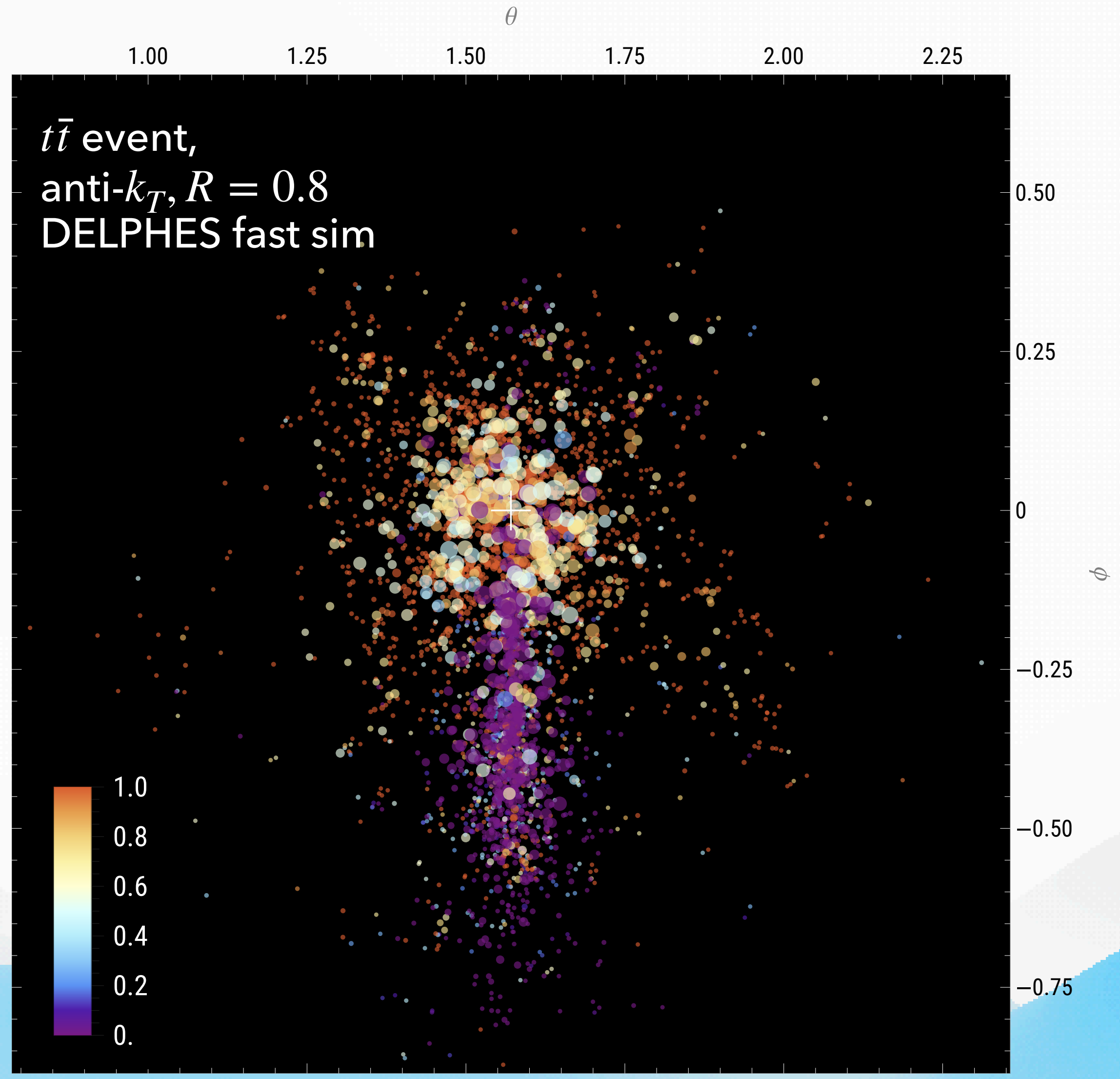
BOOST 2023 Indico

PELICAN

PERMUTATION- AND LORENTZ-EQUIVARIANT NETWORKS FOR PARTICLE PHYSICS



Identifying constituent-level W-boson decay products within a top quark jet!

