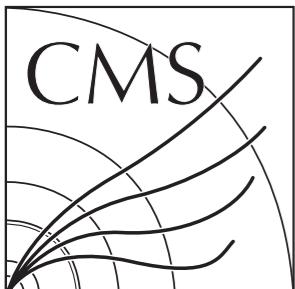


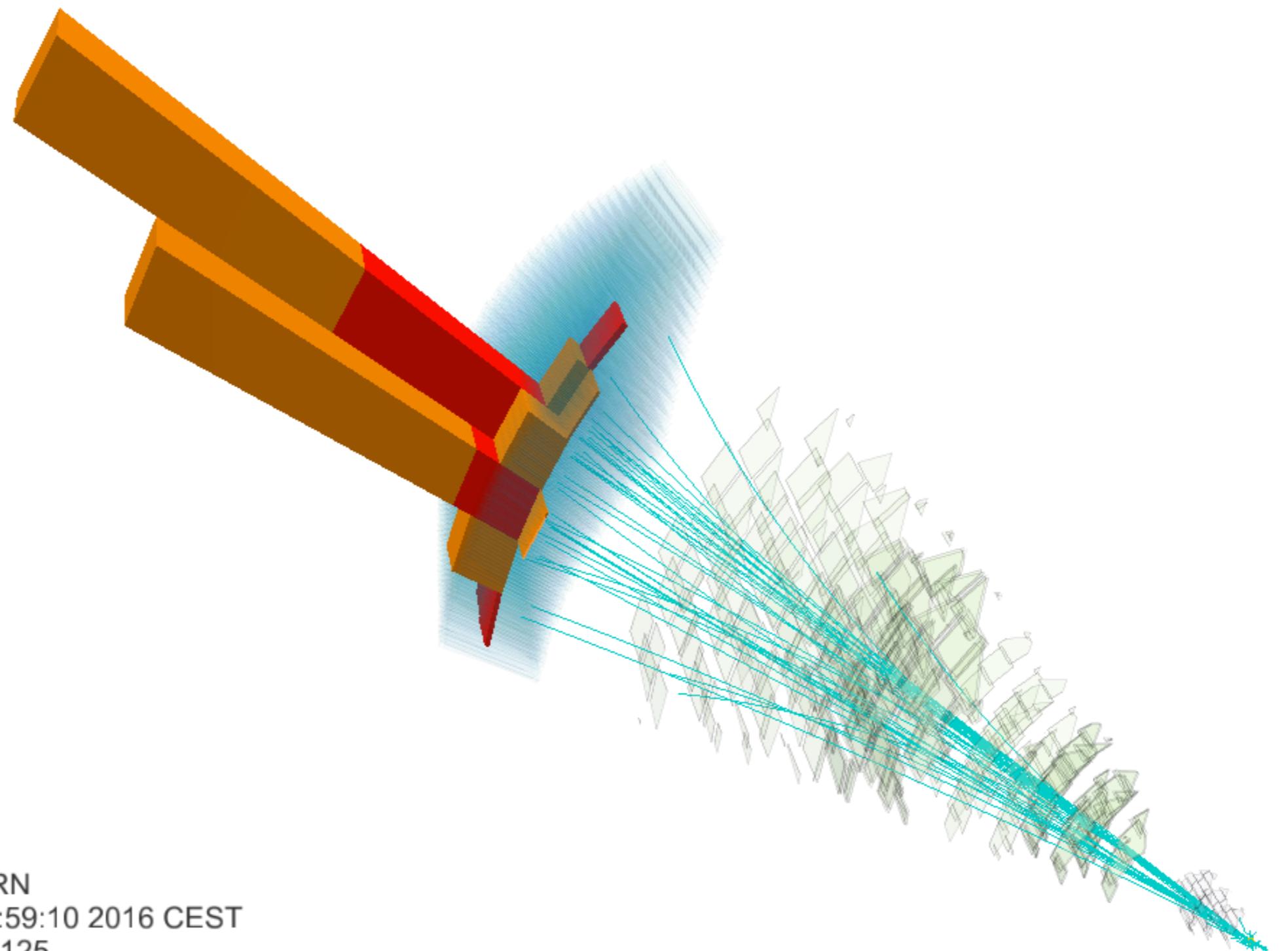
Lorentz Invariance Based DNN for W-tagging



Thea Klæboe Årrestad

Joint CMS/LHCb Seminar
Physik Institut, May 4th

W/Z-tagging in CMS



CMS-PAS-B2G-17-001

CMS Experiment at LHC, CERN

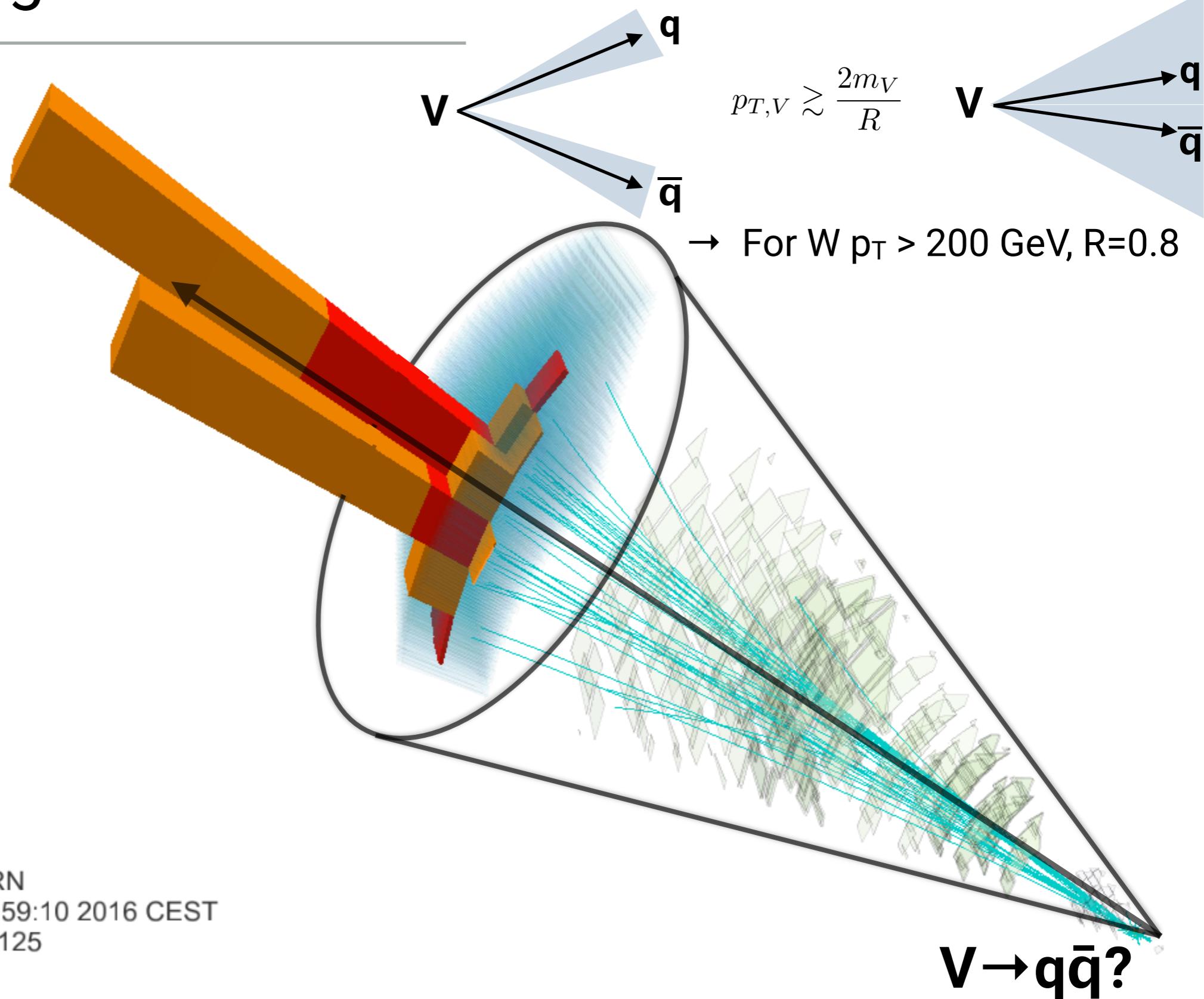
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Run/Event: 276950 / 1080730125

Lumi section: 573

$V \rightarrow q\bar{q}$?

W/Z-tagging in CMS



[CMS-PAS-B2G-17-001](#)

CMS Experiment at LHC, CERN

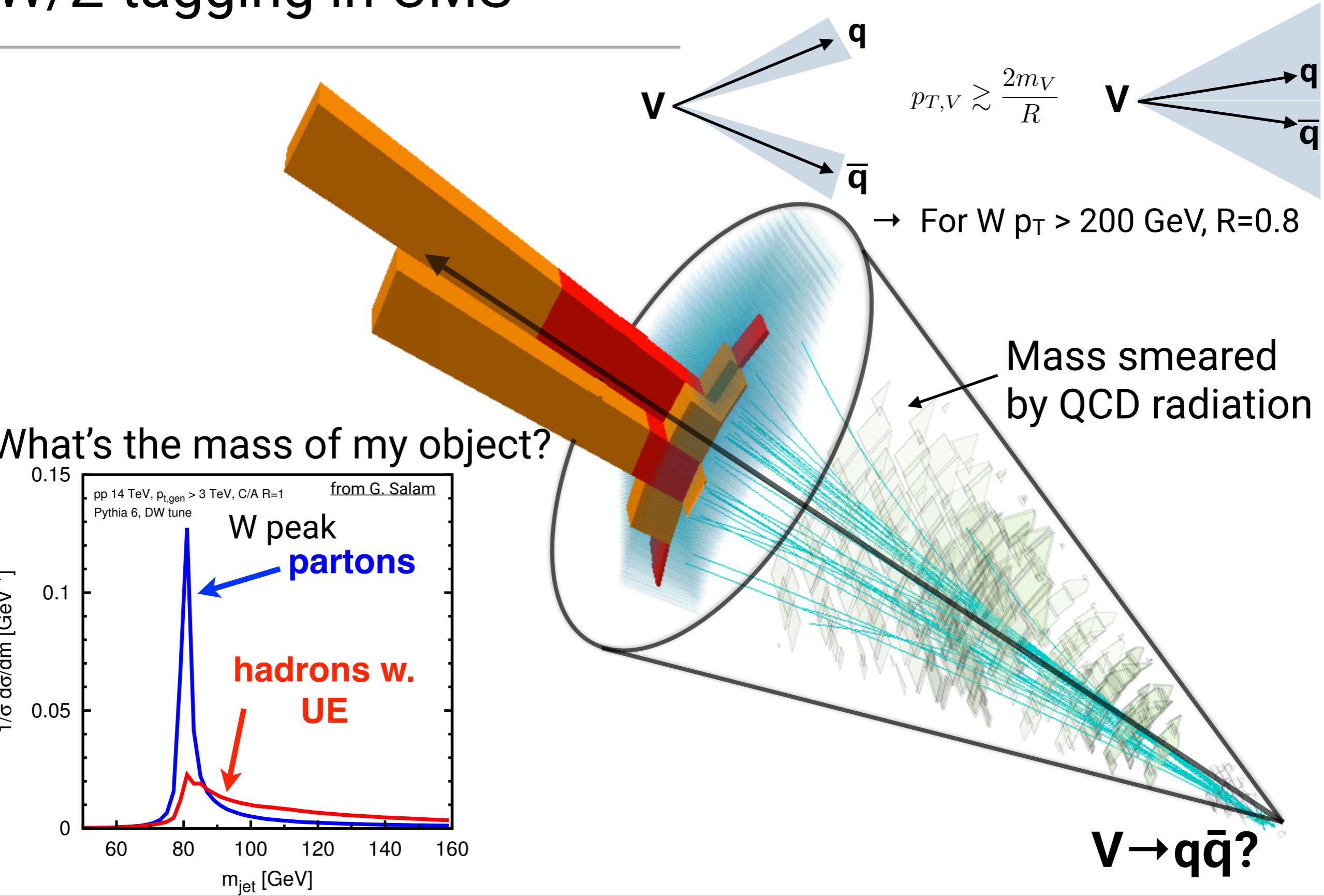
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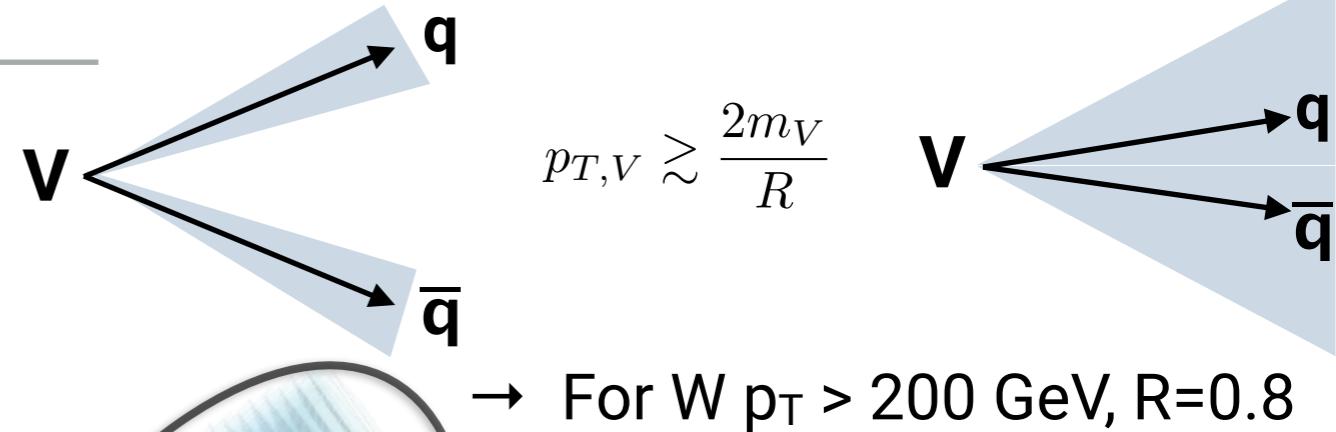
Lumi section: 573

$V \rightarrow q\bar{q}?$

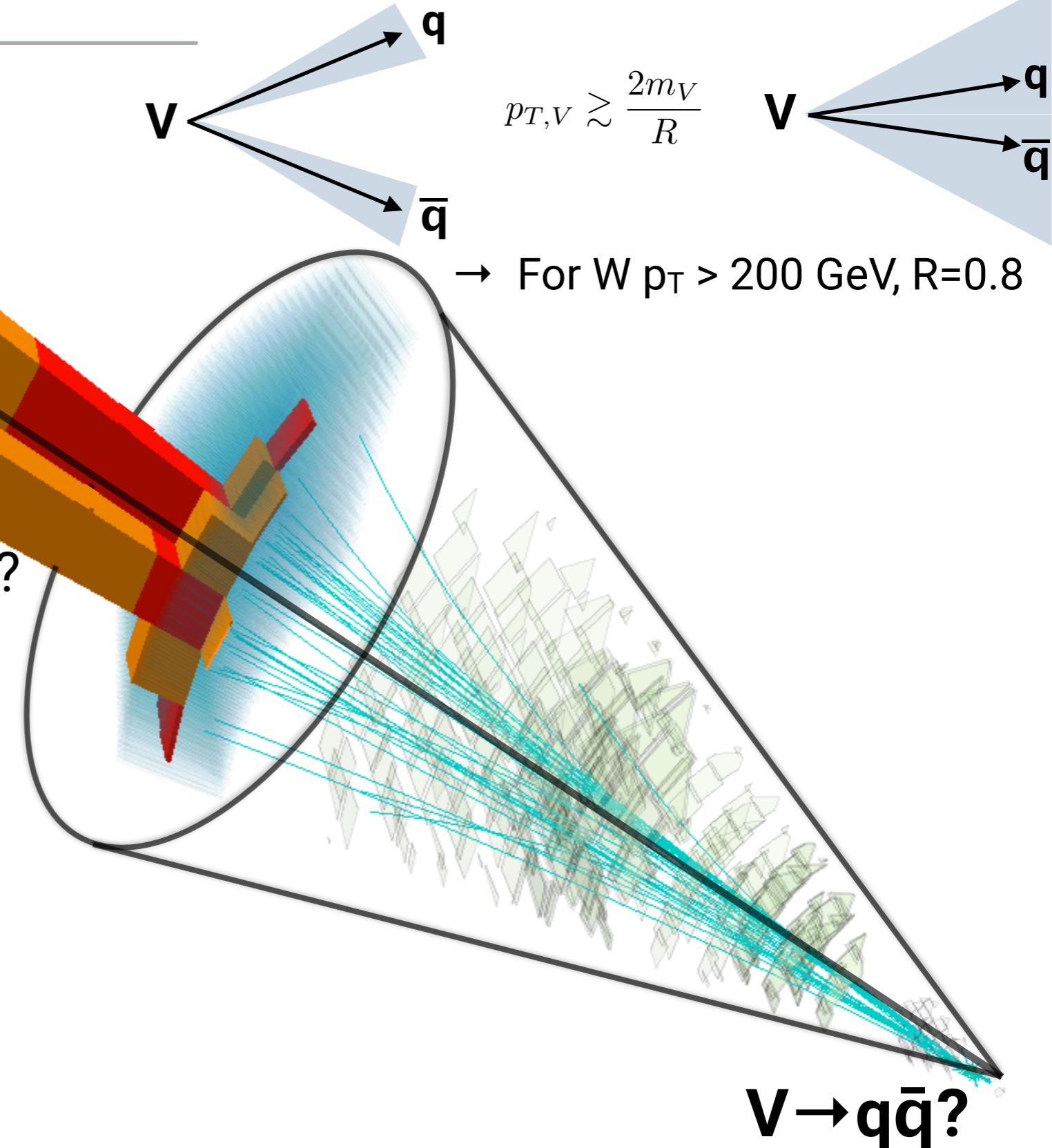
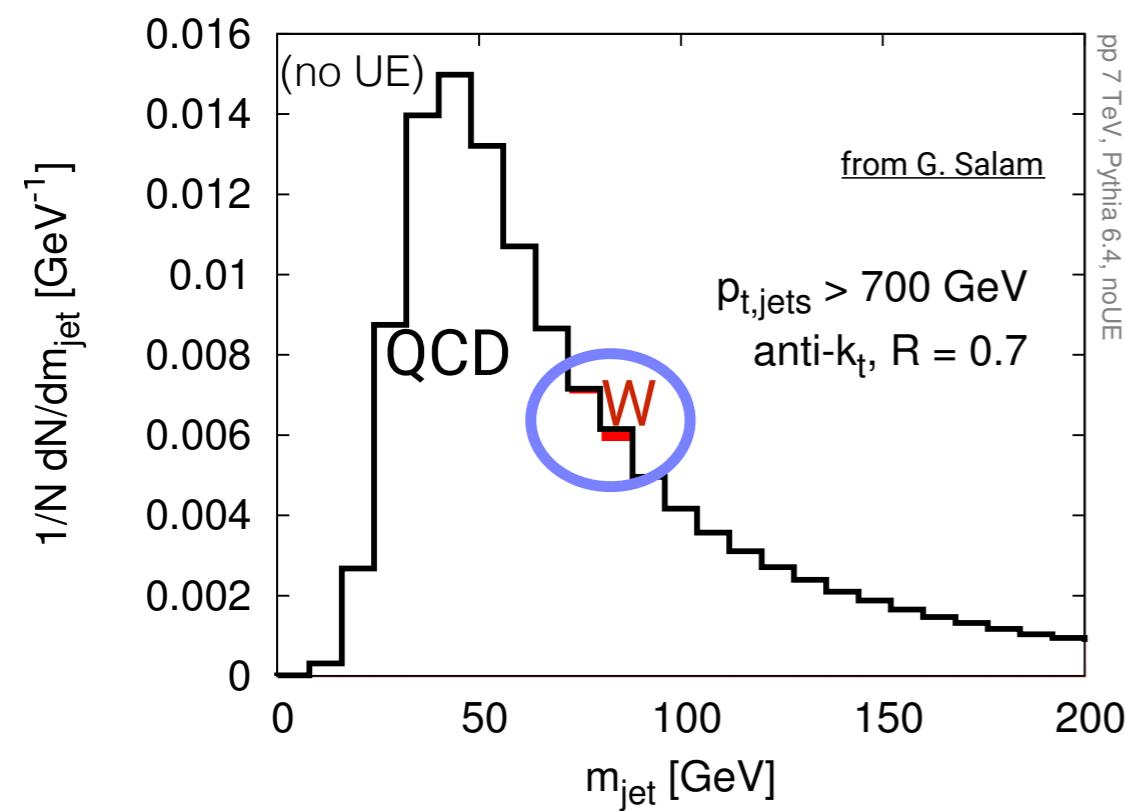
W/Z-tagging in CMS



