Experimental aspects of jet Substructure in Atlas and CMS





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Outline

- "Standard" jet constituents and calibrations
- Machine Learning for jets
- Jet taggers
- Example measurements for/with substructure

Two different detectors for the same physics



Jet reconstruction more based on calorimetry for ATLAS, more based on tracks (and PFlow) for CMS

From partons to detector: jet components



-Track jets easier to calibrate, and vertex can be used to mitigate pileup.

but harder to compare to theory, and have bad pT resolution. Just used for substruture

- Calorimeter jets good at high-pt

need to account for non-compensation, bad performanor the soft comcponent hard to control pileup

- Combined (PFlow) combine advantages of both hard to remove overlap and double counting

The basis of ATLAS jets: Topological Clusters

Z Eur. Phys. J. C 77 (2017) 490



Cell noise ratio: $\zeta_{cell}^{EM} = \frac{E_{cell}^{EM}}{\sigma_{noise,cell}^{EM}}$

Topological Clusters

- of *E* deposits in calorimeter cells \rightarrow algorithm:
 - 1 Seed: Find cells with energy $E > 4 \times |\zeta|$
 - 2 **Growth:** Neighbors with $E > 2 \times |\zeta|$ are added
 - 3 Boundary: any neighboring cells are added

 $(no \zeta requirement)$

- 4 Split: Breaks up clusters with multiple maxima
- Jets build from TopoClusters are called **EMTopo** Jets **EM:** Electromagnetic scale \rightarrow ATLAS calorimeters are non-compensating \rightarrow EM response \approx 1, hadronic response < 1

Local Cluster Weights for ATLAS TopoClusters

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- TopoClusters are identified to be EM or had by likelihood \mathcal{P}_{dus}^{EM}
- Their momenta are reweighted (ω) by
 - Difference in response due to non-compensating calorimeter
 - Energy falling in unclustered cells
 - Inactive/dead regions of the detector

Jets build from TopoClusters+LCW are called **LCTopo** Jets used for large-R (R = 1.0) jets in Run 2

Particle flow and Track-Calo Clusters in ATLAS

9/21



PFlow makes use of tracking information at constituent level shows great JER improvement over calo jets in low-*p*T



P-flow objects start from TopoClusters and assiciate tracks. Improves jet energy resolution

Resolution-based track-to-cluster matching

$$\Delta R < \sqrt{\sigma_{\rm cluster}^2 + \sigma_{\rm track}^2}$$

- resulting in 3 different constituents:
 - combined: clusters matched to tracks from primary vertex (PV)
 - charged: tracks from PV not matched to any cluster
 - neutral: clusters not matched to any track (from the PV)
 - Clusters matched to tracks from PU vertices are discarded

TCC start from tracks and consider their associations to clusters. Designed for substructure studies

The synthesis: Unified Flow Objects (UFO)



PFlow Shows best jet mass and p_T resolution at low p_T TCC performs better at high p_T UFO combines the best of both



Jet inputs in CMS



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Jet calibration in CMS



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Residual corrections for CMS calibration



phase-space

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DPNotes Legacy

CMS: jet energy scale uncertainty

MC truth correction: PU subtraction Jet response calibration Residual corrections Jet energy resolution smearing Jet energy scale uncertainties > Uncertainty ~1% for jets pt >100 GeV

- Increasing contribution from PU
- Detector degradation:
 - Ageing, damage, ...



Calibrating jets in ATLAS



- Calculate E response in bins of η and E_{true} in MC
- Numerical inversion yields calibration factors
- Origin correction corrects jet η
- Largest calibration step that brings response on average to 1



Global Sequential Calibration and In-Situ corrections



Global Sequential Calibration

- After energy scale calibrated on average, GSC corrects for small differences
- E.g. for different jet flavours
- Sequentially corrects for each variable
- Only for small (R=0.4) jets

GSC improves JER by applying different con for different population of jets (e.g. q/g in but leaves JES on average the same

In-situ calibration in data

Corrects jets with high uncertainty (e.g. forward) based on well-known (photons, central jets...) objects



