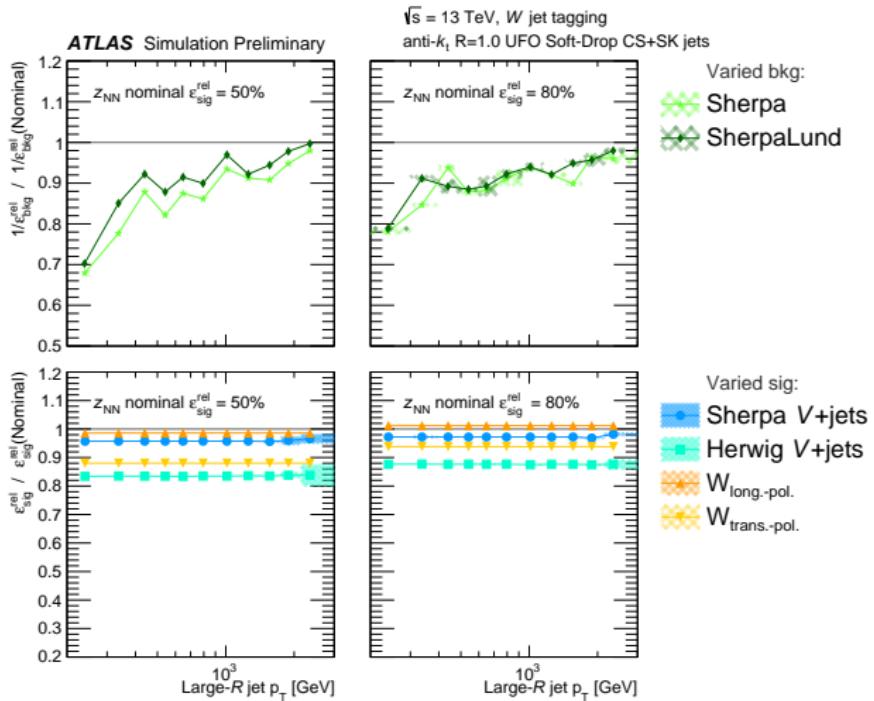
W/Z Tagger: ROC Curves



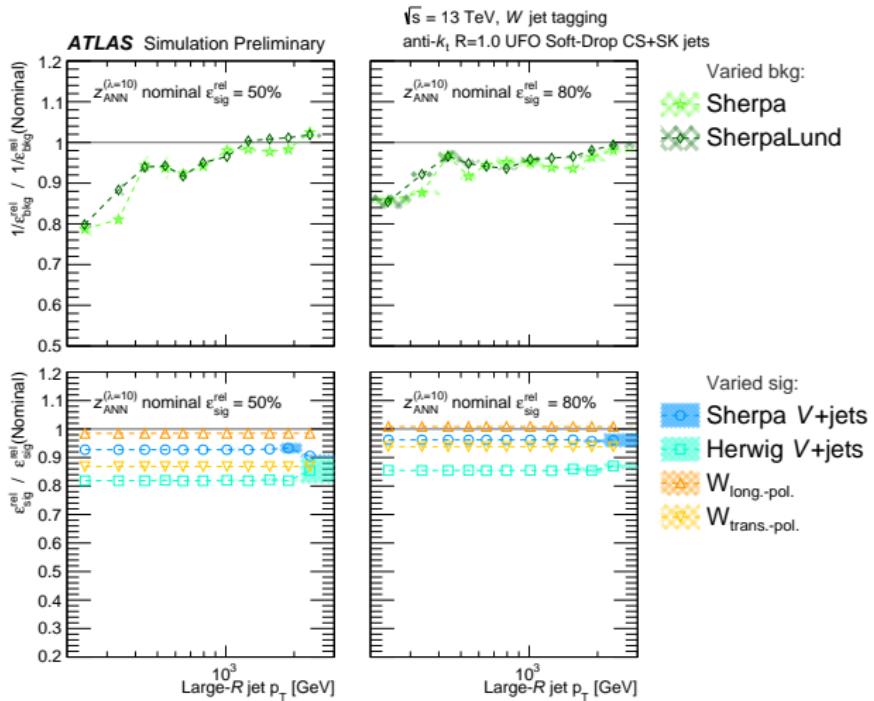
ATLAS Simulation Preliminary $\sqrt{s} = 13 \text{ TeV}$, W jet tagging
 anti- k_t R=1.0 UFO Soft-Drop CS+SK jets