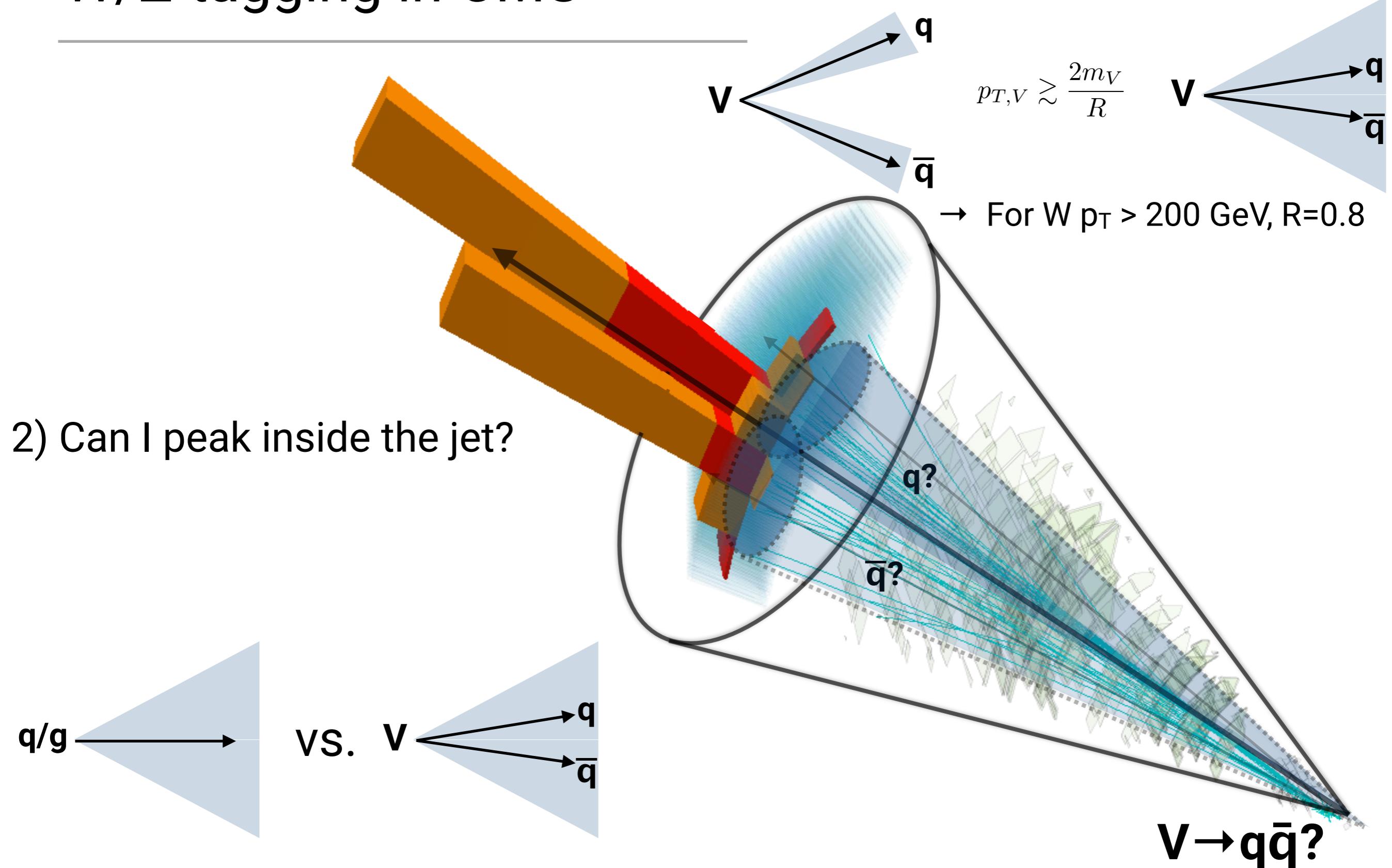
W/Z-tagging in CMS



1) What's the mass of my object?



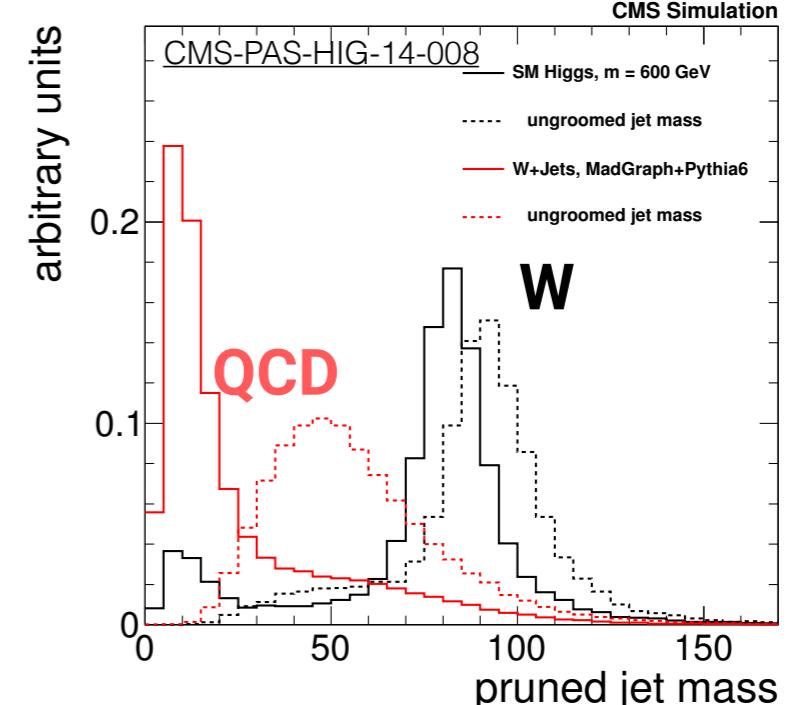
W/Z-tagging in CMS



Traditional W-tagging

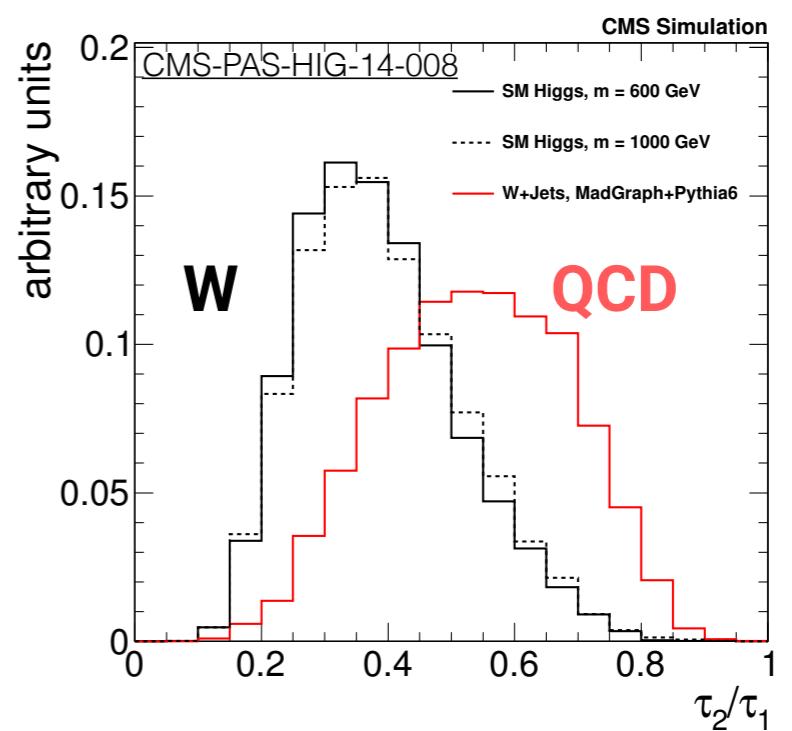
Cut-based taggers trying to answer

- Q: What's the mass of my object?
A: *Grooming (pruning/SD): Remove soft and wide angle jet constituents*
- Q: Is there substructure?
A: *N-subjettiness ++: Distance between jet constituents and hard subjet axes*



If a human can think up such algorithms, I bet a machine can too

- give DNN information it needs to design its own grooming/ substructure algorithms



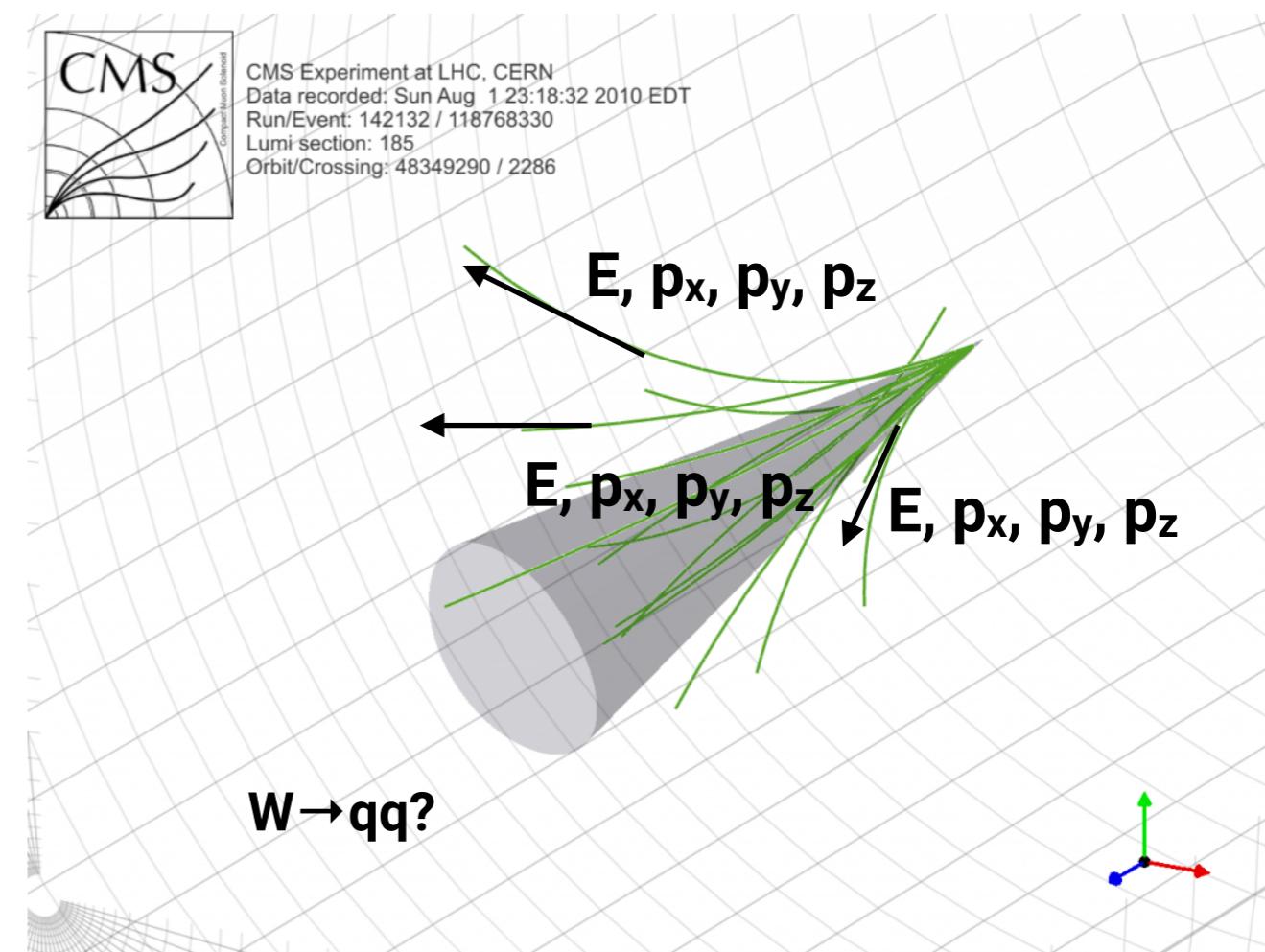
LoLa

DNN working with Lorentz vectors
introduced for top-tagging by T. Plehn,
G. Kasieczka et. Al ([arXiv:1707.08966](https://arxiv.org/abs/1707.08966))

- physics based deep neural network
- **does not**: throw huge amounts of inputs into NN and eliminate through rankings
- **does**: analyse jet constituents directly, teach NN distances in Minkowski space

All substructure/grooming algorithms in CMS based on jet constituent 4-vectors

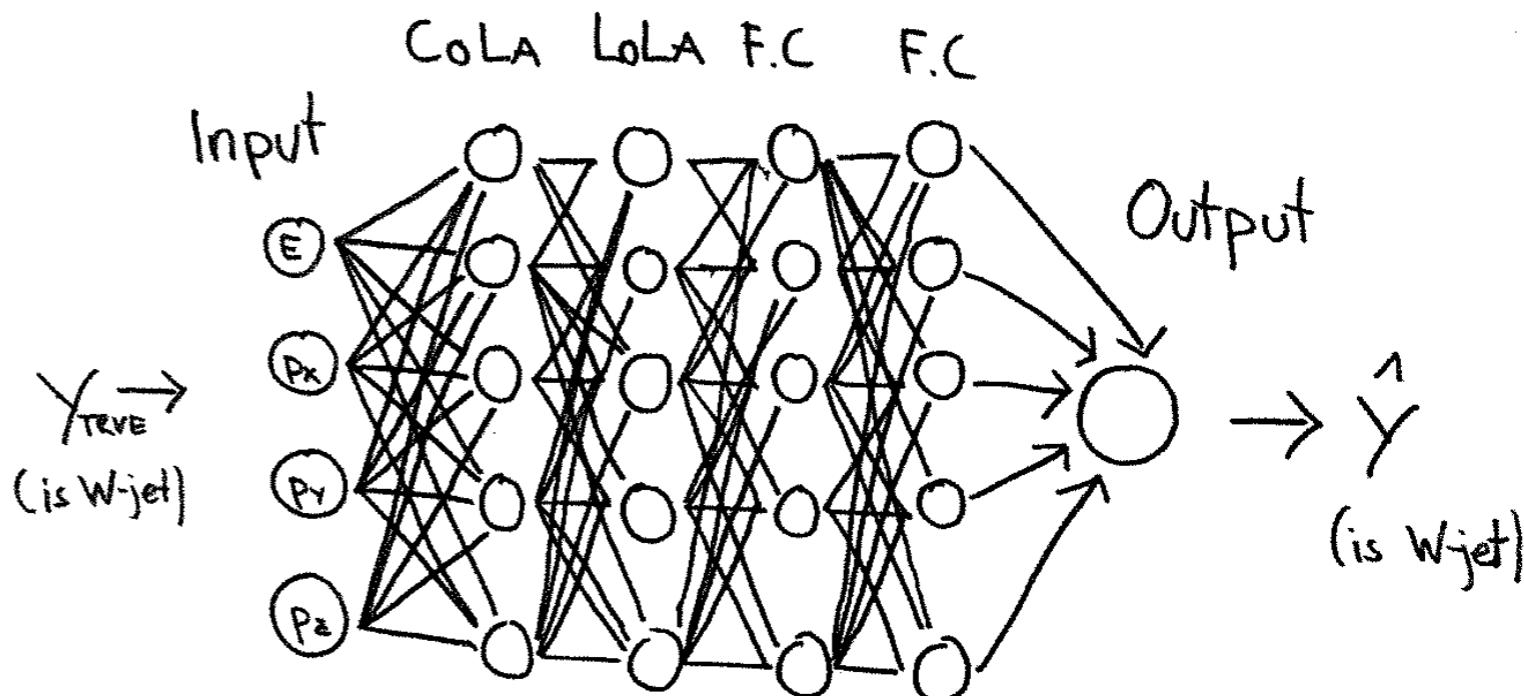
- by giving DNN tools to do jet substructure, can we learn substructure from LoLa instead of other way around