ATLAS JES resolution and uncertainty



Also 1% uncertainty after in-situ corrections

Pileup mitigation in CMS

Charged Hadron Subtraction (CHS)

- Tracker information to remove charged particles associated to PU
- Neutral particles energy subtracted
- Applicable for $|\eta| < 2.4$

Pileup Per Particle Identification (Puppi) Puppi in CMS

- Per-particle weight
 - Scale 4-momentum before clustering
- Charged particles similar to CHS
 - Redefined track-vertex association



Performance of PUPPI in CMS

- Widely used in Run 2, default in Run 3
- Improved all jet-related variables
 - Jet efficiency and purity (matched to generator-level jets)
 - Jet substructure
 - New optimation to include hadronic tau reconstruction: <u>CMS-DP-2024-043</u>



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Pileup mitigation in ATLAS: constituent subtraction and SoftKiller



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- Add ghosts in grid of $A_g = \eta \times \phi = 0.1 \times 0.1$
- With $p_T^g = A_g \times \rho$
 - $\rho = \text{med}\{\frac{\rho_{\text{T}}}{A}\}$: median energy density in event
 - Measure of PU in event
- Subtract p_T^g from p_T of constituents c within $\Delta R(g, c)$



Mass profile with CS closer to no-PU than with area-based alone _{6/21}



- CS: Scales constituents
- SK: Removes constituents
- Consider constituents in η, ϕ grid
- All constituents with $p_{\rm T} < p_{\rm T}^{\rm cut}$ are removed
- $p_{\rm T}^{\rm cut}$ determined such that half of grid cells are empty

ATLAS uses CS+SK for R=1.0 jets

Improving TopoClusters calibration with Machine learning (ATLAS)

First step in cluster calibration: Differentiate EM from hadronic clusters Non-compensating ATLAS calorimeter requires different calibrations for neutral/charged clusters



Baseline used in LCW: \mathcal{P}_{clus}^{EM}

- Binned EM-scale cluster variables
 - Total cluster energy E^{EM}_{cluster}
 - Pseudorapidity η
 - $rac{C}{C}$ Longitudinal depth λ_{clus}
 - 🖻 1st cell energy moment $\langle \rho_{\rm cell} \rangle$
- Combined into likelihood \mathcal{P}_{clus}^{EM}

Individual calorimeter cell signals

- \rightarrow As point clouds (GNN, PFN)
- \rightarrow Or projected on images (CNN)

Observations

• All point cloud methods significantly outperform baseline $\mathcal{P}_{clus}^{\mathsf{EM}}$

Topo Cluster energy calibration with ML

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2020-018



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Global Neural Network jet Calibration



Global NN Calibration (GNNC)

- GSC Does not exploit correlations of variables
- New method (GNNC) uses MLP trained to predict p_T response
- \rightarrow Improvement over full $p_{\rm T}$ range



Simultaneous calibration of energy and mass



Results for NN calibration



Improvement across the board

- DNN: better closure than standard calib. in response for E and M
- M response stable even in low and high p_T regime
- Resolution drastically improved
- Less dependence on η , pileup, MC generator for E and M
- More stable across different processes (H, W/Z, top) for E and M
- More stable across different flavours (q/g) for E and M

Pt calibration with ParticleNet (CMS)

Phys. Hev. D 101, 056019 (2020)

Graph NN with PF constituents & Secondary Vertices as inputs.

- First used for boosted resonance tagging with AK8 jets. DP-2020-002 CMS-PAS-BTV-22-001
- Extended for AK8 jet mass regression. DP-2021-017
- Commissioned for AK4 jet flavor tagging & p_T regression.



Two types of target p_T regression without & with neutrino contribution



ParticleNet response



ParticleNet resolution

DP-2024-064



Clear improvement in JER across the jet p_T range, even for forward jets.