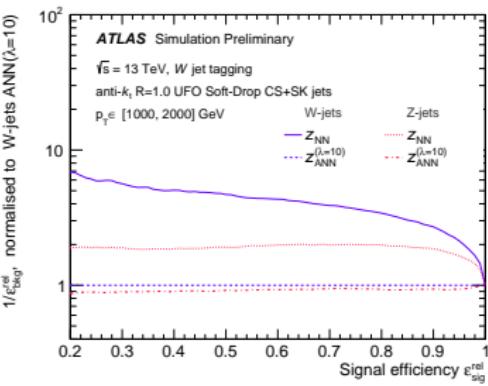
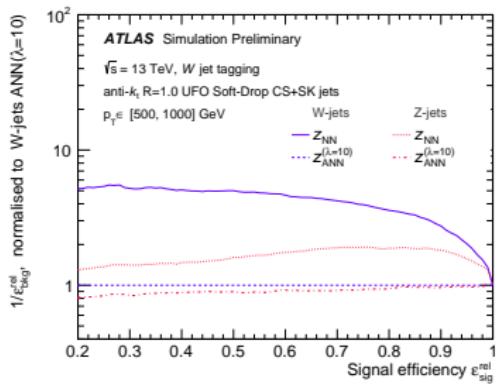
W/Z Tagger: Modelling



W/Z Tagger: Modelling



W/Z Tagger: Z vs W



Top Taggers

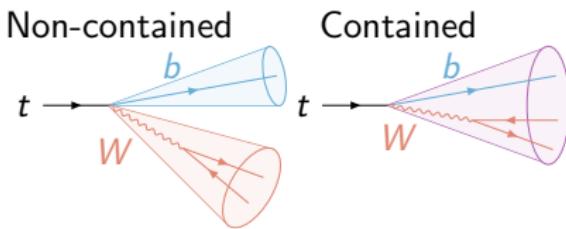
Two types of DNN-based top taggers defined:

Inclusive: Purely defined by ΔR matching:

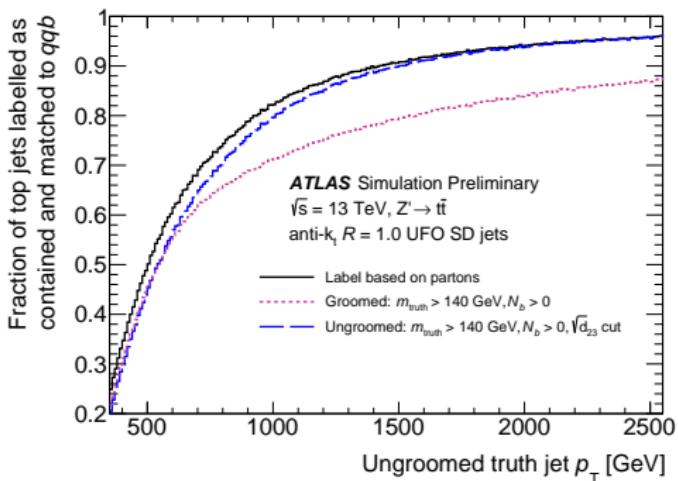
- $\Delta R(j^{\text{reco}}, j^{\text{truth}}) < 0.75$ and $\Delta R(j^{\text{truth}}, t^{\text{truth}}) < 0.75$

Contained: Extra cuts to ensure $t \rightarrow qqb$ fully contained within jet:

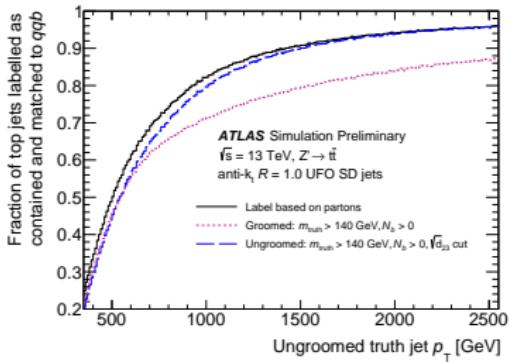
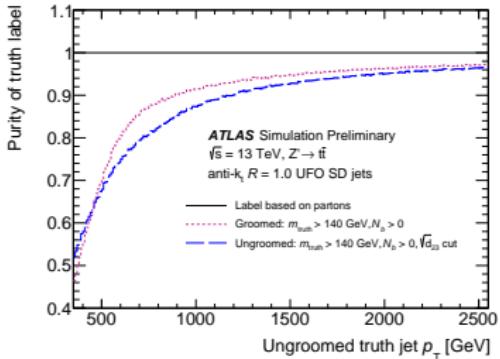
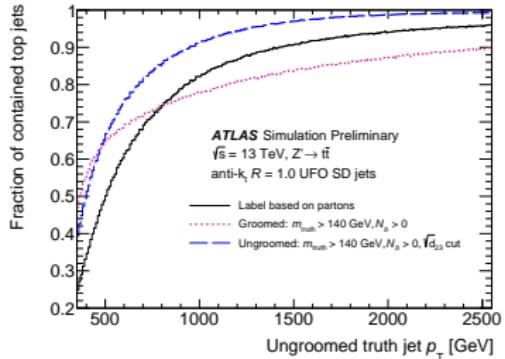
- Same ΔR requirement
- $N_B \geq 1$
- $m_{\text{ungroomed}}^{\text{truth}} > 140 \text{ GeV}$
- $\sqrt{d_{23}} > 27 e^{-\frac{p_T}{1433 \text{ GeV}}} \text{ GeV}$