Network structure

4-layer DNN doing supervised learning with fixed-size input vectors

- feed forward sequential network
- Two novel layers (CoLa and LoLa) doing jet clustering and implementing Minkowski metric



Technicalities

- Keras w/ Theano backend (on Amazon)
- Loss function: Categorical crossentropy (output :W-jet/QCD probability)
- ADAM optimiser (adapt learning rate of model parameters during training)

Input

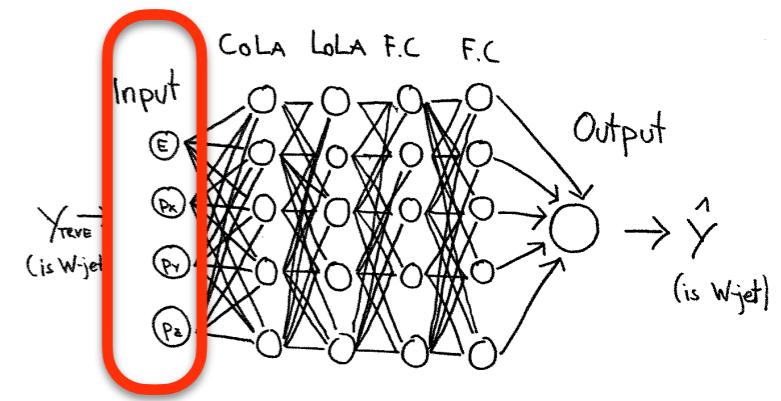
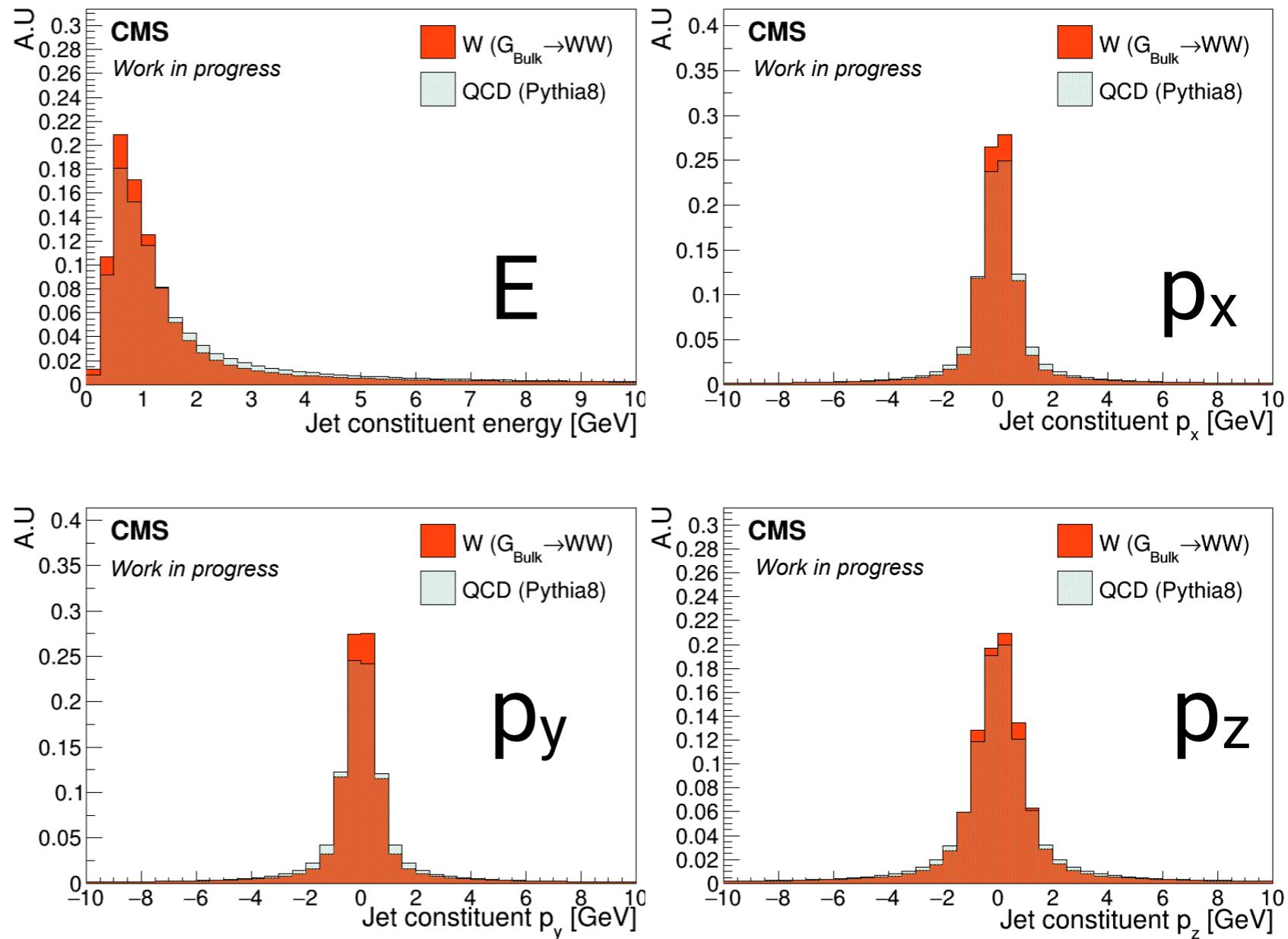
Four input features

- 4-vectors of the N=20 highest-p_T jet constituents of AK8 jets

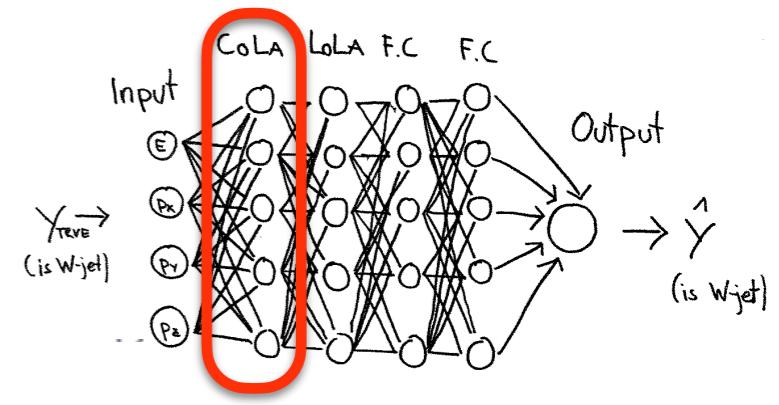
4x20 matrix $k_{\mu,i}$ for each jet

$$(k_{\mu,i}) = \begin{pmatrix} k_{0,1} & k_{0,2} & \cdots & k_{0,N} \\ k_{1,1} & k_{1,2} & \cdots & k_{1,N} \\ k_{2,1} & k_{2,2} & \cdots & k_{2,N} \\ k_{3,1} & k_{3,2} & \cdots & k_{3,N} \end{pmatrix}$$

(4 Features x 20 constituents)



Combination Layer (CoLa)



COLA: E.g for 2 constituents

$$k_{M,i} = \begin{bmatrix} E_1 & E_2 \\ P_x^1 & P_x^2 \\ P_y^1 & P_y^2 \\ P_z^1 & P_z^2 \end{bmatrix}_{(4,2)}$$

$$\tilde{k}_{M,j} = k_{M,i} \cdot C_{ij} =$$

CoLa

$$\begin{aligned} \tilde{k}_{M,j} &= \begin{bmatrix} E_1 & E_2 \\ P_x^1 & P_x^2 \\ P_y^1 & P_y^2 \\ P_z^1 & P_z^2 \end{bmatrix}_{(4,2)} \cdot \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \end{bmatrix}_{(2, M=4)} \\ &= \begin{bmatrix} E_1 + E_2 & E_1 + E_2 \\ P_x^1 + P_x^2 & P_x^1 + P_x^2 \\ P_y^1 + P_y^2 & P_y^1 + P_y^2 \\ P_z^1 + P_z^2 & P_z^1 + P_z^2 \end{bmatrix} = \begin{bmatrix} E_i & E_i \\ P_x^1 & P_x^1 \\ P_y^1 & P_y^1 \\ P_z^1 & P_z^1 \end{bmatrix} + \begin{bmatrix} W_{4,1} & W_{4,2} \\ W_{4,1} & W_{4,2} \\ W_{4,1} & W_{4,2} \\ W_{4,1} & W_{4,2} \end{bmatrix} \begin{bmatrix} E_1 & E_2 \\ P_x^1 & P_x^2 \\ P_y^1 & P_y^2 \\ P_z^1 & P_z^2 \end{bmatrix} \end{aligned}$$

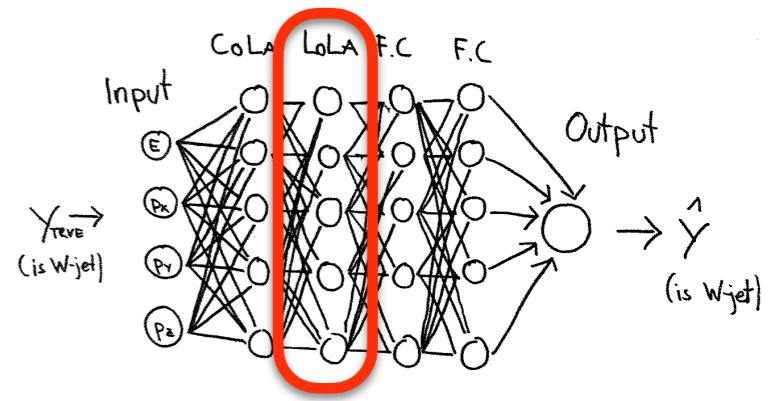
linear combinations of momenta

Linear combinations similar to jet-clustering

- Sum of all momenta
- Each original constituent momenta
- Linear combinations + **trainable weights**.
Can make subjets!

! Can “weight” constituents away, reconstruct hard subjets → groomer

Lorentz Layer (LoLa)



LoLA:

$$\tilde{k}_{uij} = \begin{bmatrix} \sum E & [E_1 E_2] w_{4,1} E_1 + w_{4,2} E_2 \\ \sum p_x & [p_x^2 p_x^2] w_{4,1} p_x^2 + w_{4,2} p_x^2 \\ \sum p_y & [p_y^2 p_y^2] w_{4,1} p_y^2 + w_{4,2} p_y^2 \\ \sum p_z & [p_z^2 p_z^2] w_{4,1} p_z^2 + w_{4,2} p_z^2 \end{bmatrix} \quad (4, 4)$$

LoLa

$$\hat{k}_j = \begin{bmatrix} m^2(\tilde{k}_j) \\ p_T(\tilde{k}_j) \\ w_{jm} E(\tilde{k}_m) \\ w_{jm} \sum d_{jm}^2 \\ w_{jm} \sum d_{jm}^2 \\ w_{jm}^{\text{min}} \min d_{jm}^2 \\ w_{jm}^{\text{sum}} \min d_{jm}^2 \end{bmatrix} \quad (7, 4)$$

$$= \frac{g_{\mu\nu} p_\mu^\nu p_\nu^\mu}{\sqrt{\sum p_x^2 + \sum p_y^2}}$$

$$w_{jm} \sum E$$

$$w_1^{\text{min}}, w_2^{\text{min}}, w_1^{\text{sum}}, w_2^{\text{sum}}$$

$$(k_\Sigma - \tilde{k}_m)_\mu g^{\mu\nu} (k_\Sigma - \tilde{k}_m)_\nu \dots$$

Maps CoLa output onto

- $m^2 + p_T$ of each column ("jet", constituents, hard subjets)
- Energy of all constituents (with trainable weight)
- Distance between all particles ($2 \cdot \text{min} + 2 \cdot \text{sum}$)
→ n-subjetiness

Minkowski metric explicitly used for m^2 and d

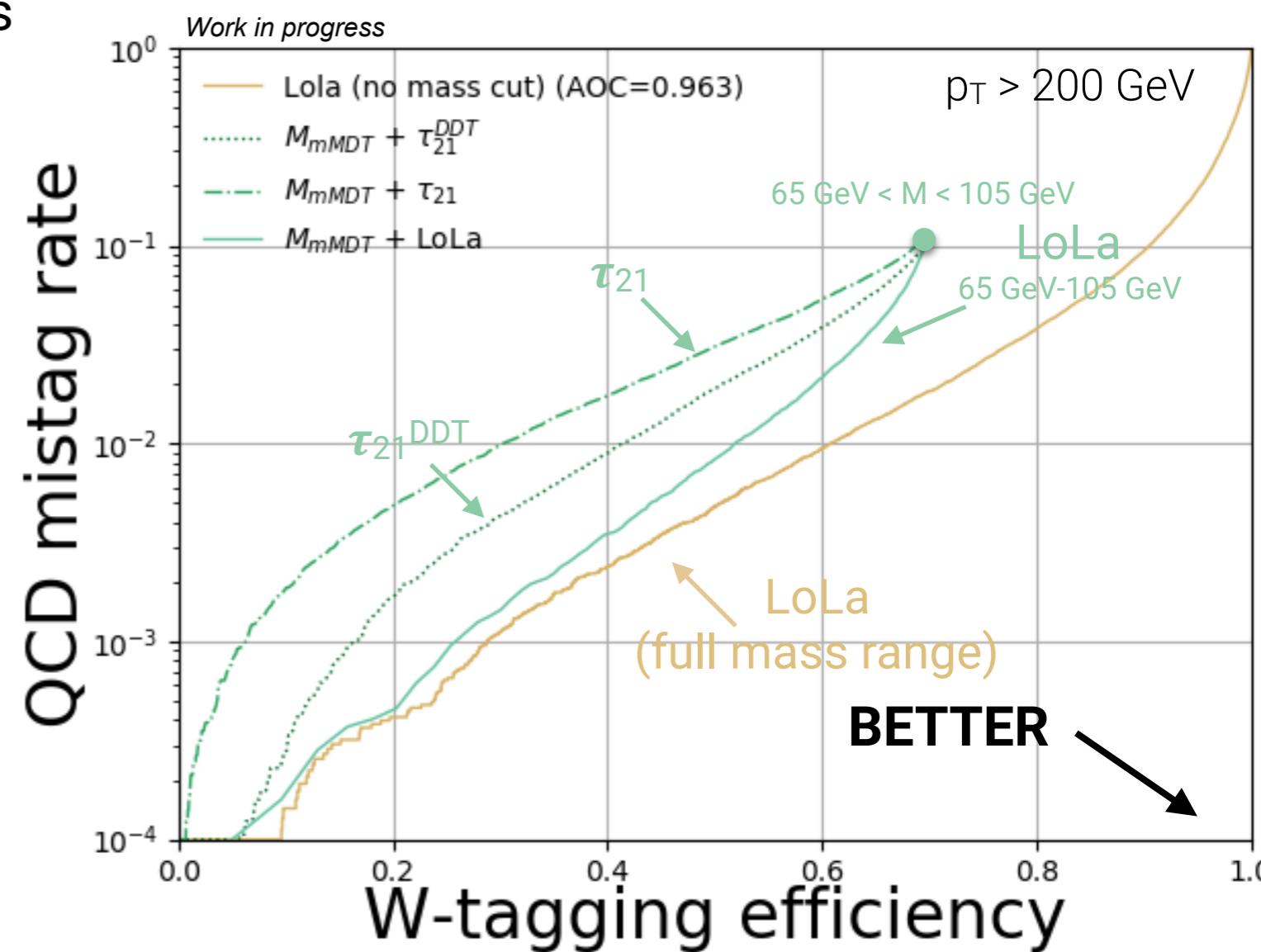
Overall performance

Compare performance to most commonly used cut based V-taggers

- LoLa performs significantly better than current baseline
 - 20% higher ϵ_S at given ϵ_B compared to best cut-based
 - no need for mass window, increased signal acceptance

For two-W final state, 43% increase in signal efficiency*

**We all know DNNs do better.
Whats next?**



*B2G-17-001



Beyond performance

Beyond performance

Three things to consider when making a DNN tagger:

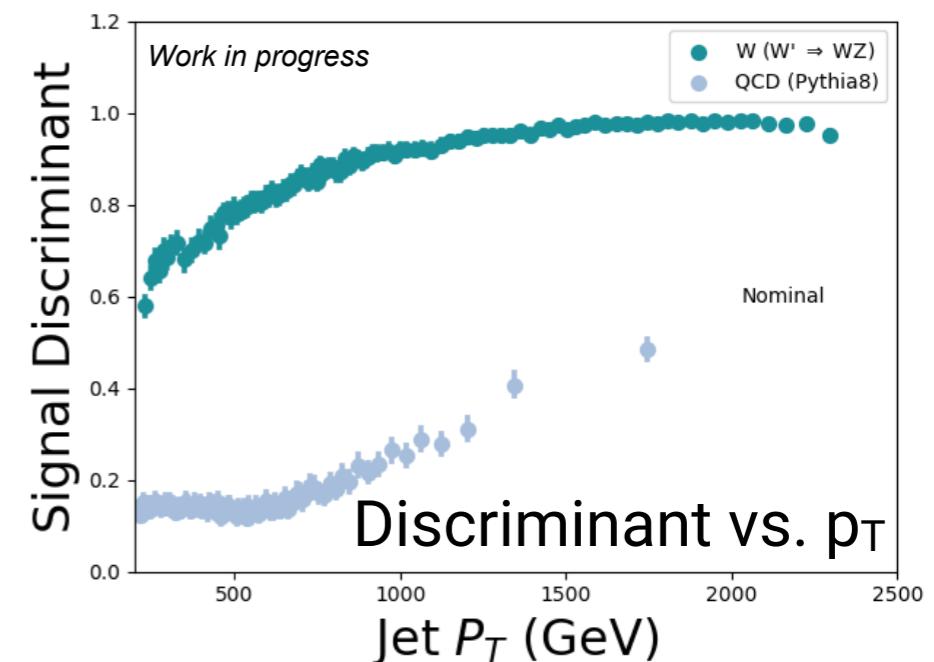
- is the absolute performance better (compared to common methods, a standard BDT)?

Beyond performance

Three things to consider when making a DNN tagger:

- is the absolute performance better (compared to common methods, a standard BDT)?
- is the tagger p_T -dependent?

