

Beyond Kinematics: Generating Jets with Particle-ID and Trajectory Displacement Information

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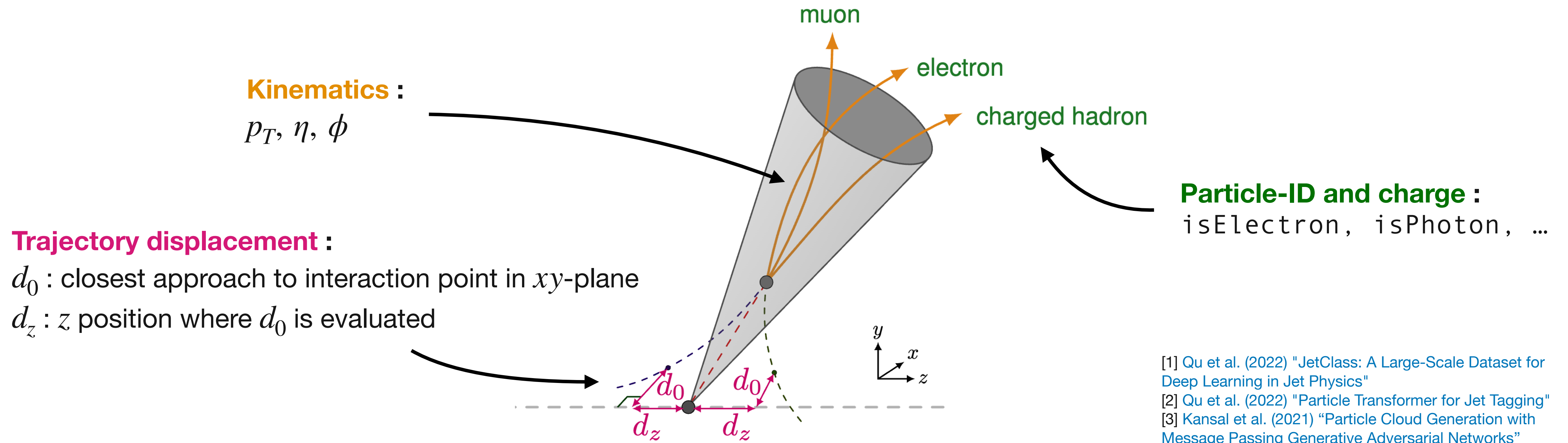
ML4Jets 2023

November 7, 2023

Motivation and dataset overview

- JetClass: public dataset [1] introduced in ParT [2] paper
- **Motivation:** can we generate all jet types from the JetClass dataset with these additional features?

	JetNet [3]	JetClass [1]
Jet types	5 types	10 types (several decay channels for top and H jets)
Dataset size	180 thousand jets per class	12.5 million jets per class (70x more than JetNet)
Features	Kinematics	Kinematics, Particle-ID and charge, trajectory displacement



Model overview

- Training on the **flow matching objective** [1]

→ model represents the vector field $v(x, t) = \frac{dx_t}{dt}$

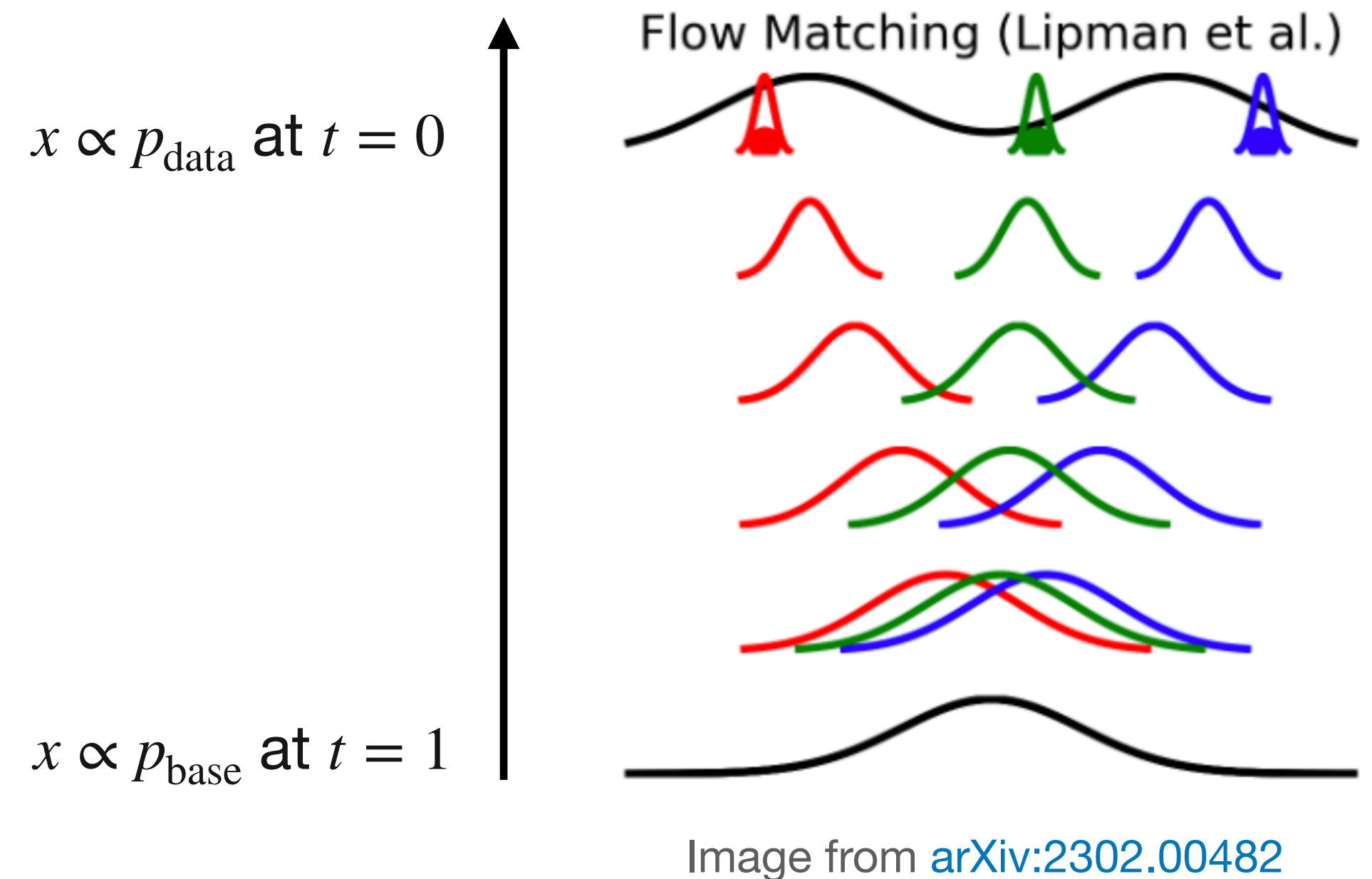
- **Generation**: sample from $p_{\text{base}}(x)$ and **integrate ODE**

- Model architecture based on EPiC layers [2] and similar to EPiC-FM model [3, 4]

- Model is **conditioned on jet type**, jet η and jet p_T

- **Model generates 13 features**:

- 3 kinematic features: p_T^{rel} , η^{rel} , ϕ^{rel}
- 4 trajectory displacement features: d_0 , d_z , σ_{d_0} , σ_{d_z}
- 6 discrete features:
isElectron, **isMuon**, **isChargedHadron**,
isNeutralHadron, **isPhoton**, **charge**



[1] Lipman et al. (2023) "Flow Matching for Generative Modeling"

[2] Buhmann et al. (2023) "EPiC-GAN: Equivariant point cloud generation for particle jets"

[3] Cedric's talk at ML4Jets

[4] Buhmann et al. (2023) "EPiC-ly Fast Particle Cloud Generation with Flow-Matching and Diffusion"

Jet mass and jet substructure

Mass distributions:

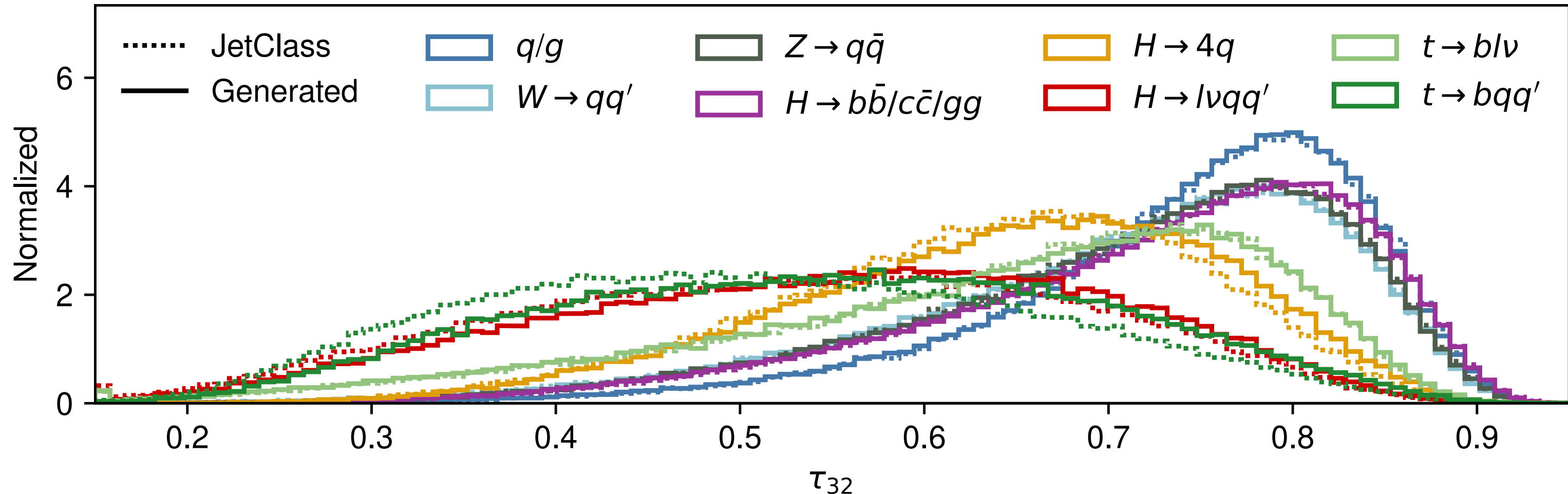
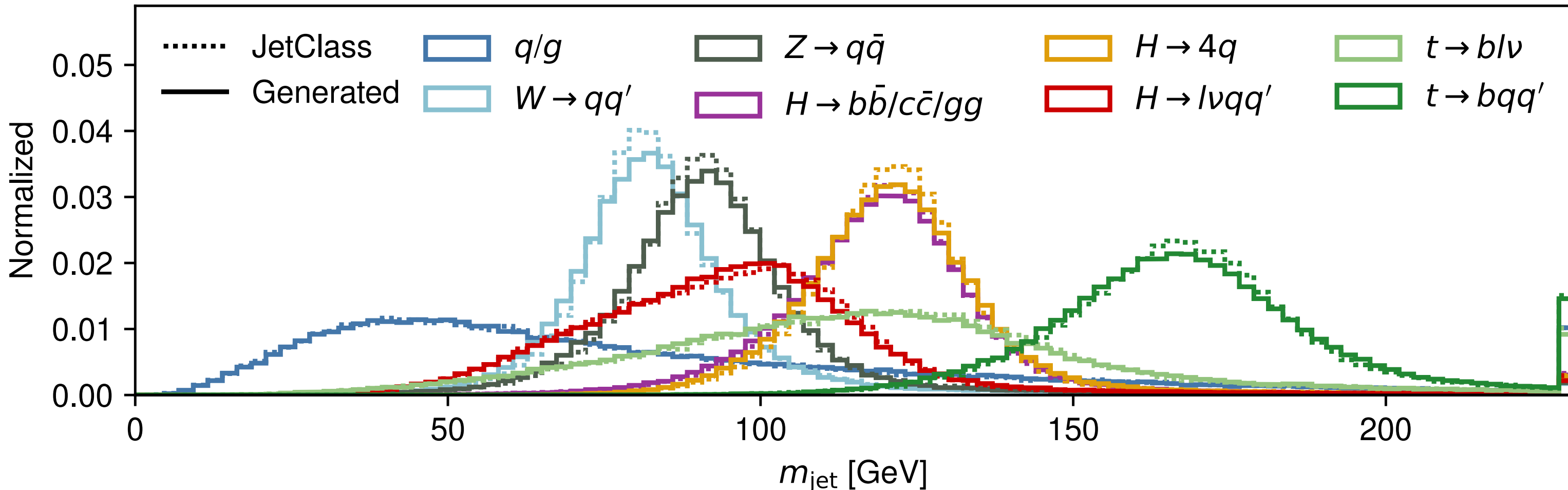
- Very good agreement!

We know:

subjettiness ratio τ_{32} hard to model

- Good agreement for most jet types
- Largest disagreement for $t \rightarrow bqq'$ and $H \rightarrow \ell\nu qq'$ jets

→ model struggles a bit with 3-prong jets



	W_1^m	$W_1^{\tau_{21}} (\cdot 10^{-3})$	$W_1^{\tau_{32}} (\cdot 10^{-3})$
Truth (q/g)	0.5 ± 0.1	1.6 ± 0.4	0.9 ± 0.2
Gen. (q/g)	0.5 ± 0.2	6 ± 1	1.3 ± 0.4
Truth ($H \rightarrow b\bar{b}$)	0.28 ± 0.09	1.6 ± 0.5	1.0 ± 0.4
Gen. ($H \rightarrow b\bar{b}$)	0.54 ± 0.09	6 ± 1	4.1 ± 0.9
Truth ($H \rightarrow \ell\nu qq'$)	0.4 ± 0.1	1.5 ± 0.7	1.5 ± 0.4
Gen. ($H \rightarrow \ell\nu qq'$)	0.67 ± 0.09	5.2 ± 0.7	19 ± 1
Truth ($Z \rightarrow q\bar{q}$)	0.32 ± 0.07	1.3 ± 0.4	1.0 ± 0.3
Gen. ($Z \rightarrow q\bar{q}$)	0.64 ± 0.05	9.1 ± 0.8	1.3 ± 0.2
Truth ($t \rightarrow bqq'$)	0.29 ± 0.08	1.7 ± 0.4	1.7 ± 0.5
Gen. ($t \rightarrow bqq'$)	0.9 ± 0.1	7.9 ± 0.5	35.4 ± 0.8