Contained top labelling efficiency:

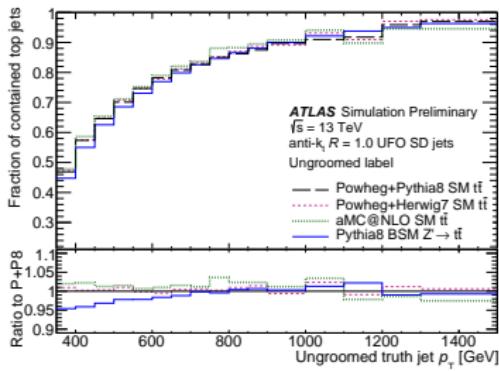
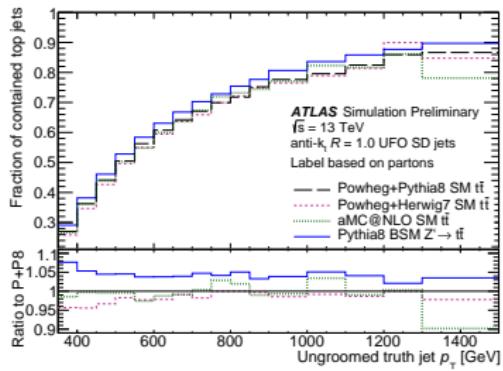


DNN Top Tagger: Truth Labelling

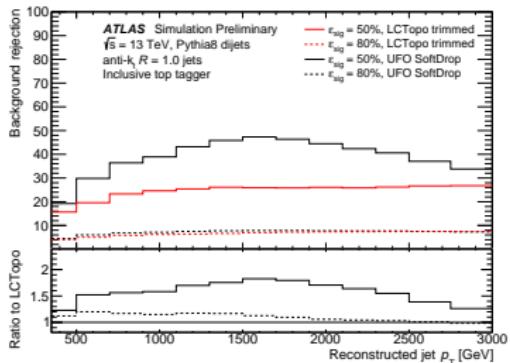
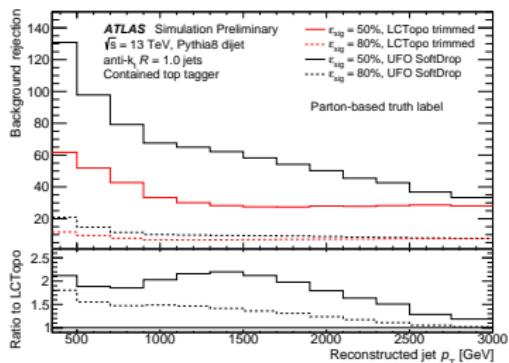
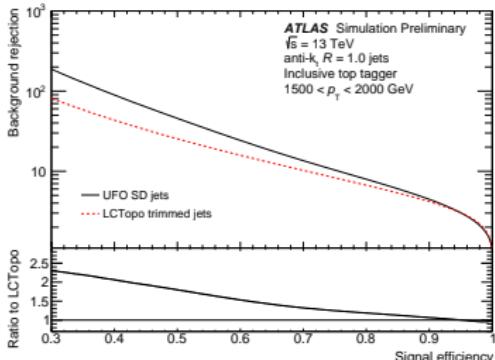
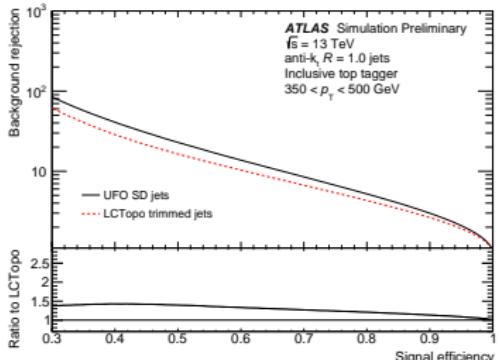