Output strongly correlated
with p_T /mass

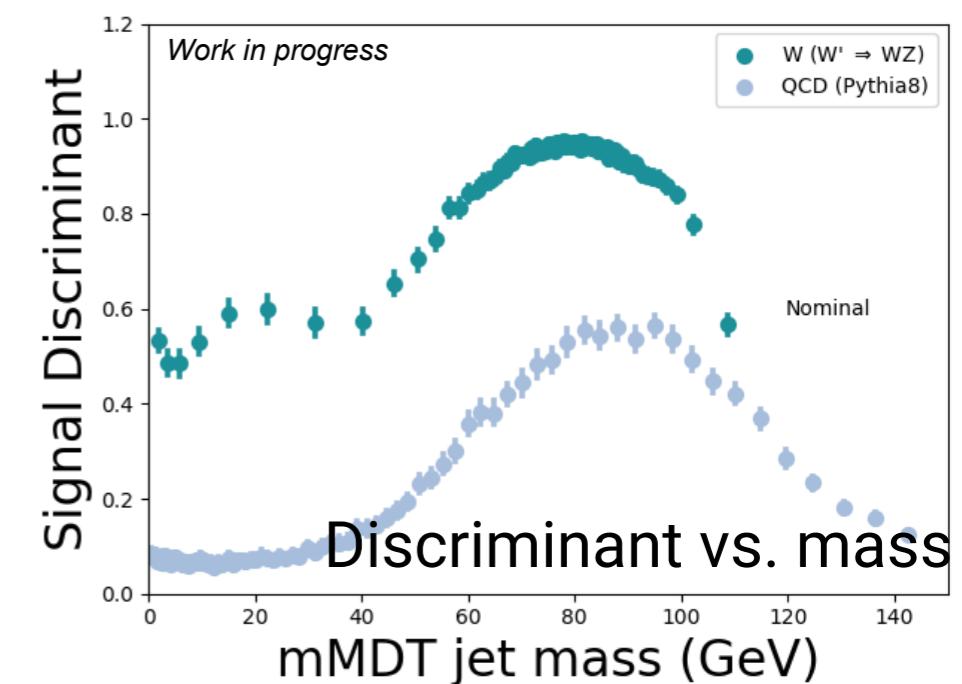
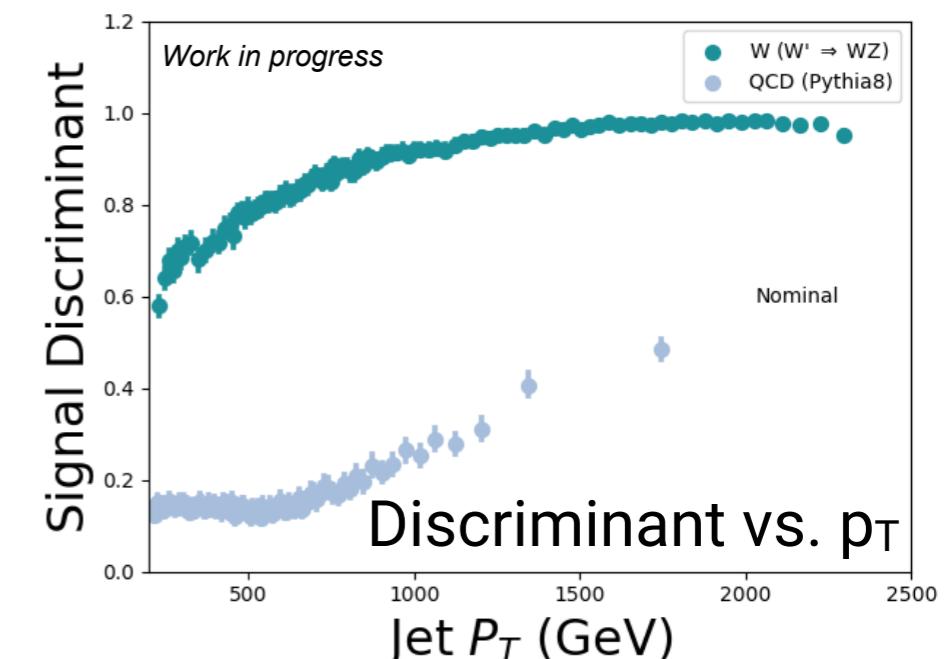


Beyond performance

Three things to consider when making a DNN tagger:

- is the absolute performance better (compared to common methods, a standard BDT)?
- is the tagger p_T -dependent?
- does the tagger sculpt the mass spectrum?

Output strongly correlated with p_T /mass



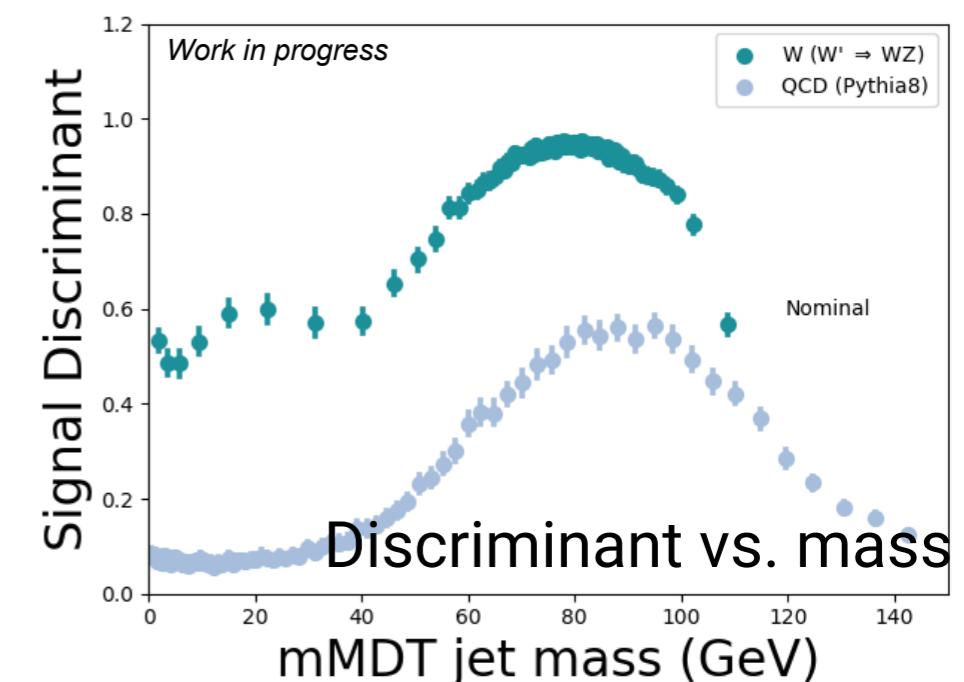
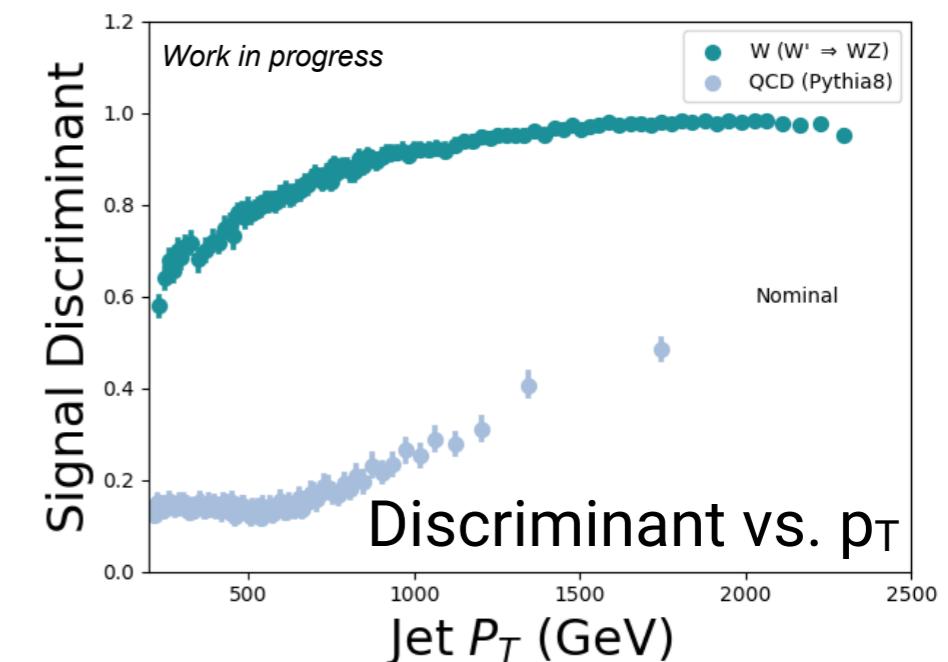
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These three measures are equally important in quantifying performance

Output strongly correlated with p_T /mass



Beyond performance

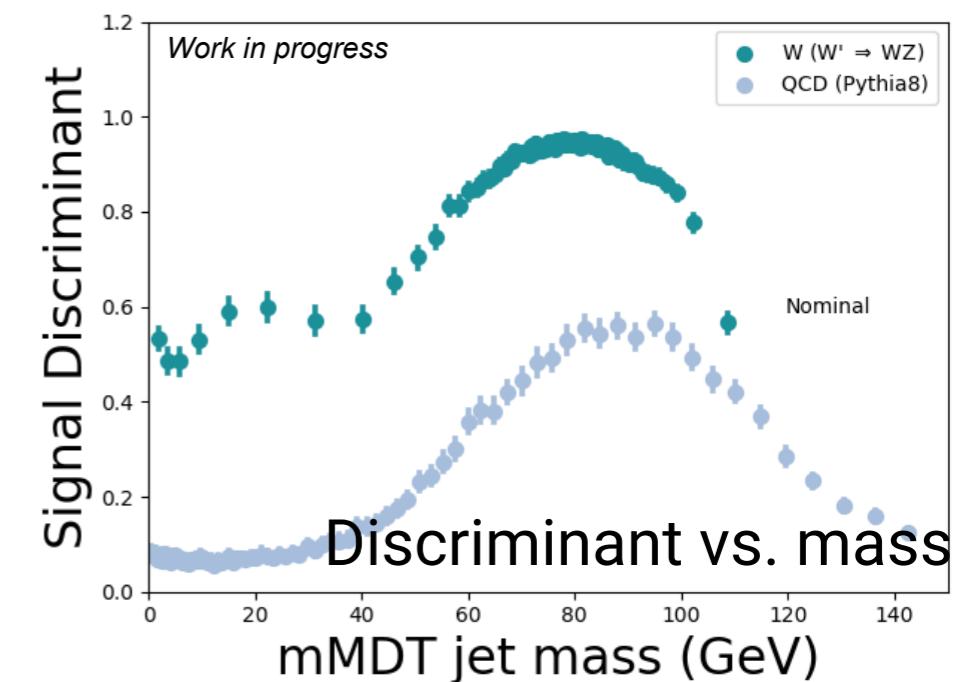
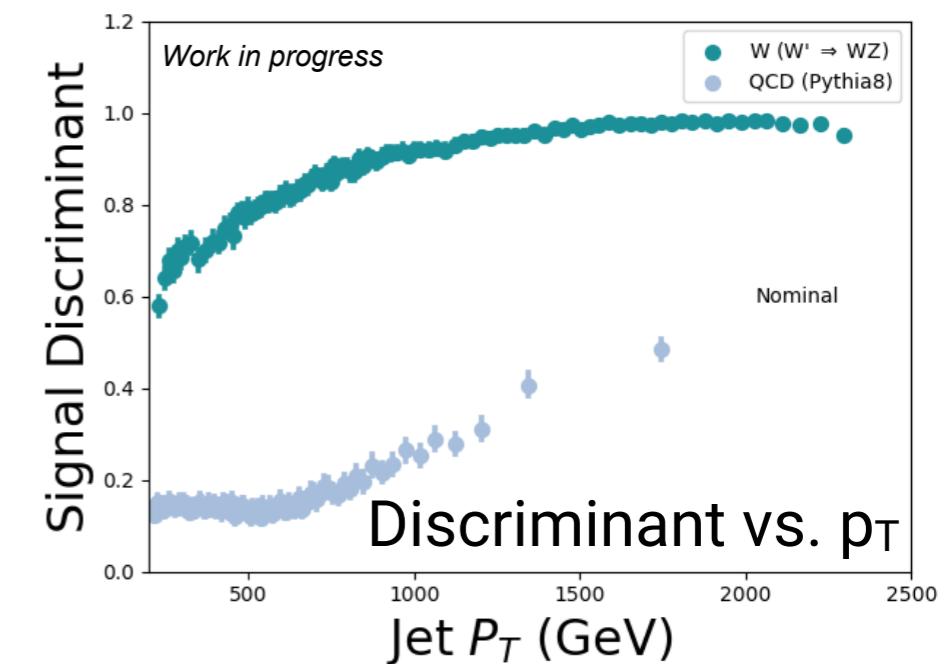
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A DNN will naturally learn that p_T and mass are discriminating variables unless you penalise it for it!

Output strongly correlated with p_T /mass



Beyond performance

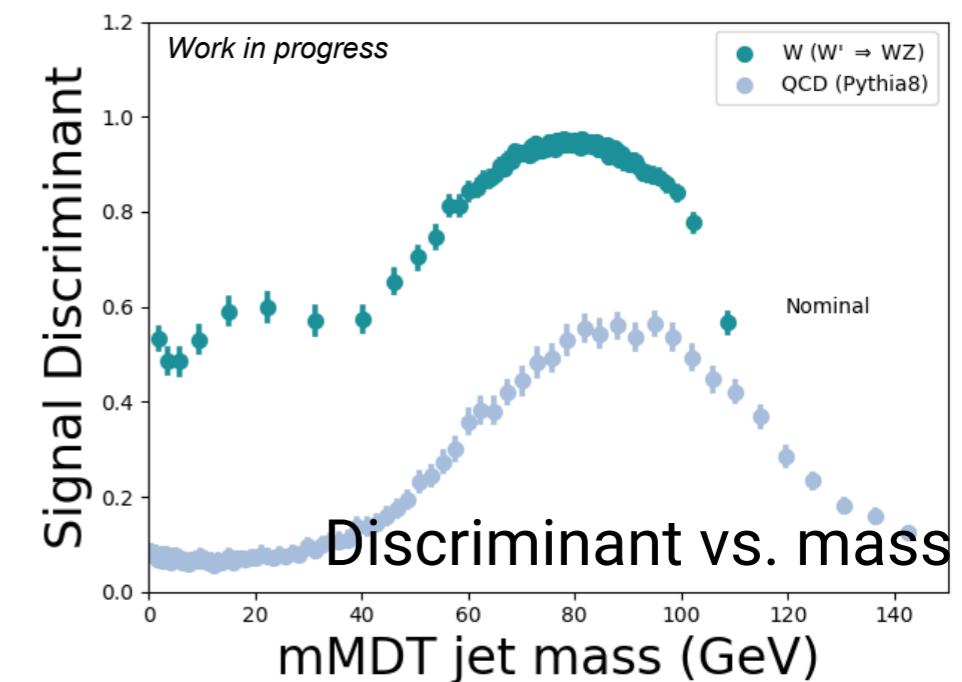
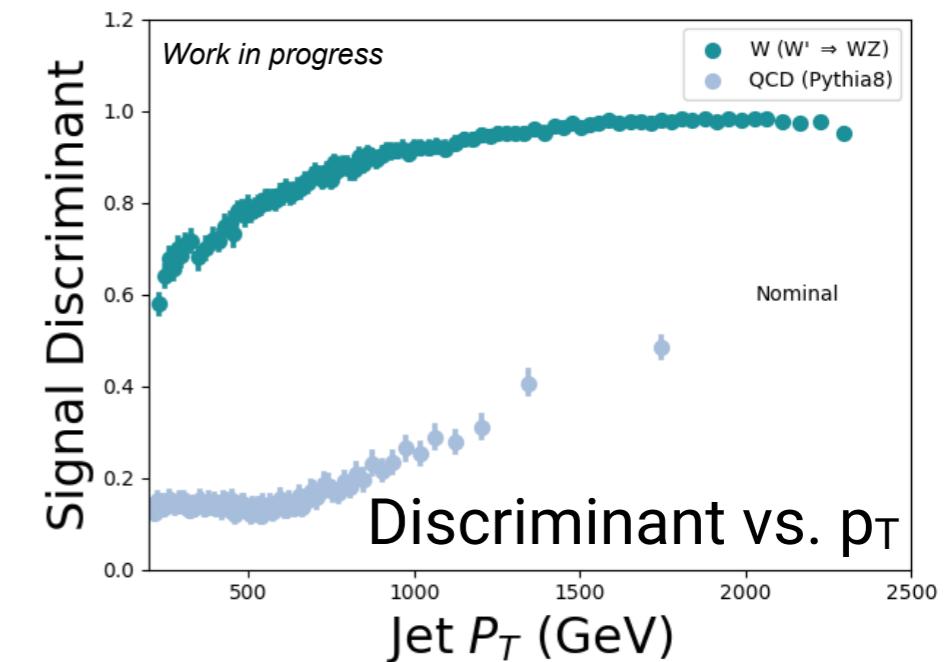
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Output strongly correlated with p_T /mass