Jet mass and jet substructure

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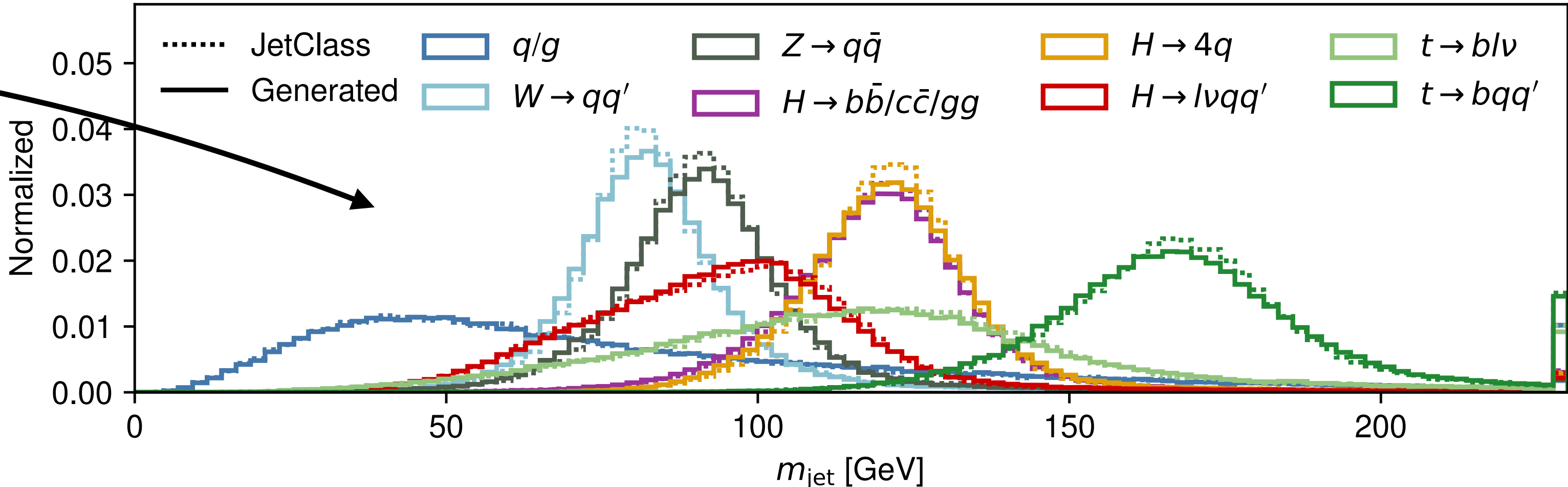
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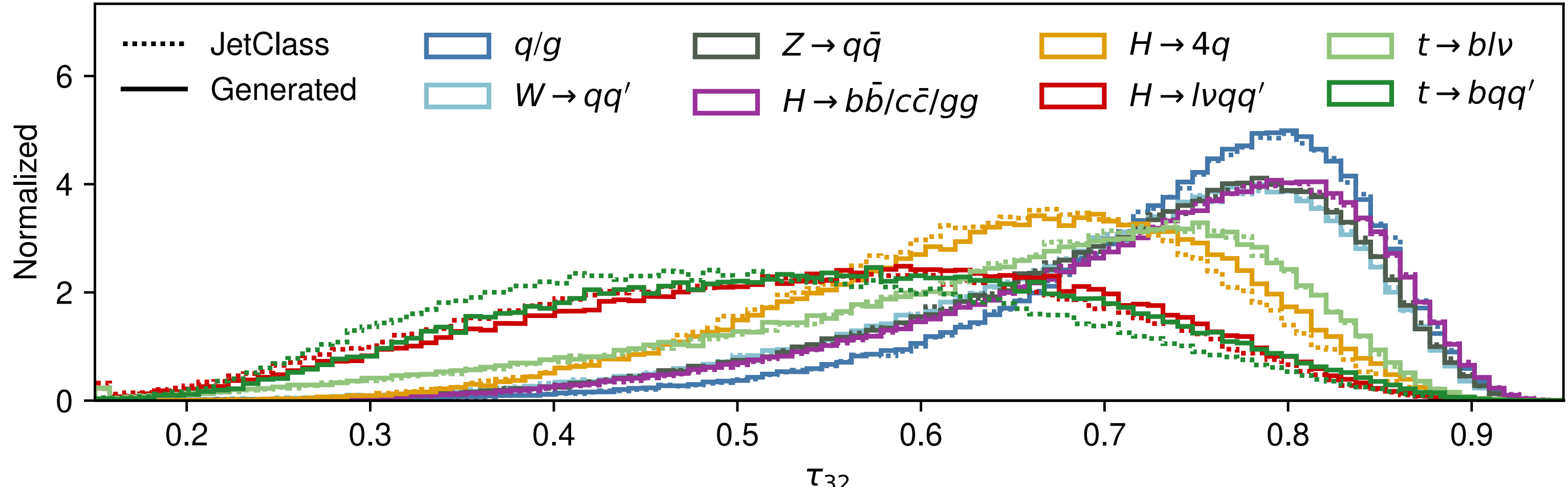
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Jet mass and jet substructure

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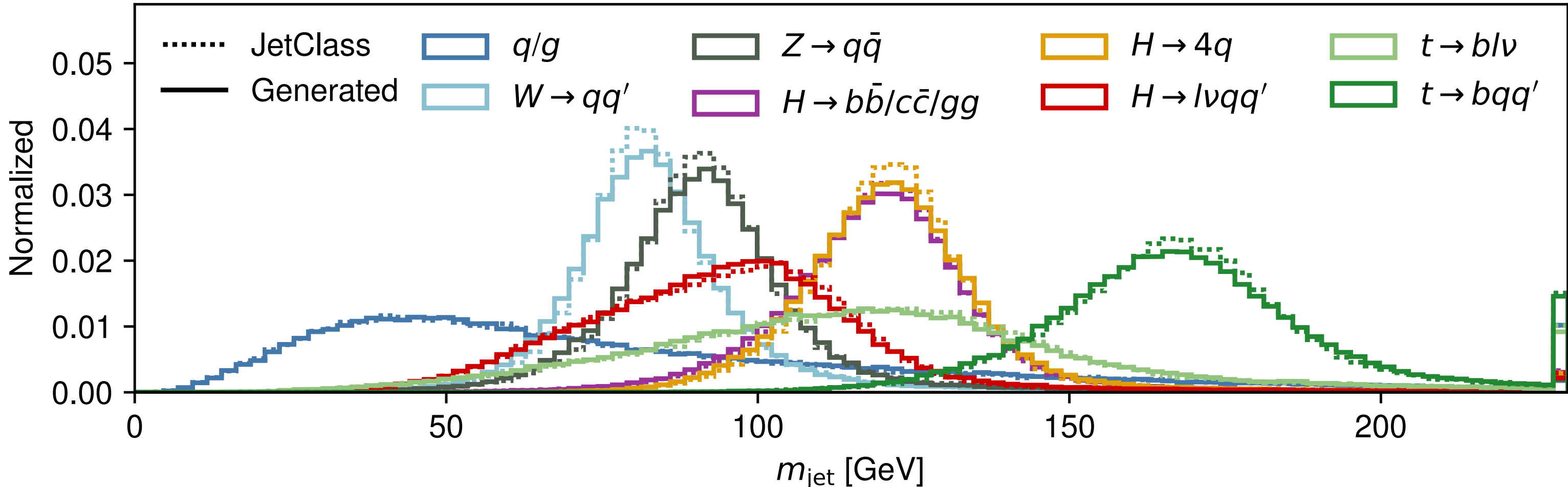
- Very good agreement!

We know:

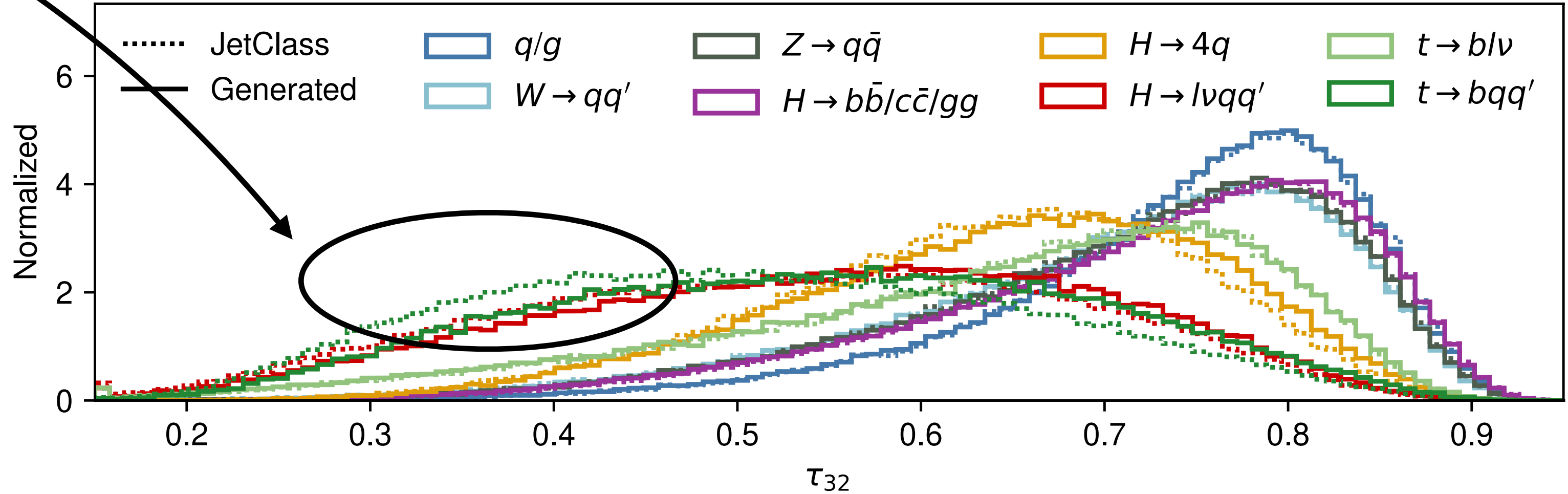
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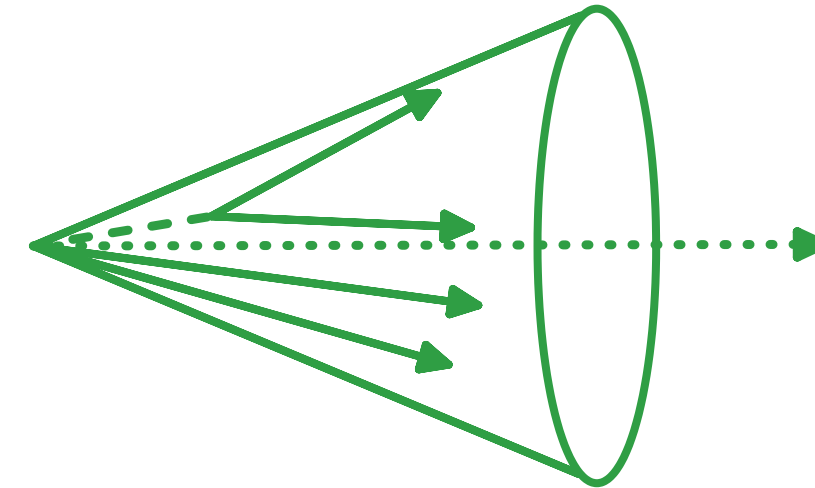


Kinematic particle features

- Looking at two very different types of jets here

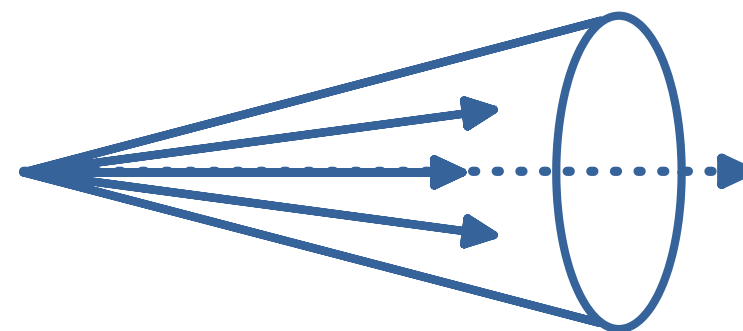
- $t \rightarrow bqq'$ jets:

- Wider: larger η^{rel}
 - More constituents: smaller $p_{\text{T}}^{\text{rel}}$



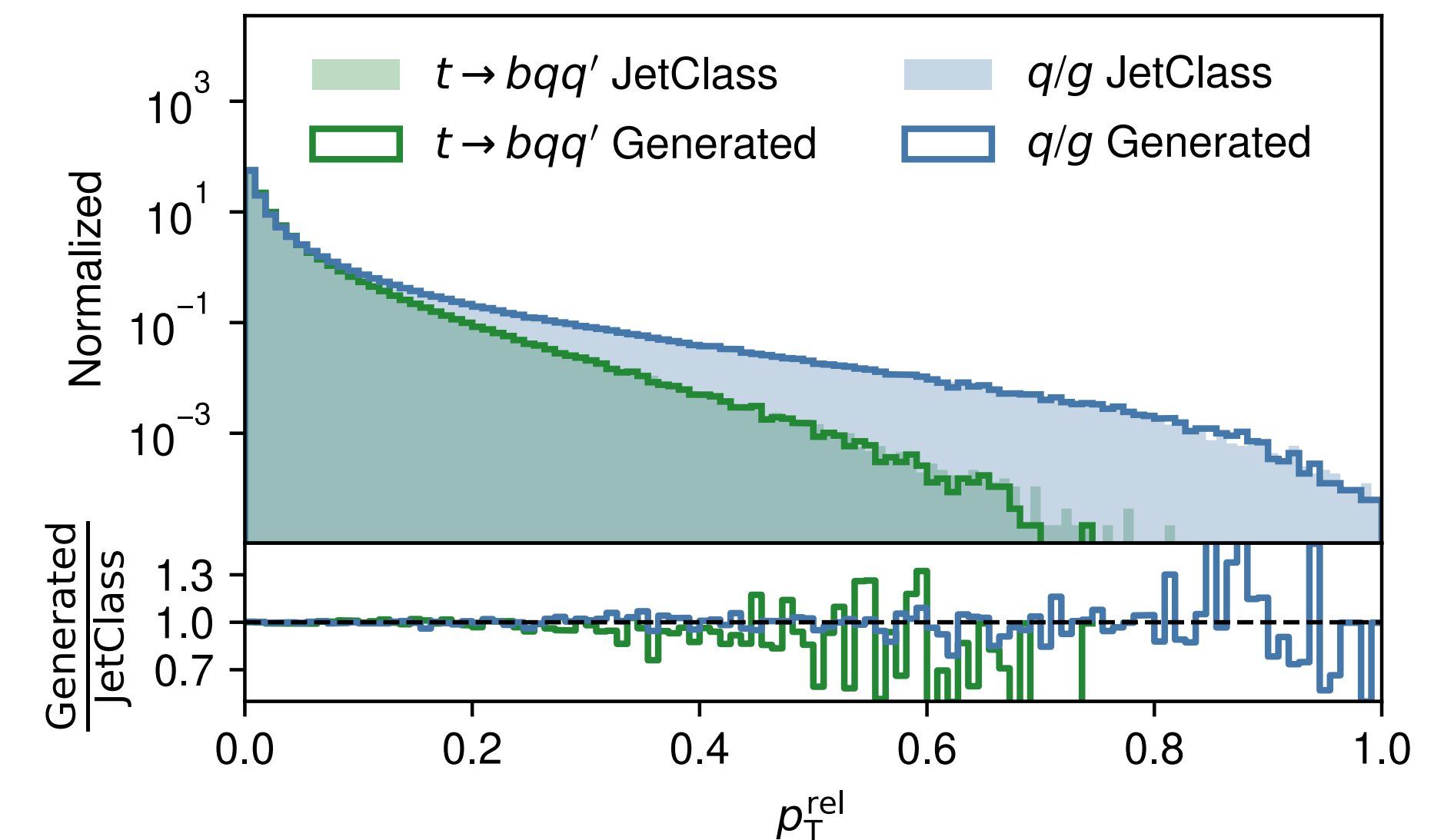
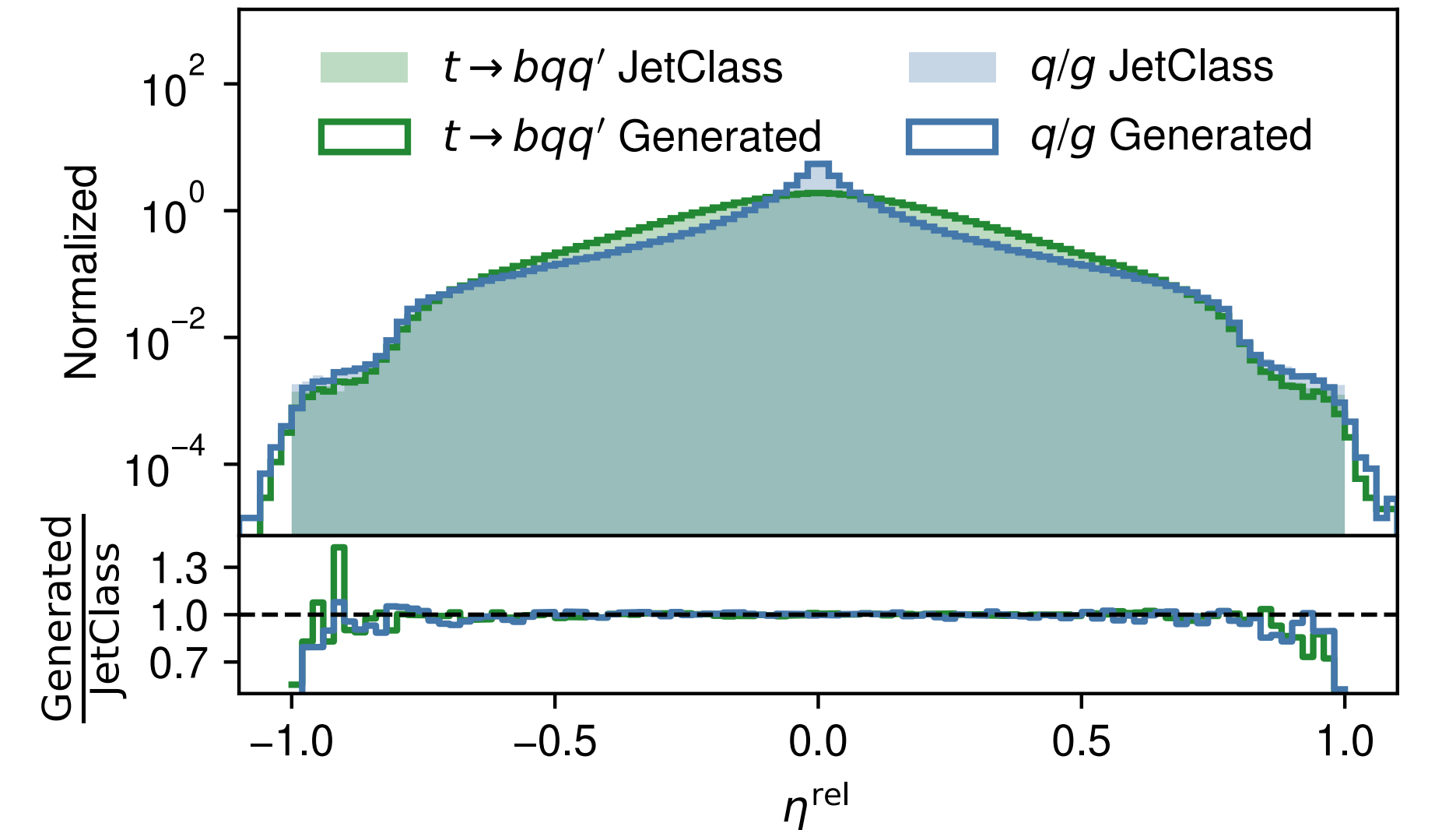
- q/g jets:

- Narrow: smaller η^{rel}
 - Fewer constituents: larger $p_{\text{T}}^{\text{rel}}$



- Very good agreement in W1-distances:

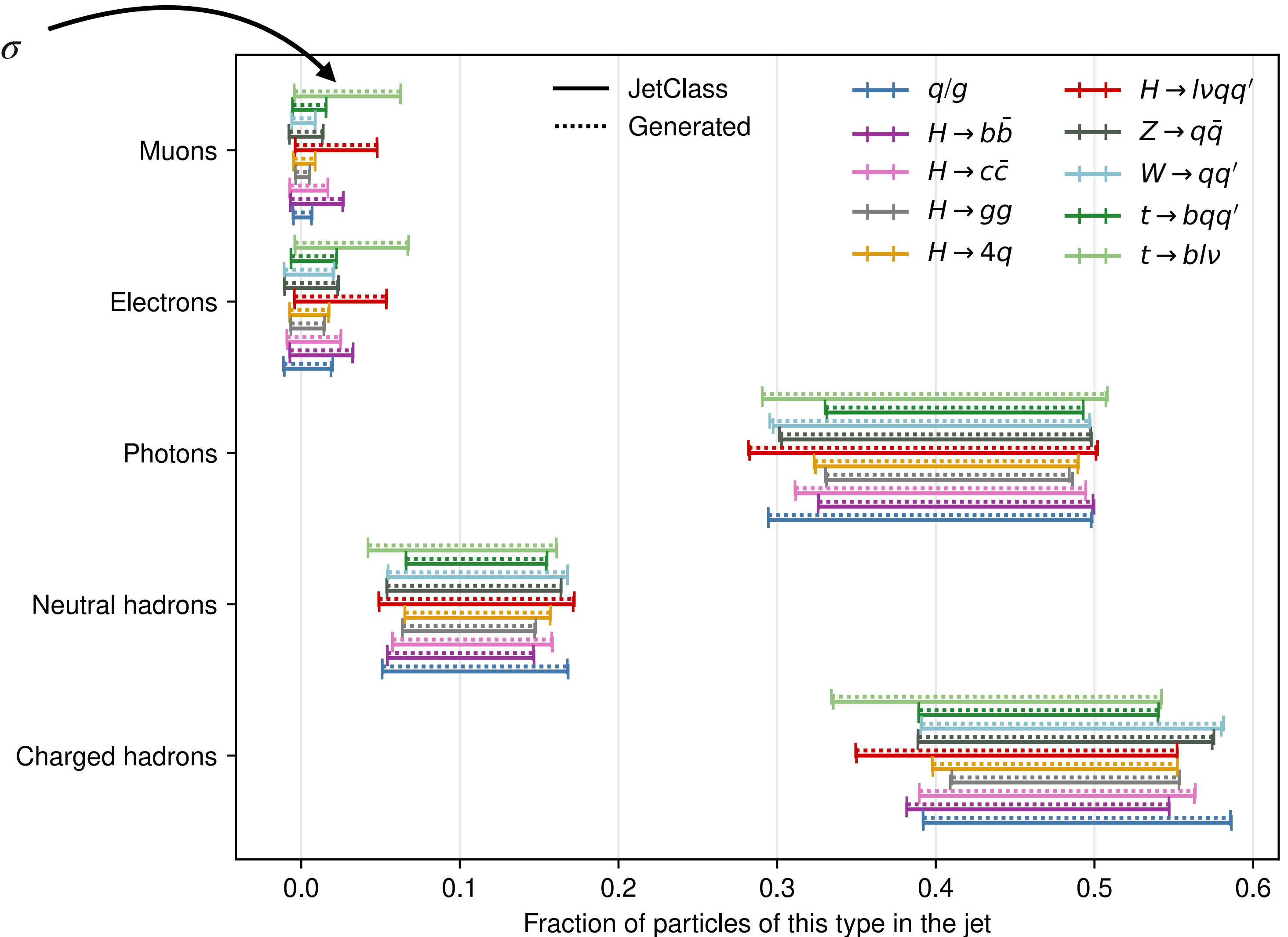
	$W_1^{p_{\text{T}}^{\text{rel}}} (.10^{-3})$	$W_1^{\eta^{\text{rel}}} (.10^{-3})$	$W_1^{\phi^{\text{rel}}} (.10^{-3})$
Truth (q/g)	0.12 ± 0.03	0.7 ± 0.2	0.8 ± 0.3
Gen. (q/g)	0.11 ± 0.02	0.8 ± 0.2	0.7 ± 0.2
Truth ($t \rightarrow bqq'$)	0.05 ± 0.01	0.7 ± 0.2	0.8 ± 0.1
Gen. ($t \rightarrow bqq'$)	0.10 ± 0.02	0.9 ± 0.3	1.1 ± 0.3



Particle-ID features

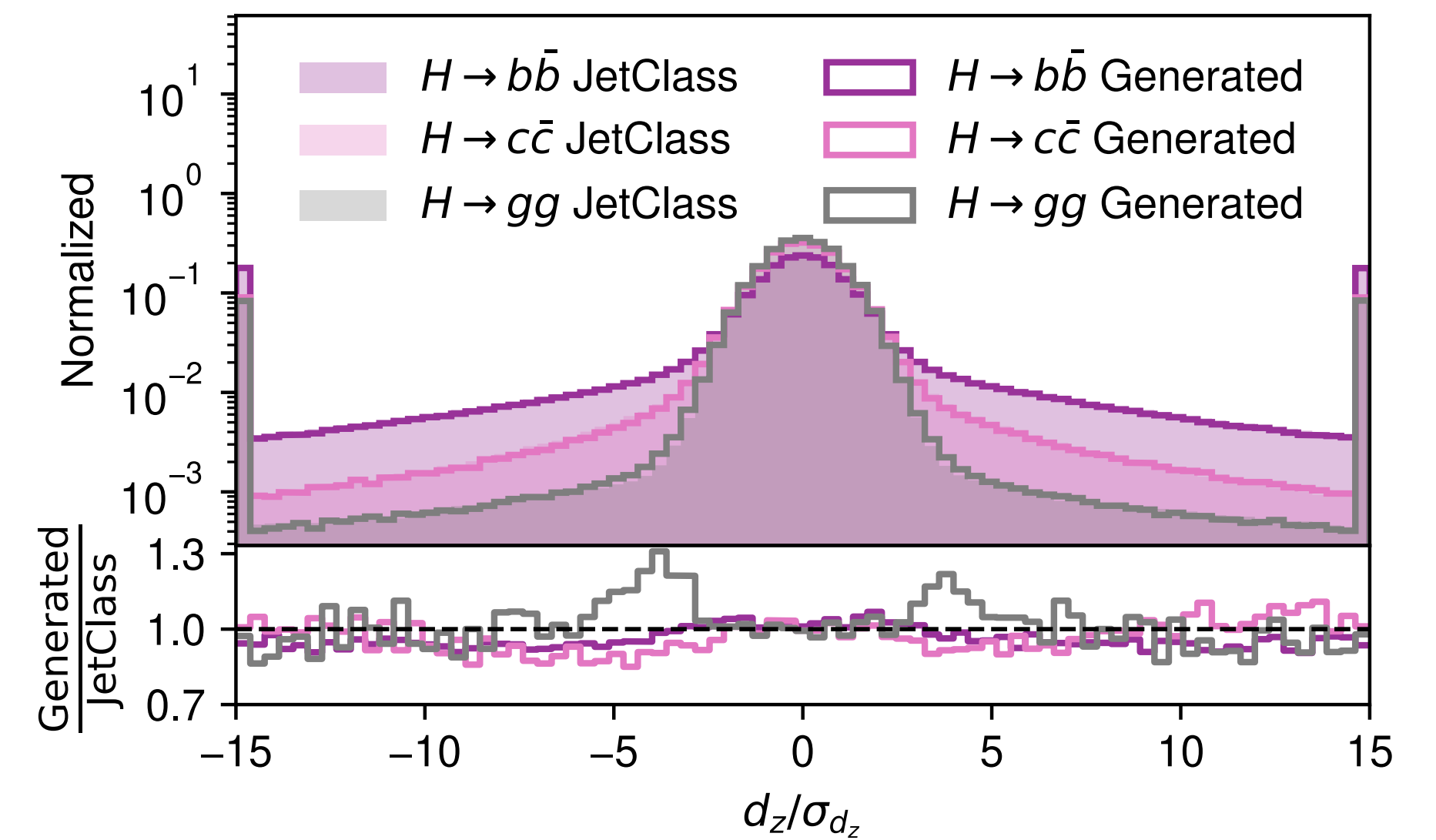
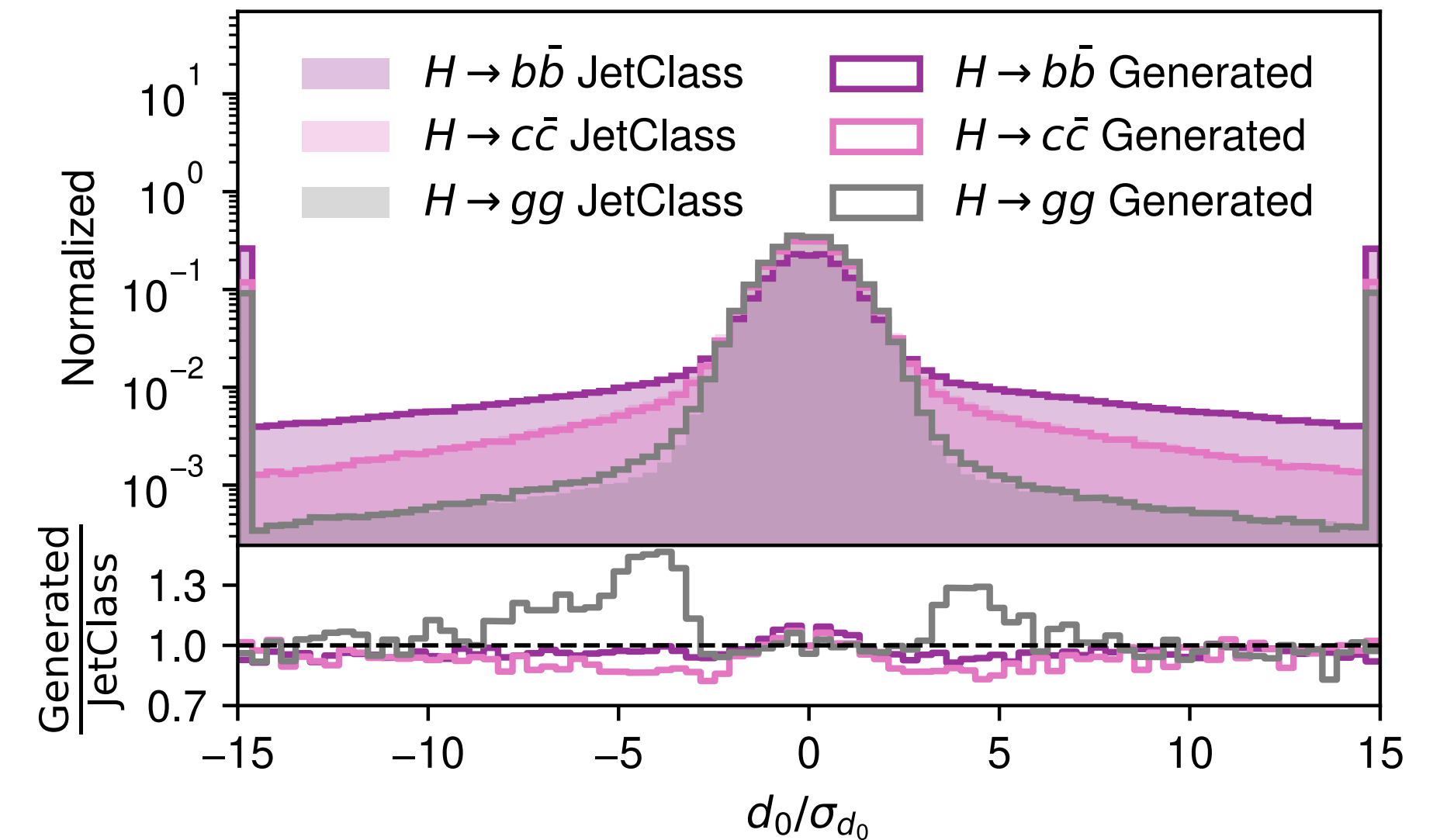
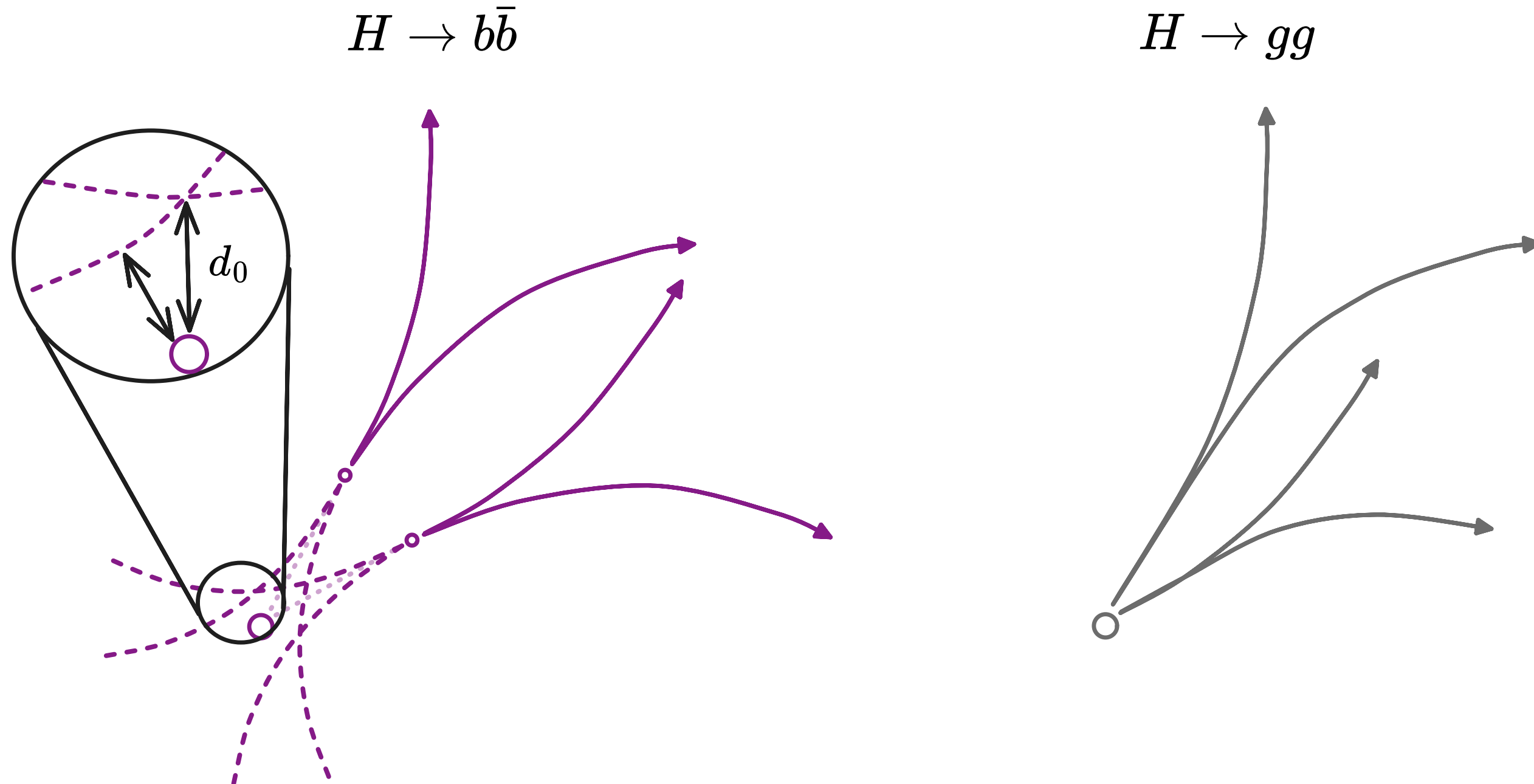
- **Post-processing** for discrete features:
 - Particle-ID: argmax
 - Charge: rounded
- Particle-ID is **very well modeled**