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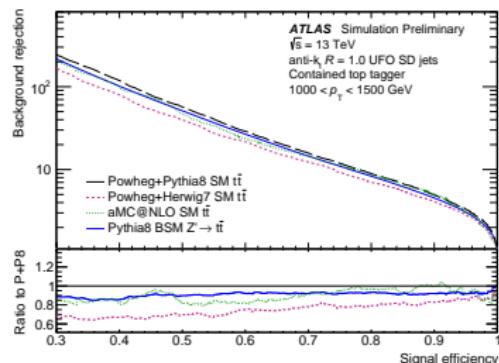
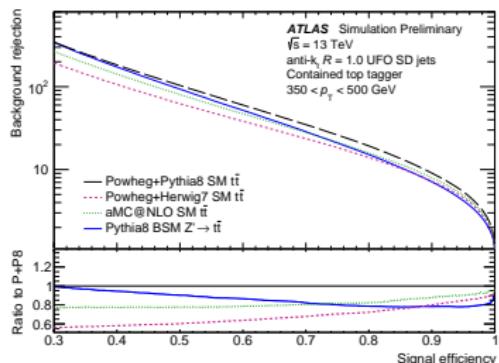
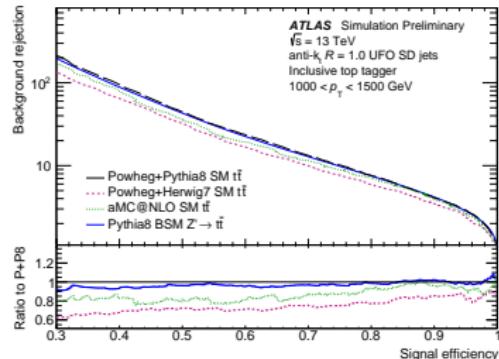
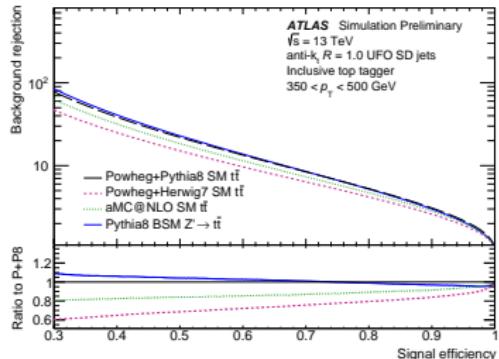
DNN Top Tagger: Truth Labelling



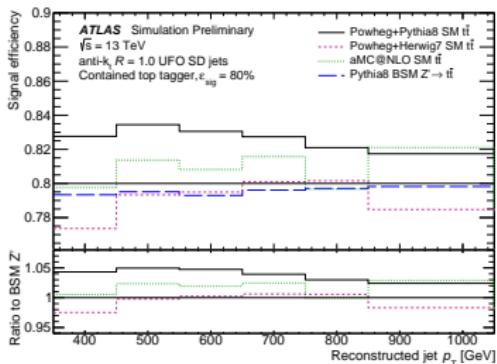
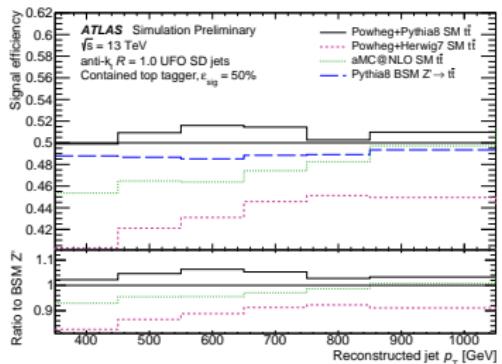
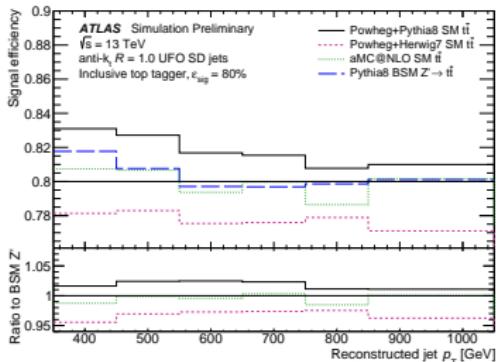
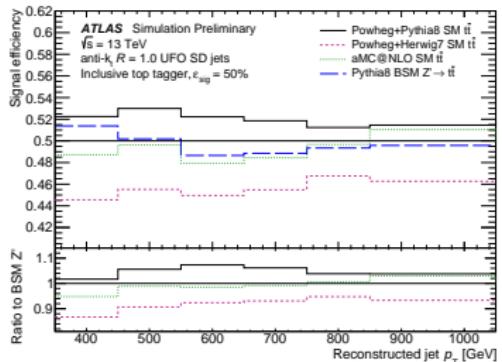
DNN Top Tagger: ROC Curves