Alexander Bogatskiy, Timothy Hoffman,
Xiaoyang Liu, David W. Miller, Jan T. Offermann

BOOST 2023

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DATA SCIENCE INSTITUTE

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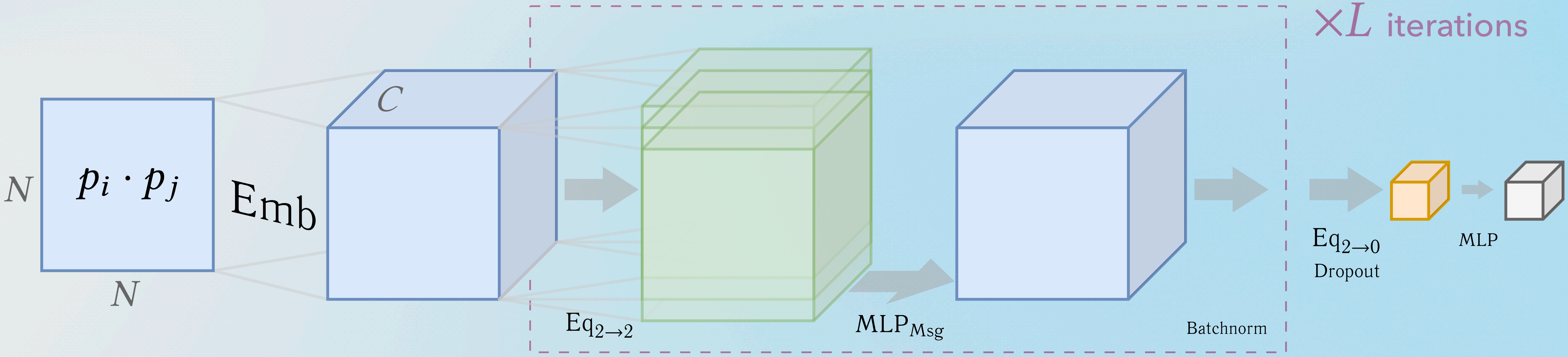
- Tagging jets is fundamentally important for measurements and searches! Neural networks have proven useful for this.
- *Equivariant* networks are strong, robust and lean.
  - Relevant here: permutation & Lorentz equivariance. [a,b]
  - Beyond tagging: subjet structure and constituent info!
- Growing interest in general approaches for Lorentz-equivariant NN's. [c] *(low parameterization, explainability)*
- For today: PELICAN for top-tagging, and measuring W-boson four-momentum *within* top quark jets.

[a] A Bogatskiy, T. Hoffman, D. W. Miller, J. T. Offermann, PELICAN (2022).
[b] S. Gong et. al., An Efficient Lorentz Equivariant Graph Neural Network for Jet Tagging (2022).
[c] A. Bogatskiy et. al., Symmetry Group Equivariant Architectures for Physics (2022).

- PELICAN is a network architecture that…
  - is permutation- and Lorentz-equivariant,
  - acts on collections of four-momenta, (c.f. point clouds)
  - and can predict Lorentz-*invariants*, e.g. tagging…
    - ***or Lorentz-covariants*, e.g. p^μ regression!**



THE PELICAN ARCHITECTURE: LORENTZ EQUIVARIANCE

- Lorentz equivariance is achieved by constructing functions of inner products of the four-momenta.

Invariants (output for PELICAN's "scalar form")

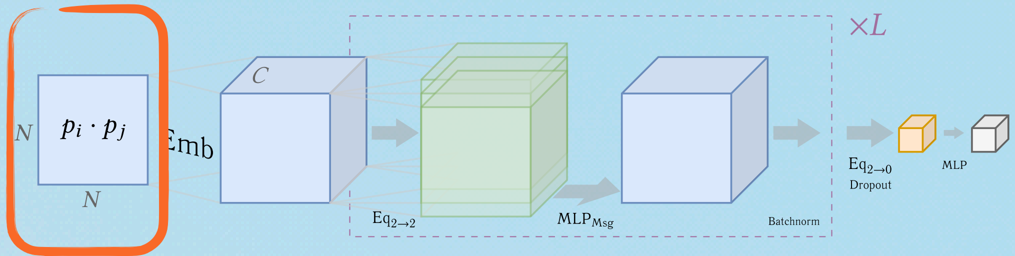
$$I_k\left(p_1, \ldots, p_N\right) = I_k\left(\left\{d_{ij}\right\}_{i,j}\right) \quad , \qquad d_{ij} \equiv p_i^\mu p_{j,\mu}$$