Mean values $\pm 1\sigma$



Trajectory displacement modeling

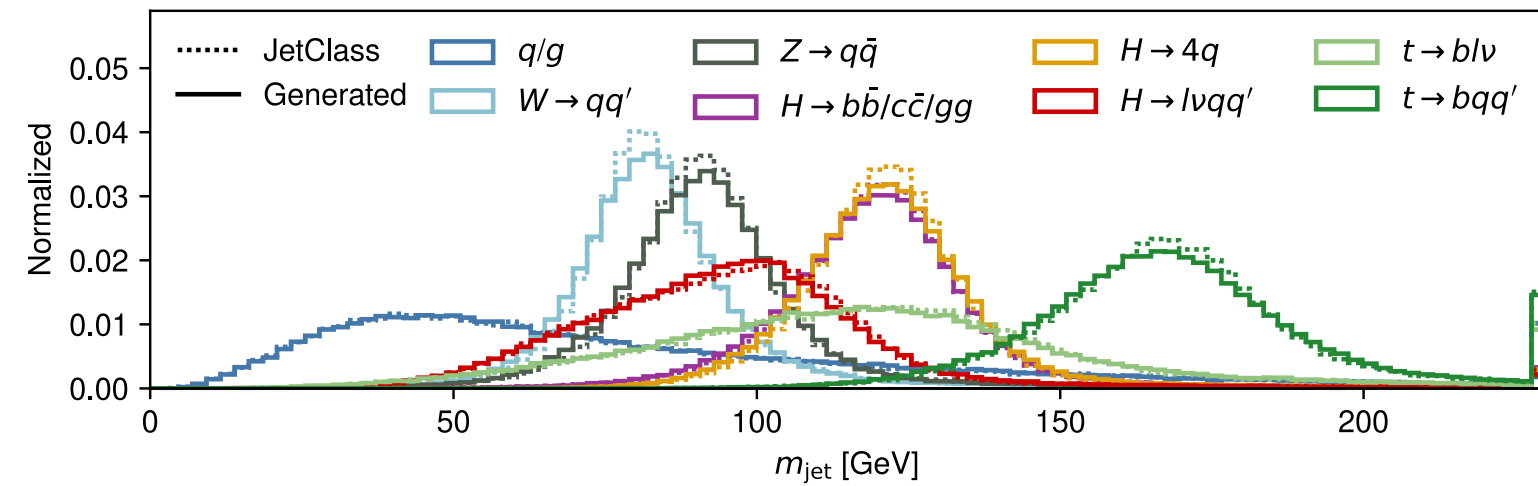
- Impact parameter (IP) d_0 and d_z :
closest approach to the interaction point
- IP of neutral particles is set to 0
- Depending on jet type, we expect wide / narrow IP distribution
 - $H \rightarrow b\bar{b}$ and $H \rightarrow c\bar{c}$: hadrons with long lifetime \rightarrow large IP
 - $H \rightarrow gg$: tracks start very close to the interaction point \rightarrow small IP



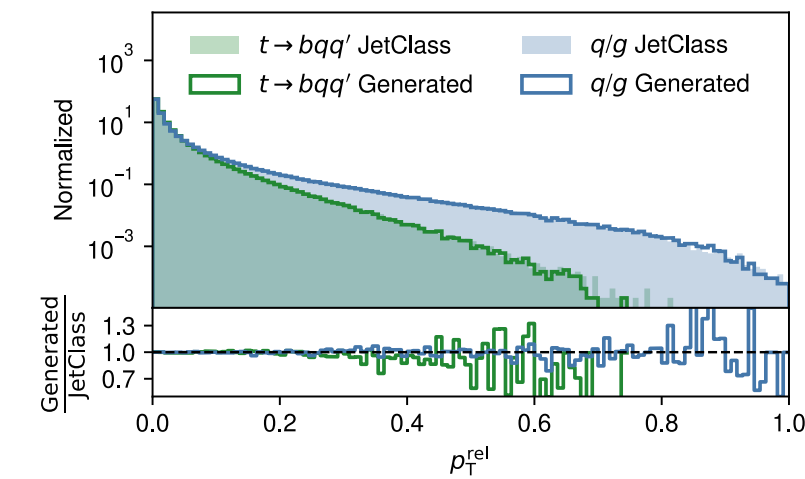
Performance overview

Overall, we see very good performance!

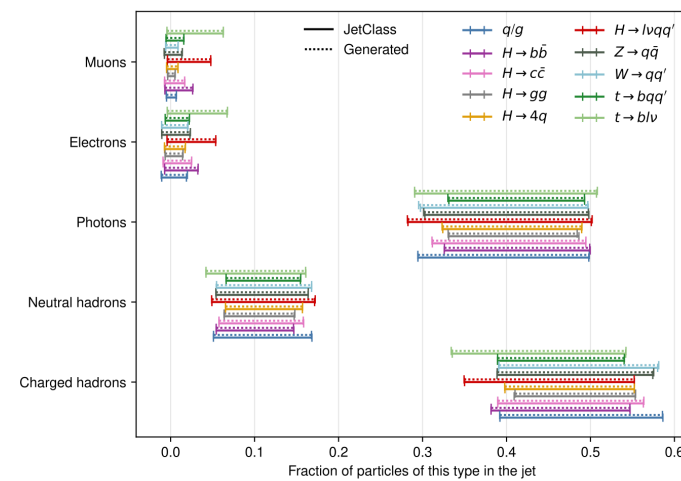
All 10 jet types in one model ✓



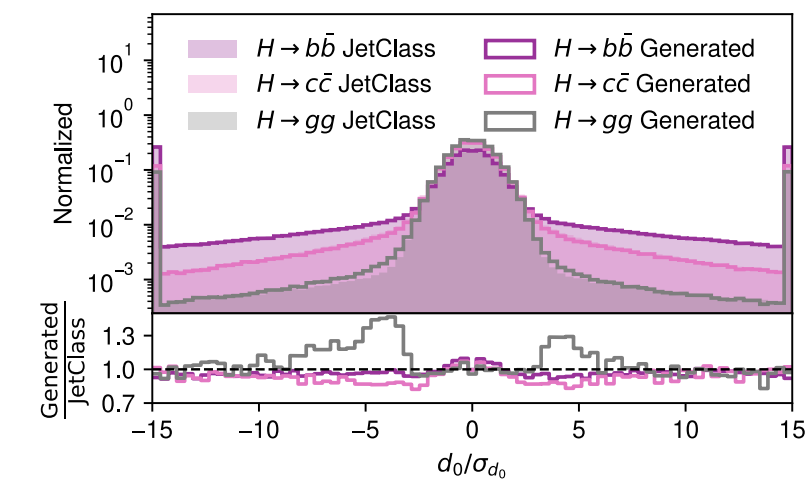
Kinematic features of jet constituents ✓



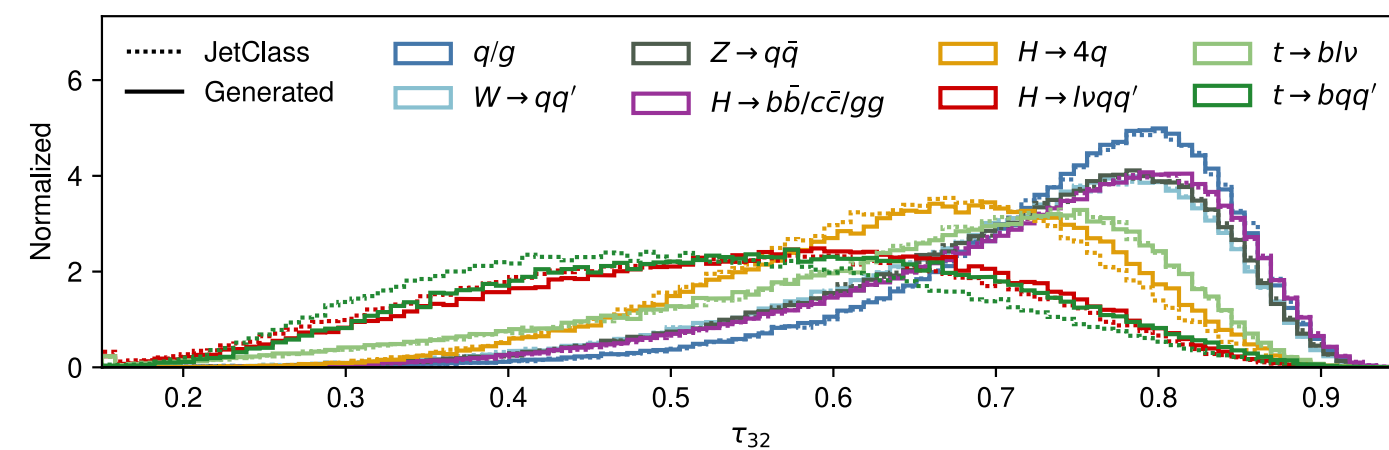
Particle-ID features accurately modeled ✓



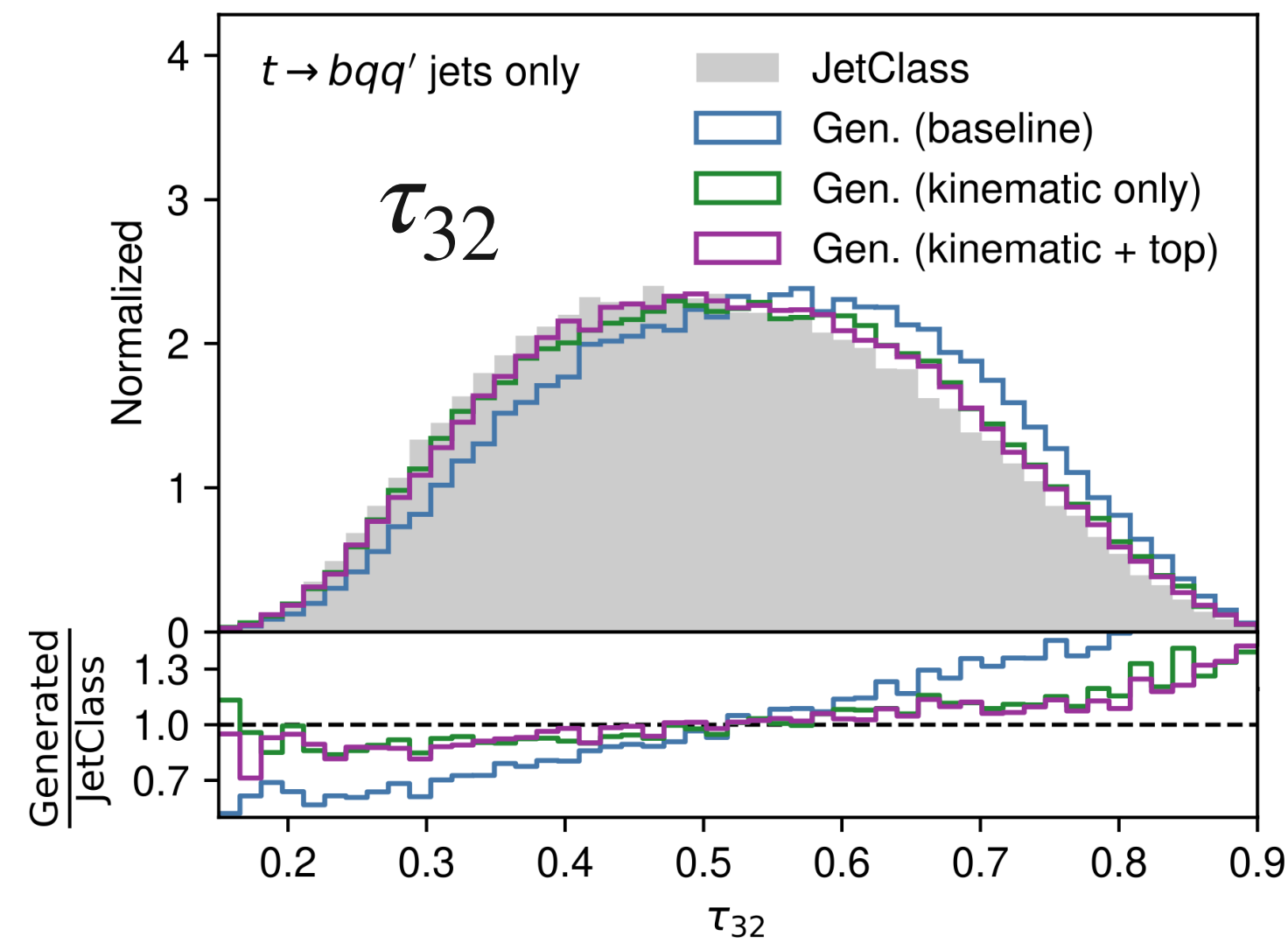
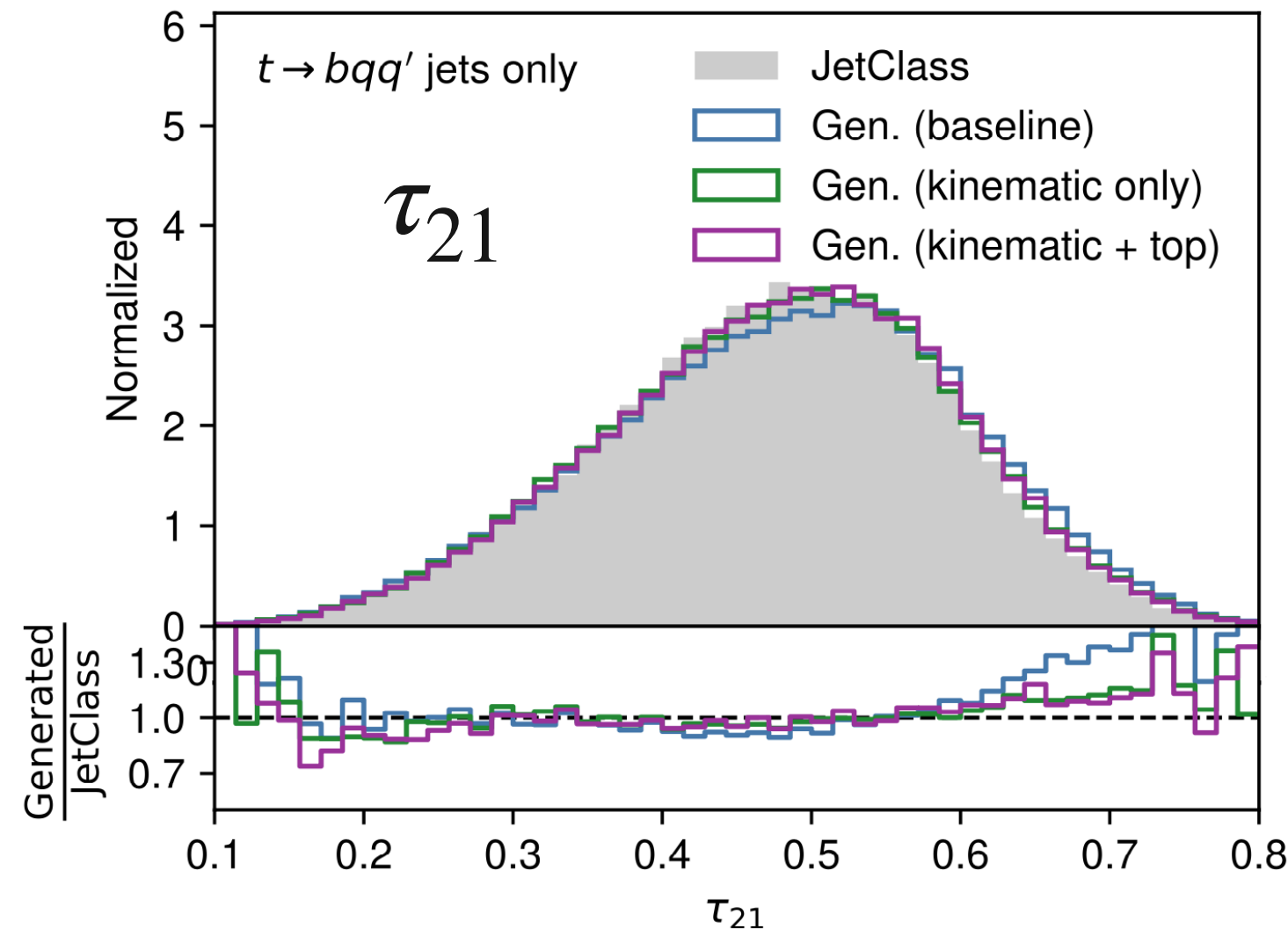
Trajectory displacement well modeled ✓