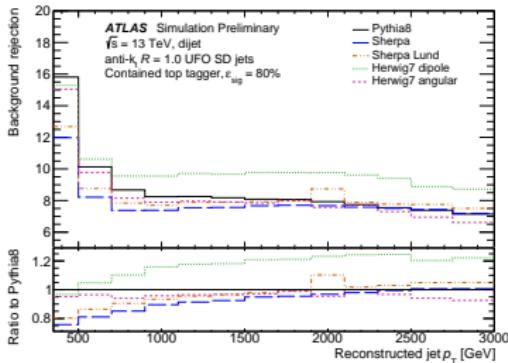
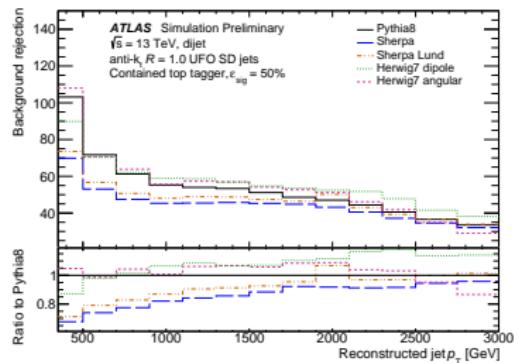
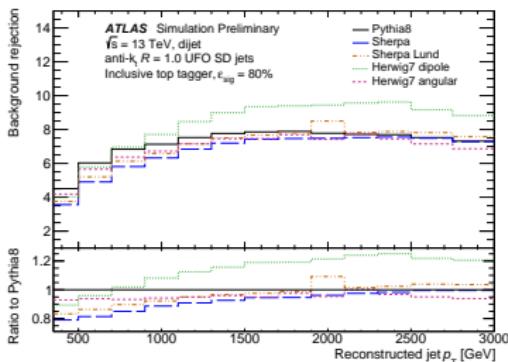
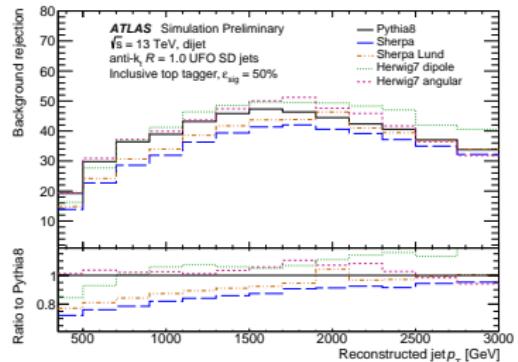
DNN Top Tagger: Modelling



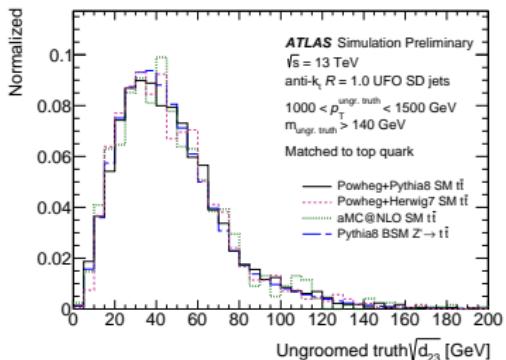
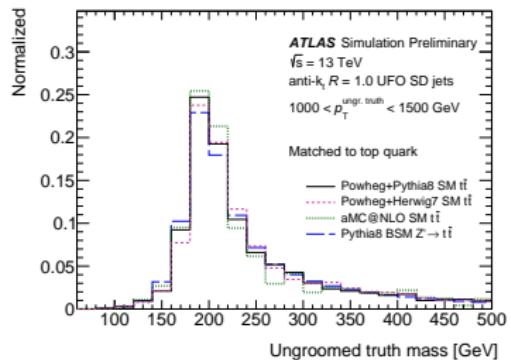
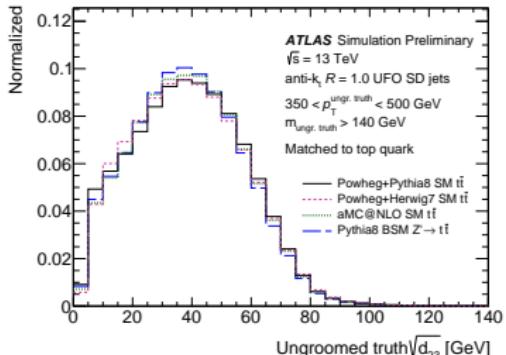
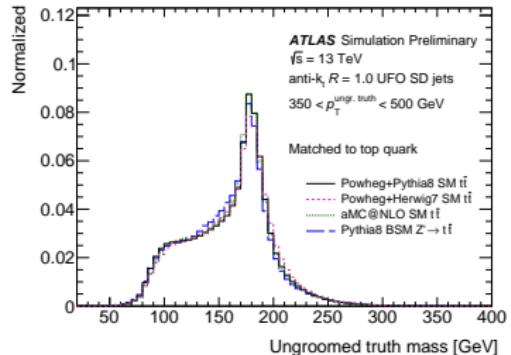
DNN Top Tagger: Modelling