Lorentz-invariant

Covariants (output for PELICAN's "vector form")

$$F^\mu = \sum_k I_k\left(p_1, \ldots, p_N\right) p_k^\mu$$

Lorentz-covariant



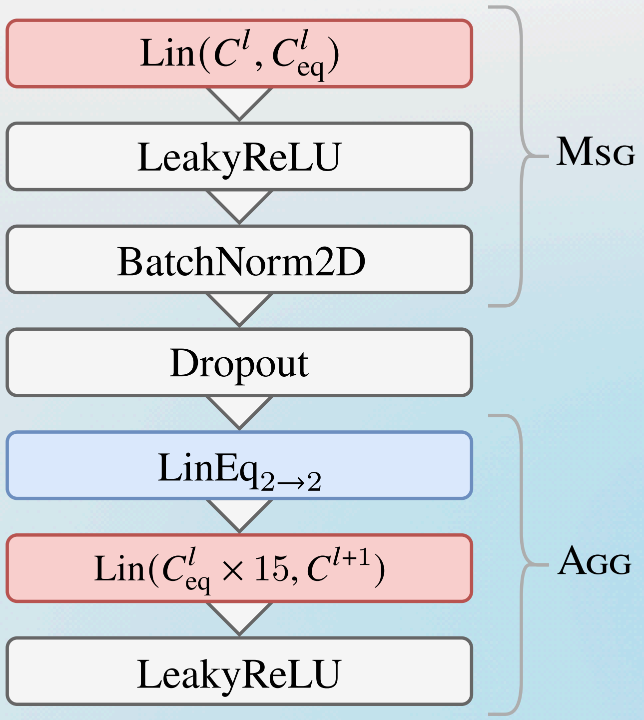
THE PELICAN ARCHITECTURE: PERMUTATION EQUIVARIANCE

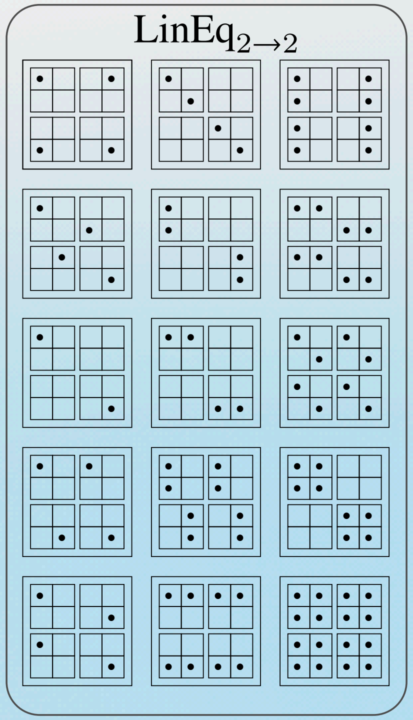
- Operations are equivariant w.r.t. particle permutations.

Equivariant $2 \to 2$ block:

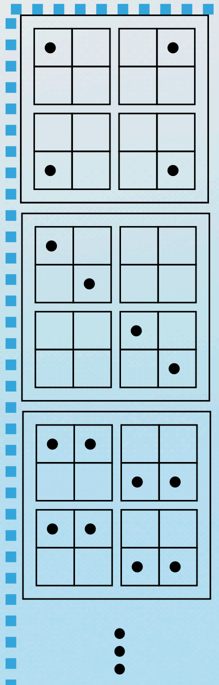
$$T^{(l+1)} = \text{Agg} \circ \text{Msg}\left(T^{l}\right)$$

- 15-dimensional linear permutation-equivariant map.
- Output tensor elements are aggregated from input tensor elements.





where…

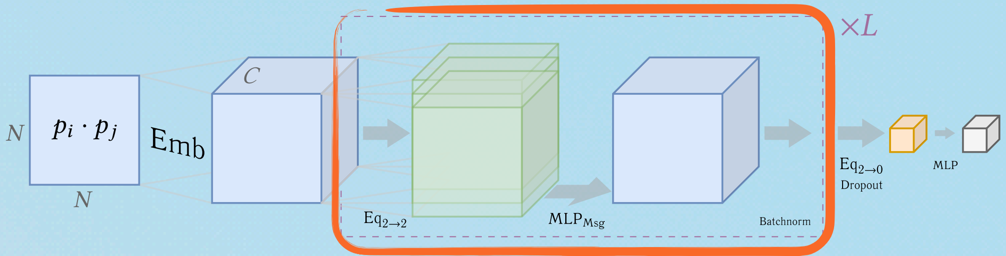


= identity

= trace (on diagonal)