Like seen in other models, jet substructure is hard to model perfectly → further studies for $t \rightarrow bqq'$ jets



Improved models for $t \rightarrow bqq'$ jets

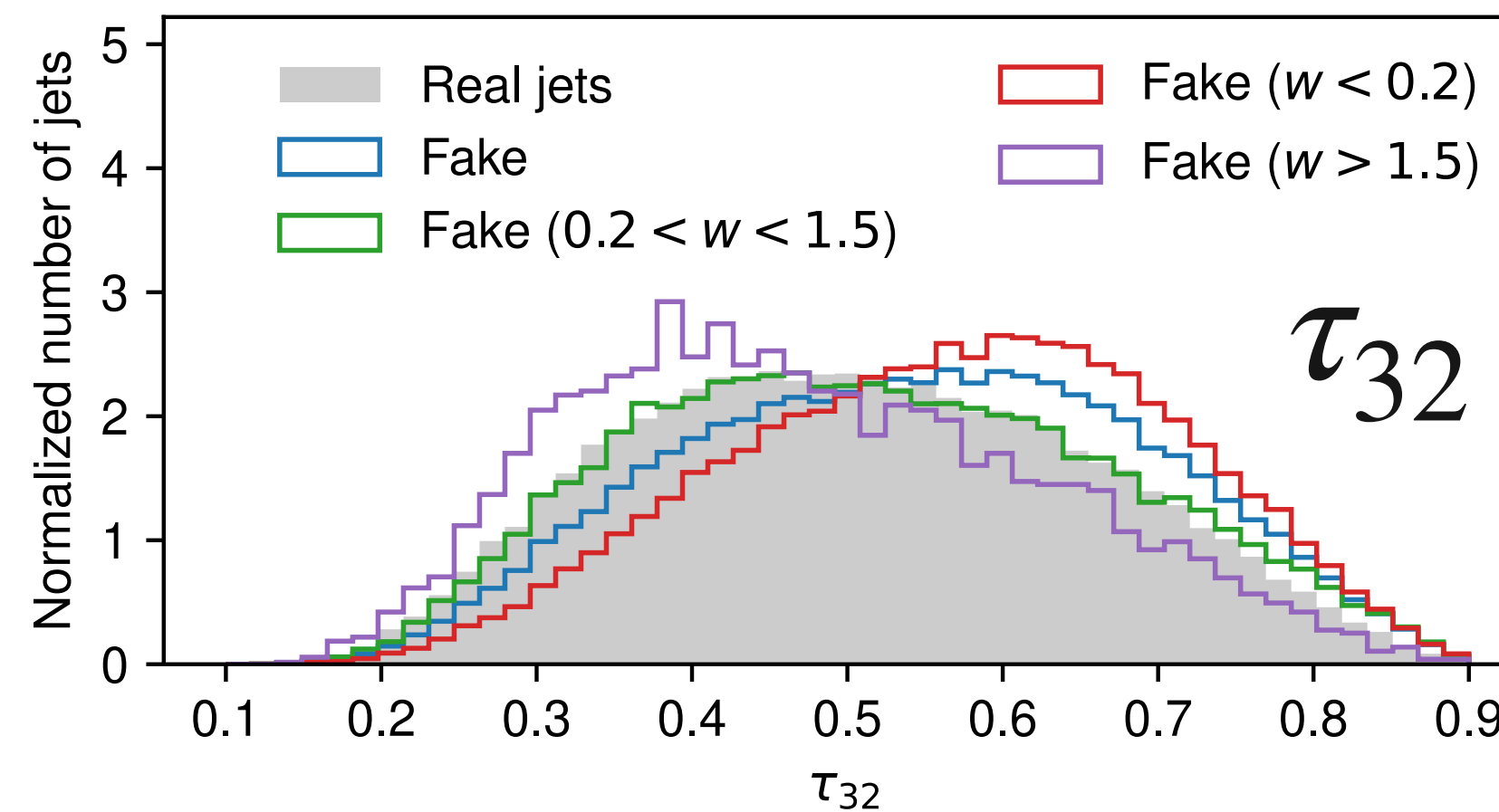
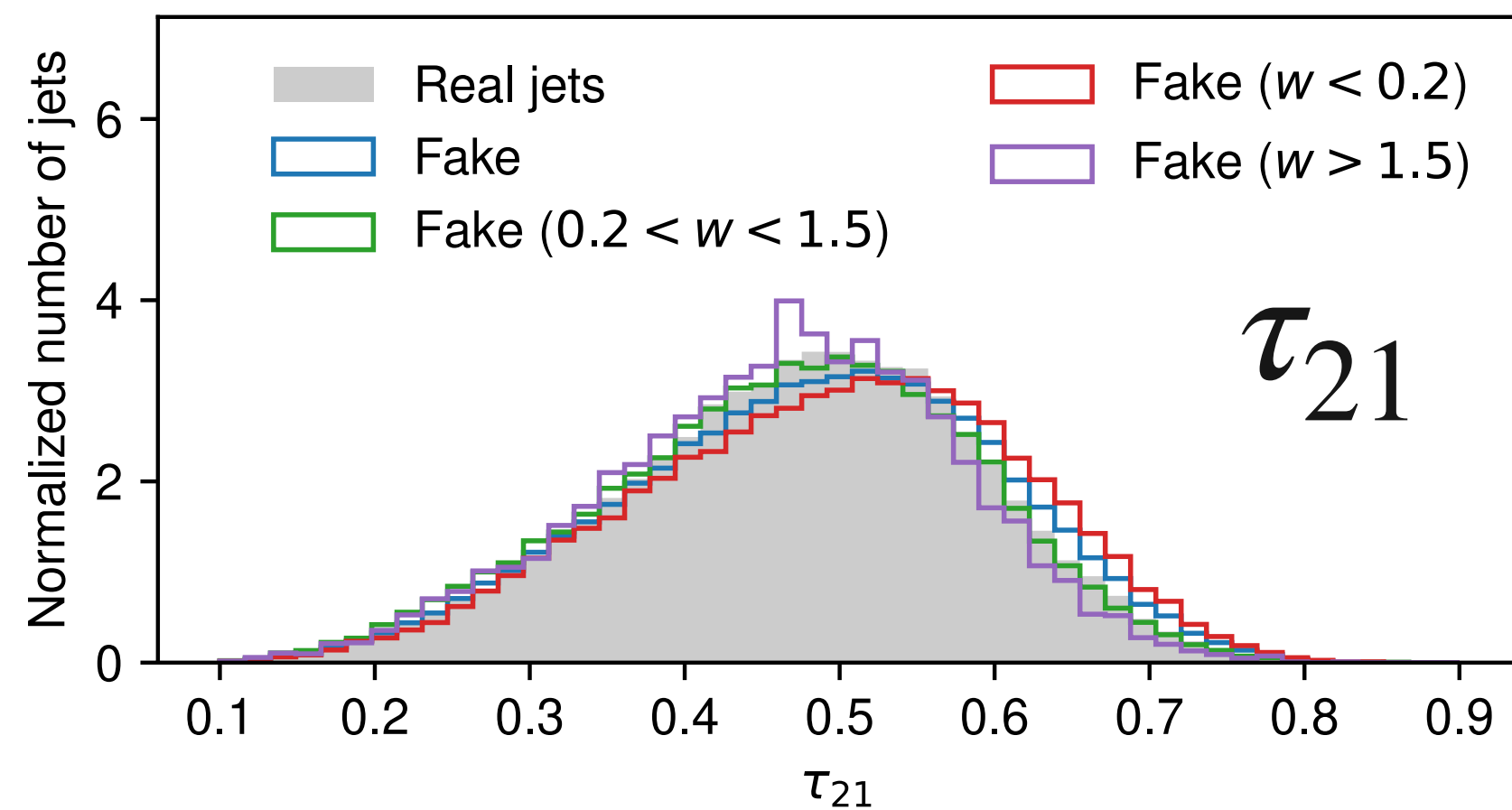
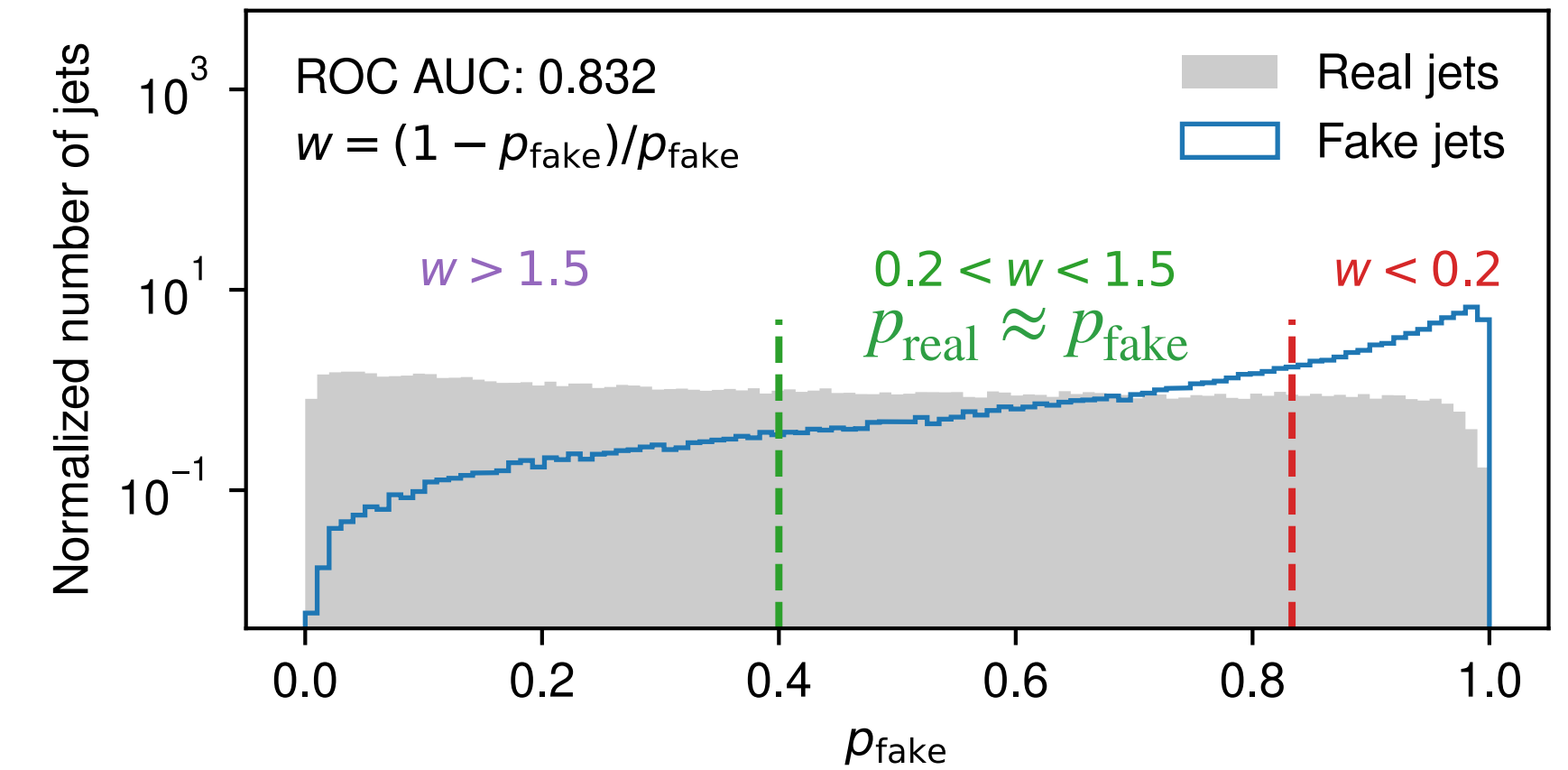


	$W_1^{\tau_{21}} (\cdot 10^{-3})$	$W_1^{\tau_{32}} (\cdot 10^{-3})$
Truth	1.7 ± 0.4	1.7 ± 0.5
Gen. (all features)	7.9 ± 0.5	35.4 ± 0.8
Gen. (kin. features)	3.6 ± 0.7	13.0 ± 0.7
Gen. (kin. features + top only)	4.8 ± 0.7	11.1 ± 0.9

- Trained two modified versions of our model:
 1. Generating **kinematic features only** ($\eta^{\text{rel}}, \phi^{\text{rel}}, p_{\text{T}}^{\text{rel}}$)
 2. Generating **kinematic features only** ($\eta^{\text{rel}}, \phi^{\text{rel}}, p_{\text{T}}^{\text{rel}}$) + trained on $t \rightarrow bqq'$ only
- **Kinematic features only improves modeling of jet substructure**
- Training on **top jets only increases agreement in τ_{32} but decreases agreement in τ_{21}**
 → training on different jet types simultaneously seems to help

Investigate $t \rightarrow bqq'$ jets with a classifier test

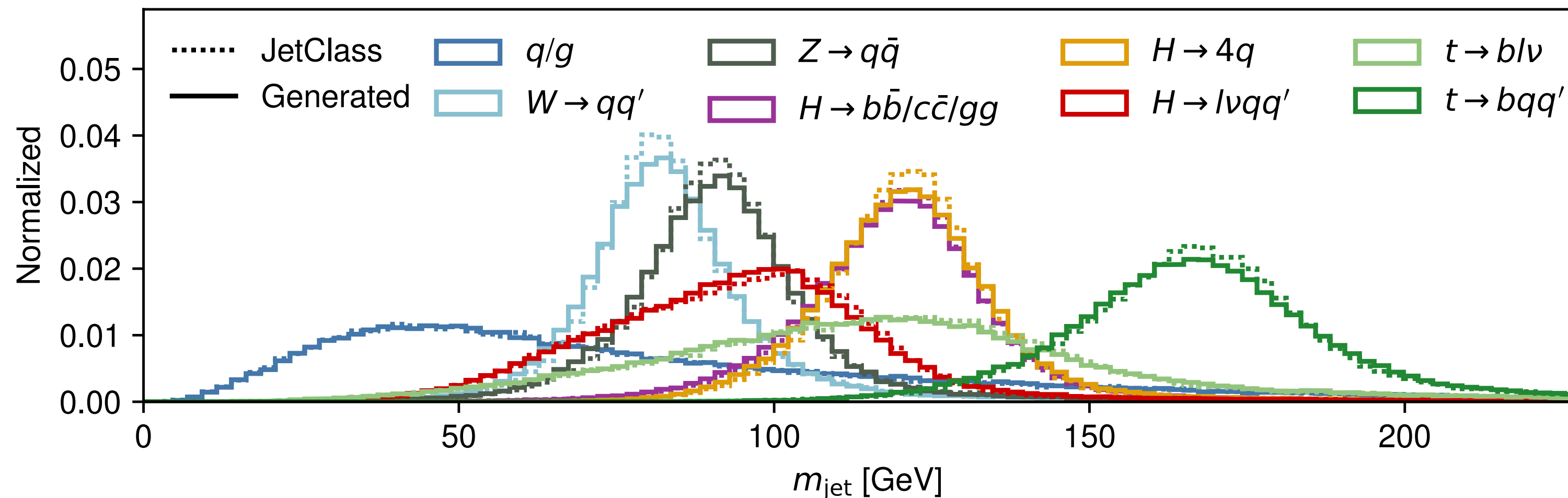
- Train **ParT-kin** [1] to distinguish between real and fake jets ($t \rightarrow bqq'$ only)
 - Split into three regions: $p_{\text{real}} \gg p_{\text{fake}}$, $p_{\text{real}} \approx p_{\text{fake}}$, $p_{\text{real}} \ll p_{\text{fake}}$
 - Substructure for fake jets from different regions:
 - **Fake jets with $p_{\text{real}} \approx p_{\text{fake}}$ show good agreement in jet substructure**
 - Especially fake jets with $p_{\text{real}} \ll p_{\text{fake}}$ lead to disagreement in **inclusive** τ_{21} and τ_{32} distributions
- Classifier output is consistent with the mis-modeling we see in the jet substructure



[1] Qu et al. (2022) "Particle Transformer for Jet Tagging"