DNN Top Tagger: Modelling



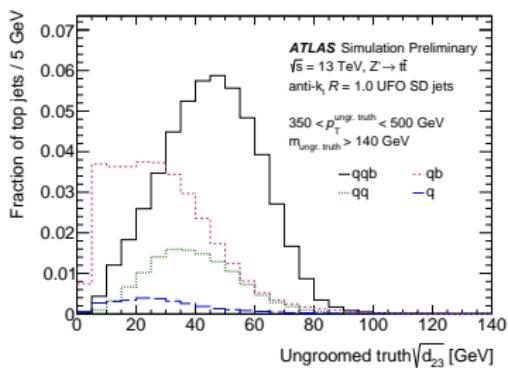
DNN Top Tagger: Modelling for Truth Labelling



DNN Top Tagger: Truth Labelling

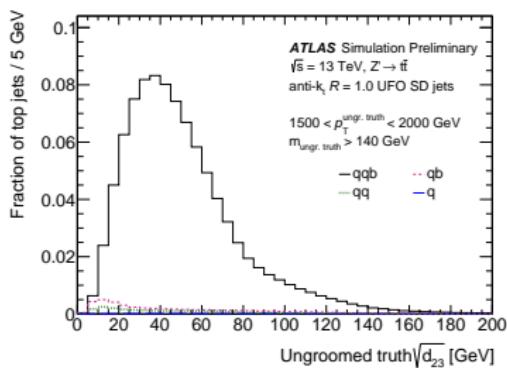
Low p_T :

→ optimal cut: $\sqrt{d_{23}} \approx 21$ GeV



High p_T :

→ optimal cut: $\sqrt{d_{23}} \approx 7$ GeV



Constituent-Based Top Tagger: Performance



Model	AUC	ACC	ε_{bkg}^{-1} @ $\varepsilon_{sig} = 0.5$	ε_{bkg}^{-1} @ $\varepsilon_{sig} = 0.8$	# Params	Inference Time
ResNet 50	0.885	0.803	21.4	5.13	1,486,209	9 ms
EFN	0.901	0.819	26.6	6.12	1,670,451	4 ms
hIDNN	0.938	0.863	51.5	10.5	93,151	3 ms
DNN	0.942	0.868	67.7	12.0	876,641	3 ms
PFN	0.954	0.882	108.0	15.9	689,801	4 ms
ParticleNet	0.961	0.894	153.7	20.4	764,887	38 ms

Substructure Variables

W/Z tagger (NN/ANN)		Top tagger (DNN)	
D_2 , C_2	Energy correlation ratios	τ_1 , τ_2 , τ_3 , τ_4	N -subjettiness
τ_{21}	N -subjettiness	$\sqrt{d_{12}}$, $\sqrt{d_{23}}$	Splitting scales
R_2^{FW}	Fox-Wolfram moment	ECF_1 , ECF_2 , ECF_3	Energy correlation (EC) functions
\mathcal{P}	Planar flow	C_2 , D_2	EC ratios
a_3	Angularity	L_2 , L_3	Generalised EC ratios
A	Aplanarity	Q_W	Invariant mass / virtuality
Z_{cut}	Z -Splitting scales	T_M	Thrust major
$\sqrt{d_{12}}$	d -Splitting scales		
$Kt\Delta R$	k_t -subjett ΔR		
n_{trk}	number of tracks		

arxiv.org/abs/1305.0007

$$\text{ECF}(N, \beta) = \sum_{i_1 < i_2 < \dots < i_N \in J} \left(\prod_{a=1}^N p_{T,i_a} \right) \left(\prod_{b=1}^{N-1} \prod_{c=b+1}^N R_{i_b i_c} \right)^\beta$$