= aggregate rows

et cetera…

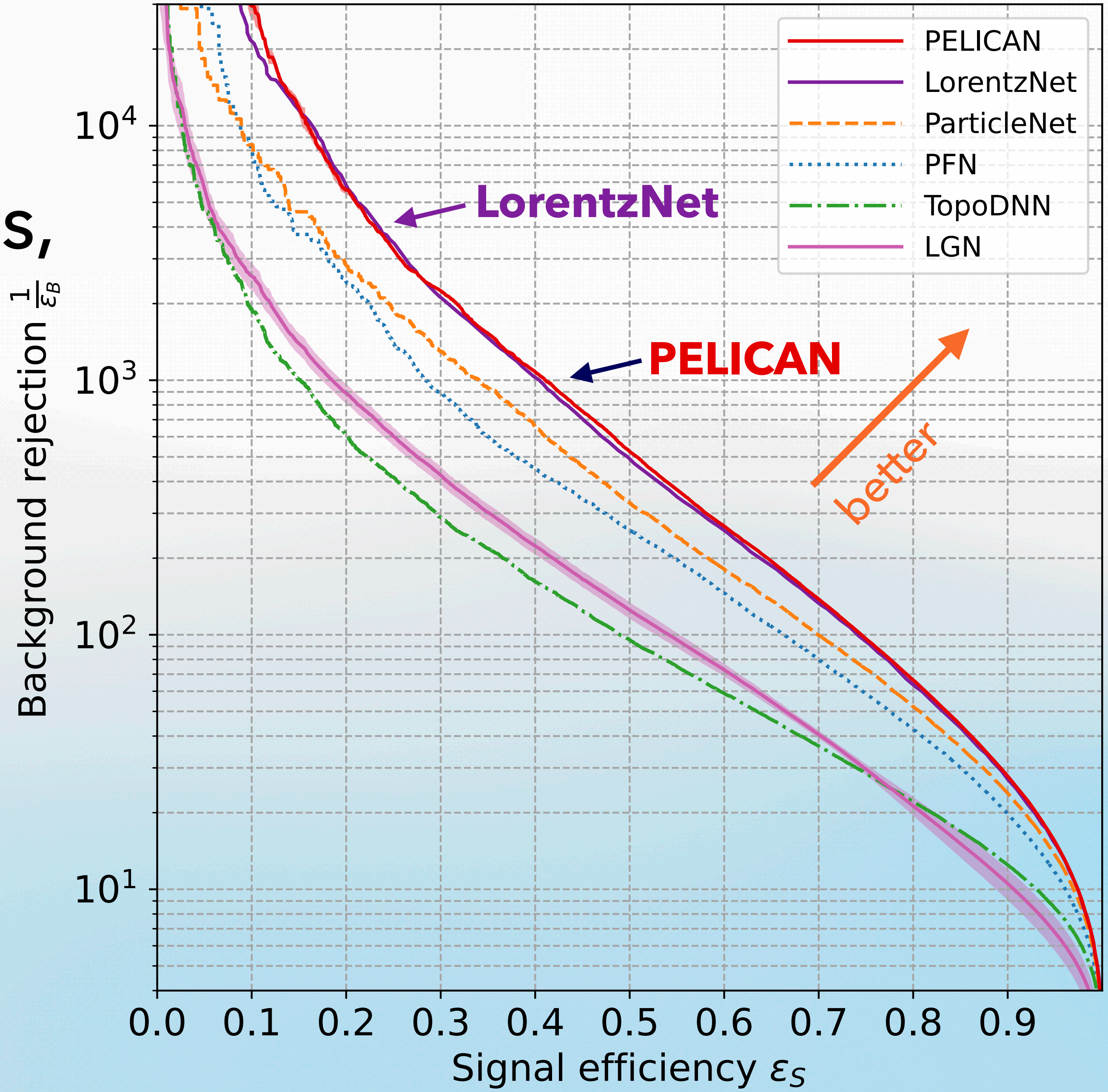


PELICAN: TOP-TAGGING

First task: top tagging!

- Hadronic tops vs. QCD dijets, anti-k_T $R = 0.8$ jets. [d]
- Interesting problem with existing ML benchmarks.
- Use PELICAN's scalar form.
    - State-of-the-art performance, even with low parameterization! [a]

Scalar form: $I\left(p_1, \ldots, p_N\right) = I\left(\left\{d_{ij}\right\}_{i,j}\right)$