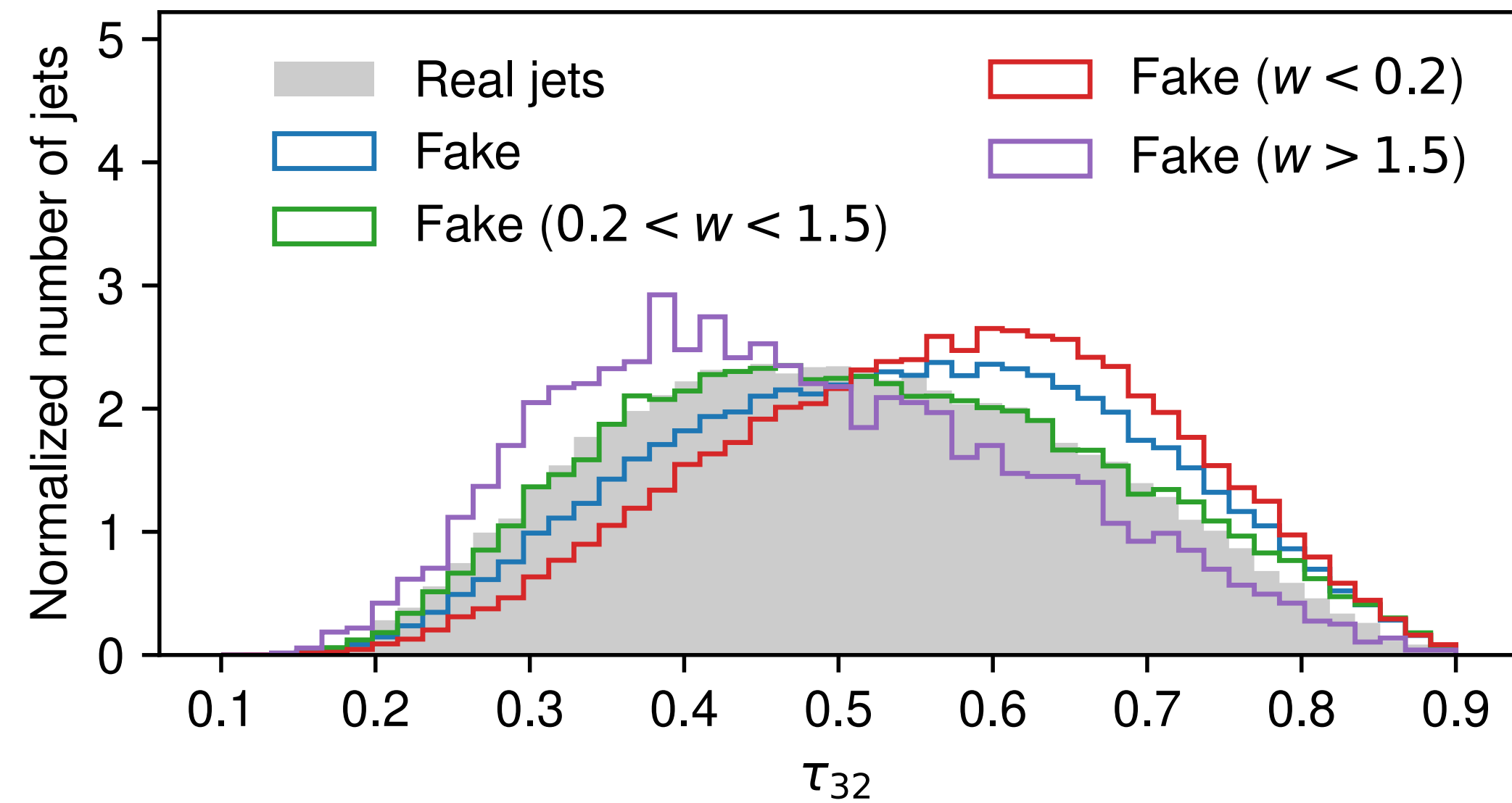
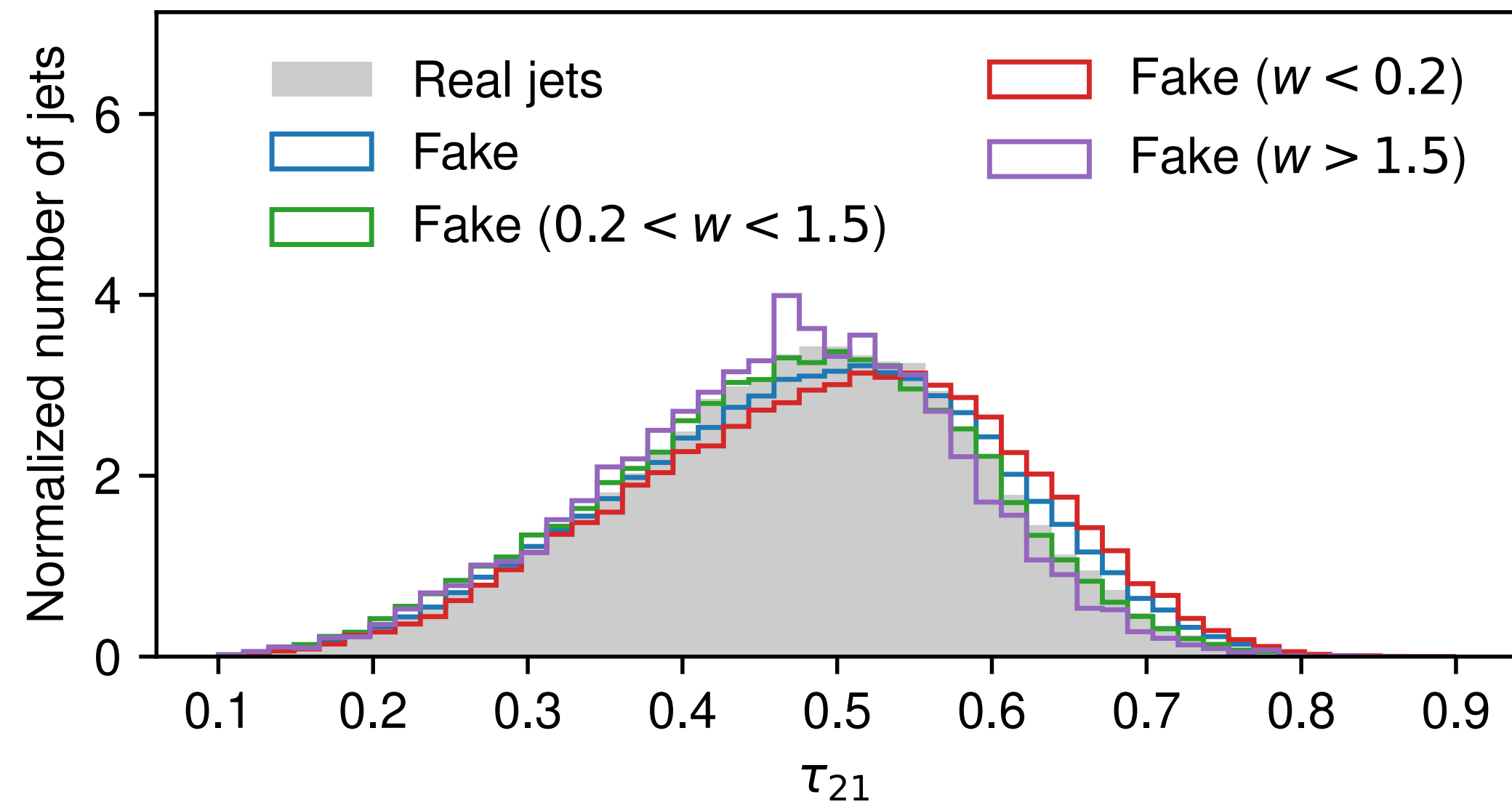
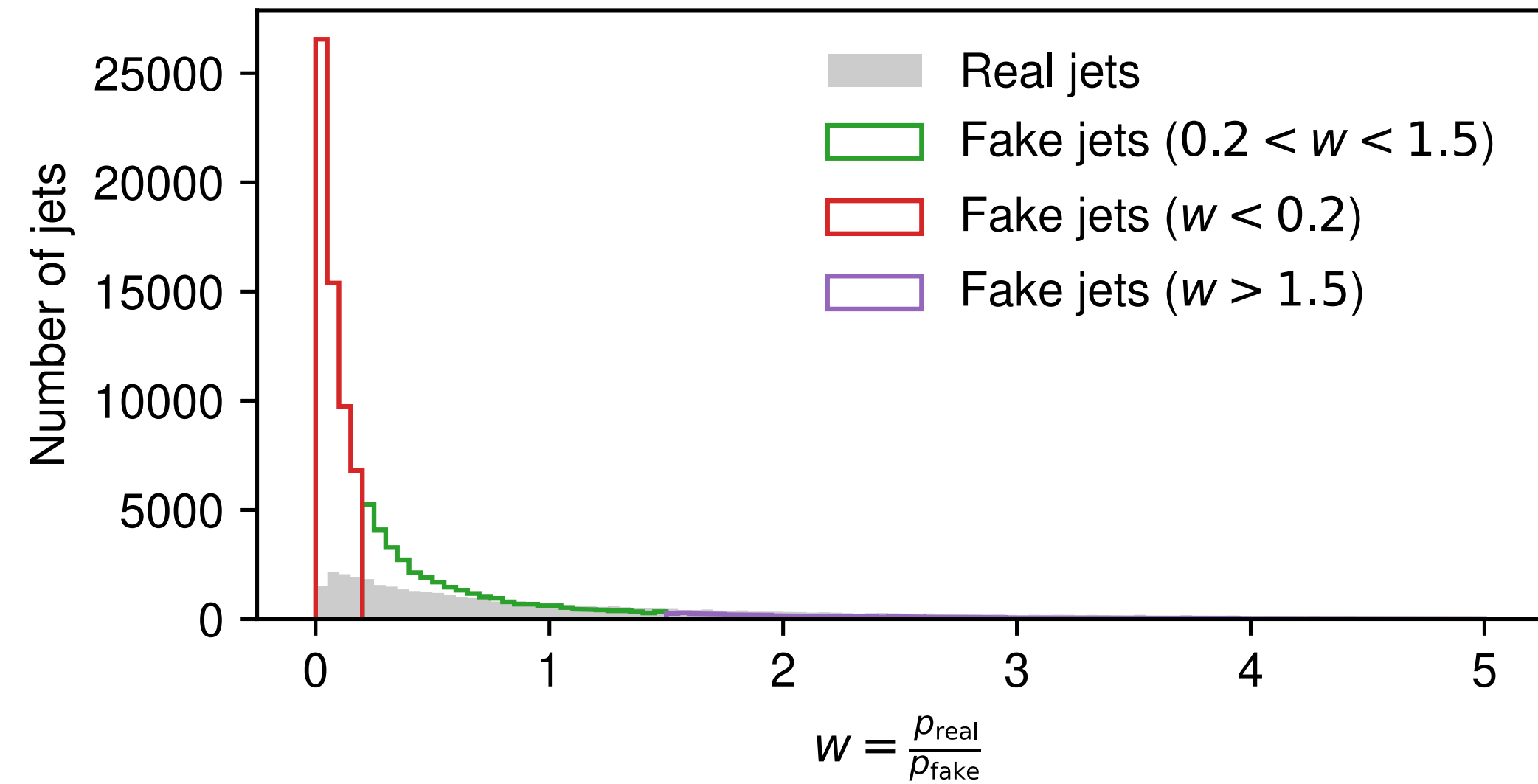
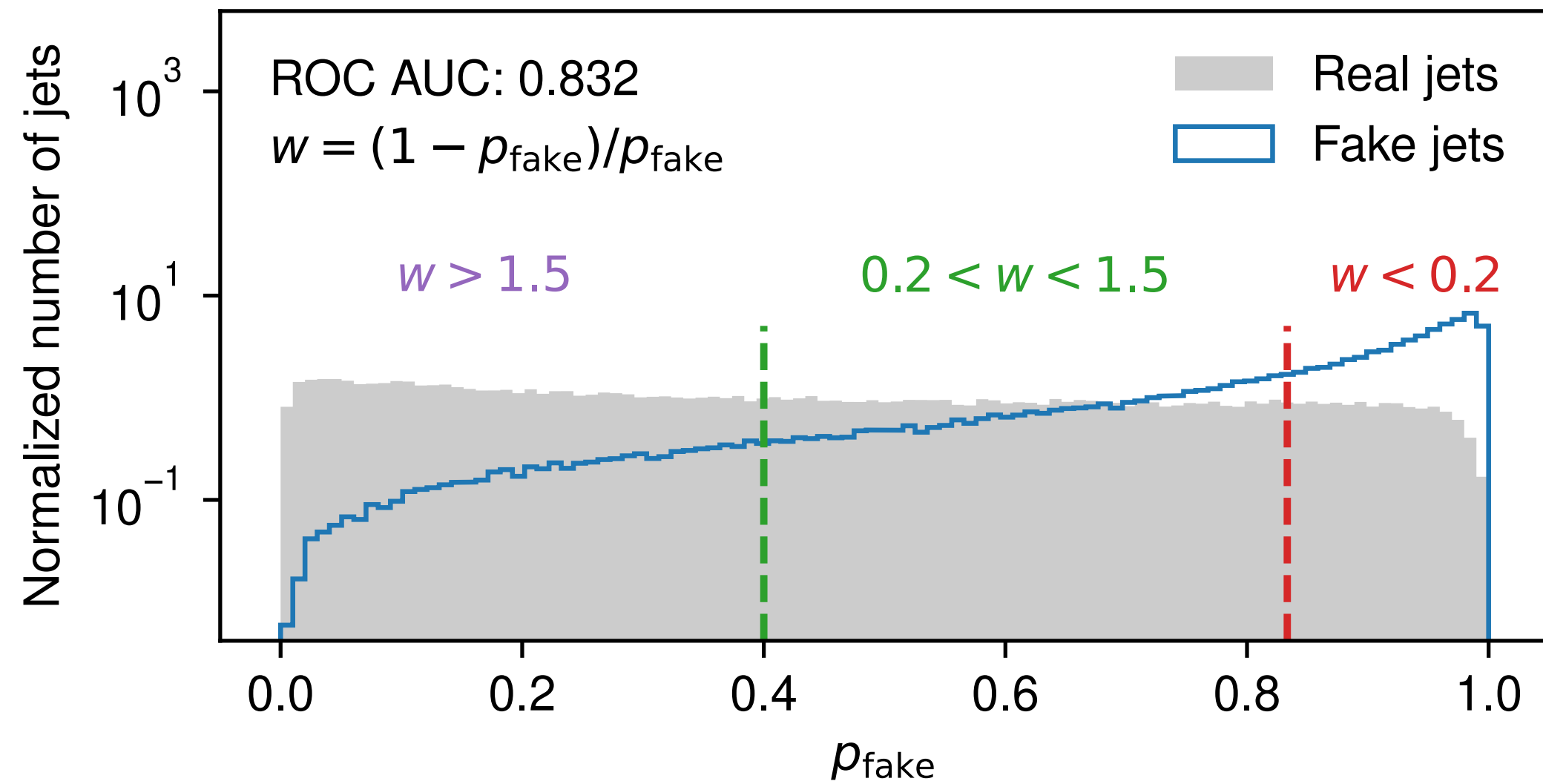
Summary

- **JetClass dataset [1] opens new possibilities for generative modeling prototyping**
 - significantly larger dataset than JetNet
 - more features that can be investigated
- **Our flow-matching based model accurately generates jets from the JetClass dataset**
 - **One model for all 10 jet types**
 - **Generated jet constituents include Particle-ID and trajectory displacement information**



[1] Qu et al. (2022) "JetClass: A Large-Scale Dataset for Deep Learning in Jet Physics"

Investigate $t \rightarrow bqq'$ jets with a classifier test



N -subjettiness calculation and visualization

- Cluster into N exclusive subsets
- Calculate p_T -weighted sum of distances to closest subset axis

