Resolving Extreme Jet Substructure

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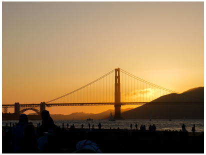


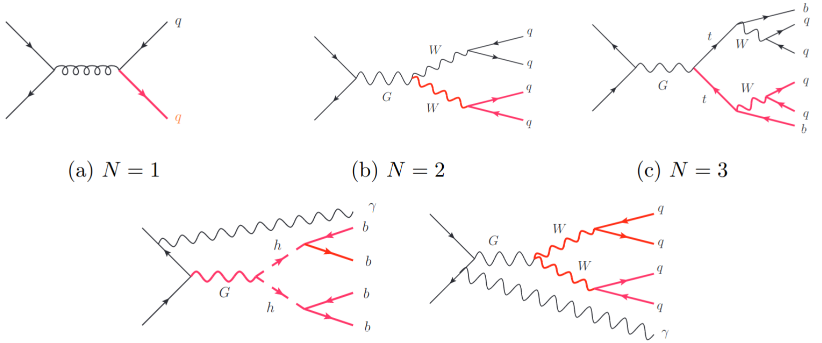
Motivation

- We know that jet taggers based on low level info usually can outperform high level features, at least for W/Z/top jets
  - But these low level taggers are hard to calibrate and use in practice
- Most large radius jet tagging studies have focused on those with $N = 2, 3$ hard subjets (ie W/Z/H or top)
  - are existing methods enough in extreme ($N > 3$) conditions to do jet tagging?
  - can we learn from the "low level" taggers, which directly use jet constituents, some "high level" features that we can use?

I consider myself something of a moral relativist.

- We compare the performance of various taggers, using either using high level observables or low level constituents, and then attempt to bridge the gap between them
- This work contributes to a growing body of work in HEP that uses ML to teach ourselves something, instead of the more usual inverse

Datasets

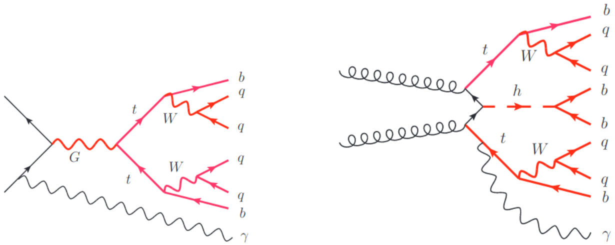


(a) $N = 1$ (b) $N = 2$ (c) $N = 3$

(d) $N = 4b$ (e) $N = 4q$

- We generate 7 classes of dataset that we classify by their ‘pronginess’ (how many hard sub-jets there are) using aMC@NLO+Pythia8+Delphes
  - We use a uniform granularity of 0.0125 in η and ϕ for the calorimeter
- We have two classes for N=4, which we call N=4q and N=4b, to investigate dependence on heavy flavor (more on this later)

Datasets

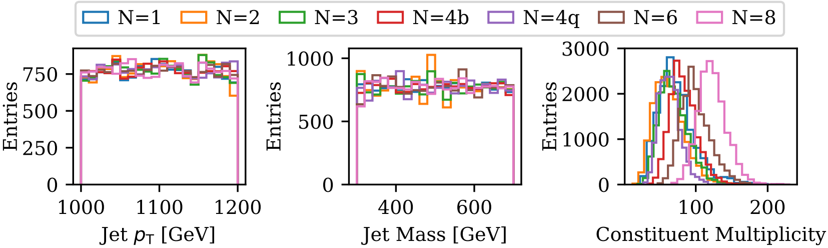


(f) $N = 6$ (g) $N = 8$

- We require a high p_T photon to recoil off the system to give it sufficient boost to be fully captured by a single R=1.2 anti-kT jet
- We also require that all quarks are ΔR matched to the jet
- We use the first 230 input constituents, more than enough for all of the jets, and zero-pad as necessary