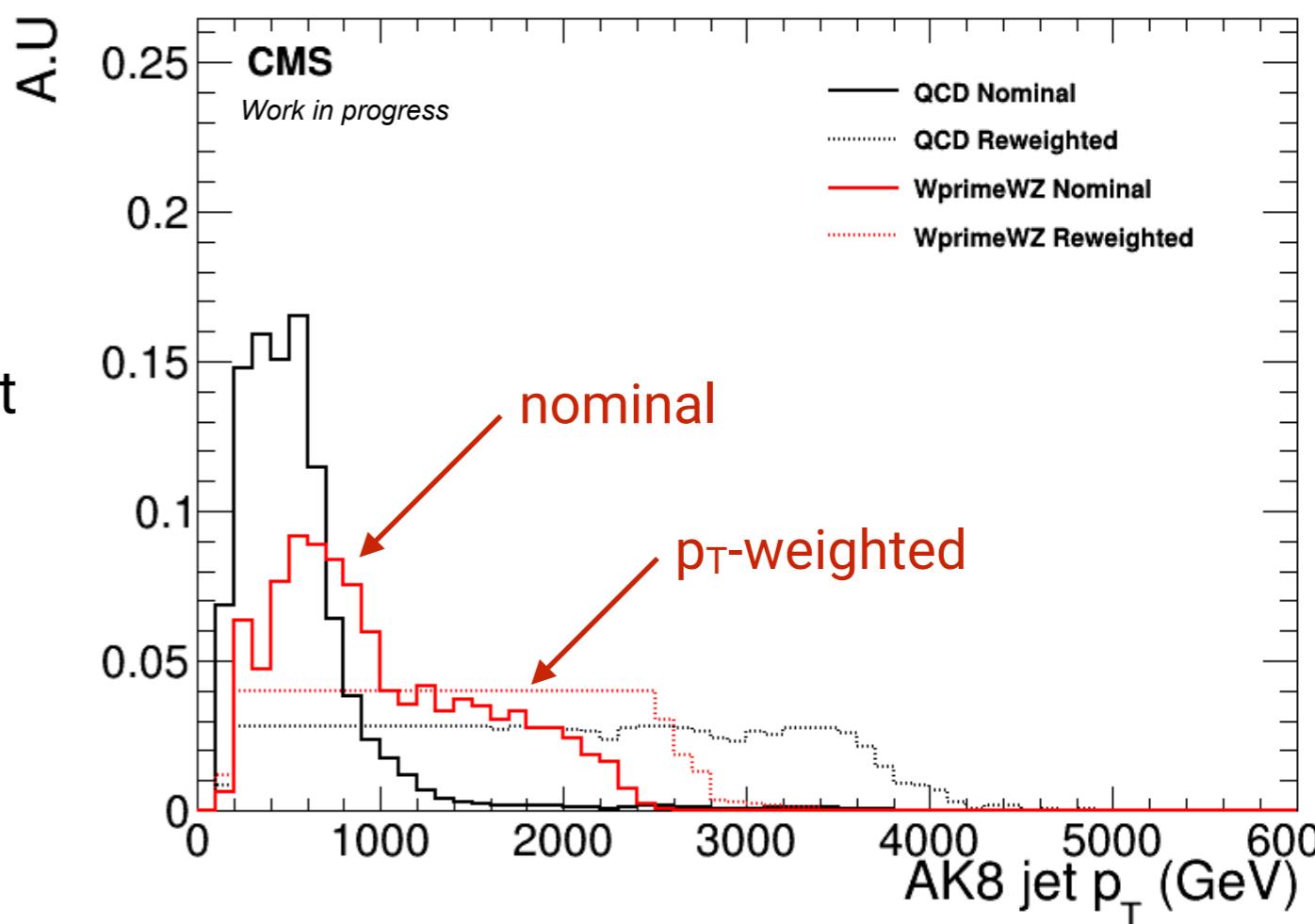
p_T dependence

p_T -dependence is a problem because

- signal efficiency is variable, requires working point scaling with p_T
- p_T (tagger validation region) \neq p_T (signal region)

One method to cope: reweight training set event-by-event to be flat in p_T -space

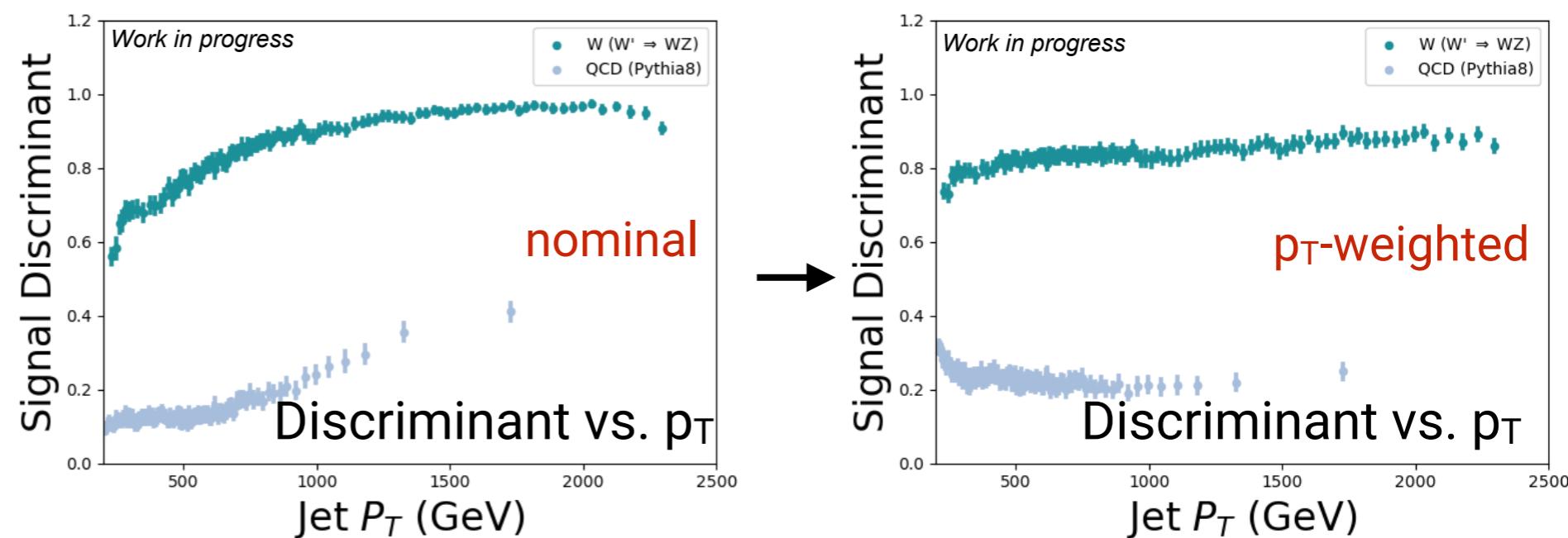
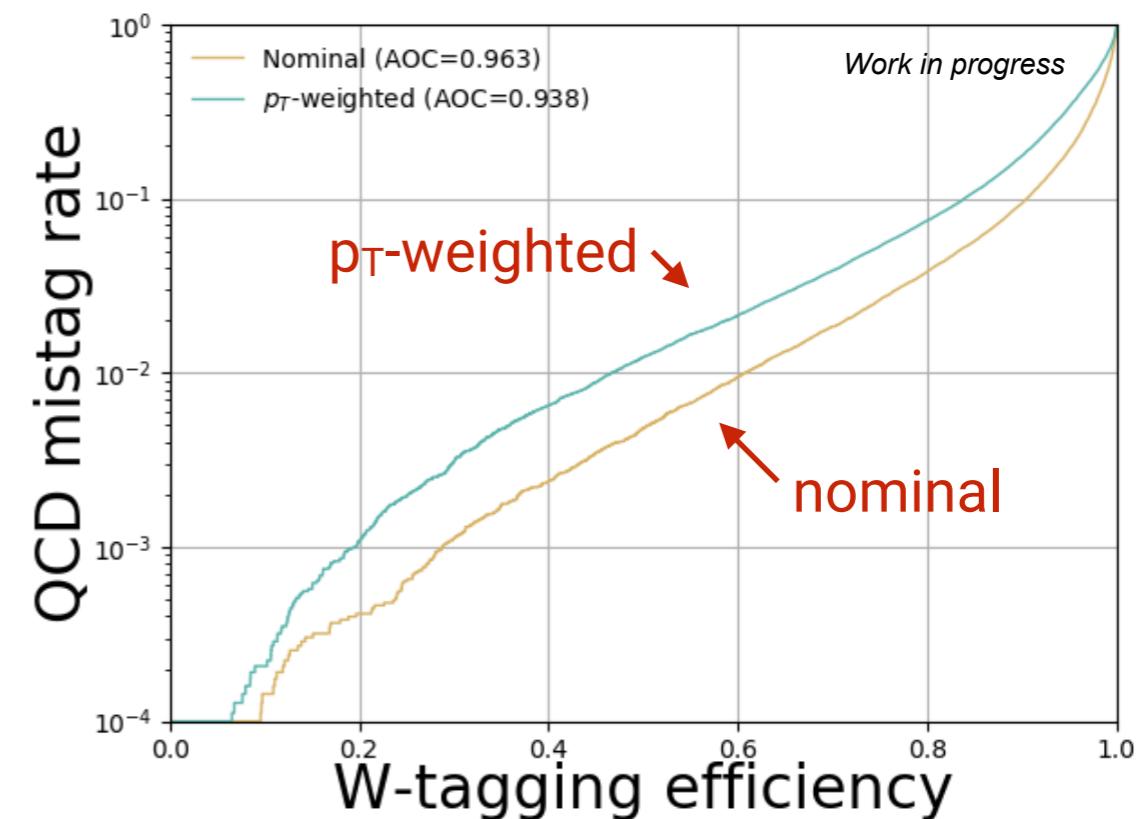
- passed as sample weights to training



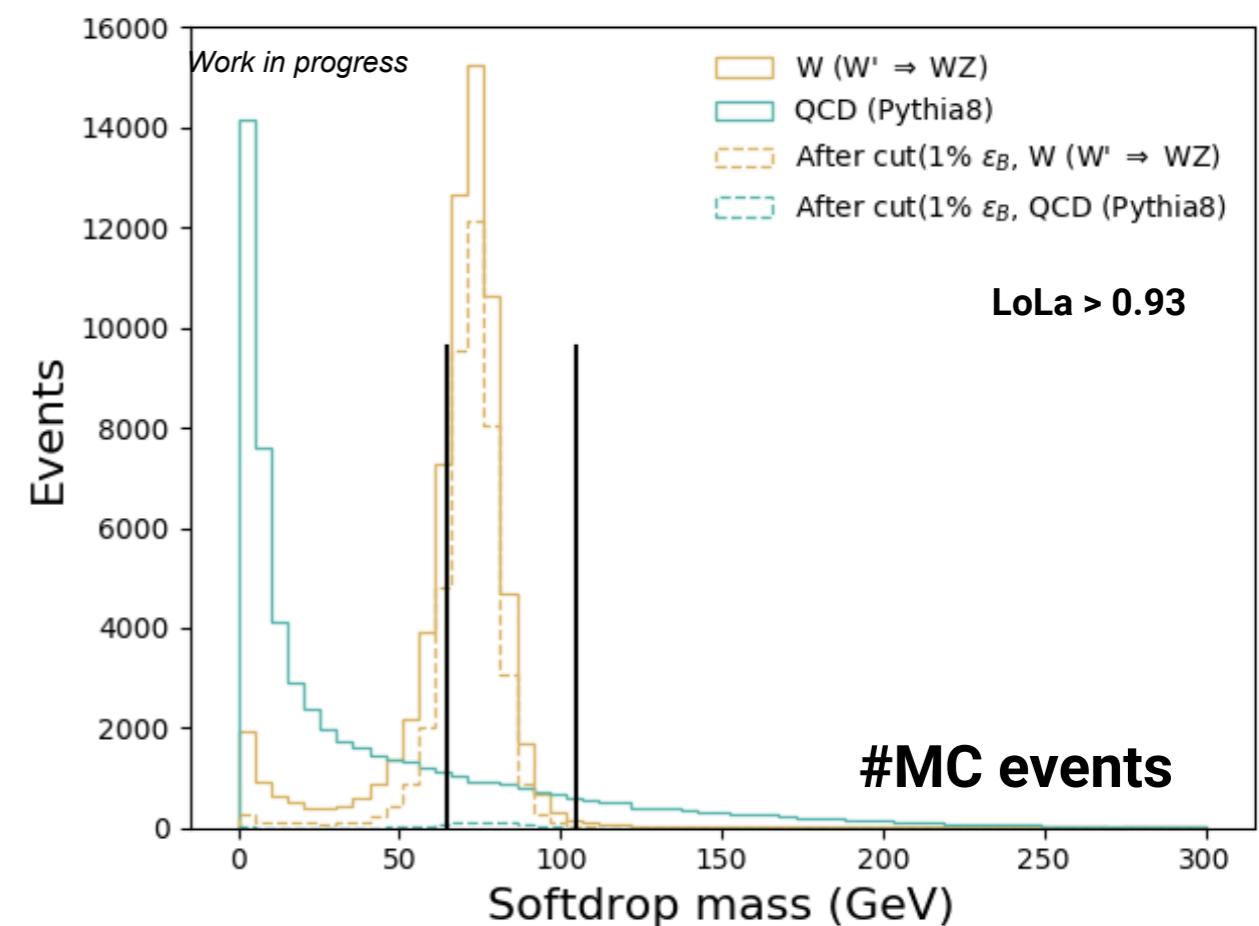
p_T dependence

Such strategies yields loss in overall performance, but reduced p_T -dependence

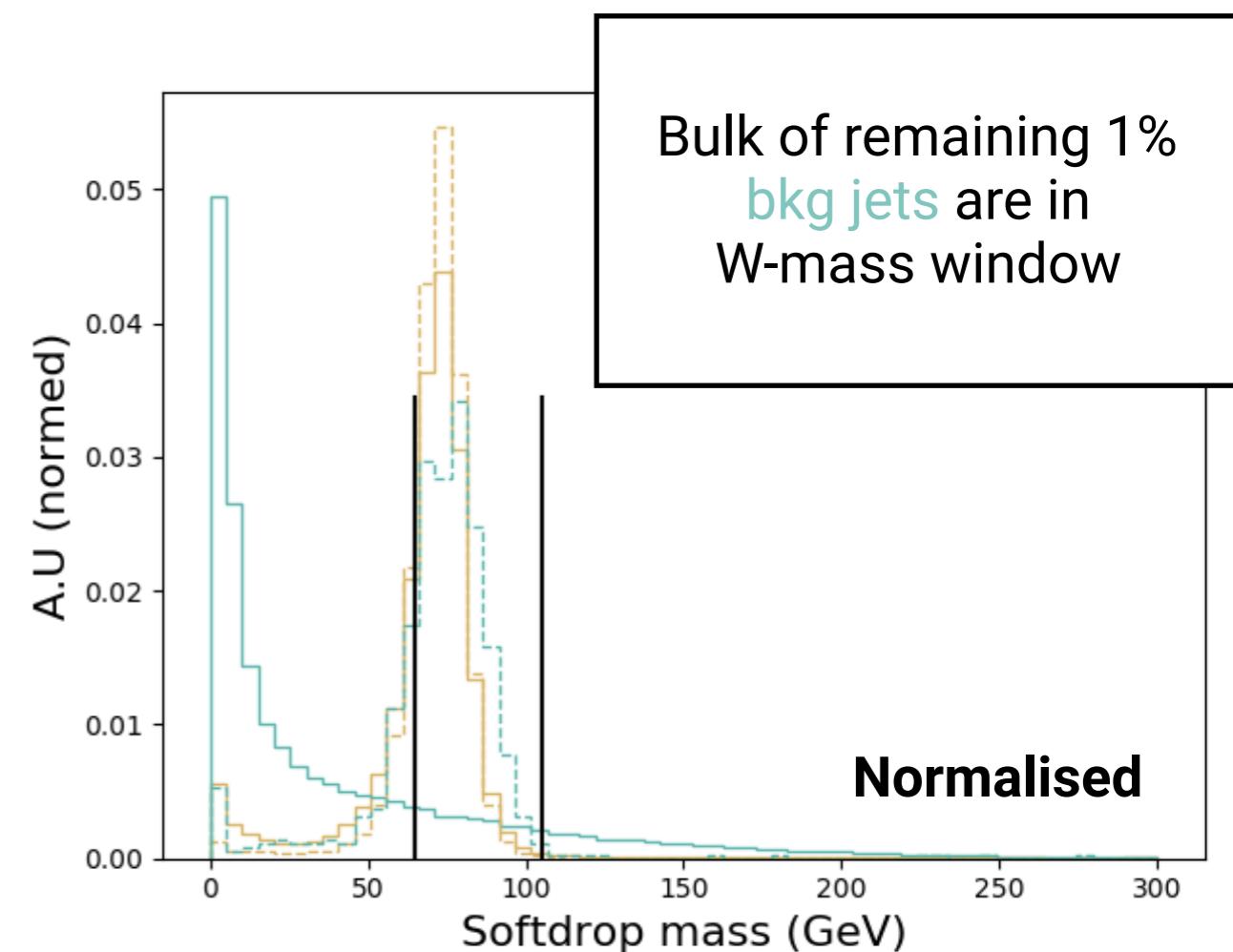
No “truth” for which solution is better before running full analysis including systematics for p_T -dependent tagging



Mass sculpting



Mass sculpting



Mass sculpting

I smart DNN will learn W-mass

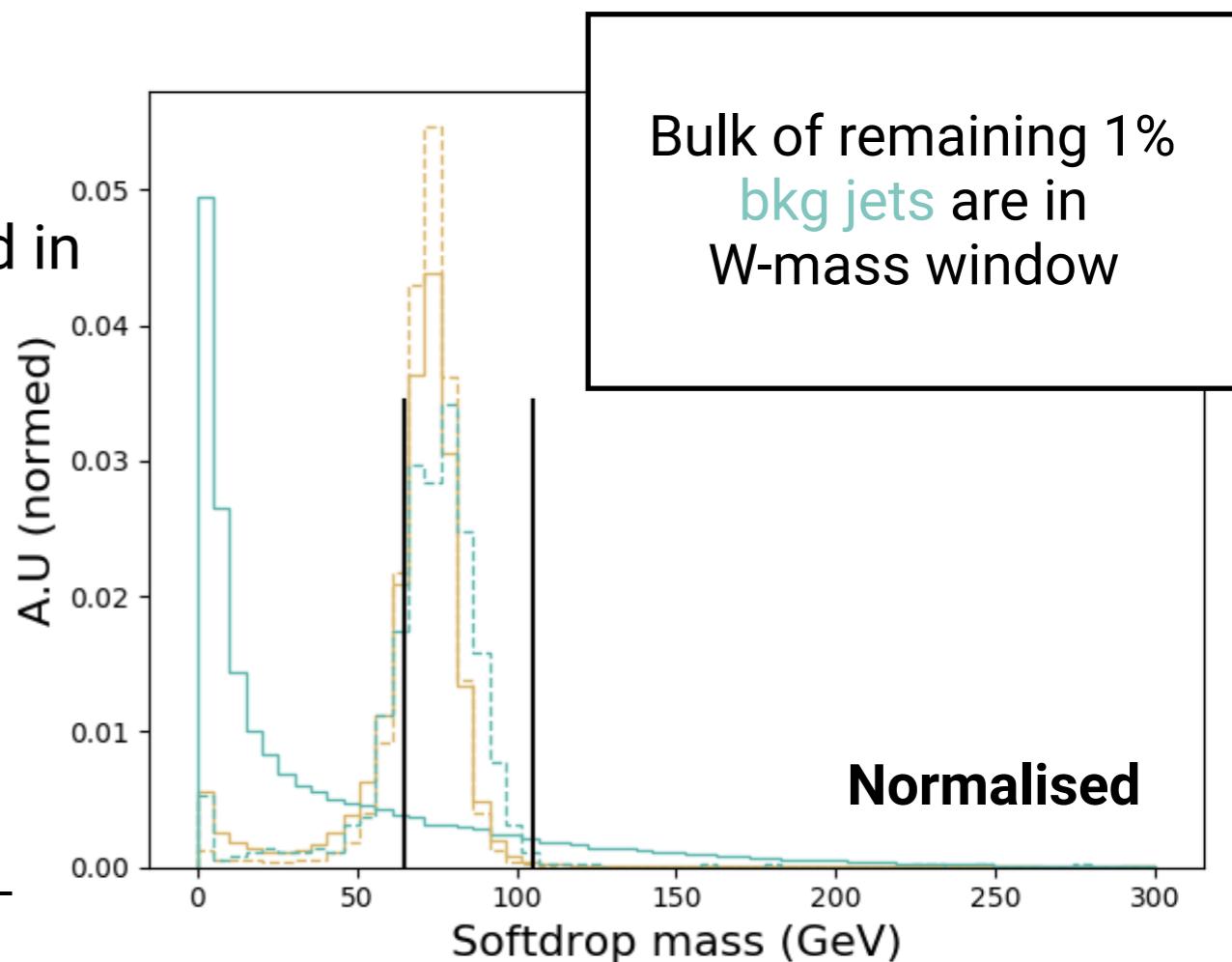
- good! Clearly W-mass \neq q/g-jet mass

Unfortunately, we often estimate background in mass sidebands

- bad! After cut on tagger, mass is sculpted making background difficult to constrain

Mass-dependence in itself not a problem, background rate uncertainties are

- trade-off between efficiency and (analysis-dependent) systematics.