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Jet tagging

Tagging b-jets using impact parameter or secondary vertex as old as precision silicon tracking (or even older)

Tagging jets using its substructure started at the LHC due to the large boost that even massive particles can reach

Techniques evolved with time:

- physics-inspired variables
- combination of variables into MLP or DNN
- constituents into CNN (imaging), DNN or Transformers (ParticleNet)
- Lund Plane into GNN (LundNet)

At the same time, also b-tagging embraced Machine Learning



Graph Neural Network for Flavour tagging



- GN1 <u>ATL-PHYS-PUB-2022-027</u>: All-in-one GNNbased (Inspired by J. Shlomi's work -<u>arXiv:2008.02831</u>)
- Use track information and jet kinematics directly ⇒ naturally adapts to variable #unordered input tracks
- Tasks include jet flavour, vertexing, and track origin prediction, trained simultaneously
 - Auxiliary targets enhance interpretability
- Easily optimised for diverse use cases and track/jet improvements.



GN2 is an upgraded version of GN1: all-in-one transformer network with significant state-of-Art performance enhancements

GN2 is based on GN1 architecture with Optimised training, Updated architecture, Increased training statistics

Architecture of GN2

GN2 Inputs:

- Tracks + jets variables
- pT & η resampled for each flavour

Large Multimodal Multitask Transformer Model with over 2600k parameters (GN1: 800K, DL1d: 130k)



Performance and future developments



Better performance than any previous tagger



Transformer architecture can be used for other kinds of tagging, vertexing, trigger etc.

Double b-tagging for boosted jets in CMS

ParticleNet-MD state-of-art for CMS boosted jet tagging.

- Graph based architecture describing the jet as a particle cloud (unordered sample).

EdgeConv block:

- NN module part of the ParticleNet architecture;
- New features vector associated to each jet constituent and based on the features of the k-nearest neighbors.

Mass decorrelation:

 Trained on Monte Carlo (MC) simulations containing boosted resonances (X) with a flat distributions in both of p_t and mass, as the signal sample, and the QCD multijet sample (reweighted to yield flat distributions) as the background sample.



bb tagger evolution, architecture and performance



k = 16, C = (256, 256, 256)

Global Average Pooling

Fully Connected

256, ReLU, Dropout = 0.1

Fully Connected

Softmax

Linear

BatchNorm

ReLU

Linear

BatchNorm

ReLU





Boosted object tagging with substructure in the ML era

Machine-learning/pheno community is developing faster then we can test on data!

- Normal dense neural networks
- ResNet: CNN Architecture representing jet as image
- Energy/Particle Flow networks (EFN/PFN): General decomposition of IRC-safe observables
- ParticleNet: Graph network on point cloud
- ParticleTransformer: Transformer
- GN2X: Transformer with auxiliary tasks
- LundNet: Graph on declustering history
- PELICAN: Lorentz invariant network





DNN tagger in ATLAS ATL-PHYS-PUB-2021/28-29

Baseline DNN top-taggers / W-tagger at 50/80% signal efficiency over 15/10 substructure observables

- Factor $\sim 1.6/6$ gain for W/top-tagging vs single substructure variable

Tagger performance deeply connected to jet definition!

- Over Run2 moved from calorimeter \rightarrow calorimeter+tracking information
- Factor 2 gains in background rejection
 - Due to better mass+substructure resolution



Constituent-based taggers ATL-PHYS-PUB-2021-039/2023-020

- Constituent based top-tagger / W-tagger outperform high-level features ones:
- Provide network the lowest level information available: the jet constituents themselves
- Another factor 2-3 improvement!
- ResNet/EFN under-perform w.r.t theoretical performance
 - Real simulation studies important!



Model	AUC	ACC	$\varepsilon_{\rm the}^{-1}$ @ $\varepsilon_{\rm sig} = 0.5$	$\varepsilon_{i,i}^{-1} @ \varepsilon_{sig} = 0.8$	# Params	Inference Time	
EFN	0.920	0.835	35.1	7.95	56.73k	0.065 ms	
PFN	0.931	0.853	44.7	9.50	57.13k	0.11 ms	
ParticleNet	0.933	0.826	46.2	9.76	366.16k	0.36 ms	
ParticleTransformer	0.951	0.880	77.9	14.6	2.14M	0.28 ms	

W-tagging summary table

(A parenthesis: the Lund Jet Plane)

- · Idea: reconstruct distribution of QCD radiation inside jet by constructing Lund Planes from proto-jets in CA algorithm.
- To reconstruct: calculate kinematic variables, eg

$$\underline{z} = \frac{p_T^e}{p_T^e + p_T^c}; \qquad \underline{\Delta R} = \sqrt{(y_e - y_c)^2 + (\phi_e - \phi_c)^2}; \qquad k_t = p_T^e \Delta R,$$

for proto-jets e, c in each step where $p_T^e < p_T^c$.