Dataset Balancing

- In order to keep performance ∼flat against mass and p_T, we selectively reject events until we have ∼flat distributions
- This ensures that the ML methods do not learn residual effects due to these kinematics



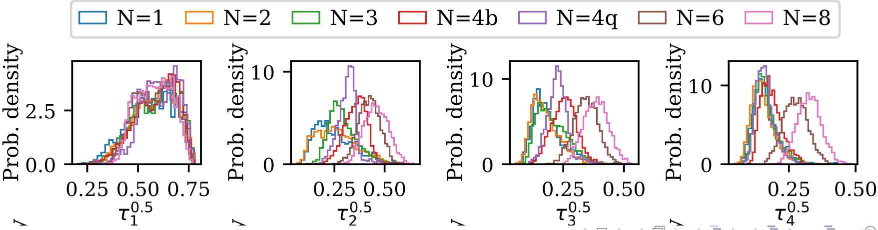
High Level Observables

- We use N-subjettiness ▸ Thaler et al

$$\tau_N = \frac{1}{d_0} \sum_k p_{T,k} \min\left\{\Delta R_{1,k}, \Delta R_{2,k}, \cdots, \Delta R_{N,k}\right\}^{\beta}$$

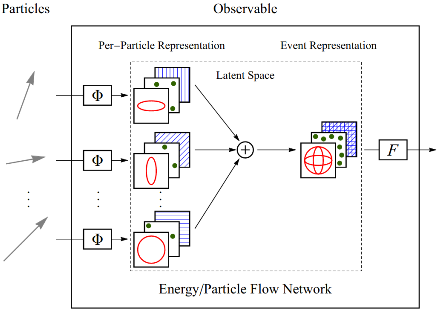
  as a basis of easily interpretable & familiar substructure variables that forms our baseline

- We input a total of 135 of these variables, with $N = 1, ..., 45$, $\beta = \{1/2, 1, 2\}$, as well as jet mass, into a fully connected dense NN, which we label DNN_{136}



Particle Flow Networks ▸ Komiske et al

$$\text{PFN}: F\left(\sum_{i\in\text{jet}} \Phi(p_{\mathrm{T}i}, \eta_i, \phi_i)\right)$$



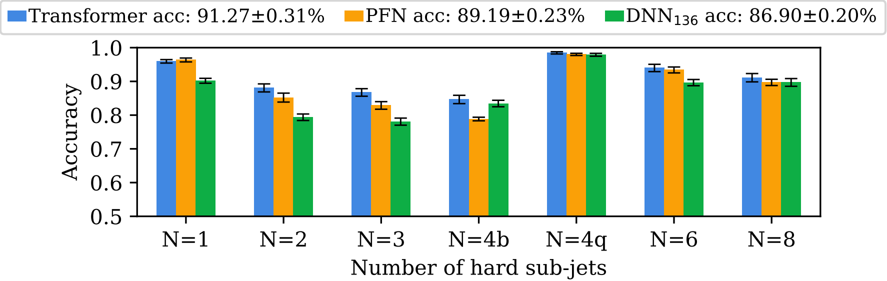
where ϕ is the latent space acting on the constituent 3-vectors and F the jet level latent space

- Based on DeepSets (▸ Zaheer et al), PFNs operate directly on **jet constituents**
- Naturally permutation invariant and capable of handling variable-length sets