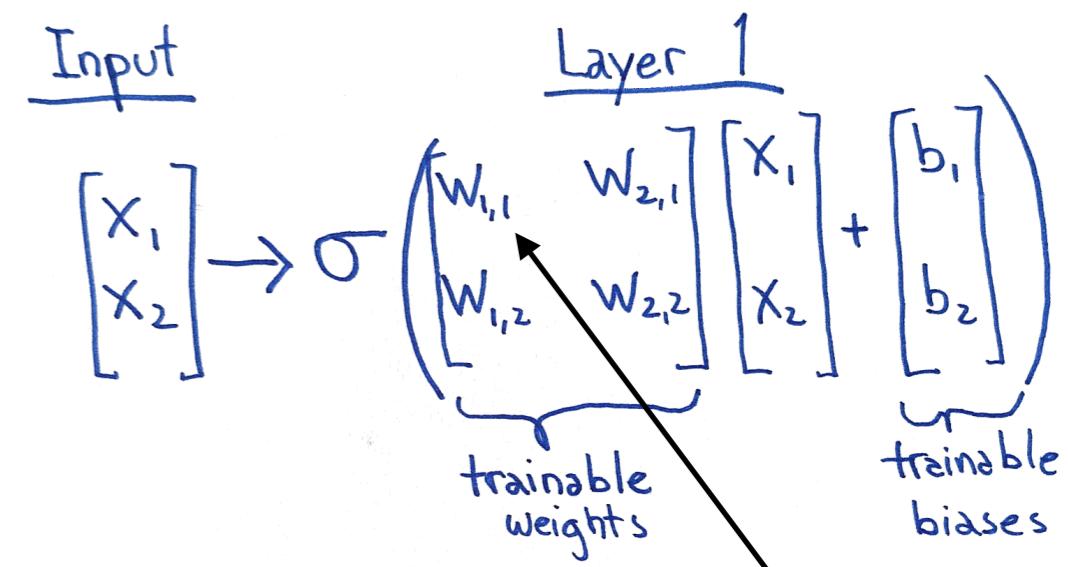
Hot topic in ML: adversarial NNs that penalise loss if mass is learned (see C. Shimmin et. Al)

- loss in efficiency, gain in analysis sensitivity

Model grooming

Despite common beliefs, a DNN is NOT a black box

- series of multiplications/additions and pre-computed activation functions
- you can (and should) read out the weights of your model for each layer (or feature)*



Does network learn something (un)expected?

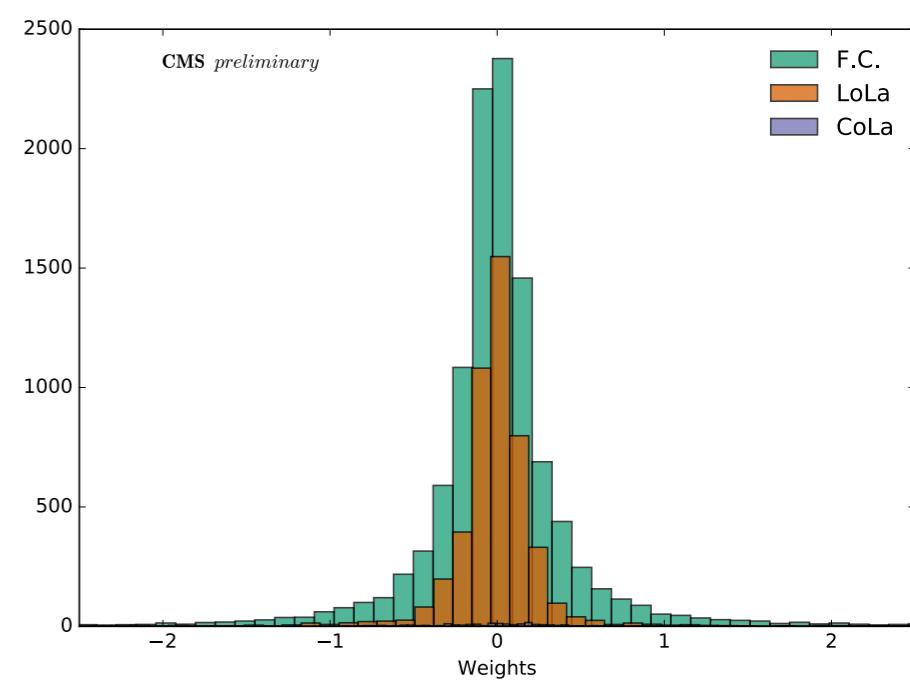
- with physics-based trainable weights like in LoLa, easier to disentangle

Also allows you to prune your DNN

- remove ~zero-weights from network. Reduces processing time with same performance

*model.layers[i].output
model.get_layer(layer_name).output

How are my features x weighted?



Summary and outlook

The idea behind LoLa is to give DNN the rules of Minkowski space, jet clustering and substructure and let it do the rest

analyse constituents directly with large set of trainable weights

For use in tagging, absolute performance is not a sufficient measure

- p_T -dependence + mass-sculpting resilience may be equally important depending on the analysis performed
- should strive to implement taggers in a full analysis chain before making final decisions (p_T -reweighting, mass penalising, etc.)

The question “What can we learn from the machine?” is getting more interesting than “What can we teach the machine?”

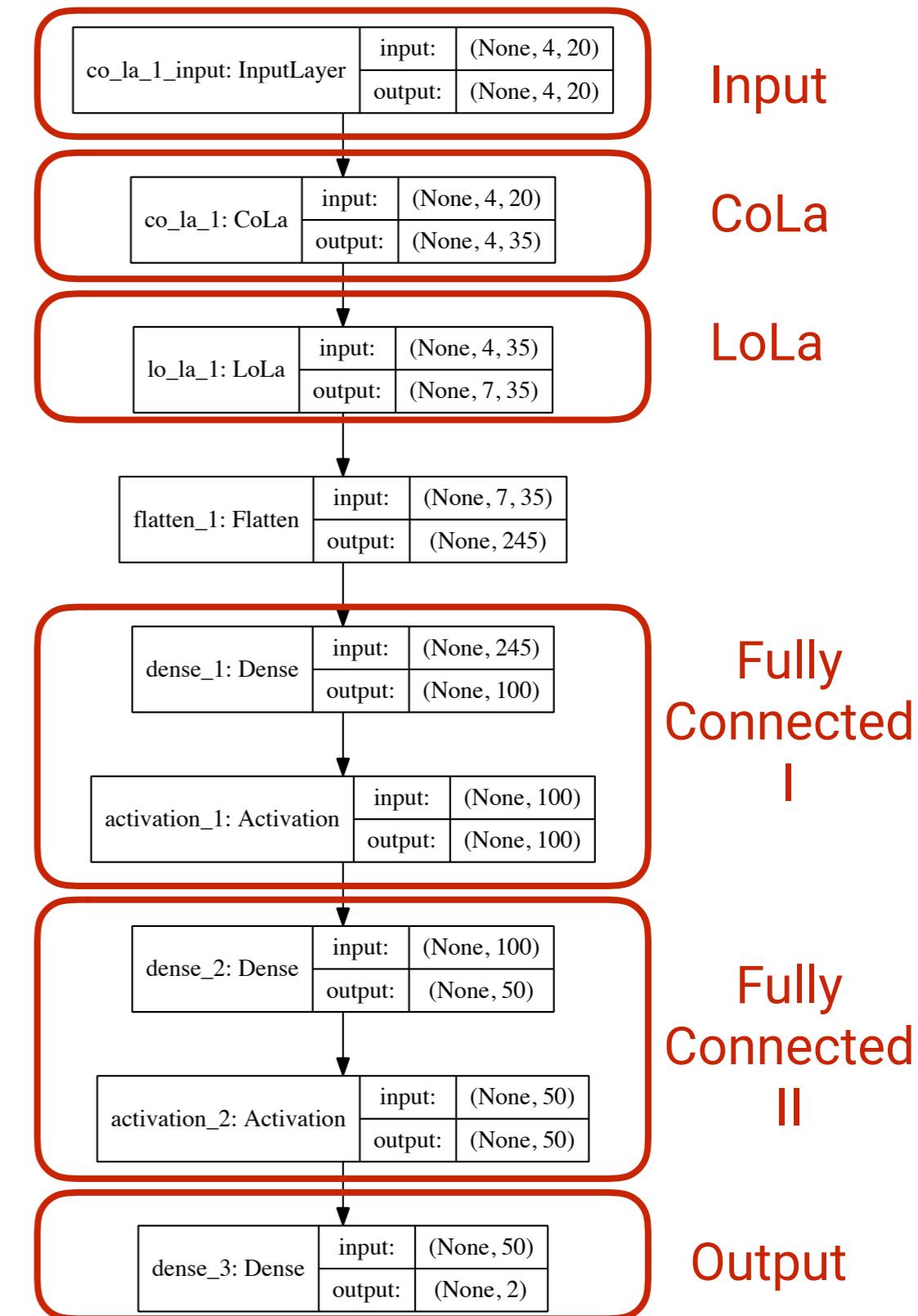
- by probing layer-wise LoLa output, hope to learn something new about substructure!



Backup

Model

- 4 layer DNN doing supervised learning with fixed-size input vectors
 - feed forward sequential network
 - Two novel layers (CoLa and LoLa) implementing Minkowski metric and “substructure” calculations (see later) and two fully connected layers
- Technicalities
 - Keras with Theano backend
 - Loss function: categorical crossentropy
 - ADAM optimiser (adapt learning rate of model parameters during training)
- Train 200k + Test 60k + Val 60k on AWS



Model summarised

Input:

4-vectors of $N = 20$
highest p_T jet
constituents
of AK8 jets

$$(k_{\mu,i}) = \begin{pmatrix} k_{0,1} & k_{0,2} & \cdots & k_{0,N} \\ k_{1,1} & k_{1,2} & \cdots & k_{1,N} \\ k_{2,1} & k_{2,2} & \cdots & k_{2,N} \\ k_{3,1} & k_{3,2} & \cdots & k_{3,N} \end{pmatrix} C = \begin{pmatrix} 1 & 1 & 0 & \cdots & 0 \\ 1 & 0 & 1 & & \vdots \\ \vdots & \vdots & \vdots & \ddots & 0 \\ 1 & 0 & 0 & \cdots & 1 \end{pmatrix} \begin{pmatrix} C_{1,N+2} & \cdots & C_{1,M} \\ C_{2,N+2} & \cdots & C_{2,M} \\ \vdots & & \vdots \\ C_{N,N+2} & \cdots & C_{N,M} \end{pmatrix}$$

$$k_{\mu,i}$$

 (4×20)

Combination layer(CoLa):

- Sum of all momenta
- Each original momentum
- 15 trainable weights C

$$k_{\mu,i} \xrightarrow{\text{CoLa}} \tilde{k}_{\mu,j} = k_{\mu,i} C_{ij}$$

 (4×35)

Summing and weighting all constituent should allow network to calculate subject axes

Lorentz layer(LoLa):

Compute kinematics for CoLa output.
1+4 additional trainable weights

$$\tilde{k}_j \xrightarrow{\text{LoLa}} \hat{k}_j = \begin{pmatrix} m^2(\tilde{k}_j) \\ p_T(\tilde{k}_j) \\ w_{jm}^{(E)} E(\tilde{k}_m) \\ w_{jm}^{(d)} d_{jm}^2 \end{pmatrix}$$

$$\tilde{k}_j \xrightarrow{\text{LoLa}} \hat{k}_j$$

 (7×35)

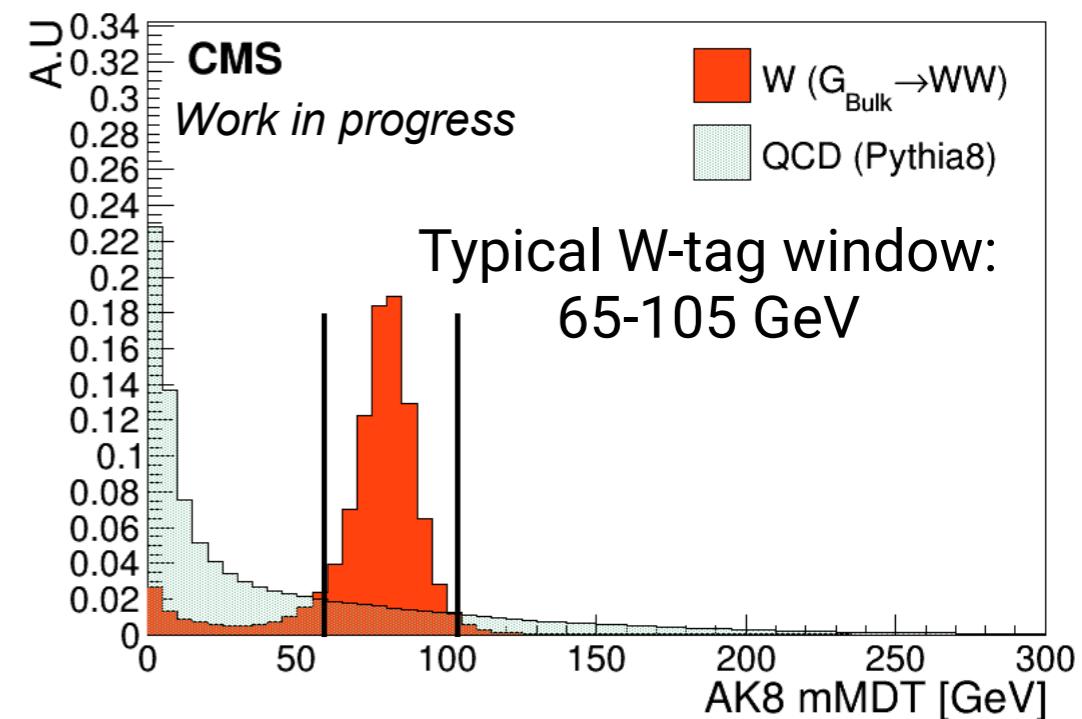
d_{jm}^2 and m^2 use Minkowski distance

$$d_{jm}^2 = (\tilde{k}_j - \tilde{k}_m)_\mu g^{\mu\nu} (\tilde{k}_j - \tilde{k}_m)_\nu$$

The basic setup

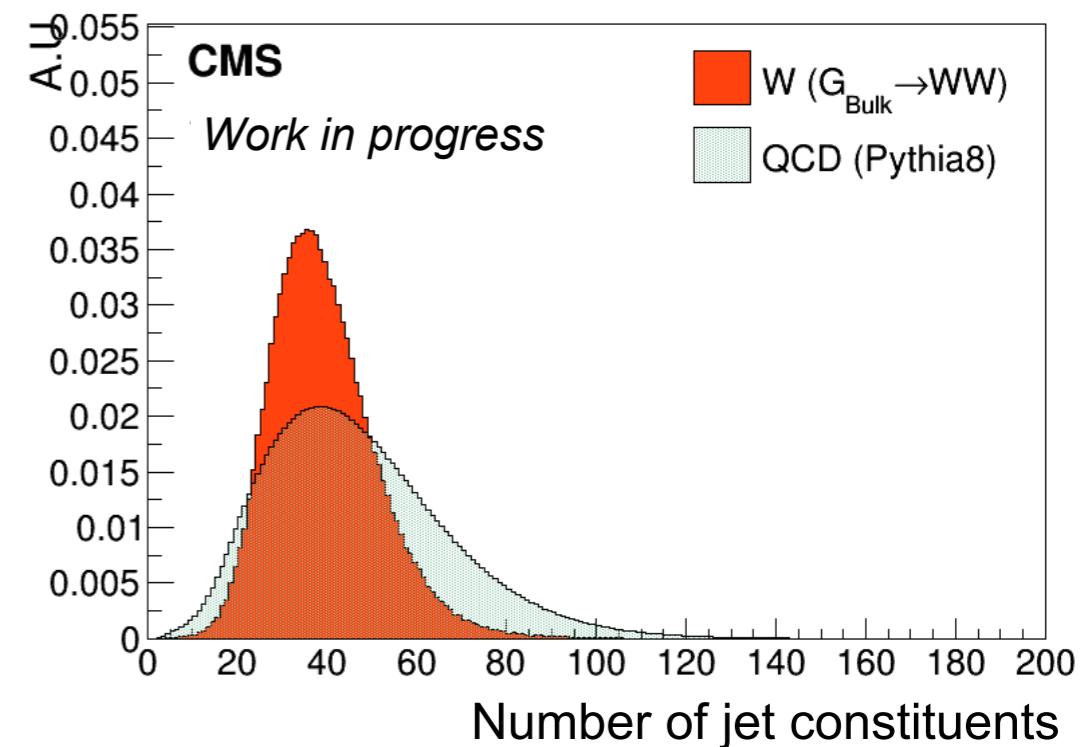
Signal

- 320k fully merged hadronic W-jets (AK8) from $W' \rightarrow WZ \rightarrow 4q$ ($M_{W'} = 0.6\text{-}4.5 \text{ TeV}$)
- why small training set? → Do not mix signal samples until one is understood (can change with W polarisation etc.)