- Plot LJP for angular + momentum variable. (Total number of emissions) / (total number of jets) gives the average emission density ρ_{LJP}.
- These Lund Jet Planes [Dreyer, 1807.04758] have many interesting features. Radiation of different origins is factorised across the plane.
- LJP relates closely to other jet substructure observables that are built from CA clustering sequences, e.g. the Soft Drop [Larkoski, 1402.2657,ATLAS, 1912.09837] jet mass which show similar behaviour.
- To leading order in QCD, the emission density is proportional to α_s(k_t).



Why is the LJP impotant in QCD?

ATLAS Simulation

Parton shower

(Ang. ord. / Dipole)

Herwig 7.1.3 (Ang. ord.) / Herwig 7.1.3

Vs = 13 TeV, p, > 675 GeV

Hadronization

(Lund string / AHADIC)

ATLAS Simulation Sherpa 2.2.5 (String) / Sherpa 2.2.5 (AHADIC)

 Emissions of different scales and origins enter in different regions of the plane



Using the LJP as a Physics-aware tagger

- The distinctive features of the LJP make it an interesting observable for jet tagging.
- Wide-angle splittings due to heavy particle decays clearly visible in the LJP. Quark and gluon jets can also be distinguished [Dreyer, 2112.09140].
- Can apply different types of neural networks to take advantage of these input shapes eg. conv. nets [Oliveira, 1511.05190], LSTMs [Dreyer, 1807.04758].
- Latest developments: graph neural networks [Dreyer, 2112.09140, Qu, 1902.08570] using the LJP coordinates on the full CA clustering tree as input features
- LundNet uses EdgeConv [Wang, 1801.07829] layers to perform convolutions along edges of graphs.







Comparison of W and Top taggers in ATLAS

The more information you feed into the network, the better the network classification power will be





However, the most sophisticated the tagger, the larger will be the modeling systematics

Can have > 20% difference in performance using a MC model different from the one used for training

Working to mitigate it (adversarial networks, mixed training, training on data, cutting away LJP etc.)

Tagger comparison in CMS CERN-EP-2020-037 2020/06/09

	Algorithm	Subsection	jet $p_{\rm T}$ [GeV]	t quark	W boson	Z boson	H boson				
substructure	$m_{\rm SD} + \tau_{32}$	6.1	400	\checkmark							
variables	$m_{\rm SD} + \tau_{32} + b$	6.1	400	\checkmark							
Heavy Objects Variable R Tagger Energy Correlation Boosted Event Shape CNN imaging	$m_{\rm SD} + \tau_{21}$	6.1	200	\checkmark	\checkmark						
	HOTVR	6.2	200	\checkmark							
	N_3 -BDT (CA15)	6.3	200	\checkmark							
	$m_{\rm SD} + N_2$	6.3	200		\checkmark	\checkmark	\checkmark				
	BEST	6.5	500	\checkmark	\checkmark	\checkmark	\checkmark				
	ImageTop	6.6	600	\checkmark							
"Particle "and "Vertex"	DeepAK8 ^(*)	6.7	200	\checkmark	\checkmark	\checkmark	\checkmark				
lists into a DNN	Jet mass decorrelated algorithms										
	$m_{\rm SD} + N_2^{\rm DDT}$	6.3	200	0	\checkmark	\checkmark	\checkmark				
	double-b	6.4	300			\checkmark	\checkmark				
	ImageTop-MD	6.6	600	\checkmark							
	DeepAK8-MD ^(*)	6.7	200	\checkmark	\checkmark	\checkmark	\checkmark				

mostly multi-class taggers combining b-tagging and substructure

Taggers performance on MC



Deep AKT8 architecture



Use CNN to reduce dimentionality and extract features from list of particles and secondary vertices

Mass-decorrelated version has a mass predictor that can be used in the loss function to avoid shaping the BG around the signal mass

Variable- Radius top taggers

Heavy Object Tagger with Variable Radius

- $R = 600 / p_t$ (R min 0.1, R max 1.5).
- Useful for 4 top final states where the top quark is not completely boosted (200 < p_t < 800 GeV).
- Efficiency as the ratio between the generated top quarks matching a reconstructed jet within ΔR and all the generated top quarks.