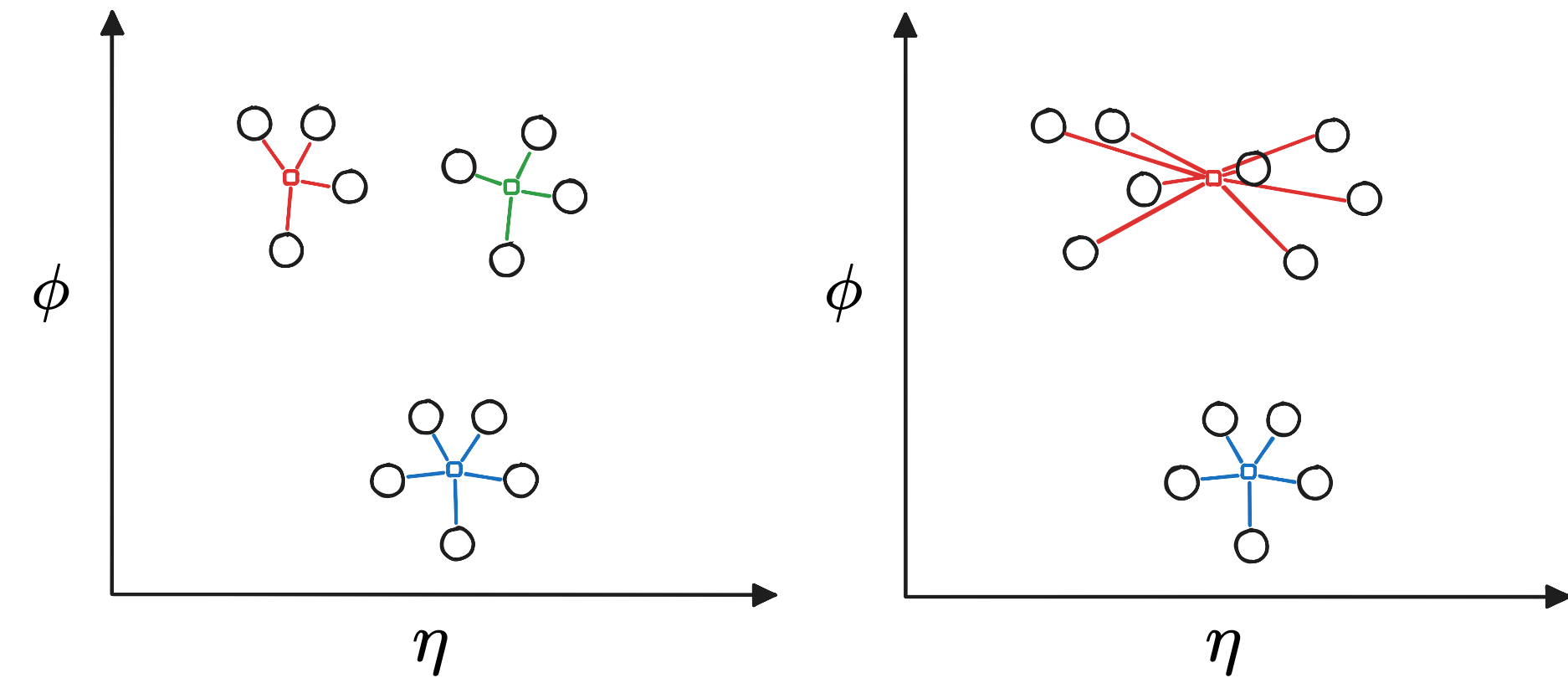
$$\tau_2 = \frac{1}{d_0} \sum_i p_{T,i} \min\{\Delta R_{1,i}, \Delta R_{2,i}\}$$

$$\tau_3 = \frac{1}{d_0} \sum_i p_{T,i} \min\{\Delta R_{1,i}, \Delta R_{2,i}, \Delta R_{3,i}\}$$

- We then look at ratio $\tau_{32} = \tau_3/\tau_2$
- **3-prong jets:** expect τ_{32} to **peak at small value**
- **2-prong jets:** expect τ_{32} to **peak at larger value**

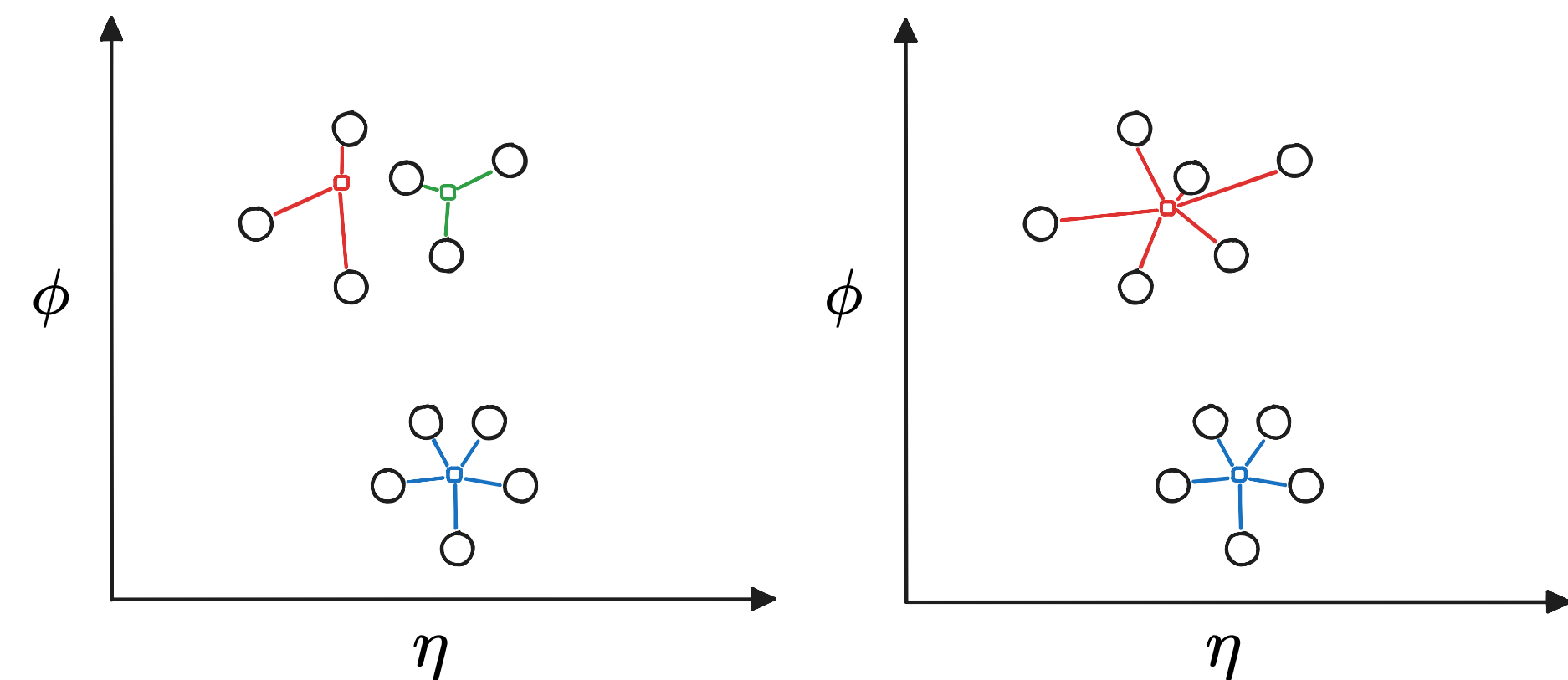
$t \rightarrow bqq'$

Here, τ_3 will be much smaller than τ_2

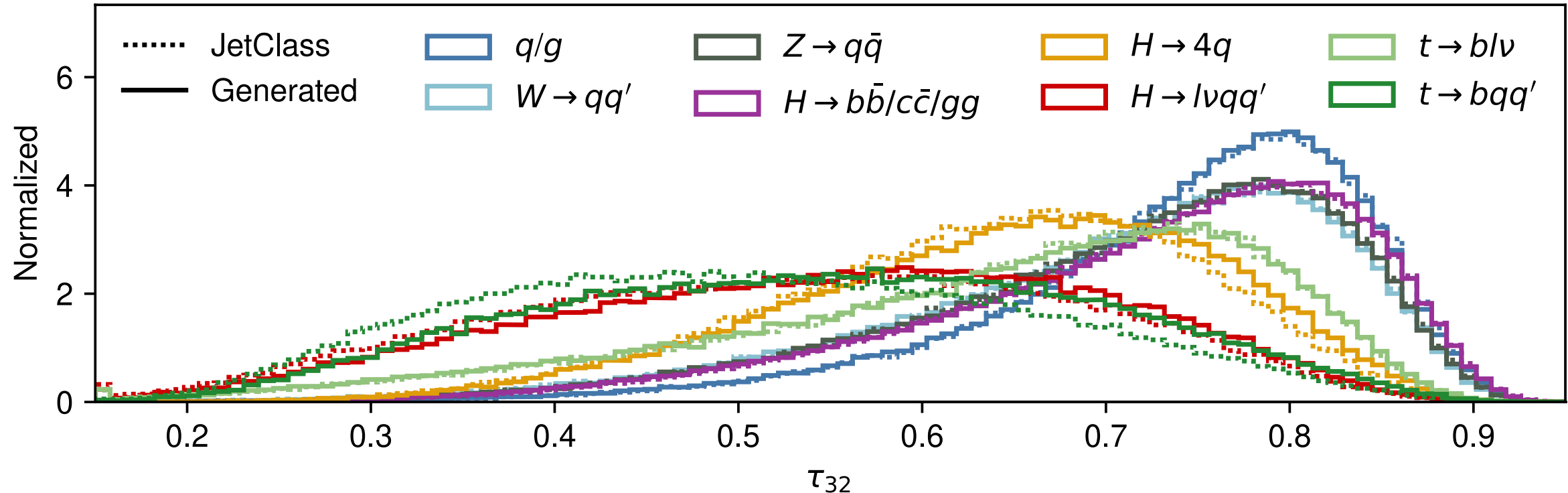
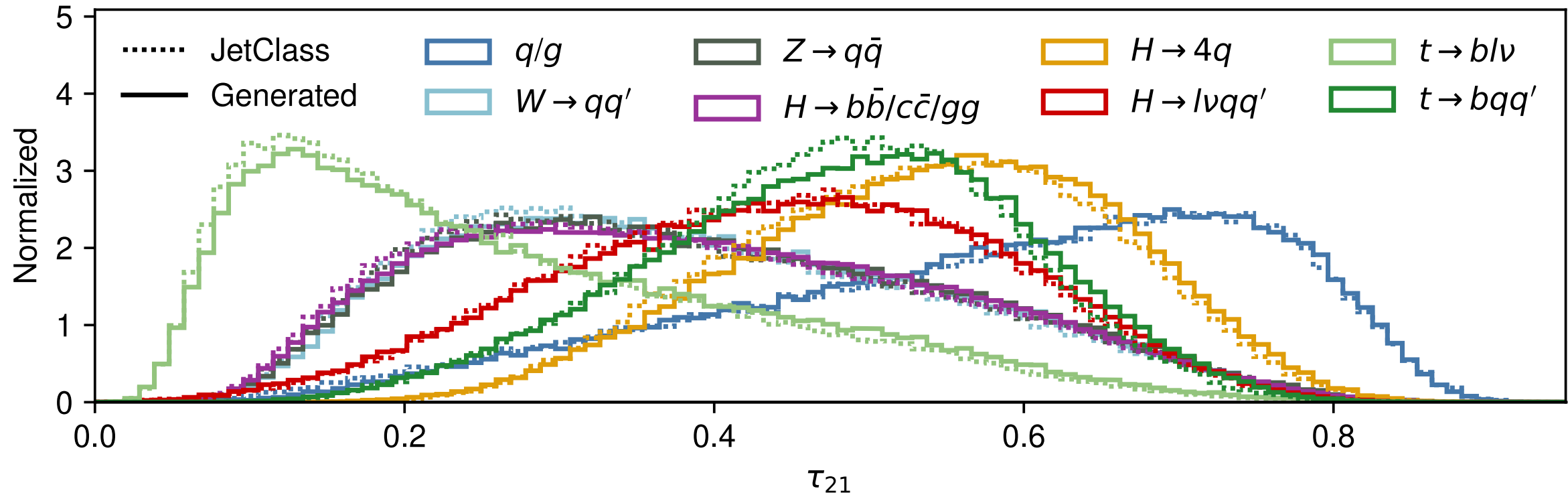
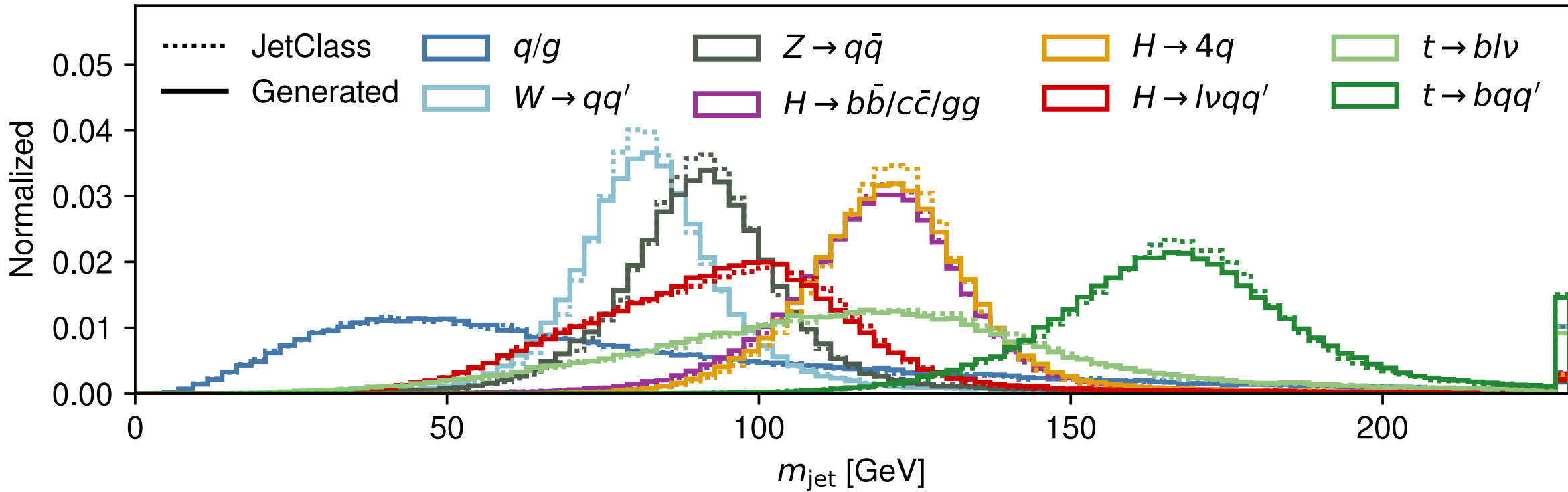


$H \rightarrow b\bar{b}$

Here, τ_3 will be only slightly smaller than τ_2



Jet substructure



Constituent features definitions

Table 2: Jet constituent features used for the studies in this paper. All features are either taken directly from the JETCLASS dataset or calculated from existing entries in the JETCLASS dataset.

Category	Variable	Definition
Kinematics	η^{rel}	Difference in pseudorapidity η between the particle and the jet axis
	ϕ^{rel}	Difference in azimuthal angle ϕ between the particle and the jet axis
	$p_{\text{T}}^{\text{rel}}$	Fraction of the particle p_{T} and the jet p_{T}
Trajectory displacement	d_0	Transverse impact parameter value
	d_z	Longitudinal impact parameter value
	σ_{d_0}	Error of measured transverse impact parameter
	σ_{d_z}	Error of measured longitudinal impact parameter
Particle identification	charge	Electric charge of the particle
	isChargedHadron	Flag if the particle is a charged hadron ($ \text{pid} ==211$ or 321 or 2212)
	isNeutralHadron	Flag if the particle is a neutral hadron ($ \text{pid} ==130$ or 2112 or 0)
	isPhoton	Flag if the particle is a photon ($\text{pid}==22$)
	isElectron	Flag if the particle is an electron ($ \text{pid} ==11$)
	isMuon	Flag if the particle is a muon ($ \text{pid} ==13$)

Metrics for constituent-level features

Table 4: W_1 distances of the constituent features for the baseline model.