Attention Is All You Need ▸ Vaswani et al

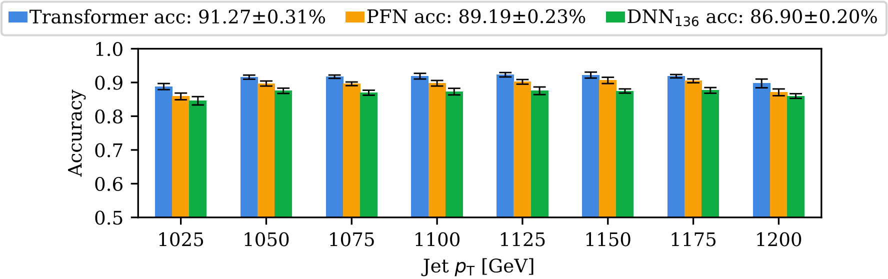
- In NLP, "Attention" mechanisms are now dominant, replacing RNNs / LSTMs in most applications
  - Process sentences as a sequence of words to perform translation, prediction, etc.
  - Reordering the inputs results in the same reordering of the attention matrices: **permutation invariant**
- In our case; input the full sequence of **jet constituents** to multiple self-attention heads in parallel
  - In principle these networks can become large, but we focus on architectures with similar numbers of free parameters ($\mathcal{O}(1M)$) as the other methods
- Transformer based architectures are now state of the art on many tasks in HEP, including event reconstruction ▸ Fenton et al, top-tagging ▸ Qu et al, and pileup mitigation ▸ Maier et al

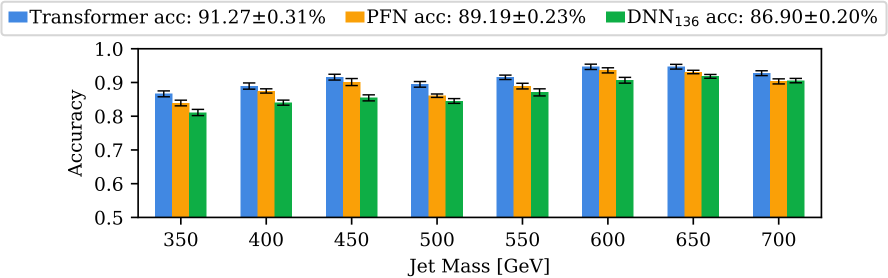
Initial Performance (1/3)



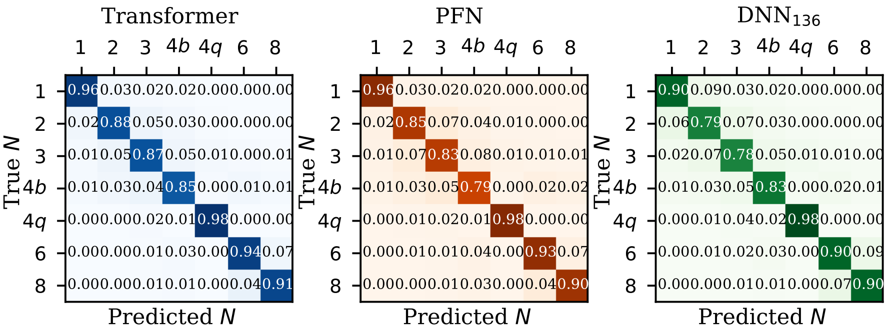
- We see good performance for all categories and a consistent story between architectures
- Transformer > PFN > DNN

Initial Performance (2/3)





Initial Performance (3/3)



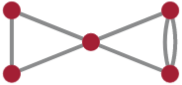
- Confusion matrices; ie which categories are mistaken for each other?
- Perhaps surprisingly, 4b and 4q are confused less often than 4b and 3, suggesting more is being learned than just "pronginess", even for DNN that takes τ variables as input
- Can we understand what information the networks are relying on?

Energy Flow Polynomials ▸ Komiske et al

- A complete basis for jet substructure, easily represented by simple graphs

$$\mathrm{EFP}_G = \sum_{i_1=1}^{M} \cdots \sum_{i_N=1}^{M} z_{i_1} \cdots z_{i_N} \prod_{(k,\ell)\in G} \theta_{i_k i_\ell},$$

ie



$$= \sum_{i_1=1}^{M}\sum_{i_2=1}^{M}\sum_{i_3=1}^{M}\sum_{i_4=1}^{M}\sum_{i_5=1}^{M} z_{i_1} z_{i_2} z_{i_3} z_{i_4} z_{i_5} \theta_{i_1 i_2}\theta_{i_2 i_3}\theta_{i_1 i_3}\theta_{i_1 i_4}\theta_{i_1 i_5}\theta_{i_4 i_5}^2.$$