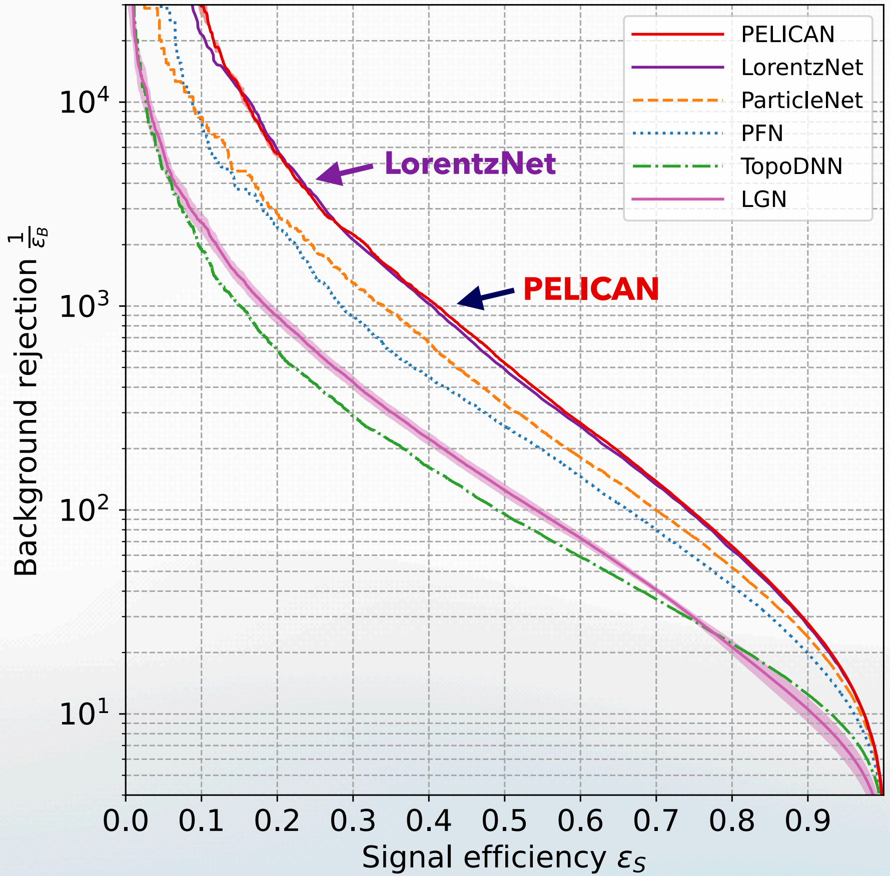
Architecture	Accuracy	AUC	# Params
PELICAN	0.9425(1)	0.9869(1)	45k
LorentzNet	0.942	0.9868	220k
ParticleNet	0.938	0.985	498k
PFN	0.932	0.982	82k
TopoDNN	0.916	0.972	59k
LGN	0.929	0.964	4.5k

[a] A Bogatskiy, T. Hoffman, D. W. Miller, J. T. Offermann, PELICAN (2022).

[d] G. Kasieczka, T. Plehn, J. Thompson, and M. Russel (2019).

PELICAN: TOP-TAGGING

- State-of-the-art performance, even with low parameterization!