	$W_1^{p_T^{\text{rel}}} (\cdot 10^{-3})$	$W_1^{\eta^{\text{rel}}} (\cdot 10^{-3})$	$W_1^{\phi^{\text{rel}}} (\cdot 10^{-3})$	$W_1^{d_0} (\cdot 10^{-3})$	$W_1^{d_z} (\cdot 10^{-3})$	$W_1^{\text{charge}} (\cdot 10^{-3})$
Truth (QCD)	0.12 ± 0.03	0.7 ± 0.2	0.8 ± 0.3	27 ± 4	18 ± 3	0.5 ± 0.3
Gen. (QCD)	0.11 ± 0.02	0.8 ± 0.2	0.7 ± 0.2	90 ± 10	50 ± 9	0.7 ± 0.4
Truth (Hbb)	0.07 ± 0.02	0.7 ± 0.1	0.7 ± 0.2	23 ± 5	12 ± 1	0.5 ± 0.2
Gen. (Hbb)	0.08 ± 0.02	1.0 ± 0.2	1.0 ± 0.2	100 ± 10	57 ± 6	0.7 ± 0.4
Truth (Hcc)	0.07 ± 0.02	0.7 ± 0.2	1.0 ± 0.3	22 ± 4	17 ± 3	0.6 ± 0.6
Gen. (Hcc)	0.12 ± 0.04	0.7 ± 0.3	1.0 ± 0.2	80 ± 10	42 ± 7	0.6 ± 0.2
Truth (Hgg)	0.031 ± 0.008	0.5 ± 0.2	0.6 ± 0.2	25 ± 6	14 ± 2	0.5 ± 0.3
Gen. (Hgg)	0.039 ± 0.007	0.6 ± 0.1	0.7 ± 0.2	100 ± 10	53 ± 6	0.9 ± 0.3
Truth (H4q)	0.05 ± 0.01	0.4 ± 0.1	0.6 ± 0.2	27 ± 8	14 ± 3	0.5 ± 0.3
Gen. (H4q)	0.06 ± 0.02	0.7 ± 0.2	0.8 ± 0.2	110 ± 20	66 ± 8	0.6 ± 0.2
Truth (Hqql)	0.11 ± 0.03	0.8 ± 0.3	0.7 ± 0.3	30 ± 10	15 ± 4	0.7 ± 0.5
Gen. (Hqql)	0.38 ± 0.05	1.2 ± 0.3	1.5 ± 0.3	88 ± 7	55 ± 7	0.6 ± 0.3
Truth (Zqq)	0.09 ± 0.02	0.7 ± 0.2	0.8 ± 0.2	24 ± 6	16 ± 4	0.7 ± 0.2
Gen. (Zqq)	0.10 ± 0.02	0.8 ± 0.2	0.9 ± 0.2	81 ± 7	44 ± 5	1.0 ± 0.3
Truth (Wqq)	0.09 ± 0.02	0.8 ± 0.3	0.7 ± 0.2	29 ± 8	18 ± 4	1.0 ± 0.3
Gen. (Wqq)	0.10 ± 0.02	0.8 ± 0.2	0.8 ± 0.2	110 ± 20	56 ± 8	0.9 ± 0.3
Truth (Tbqq)	0.05 ± 0.01	0.7 ± 0.2	0.8 ± 0.1	23 ± 5	14 ± 2	0.6 ± 0.2
Gen. (Tbqq)	0.10 ± 0.02	0.9 ± 0.3	1.1 ± 0.3	68 ± 9	44 ± 3	0.7 ± 0.3
Truth (Tbl)	0.17 ± 0.04	0.9 ± 0.3	1.2 ± 0.2	25 ± 4	17 ± 3	0.5 ± 0.2
Gen. (Tbl)	0.41 ± 0.09	1.6 ± 0.4	1.8 ± 0.5	80 ± 10	41 ± 3	0.6 ± 0.4

Metrics for jet-level features

Table 8: Wasserstein metrics for the baseline model and the model that is restricted to kinematic features only. For hadronic top jets, also two models were trained on hadronic top jets only.

	W_1^m	$W_1^{m_{\text{rel}}} (\cdot 10^{-3})$	$W_1^P (\cdot 10^{-3})$	$W_1^{\tau_{21}} (\cdot 10^{-3})$	$W_1^{\tau_{32}} (\cdot 10^{-3})$	$W_1^{D^2} (\cdot 10^{-2})$
Truth (QCD)	0.5 ± 0.1	0.6 ± 0.1	0.5 ± 0.2	1.6 ± 0.4	0.9 ± 0.2	3.5 ± 0.9
Gen. (QCD)	0.5 ± 0.2	1.0 ± 0.2	0.5 ± 0.2	6 ± 1	1.3 ± 0.4	7 ± 2
Gen. kin (QCD)	0.6 ± 0.2	0.8 ± 0.2	0.6 ± 0.2	4.0 ± 0.6	1.2 ± 0.3	4 ± 1
Truth (Hbb)	0.28 ± 0.09	0.42 ± 0.08	0.5 ± 0.1	1.6 ± 0.5	1.0 ± 0.4	0.9 ± 0.2
Gen. (Hbb)	0.54 ± 0.09	0.8 ± 0.2	0.7 ± 0.2	6 ± 1	4.1 ± 0.9	2.7 ± 0.3
Gen. kin (Hbb)	0.5 ± 0.1	0.8 ± 0.2	0.6 ± 0.1	1.5 ± 0.6	1.4 ± 0.4	1.5 ± 0.3
Truth (Hcc)	0.20 ± 0.03	0.6 ± 0.2	0.6 ± 0.2	1.5 ± 0.5	1.0 ± 0.4	0.9 ± 0.2
Gen. (Hcc)	0.76 ± 0.07	1.0 ± 0.2	0.6 ± 0.2	14.7 ± 0.7	4.2 ± 0.5	3.4 ± 0.3
Gen. kin (Hcc)	0.26 ± 0.04	0.5 ± 0.2	0.6 ± 0.1	5.1 ± 0.7	3.0 ± 0.5	1.3 ± 0.3
Truth (Hgg)	0.31 ± 0.04	0.5 ± 0.1	0.44 ± 0.09	1.2 ± 0.4	1.0 ± 0.3	0.7 ± 0.3
Gen. (Hgg)	0.67 ± 0.06	0.9 ± 0.3	0.5 ± 0.2	7.9 ± 0.8	3.3 ± 0.5	2.0 ± 0.2
Gen. kin (Hgg)	0.30 ± 0.06	0.5 ± 0.2	0.4 ± 0.1	2.4 ± 0.6	2.0 ± 0.5	0.8 ± 0.3
Truth (H4q)	0.26 ± 0.08	0.4 ± 0.1	0.34 ± 0.07	1.1 ± 0.3	0.9 ± 0.2	0.5 ± 0.1
Gen. (H4q)	0.84 ± 0.08	0.9 ± 0.2	0.5 ± 0.1	9.0 ± 0.8	10.3 ± 0.6	1.12 ± 0.09
Gen. kin (H4q)	0.31 ± 0.06	0.6 ± 0.1	0 ± 1	2.9 ± 0.7	4.0 ± 0.4	0.6 ± 0.1
Truth (Hqql)	0.4 ± 0.1	0.6 ± 0.2	0.6 ± 0.2	1.5 ± 0.7	1.5 ± 0.4	1.4 ± 0.4
Gen. (Hqql)	0.67 ± 0.09	0.9 ± 0.2	0.9 ± 0.2	5.2 ± 0.7	19 ± 1	2.5 ± 0.5
Gen. kin (Hqql)	0.53 ± 0.08	0.8 ± 0.2	0.8 ± 0.2	2.9 ± 0.7	12.5 ± 0.8	2.2 ± 0.5
Truth (Zqq)	0.32 ± 0.07	0.5 ± 0.1	0.5 ± 0.1	1.3 ± 0.4	1.0 ± 0.3	1.2 ± 0.3
Gen. (Zqq)	0.64 ± 0.05	1.0 ± 0.2	0.6 ± 0.2	9.1 ± 0.8	1.3 ± 0.2	2.1 ± 0.3
Gen. kin (Zqq)	0.32 ± 0.06	0.5 ± 0.1	0.6 ± 0.1	3 ± 2	3.2 ± 0.5	1.2 ± 0.6
Truth (Wqq)	0.36 ± 0.09	0.4 ± 0.1	0.5 ± 0.1	1.6 ± 0.4	1.0 ± 0.2	1.0 ± 0.1
Gen. (Wqq)	0.86 ± 0.06	1.1 ± 0.2	0.6 ± 0.2	11 ± 1	2.0 ± 0.3	2.9 ± 0.5
Gen. kin (Wqq)	0.5 ± 0.1	0.5 ± 0.1	0.5 ± 0.1	5 ± 1	2.6 ± 0.5	1.6 ± 0.3
Truth (Tbqq)	0.29 ± 0.08	0.5 ± 0.2	0.5 ± 0.1	1.7 ± 0.4	1.7 ± 0.5	0.4 ± 0.1
Gen. (Tbqq)	0.9 ± 0.1	0.8 ± 0.2	0.6 ± 0.2	7.9 ± 0.5	35.4 ± 0.8	0.7 ± 0.1
Gen. kin (Tbqq)	0.41 ± 0.07	0.5 ± 0.1	0 ± 1	3.6 ± 0.7	13.0 ± 0.7	0.57 ± 0.08
Gen. allTop (Tbqq)	0.77 ± 0.05	0 ± 1	0.6 ± 0.1	11.3 ± 0.5	22 ± 1	1.07 ± 0.08
Gen. kinTop (Tbqq)	0.42 ± 0.07	0.7 ± 0.2	0.6 ± 0.2	4.8 ± 0.7	11.1 ± 0.9	0.6 ± 0.1
Truth (Tbl)	0.4 ± 0.2	0.48 ± 0.09	0.7 ± 0.2	1.1 ± 0.2	1.6 ± 0.6	1.6 ± 0.5
Gen. (Tbl)	1.2 ± 0.2	1.7 ± 0.4	1.6 ± 0.3	12.5 ± 0.8	2.6 ± 0.5	5.8 ± 0.5
Gen. kin (Tbl)	0.44 ± 0.09	0.6 ± 0.1	1.0 ± 0.2	4.8 ± 0.7	2.2 ± 0.6	2.3 ± 0.7

Training and inference

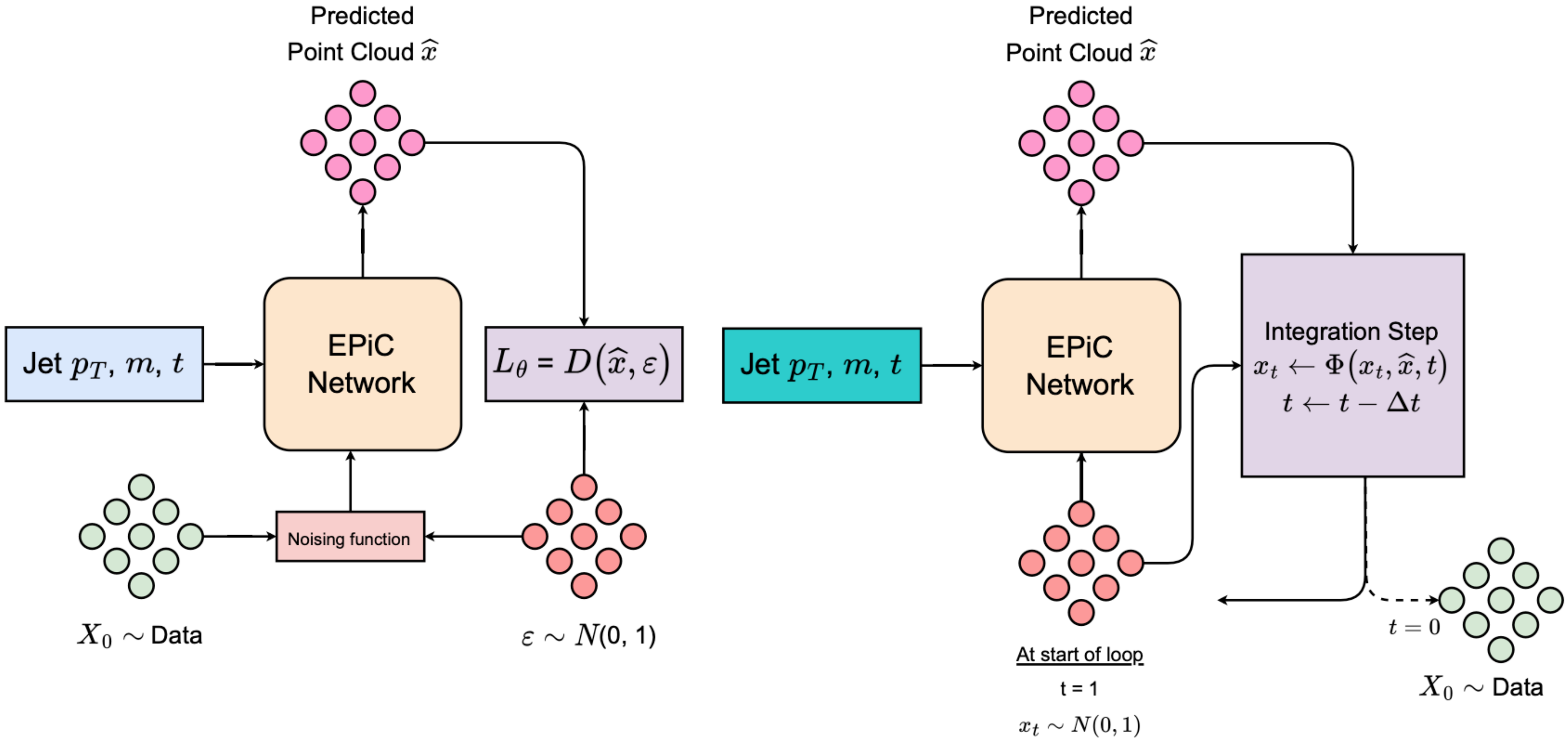


Fig. 1: Schematic overview of the EPiC-JeDi and EPiC-FM training (left) and generation (right) pipeline.

Image from [Buhmann et al. \(2023\)](#) "EPiC-ly Fast Particle Cloud Generation with Flow-Matching and Diffusion"

Model architecture sketch

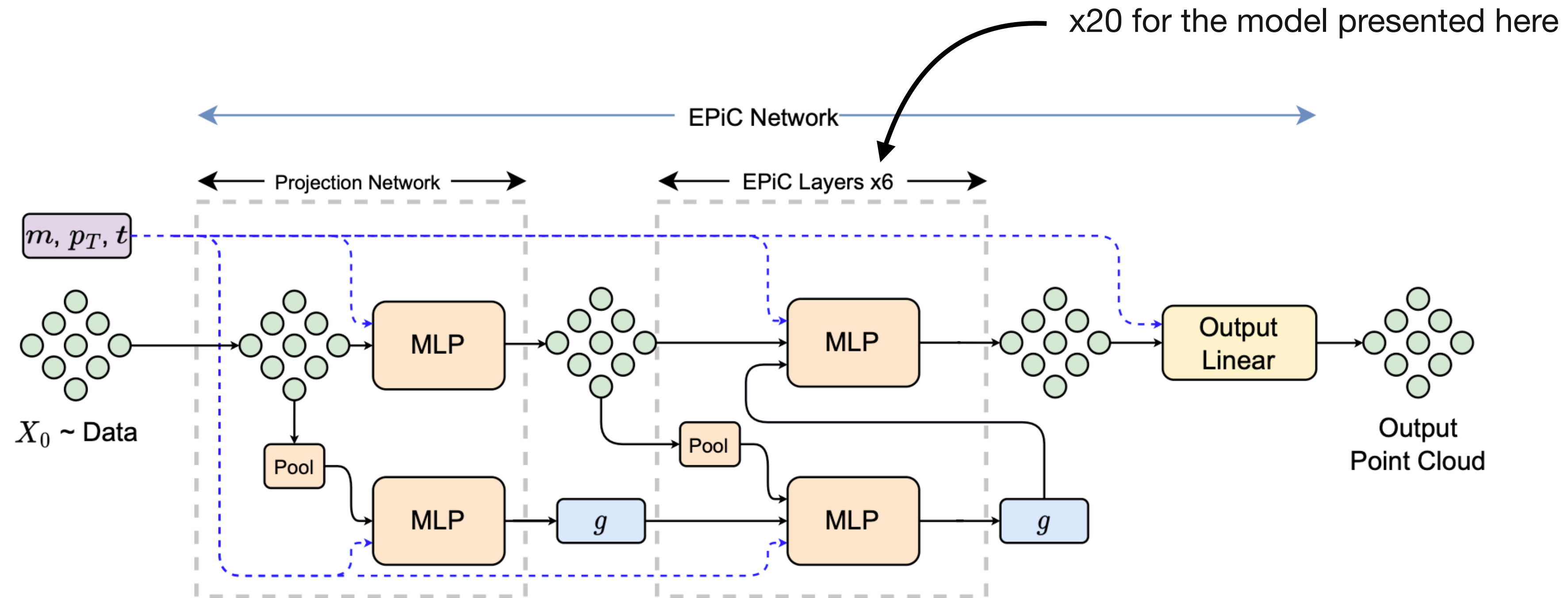


Fig. 2: Model schema of the *EPiC Network* generator architecture used in both EPiC-JeDi and EPiC-FM. Each multi-layer perceptron (MLP) is a two-layer neural network with LeakyReLU activation. The pooling operation is a concatenation of both average and summation pooling.

Image from [Buhmann et al. \(2023\) "EPiC-ly Fast Particle Cloud Generation with Flow-Matching and Diffusion"](#)