$z_i = \frac{p_{T_i}}{\sum_i p_{T_J}}$, $\theta_{ij} = (\delta\eta_{ij}^2 + \delta\phi_{ij})$

We further introduce an angular weighting factor $\beta = \{1/2, 1, 2\}$ which we attach to the θ terms for each graph with N=5 or fewer nodes, giving us a total of 162 observables

Bridging the Gap with LASSO ▸ R. Tibshirani

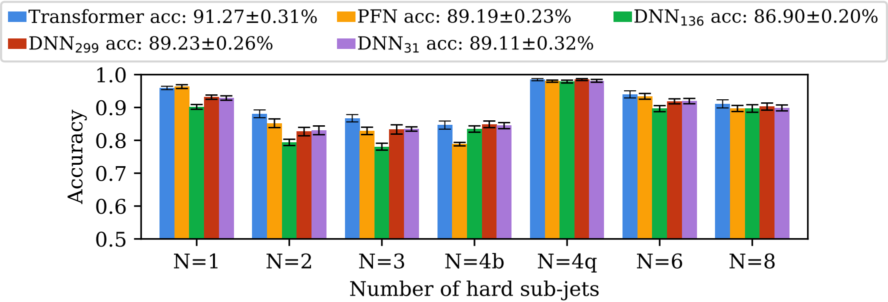
- We can then add these EFP observables to the DNN to see if we can bridge the gap to the PFN and Transformer models
- But this blunt force approach isn't that useful practically; what we want is the minimal set of observables that can match the performance

→ LASSO: "least absolute shrinkage and selection operator"

- Add a learnable parameter per input observable that shrinks to zero if the observable is not useful for classification
- Loss $L = -\log f(Y, Y_{\mathrm{pred}}) + \lambda \sum_i^{299} |g_i|$
  - where $-\log f(Y, Y_{\mathrm{pred}})$ is the negative log likelihood and λ is a hyperparameter of the network ($\lambda = 5$)

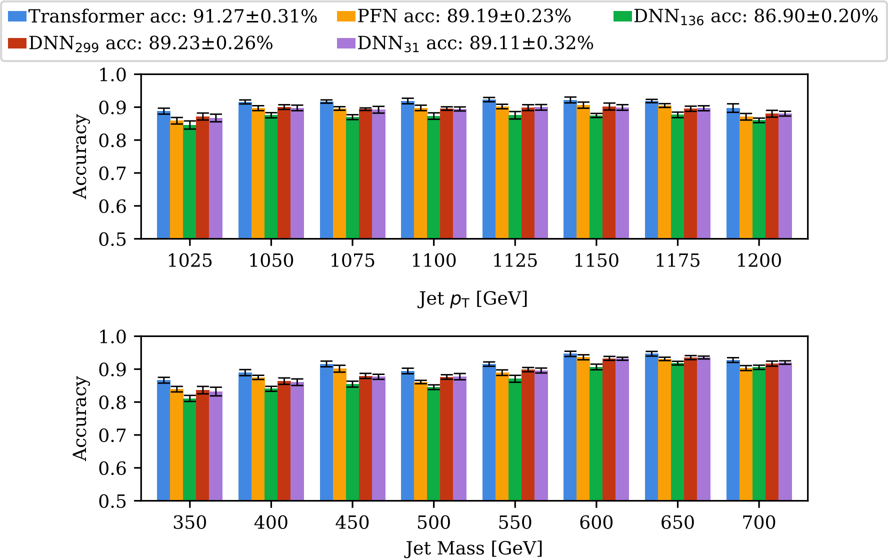
See also: Average Decision Ordering ▸ arXiv:2010.11998:

Bridging the Gap Results

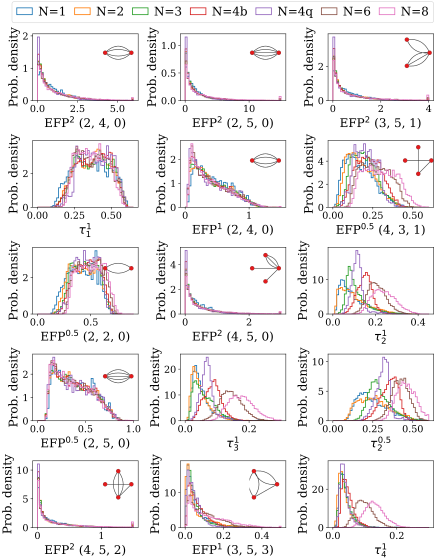


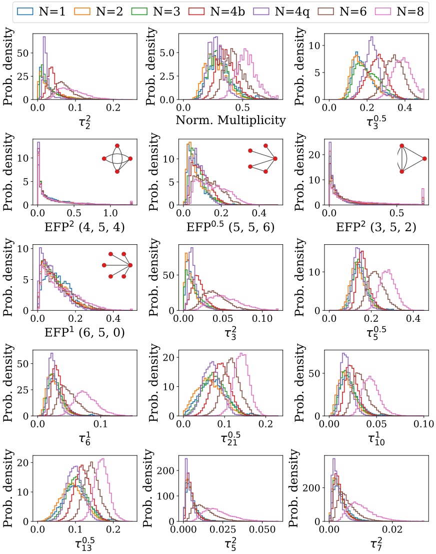
- All 299 variables achieve the ∼same performance as the PFN, but a gap to the Transformer model remains
- We find that with just 31 LASSO-selected variables, we can achieve the same overall performance as the larger model
- Note though that performance is not identical in each class!

Bridging the Gap Results (2)