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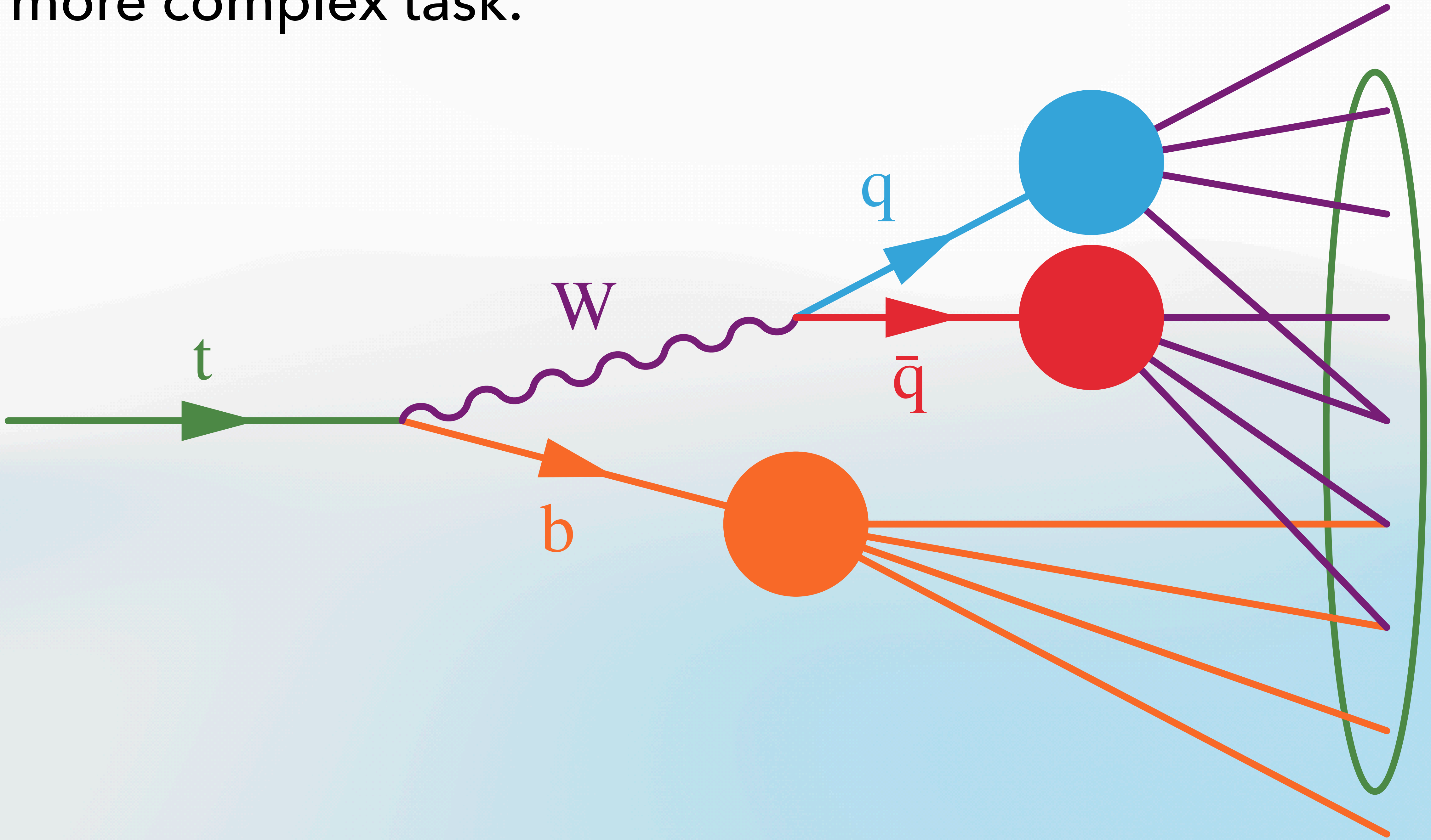
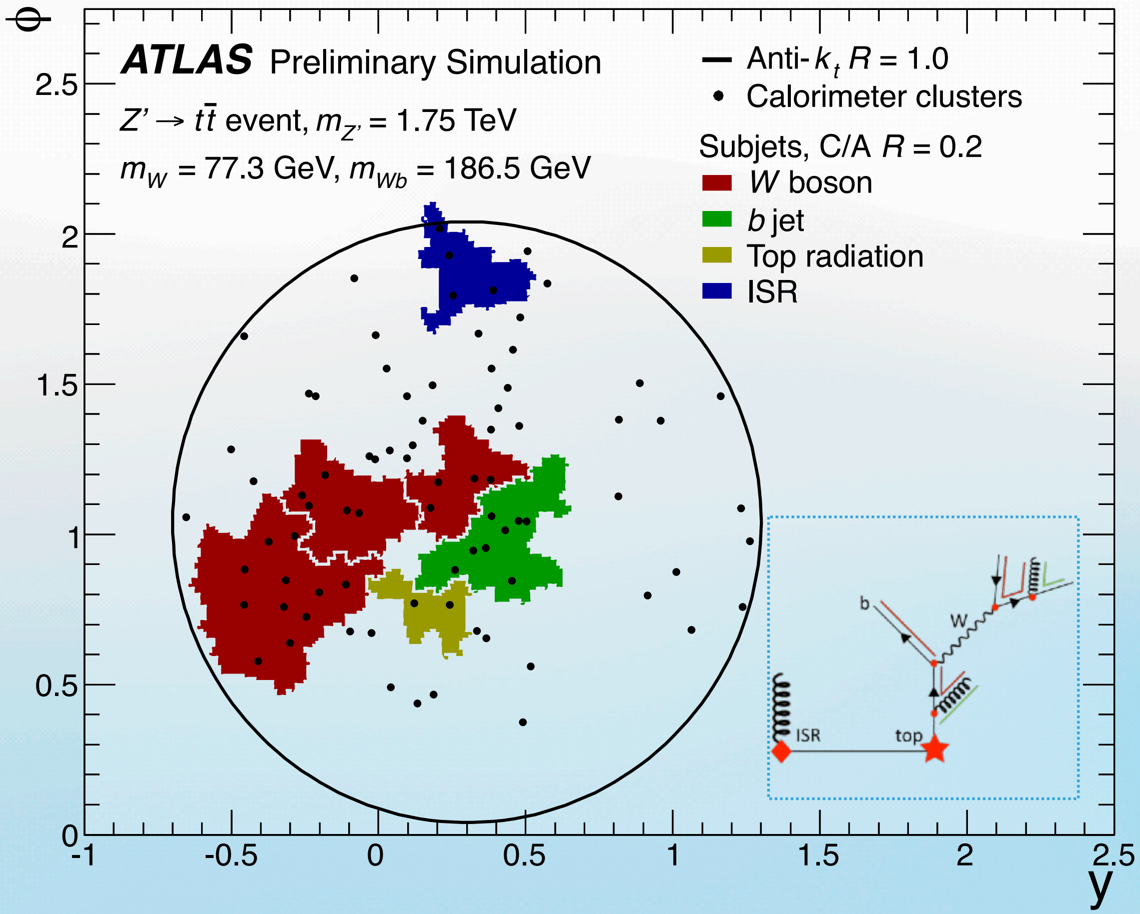
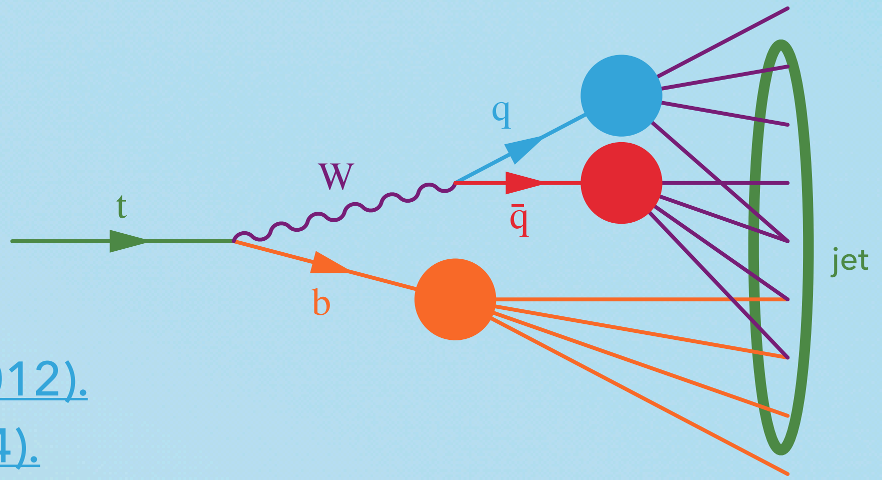
A more complex task:



Given a top quark jet from fully-hadronic top decay, can we measure properties of the *W*-boson, such as its momentum?

- Analogous to *shower deconstruction*: jet components are associated with elements of top decay/shower. [e,f]
- In our task, identifying part of the jet as the W-boson showering products is implicit.
    - Deconstruction works at the subjet level – we will work at the *constituent* level!
- Our goal is to *measure properties* of the W-boson!

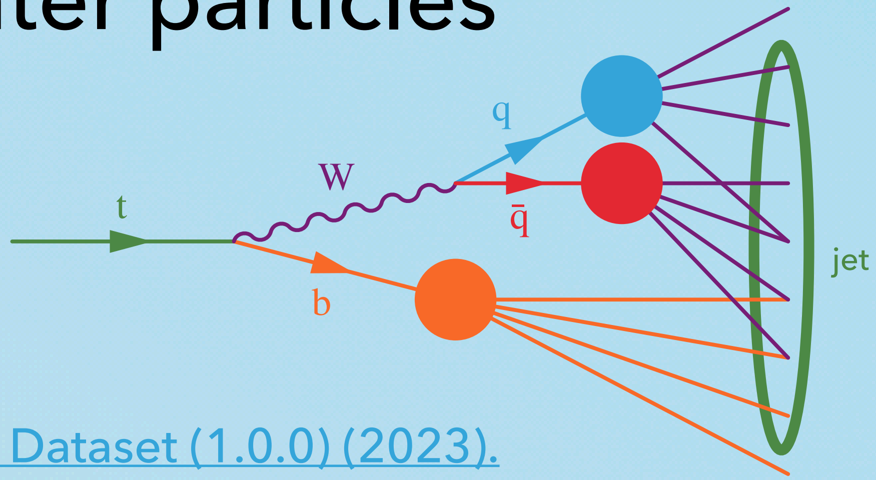




[e] D. E. Soper, M. Spannowsky, Finding top quarks with shower deconstruction (2012).

[f] The ATLAS collaboration, Performance of shower deconstruction in ATLAS (2014).