N constituents i of the jet J with Euclidian distance:

$$R_{i_b i_c} = (y_i - y_j)^2 + (\phi_i - \phi_j)^2$$

- IRC (infrared & collinear) safe $\forall \beta > 0$
 - Goes to $\rightarrow 0$ in infrared/collinear limit

Here: ECF₁, ECF₂, ECF₃;

Energy Correlation Ratios C_2 , D_2

[doi.org/10.1007/JHEP12\(2014\)009](https://doi.org/10.1007/JHEP12(2014)009)

Normalised ECFs e_n^β :

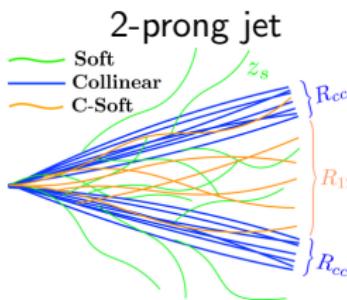
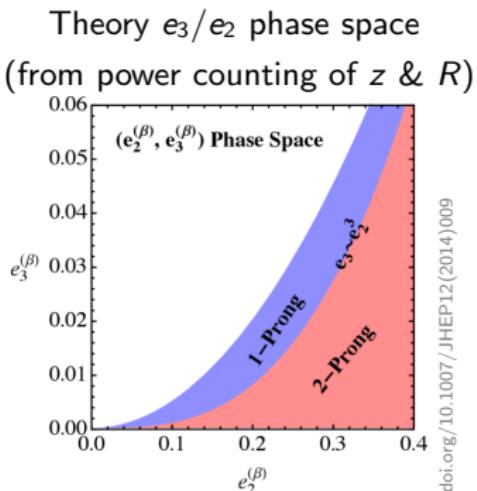
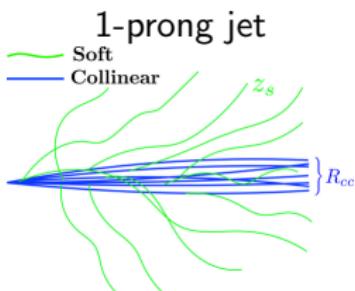
$$e_n^\beta = \frac{\text{ECF}(n, \beta)}{\text{ECF}(1, \beta)^n}; \quad z_i = \frac{p_{T_i}}{p_{T_J}}$$

$$\Rightarrow e_2^\beta = \sum_{1 \leq i \leq j \leq n_J} z_i z_j R_{ij}^\beta$$

$$\Rightarrow e_3^\beta = \sum_{1 \leq i \leq j \leq k \leq n_J} z_i z_j z_k R_{ij}^\beta R_{ik}^\beta R_{jk}^\beta$$

Ratios of e_n^β :

$$C_2 = \frac{e_3^\beta}{\left(e_2^\beta\right)^2}, \quad D_2 = \frac{e_3^\beta}{\left(e_2^\beta\right)^3}$$



→ C_2 and D_2 Separate 1- and 2-prong jets on the e_3/e_2 plane

N-Subjettiness τ_N

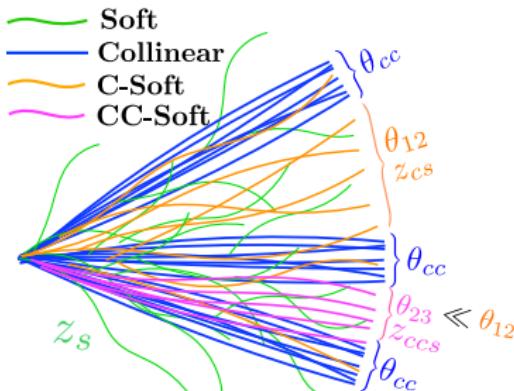
<https://arxiv.org/abs/1011.2268>

$$\tau_N^\beta = \sum_{1 \leq i \leq n_J} z_i \min \left\{ R_{i1}^\beta, \dots, R_{iN}^\beta \right\}$$

$$\text{with } z_i = \frac{p_{T_i}}{p_{T_J}}$$

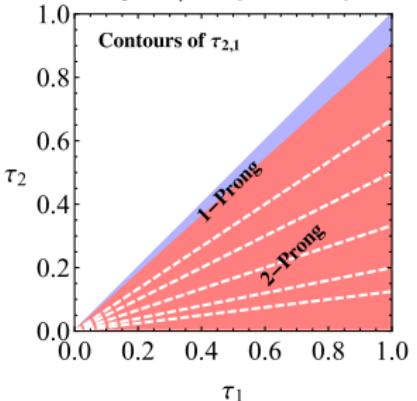
$$\rightarrow \tau_{21}^\beta = \frac{\tau_2^\beta}{\tau_1^\beta}$$