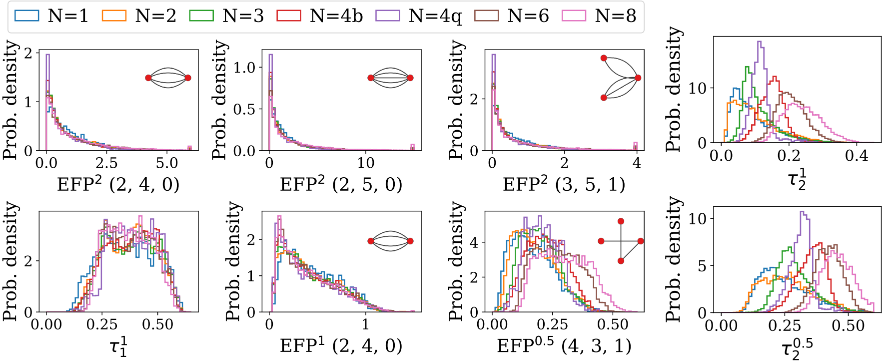


Selected Observables



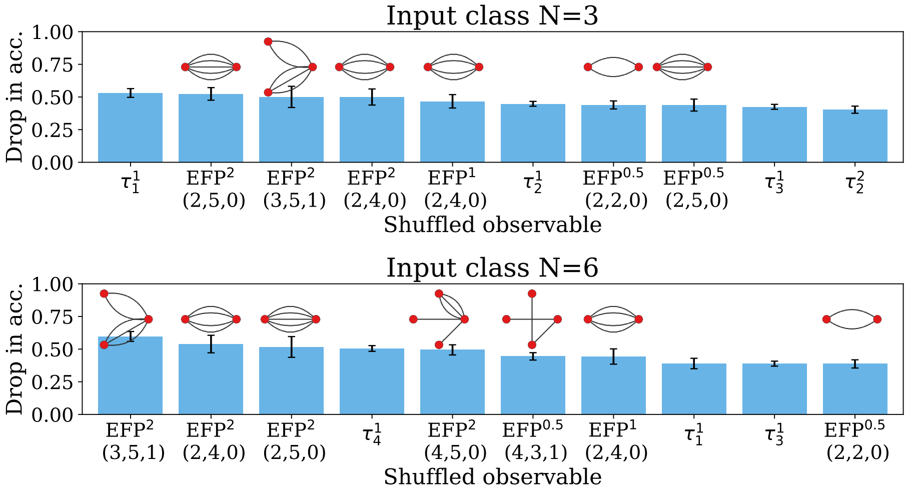


Selected Observables



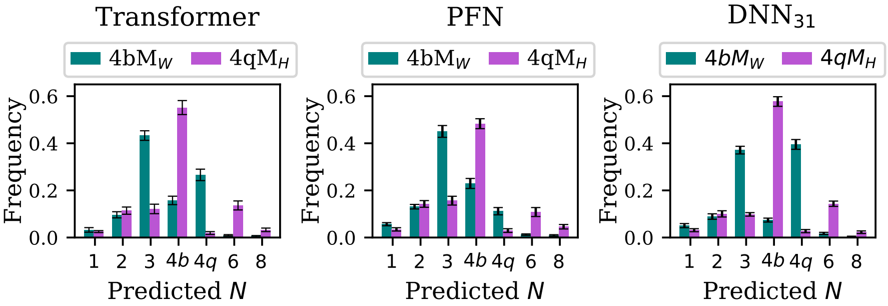
- Lots of $N = 2$ correlators
- Many EFP's do not, by themselves, show good separation between classes, yet are ranked higher than τ's which show more obvious differences
- Most important τ variable is τ_1, which is a direct measure of collimation
- Other highly ranked τ variables are mostly the "usual suspects", ie $N \leq 4$
- Lots of high angular weighting exponents

Breaking down the Selected Observables



- Ranking plot for specific classes (more in backup)

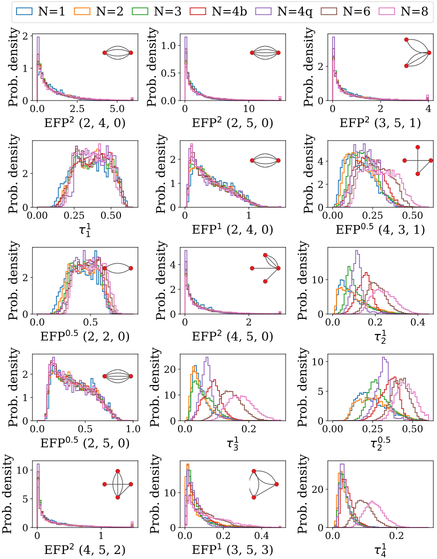
Zooming in on 4b vs 4q



- To understand the 4b vs 4q performance, we generate alternative $G \to HH$ / $G \to WW$ samples whereby the Higgs and W masses are swapped
- We see that $4\mathrm{qM}_H$ is usually classified as 4b, indicating the importance of the intermediate masses
- For $4\mathrm{bM}_W$, we find mixed results; the low-level networks often guess N=3, in which there is both a W and a b
    - Including b-tagging information directly in the networks may improve performance

Summary

- We have investigated the performance of both low level and high level jet taggers in extreme conditions, with up to $N = 8$ hard subjets
- The low level taggers typically out perform the "traditional" high level taggers
- Some of the gap can be filled by cleverly selecting/adding new variables, but still Transformer architectures maintain supremacy
- Performance is dependent on mass structures as well as heavy flavor content
- LASSO regulation a useful tool for automated feature selection