Developed a BDT to distinguish top quarks from QCD:

- Training on QCD multijet and the ttZ to simulate the background and the signal, respectively;
- Tested on a Z+jets enriched selection
 - Two opposite sign leptons ($80 < m_{\ell\ell} < 101$ GeV) + >1 HOTVR

CMS-DP-2024-038



Measuring substructure: the Lund Jet Plane for dijets

- First ever measurement of the Lund Jet Plane observable by ATLAS in dijet events [EP-2020-030].
- Uses the full ATLAS Run 2 dataset with lowest pT un-prescaled single jet triggers. More than 29 million jets!
- Jets are reconstructed from calorimeter topoclusters using anti- k_T with R = 0.4.
- Event selections:
 - ▶ 2 jets, both $|\eta| < 2.1$
 - p_T^{leading} > 675 GeV
 Dijet balance: p_T^{leading} < 1.5 × p_T^{sub-leading}
- LJPs are reconstructed for both jets. High jet p_T ensures good LJP resolution.
- Measurement was later compared to all-orger NLL resummations [Lifson, 2007.06578]. Good overall agreement, mismodelling at jet boundary due to CA-reclustering of anti-kt jet.



Running of as in a single jet, and analytical comparisons



Recall LO pocket formula for Lund density:

$$\frac{1}{N^{\text{jets}}} \frac{\mathrm{d}^2 N_{\text{emissions}}}{\mathrm{d}\ln(k_T) \mathrm{d}\ln(R/\Delta R)} \simeq \frac{2}{\pi} C_R \alpha_s(k_T)$$

Running $\alpha_{s}(k_{T})$ from few GeV to ~60 GeV qualitatively describes the data (Assuming q/g fractions from PYTHIA8)

Cute to see, but breaks down at large angles ΔR , close to the edge, etc





Lund Jet Plane for W and Top jets

- LJPs for Top jets and W jets are presented separately.
- Unfold LJP to the particle level using Iterative Bayesian Unfolding with 4 iterations.
- Structure related to the top/W mass is observed in the lower-left corner of the LJP
- Unfolded distributions of the LJP are compared to a wide range of alternative $t\bar{t}$ MC configurations.
- Results could be useful for tuning tt MCs or developing and calibrating (see CMS-DP-2023-046) heavy particle jet taggers. tt events could also be investigated in future to measure LJP for b jets.





Using jet tagging for searches



Exotic substructure for exotic Physics: example hadronic LLP: CMS-EXO-23-013



Traditional techniques (trigger and tagging) optimised for prompt jets

Special GNNd developed for displaced vertices

Additional GNNp for prompt production

Background estimated from the comparison of the two using the ABCD method



Semi-visible jets

Characterised by ratio of stable partiles in the jet R, that influence Pt balance and $\Delta \Phi$

A first fit is performed in low E^{T}_{miss} CR to get the multijet re-weighting factors.

A final fit of the [pTbalance and $\Delta \phi$] 2D distribution, with all high E_{miss}^{T} regions, is done:

 largest uncs on pTbalance and ∆¢ shapes comes from signal, Z+jets and ttbar modelling (10%)





Conclusions

- Jet physics is complex, and extremely important at the LHC
- It has been rapidly evolving, with the development of substructure and Machine Learning
- ML in obiquous, helping us reconstructing and calibrating jet constituents, reducing pileup and calibrating jets
- Sophisticated ML techniques are used for multi-class jet tagging, and exotic searches
- We are only half-way in the LHC explotation, and the next years will see many more jets, boosted objects and pileup
- Even more ingenuity and creativity will be needed