3-prong jet



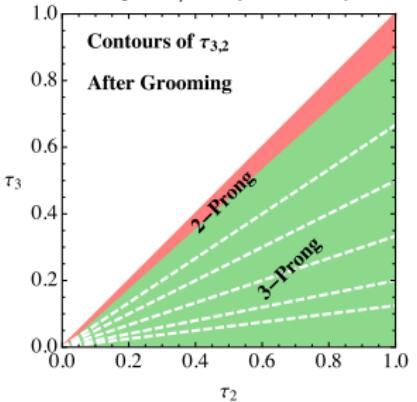
arxiv.org/abs/1609.07483

Theory τ_2/τ_1 phase space



arxiv.org/abs/1609.07483

Theory τ_3/τ_2 phase space



arxiv.org/abs/1609.07483

arxiv.org/abs/1609.07483

$${}_\nu e_N^\beta = \sum_{i_1 < i_2 < \dots < i_N \in J} \left(\prod_{a=1}^N p_{T_{i_a}} \right) \left(\prod_{m=1}^{\nu} \min_{s < t \in \{i_1, i_2, \dots, i_N\}} R_{st} \right)^\beta$$

Where $\min_X^{(m)}$ denotes the m th smallest element in the set X

Reduces to nominal ECF in the case $\nu = \binom{N}{2}$:

$$\text{ECF}(N, \beta) = \sum_{i_1 < i_2 < \dots < i_N \in J} \left(\prod_{a=1}^N p_{T_{i_a}} \right) \left(\prod_{b=1}^{N-1} \prod_{c=b+1}^N R_{i_b i_c} \right)^\beta$$

→ ${}_\nu e_N^\beta$ are sensitive to hierarchy of distinct angular (R) scales m in jet

- ECF average over them

Ratios to separate 2- & 3-prong jets: $L_2 = \frac{{}_3 e_3^{\beta=1}}{{}_1 e_2^{\beta=2}}^{\frac{3}{2}}$, $L_3 = \frac{{}_1 e_3^{\beta=1}}{{}_3 e_3^{\beta=1}}^{\frac{1}{3}}$

Number of Ghost-Associated Tracks n_{trk}



JHEP04(2008)005

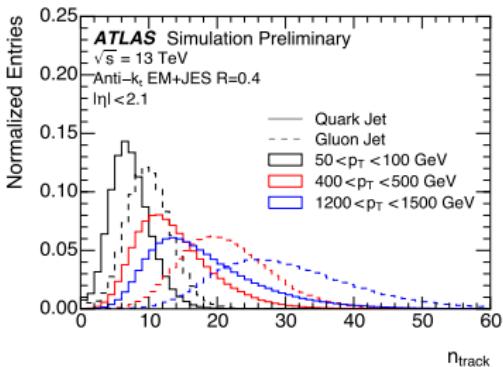
n_{trk} : number of tracks

- With $p_T > 500 \text{ MeV}$
 - Ghost-associated to jet
- Powerful q/g discriminant

Ghost-associated jet area

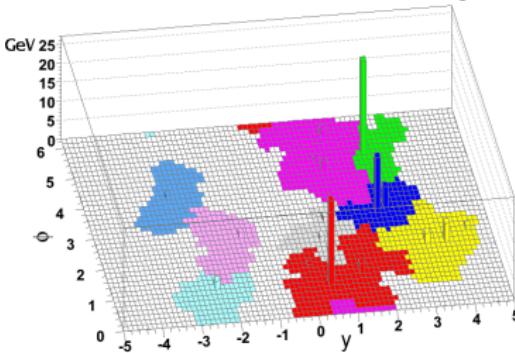
- Add dense coverage of 'infinitely' soft 'ghost' constituents
- Count how many are clustered within the jet

n_{trk} as q/g discriminant



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Ghost associated areas of k_t jets



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