Backup

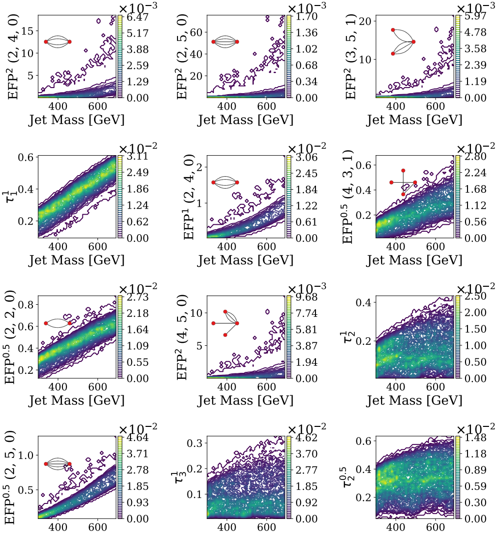
MC Details

N hard sub-jets	Process	M_W	M_h	M_t	M_G	requirements
1	$q\bar{q} \to q\bar{q}$					$p_T^q > 1000$
2	$q\bar{q} \to G \to W^+W^-$	80.4			2200	
		264.5			2200	
		440.8			2500	
		617.1			2800	
3	$q\bar{q} \to G \to t\bar{t}$			300	2200	
				500	2500	
				700	3000	
$4b$	$q\bar{q} \to \gamma G \to \gamma hh$				400	$p_T^\gamma > 1000$
					600	$p_T^\gamma > 1000$
					800	$p_T^\gamma > 1000$
$4q$	$q\bar{q} \to \gamma G \to \gamma W^+W^-$				400	$p_T^\gamma > 1000$
					600	$p_T^\gamma > 1000$
					800	$p_T^\gamma > 1000$
6	$q\bar{q} \to \gamma G \to \gamma t\bar{t}$				400	$p_T^\gamma > 1000$
					600	$p_T^\gamma > 1000$
					800	$p_T^\gamma > 1000$
8	$q\bar{q} \to \gamma t\bar{t}h$		100	125		$p_T^\gamma > 1000$
			125	175		$p_T^\gamma > 1000$

Network Details

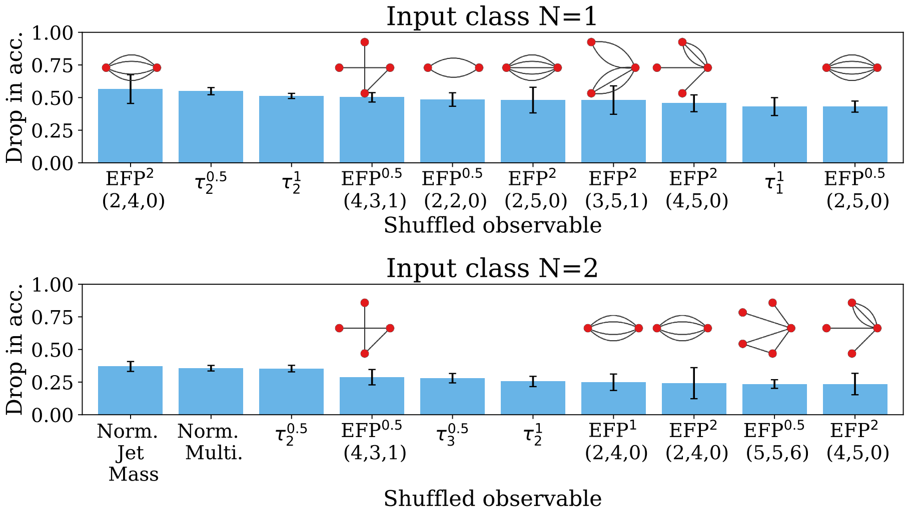
Model	Description	No. of Params.	Accuracy
Transformer	Transformer Network trained on the jet constituents.	1,388,807	91.27 ± 0.31 %
PFN	Particle-Flow Network trained on the jet constituents.	1,205,895	89.19 ± 0.23 %
DNN_{136}	Fully-connected neural network trained on the 135 N-subjettiness observables and the norm. jet mass.	2,732,519	86.90 ± 0.20 %
DNN_{299}	Fully-connected neural network trained on the 135 N-subjettiness, observables the normalized jet mass, and the full set of EFP observables.	2,862,919	89.23 ± 0.26 %
DNN_{31}	Fully-connected neural network trained on the 31 LASSO-selected observables.	2,622,663	89.11 ± 0.32 %

Why does performance increase as mass increases?