Background

- QCD Pythia8 non-W jets
- Danger: Jet substructure strongly depends on shower generators (different description of gluon radiation). Different QCD MC might yield different results



Disclaimer: The following contains student work in progress studies and not CMS approved results

What does LoLa learn?

Input:

4-vectors of $N = 20$
highest p_T jet constituents

$$\begin{matrix} E_i \dots E_N \\ p_x(k_{\mu,i}) \\ p_y \\ p_z \end{matrix} = \begin{pmatrix} k_{0,1} & k_{0,2} & \cdots & k_{0,N} \\ k_{1,1} & k_{1,2} & \cdots & k_{1,N} \\ k_{2,1} & k_{2,2} & \cdots & k_{2,N} \\ k_{3,1} & k_{3,2} & \cdots & k_{3,N} \end{pmatrix}$$

Combination layer(CoLa): Sum of all momenta

$$C = \begin{pmatrix} 1 & 1 & 0 & \cdots & 0 & C_{1,N+2} & \cdots & C_{1,M} \\ 1 & 0 & 1 & & & \vdots & C_{2,N+2} & \cdots & C_{2,M} \\ \vdots & \vdots & \vdots & \ddots & 0 & \vdots & & & \vdots \\ 1 & 0 & 0 & \cdots & 1 & C_{N,N+2} & \cdots & C_{N,M} \end{pmatrix}$$

HOW DOES THIS BIAS MASS AND P_T !?

Summing and weighting all constituent should allow network to calculate subject axes

Lorentz layer(LoLa): Compute kinematics for CoLa output.

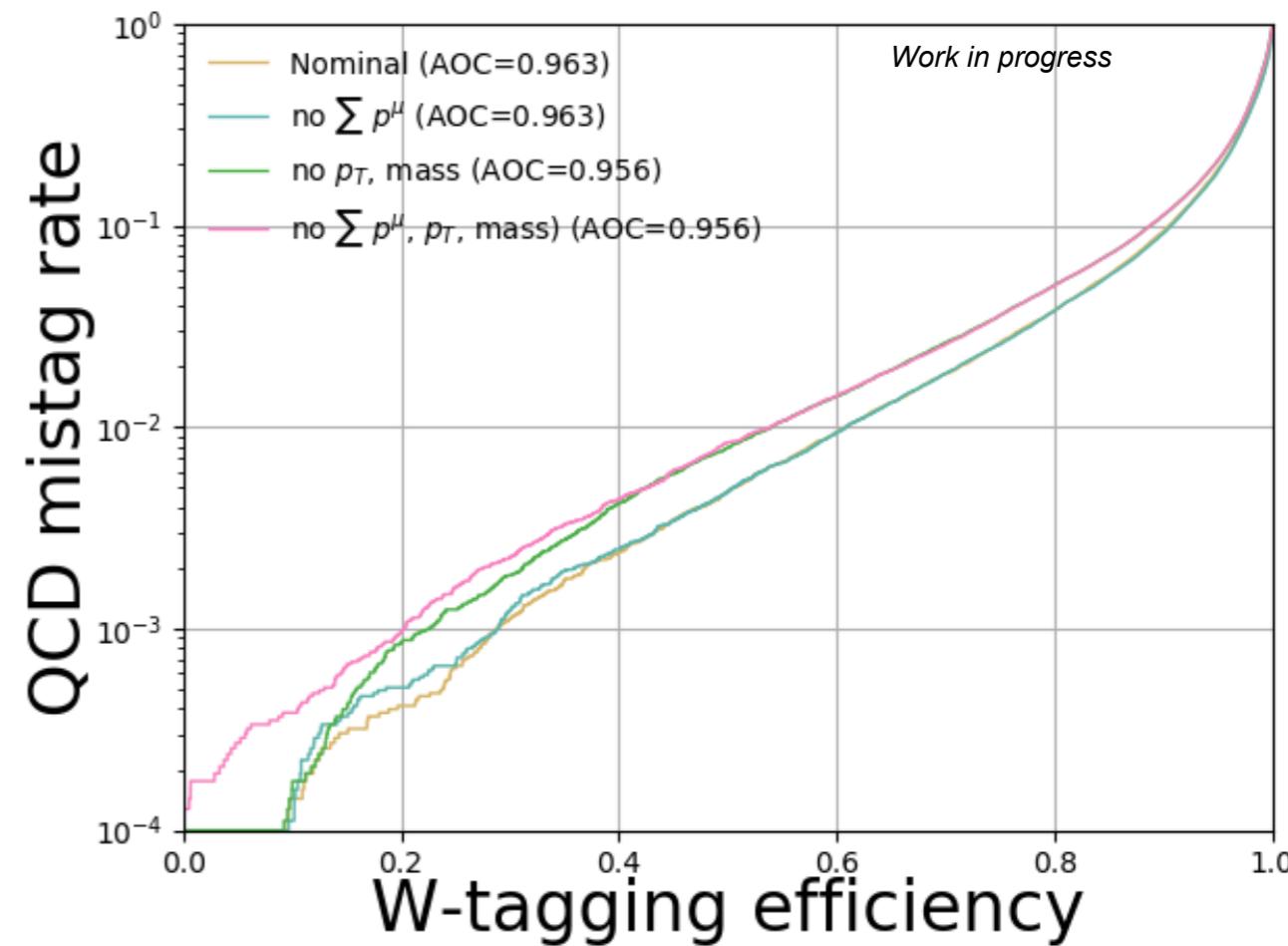
$$\tilde{k}_j \xrightarrow{\text{LoLa}} \hat{k}_j = \begin{pmatrix} m^2(\tilde{k}_j) \\ p_T(\tilde{k}_j) \\ w_{jm}^{(E)} E(\tilde{k}_m) \\ w_{jm}^{(d)} d_{jm}^2 \end{pmatrix}$$

d_{jm}^2 and m^2 use Minkowski distance

$$d_{jm}^2 = (\tilde{k}_j - \tilde{k}_m)_\mu g^{\mu\nu} (\tilde{k}_j - \tilde{k}_m)_\nu$$

What does LoLa learn?

- Compare **nominal training** to training after removing variables sensitive to mass and p_T
- Remove **CoLa column** that passes sum of all 4-momentum (“jet” 4-vector)
 - not much impact on overall performance
 - not much information taken from LoLa “n-subjettiness”
- Remove **Lola mass and p_T** variables reduce performance significantly
 - worst when removing jet 4-vector, mass and p_T



LoLas future

Study LoLa output column-wise to understand what LoLa is learning

- picking up substructure or not?

Study discriminating power for longitudinally versus transversally polarised W bosons
→ W_T vs W_L tagger?

As part of fun

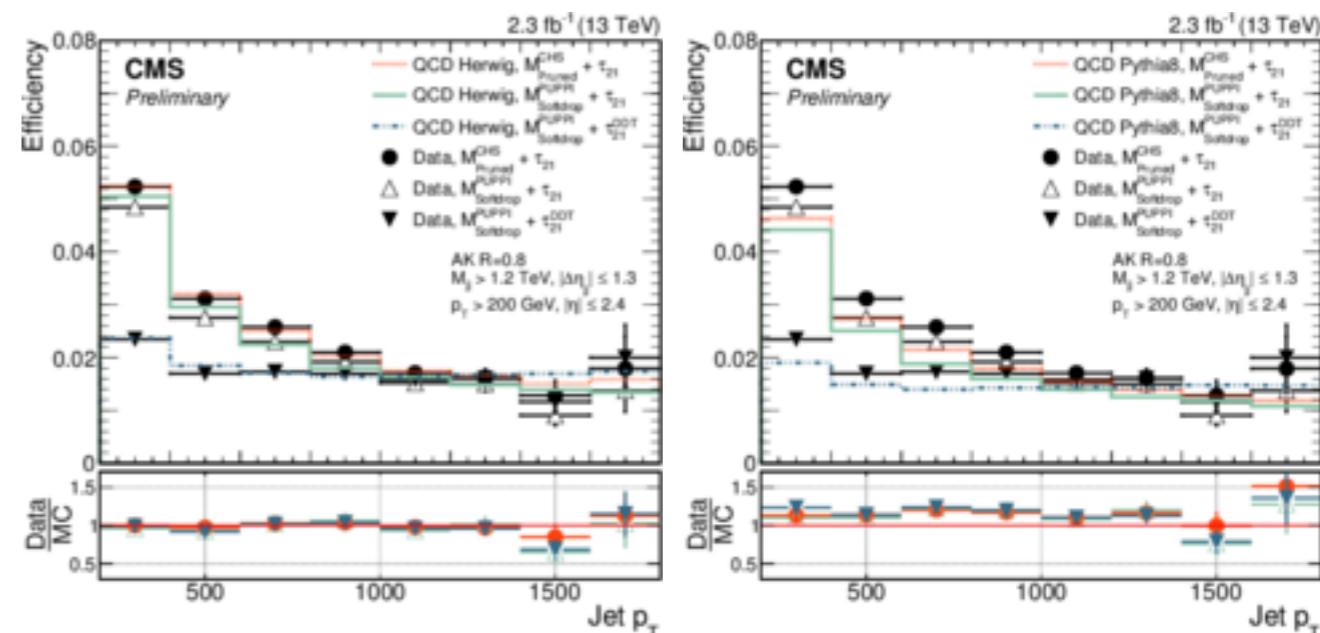
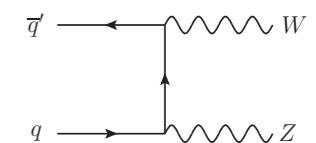
- train LoLa to do Pythia QCD vs. Herwig to understand where shower differences arise?

Energy enhanced new-physics effects in longitudinal channel

$$\frac{\mathcal{A}_{LL}^{\text{SM} + \text{BSM}}(q\bar{q} \rightarrow WZ)}{\mathcal{A}_{LL}^{\text{SM}}(q\bar{q} \rightarrow WZ)} \sim 1 + a_q^{(3)} E^2$$

... but **transverse** channels **dominate** the SM cross section

large cross section
due to t-channel singularity
(only there for transverse)



What's the mass of my object?

Pruning

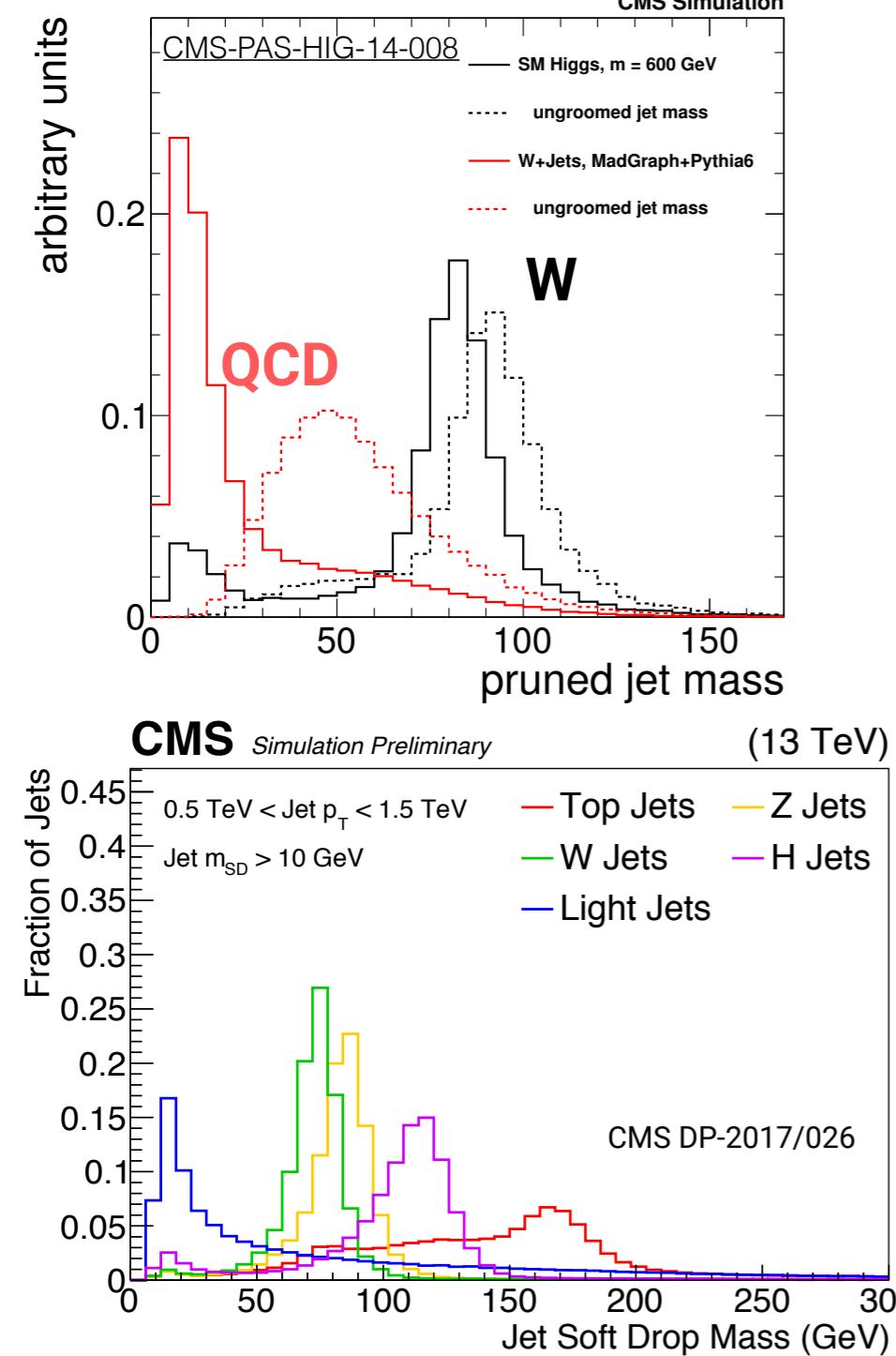
- Remove soft, wide-angle radiation
 - recluster jet with C-A, remove recombination if

$$\frac{\min(p_{T1}, p_{T2})}{p_{T1} + p_{T2}} < 0.1 \text{ and } \Delta_{1,2} > 0.5 \cdot \frac{2m}{p_T}$$

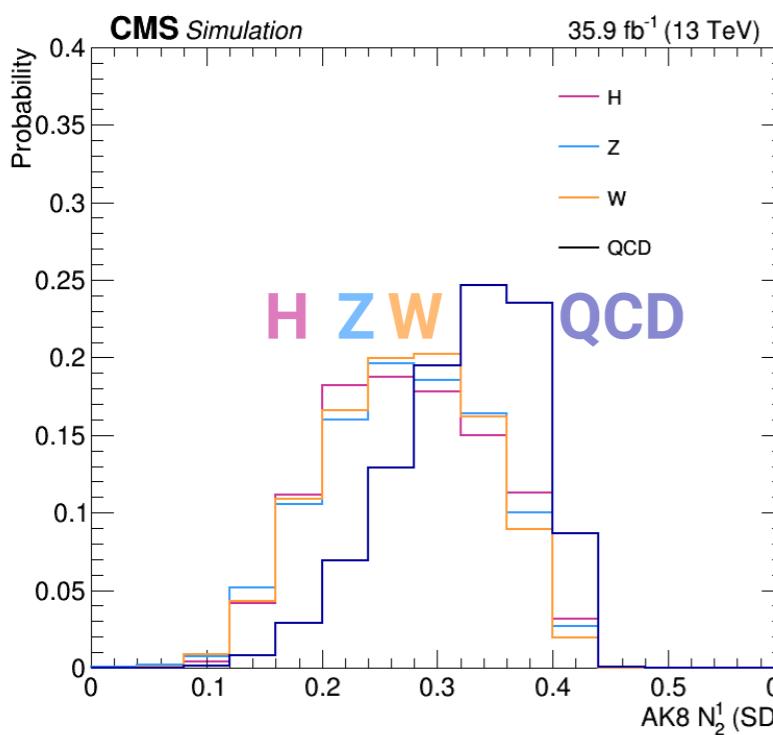
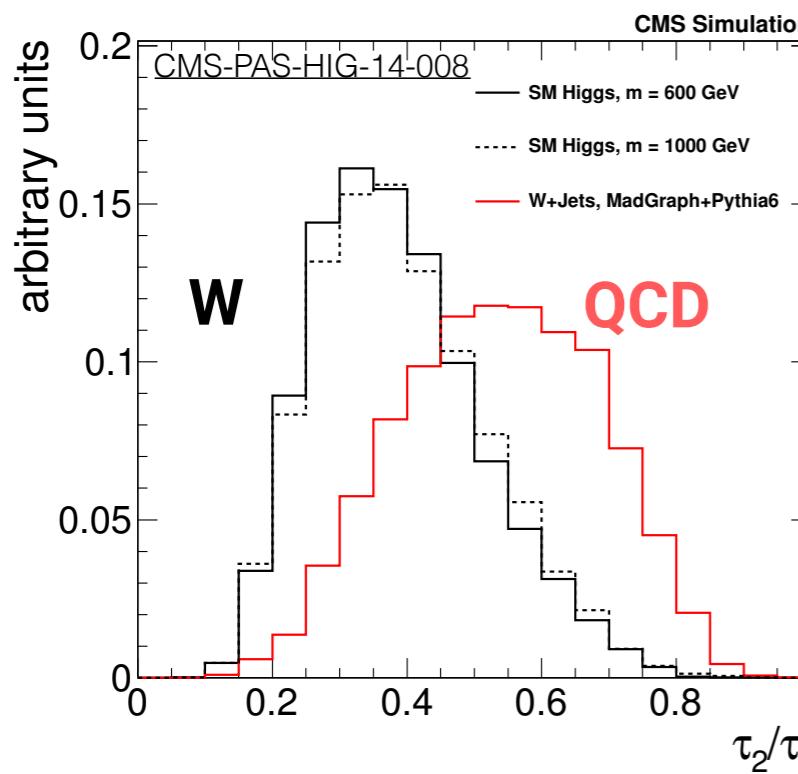
Modified Mass Drop Tagger (aka Softdrop, $\beta=0$)

- Remove all soft emission
 - decluster with C-A, remove recombination if

$$\frac{\min(p_{T1}, p_{T2})}{p_{T1} + p_{T2}} < 0.1$$



Can I peak inside the jet?