- We inspect the correlations of the highest ranked variables against the mass to understand why higher masses seem easier to classify
- τ_1, which is a measure of collimation along the jet axis, gives us a clue; this variable, ranked 4th, is highly correlated to mass
  - $\rightarrow$ more collimated jets are harder to classify, probably due to merging constituents
- Our results are consistent if we only use half of the overall (quite large) mass range

Breaking down the Selected Observables



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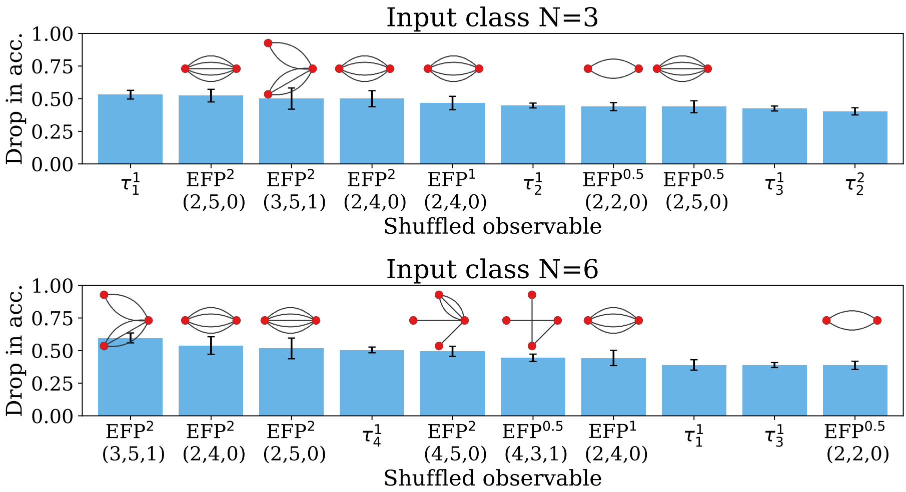

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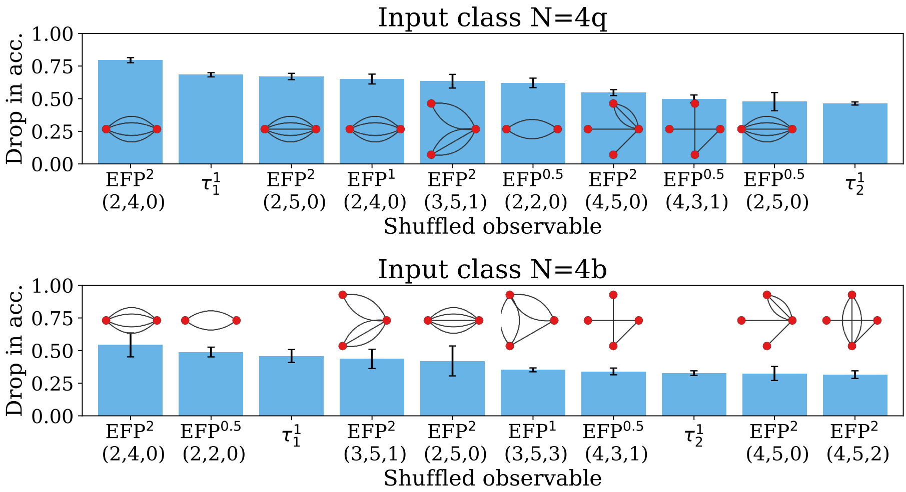

Breaking down the Selected Observables