N-subjettiness τ_{21}

arxiv:1011.2268

- How compatible jet is with having N axis
 - p_T -weighted distance between constituents and N axes
 - small τ_2/τ_1 : more two- than one-prong like

Ratio of Energy Correlation Functions N_2

arxiv:1305.0007

- Sensitive to N-particle correlations within jet
 - like τ_2/τ_1 , but avoid definition of subjet axes
 - less dependent on p_T and p_T^2/m^2

$$N_2 = \frac{2e_3}{(e_2)^2} \quad e_2 = \sum_{1 \leq i < j \leq n_J} z_i z_j \theta_{ij}$$

pairwise angles between n constituents

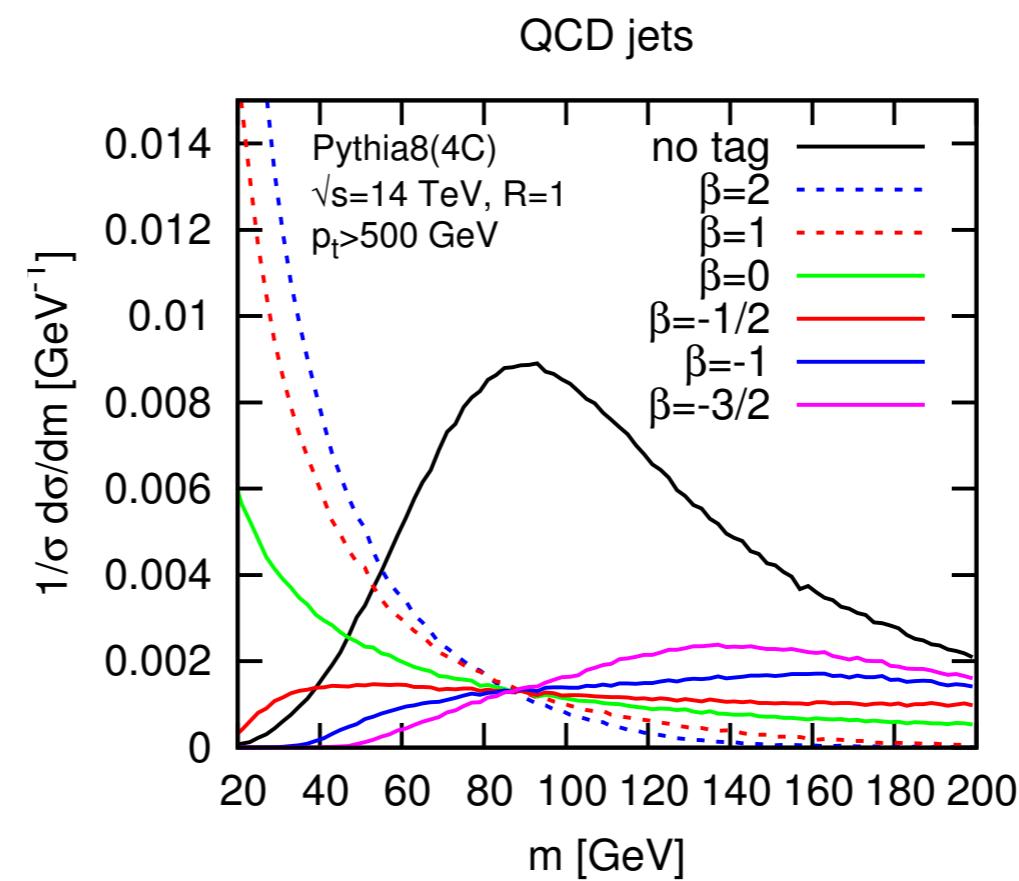
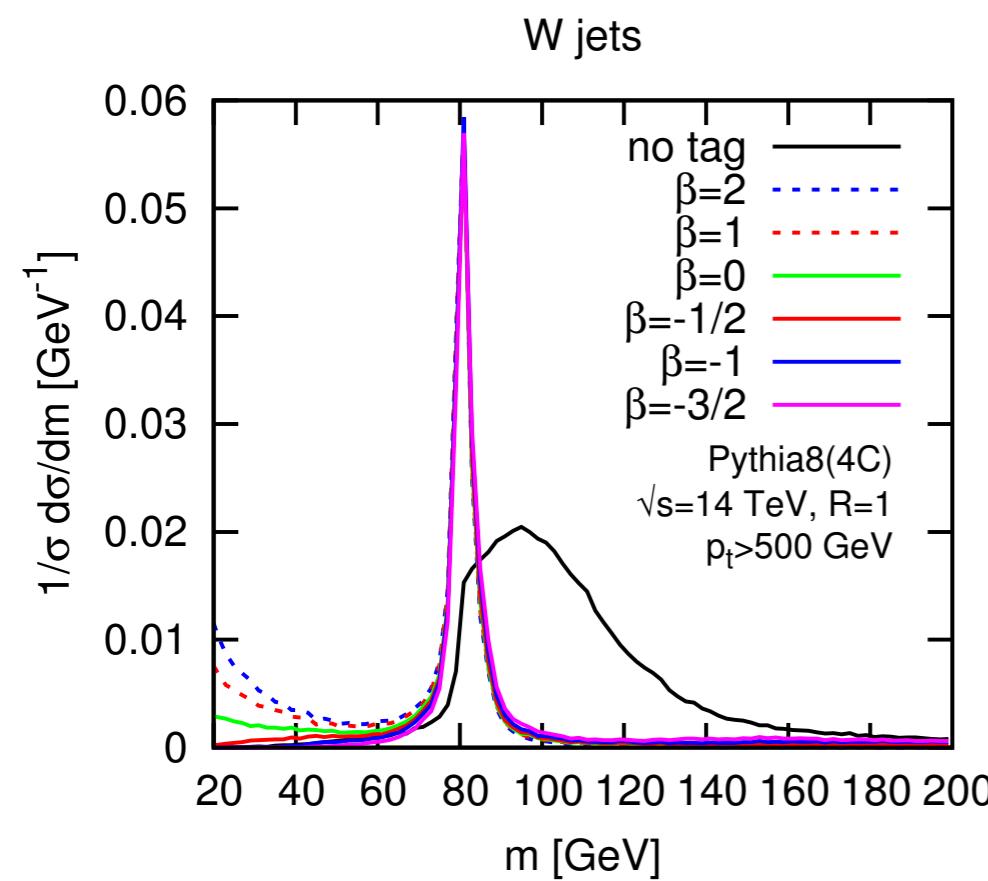
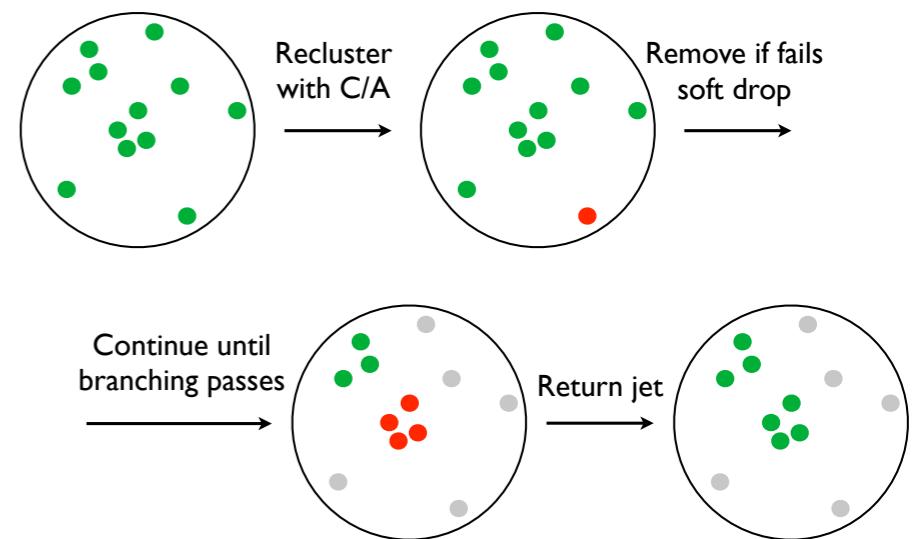
Mass: Softdrop

- Recluster jet with C-A algorithm. Then decluster and check if subjets pass

$$\frac{\min(p_{T1}, p_{T2})}{p_{T1} + p_{T2}} > z_{\text{cut}} \left(\frac{\Delta R_{12}}{R_0} \right)^\beta$$

Soft threshold
Angular exponent

- in CMS $\beta=0$, $z_{\text{cut}} = 0.1$ (modified Mass Drop)



Tuned parameters:
 Z_{cut} and β

$\beta = \infty$
no grooming

$$\beta > 0$$

soft, wide angle removed
some soft-collinear removed

$\beta = 0$
ft emissions removed
fied Mass Drop limit

$\beta < 0$ CMS default

all soft and collinear
emissions removed

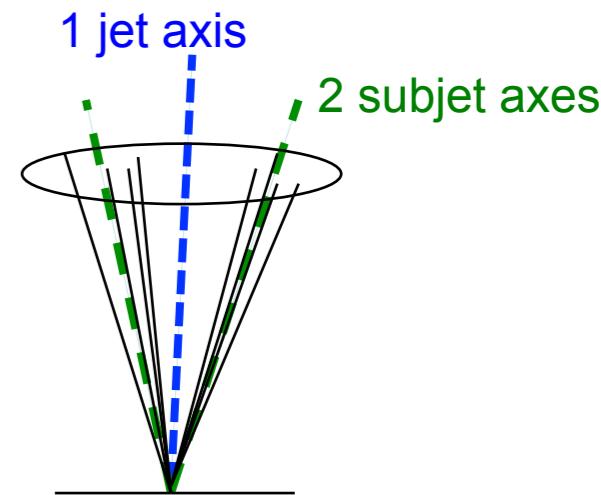
Substructure: N-subjettiness

- p_T -weighted sum over all constituents of the distance w.r.t the closest of N axes in a jet

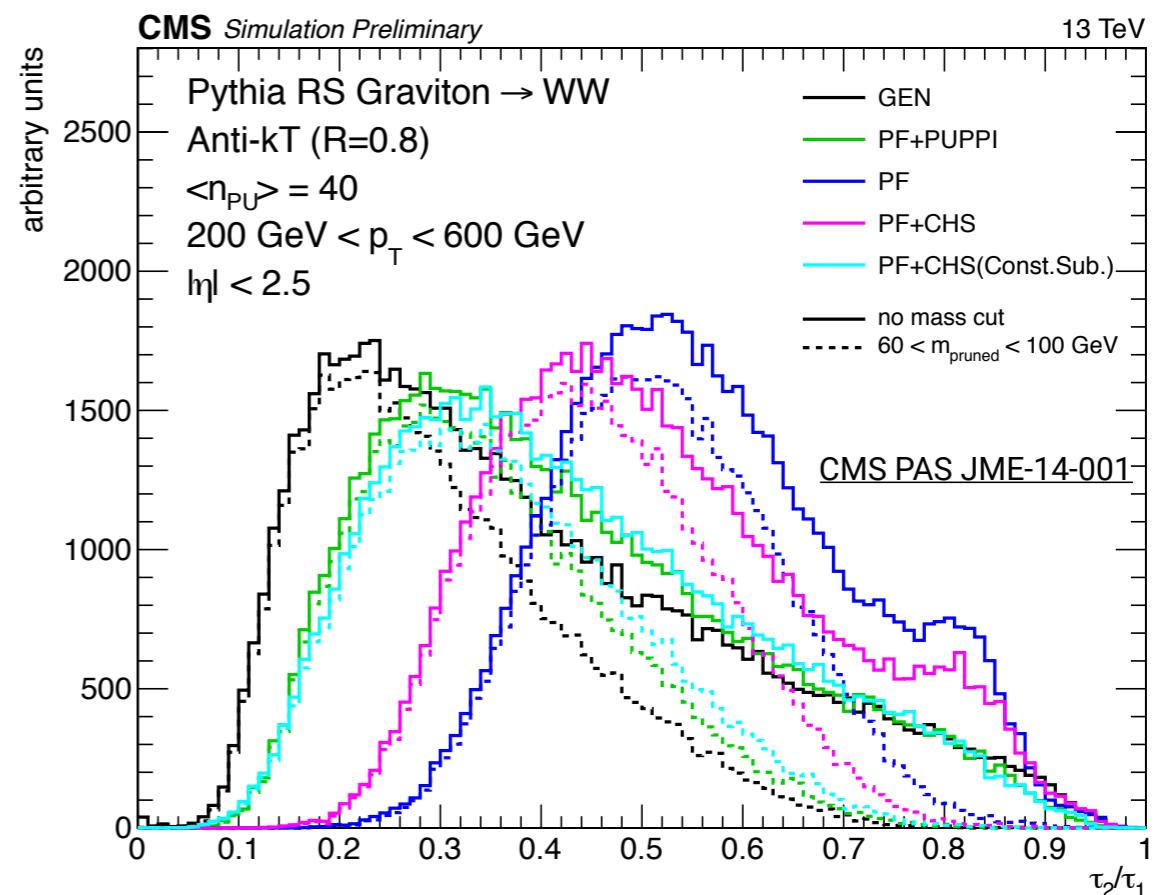
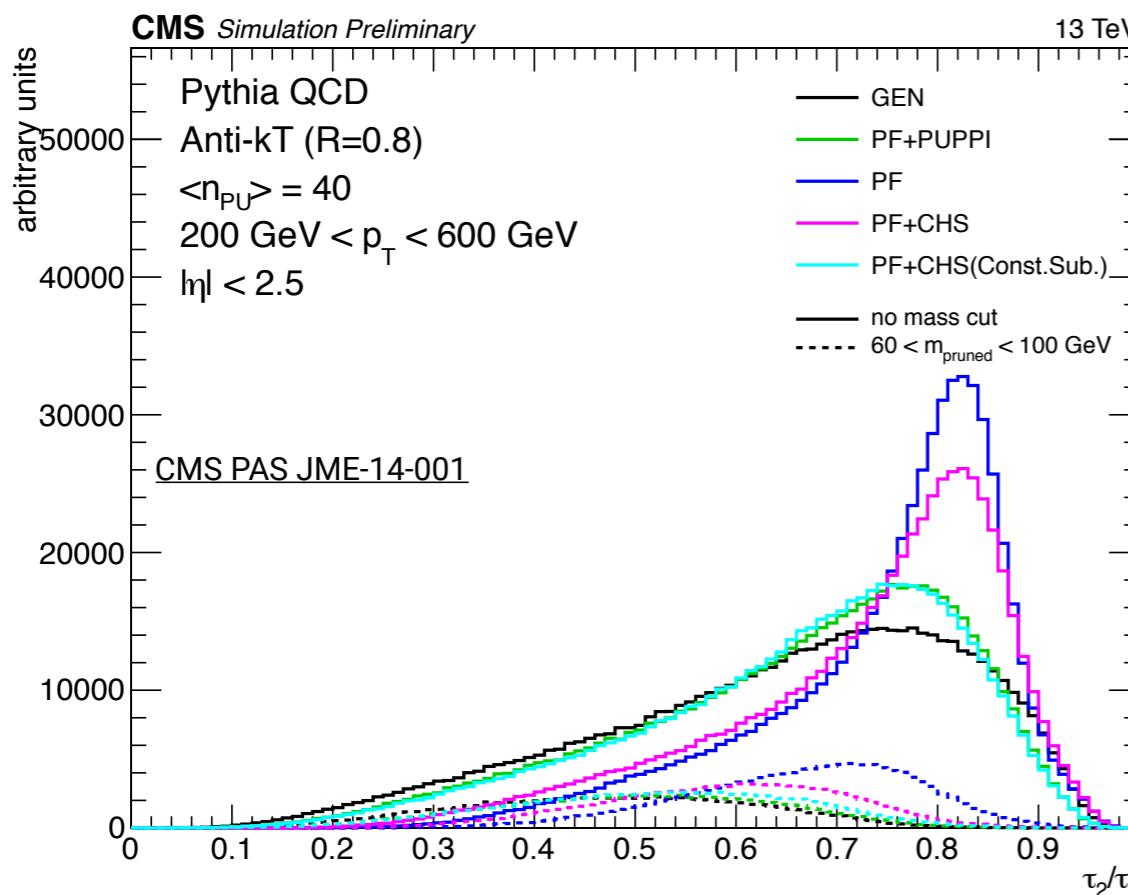
$$\tau_N = \frac{1}{d_0} \sum_k p_{T,k} \min((\Delta R_{1,k}), (\Delta R_{2,k}) \dots (\Delta R_{N,k}))$$

Distance between momentum of constituent k w.r.t momentum of rest-frame subjet N

Each constituent assigned to nearest subjet!



- axis obtained by undoing last ($N-1$) steps of clustering algorithm
- small τ_N indicates compatibility with N axes hypothesis



Energy correlation functions (EFCs)

- Signal jets satisfy the inequality ${}_2e_3 \ll (e_2)^2$, explaining the definition of the N2 observable
- Less discriminating power after grooming applied

$$N_2^\beta = \frac{2e_3^\beta}{(1e_2^\beta)^2}$$

particles
angles

$${}_1e_2^1 = \sum_{1 \leq i < j \leq n_J} z_i z_j \Delta R_{ij}$$

$${}_2e_3^1 = \sum_{1 \leq i < j < k \leq n_J} z_i z_j z_k \min\{\Delta R_{ij}\Delta R_{ik}, \Delta R_{ij}\Delta R_{jk}, \Delta R_{ik}\Delta R_{jk}\}$$