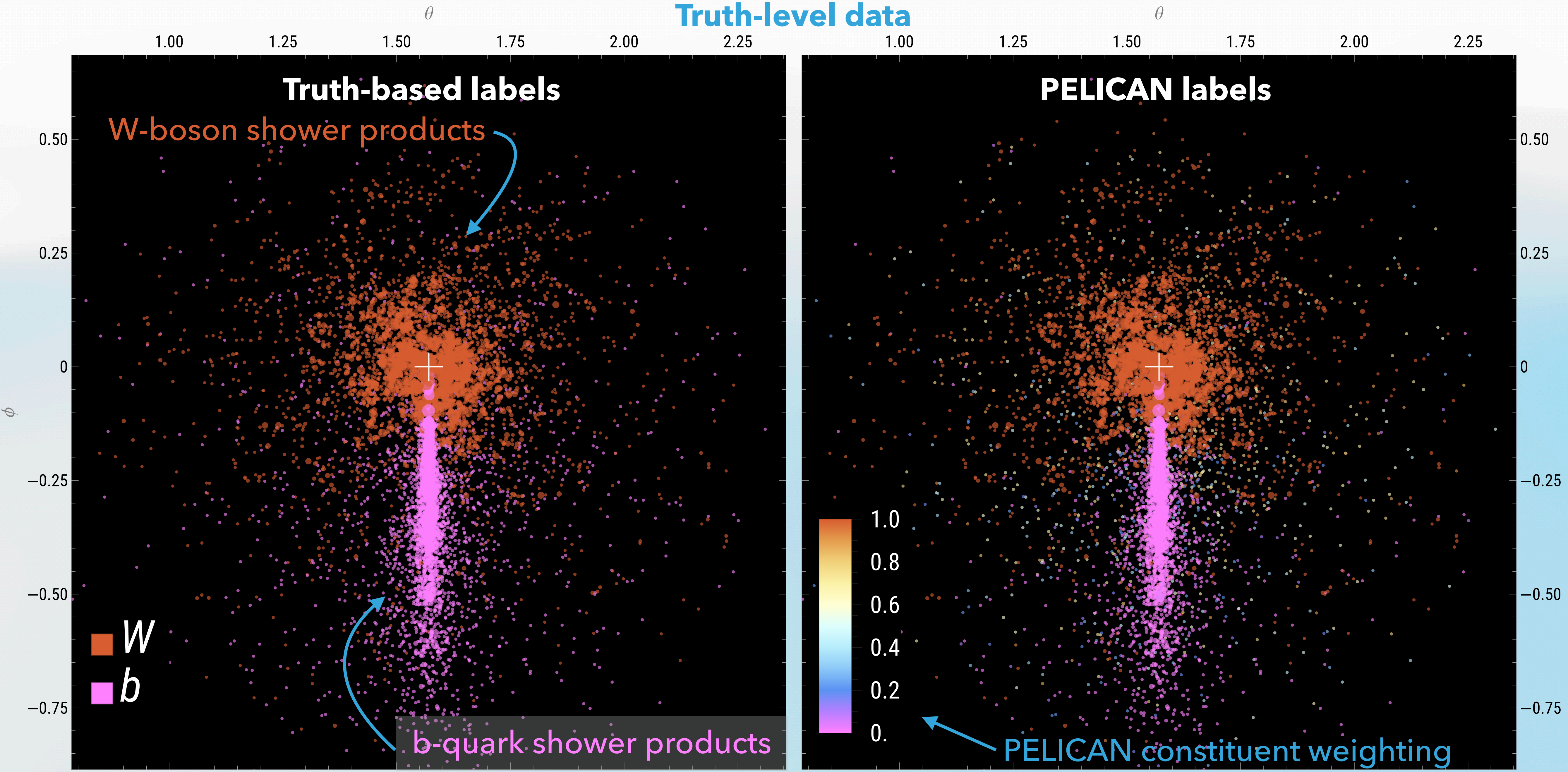
- Use PELICAN's vector form: $F^{\mu} = \sum_{k} I_k\left(p_1, \ldots, p_N\right) p_k^{\mu}$
- Fully-hadronic tops, anti-k_T $R = 0.8$ jets. [g]
  - Nominal & variable true W mass: $m_W^0 \in [64,96]$ GeV.
- Predicted W-boson momentum is a *weighted* sum of jet constituent momenta.
- At truth-level, weights I_k should be binary *(is / is not W daughter)*.
  - W momentum is the sum of its daughter particles' momenta.



[g] J. T. Offermann, T. Hoffman, A. Bogatskiy, Top Jet W-Momentum Reconstruction Dataset (1.0.0) (2023).

PELICAN: MOMENTUM REGRESSION

- Aggregated jet displays, centered on truth-level W.
- PELICAN weights each constituent in producing W 4-momentum – interpretable as likelihood of being W daughter!



Truth-level data

Truth-based labels

W-boson shower products

b-quark shower products

PELICAN labels

PELICAN constituent weighting

PELICAN: MOMENTUM REGRESSION

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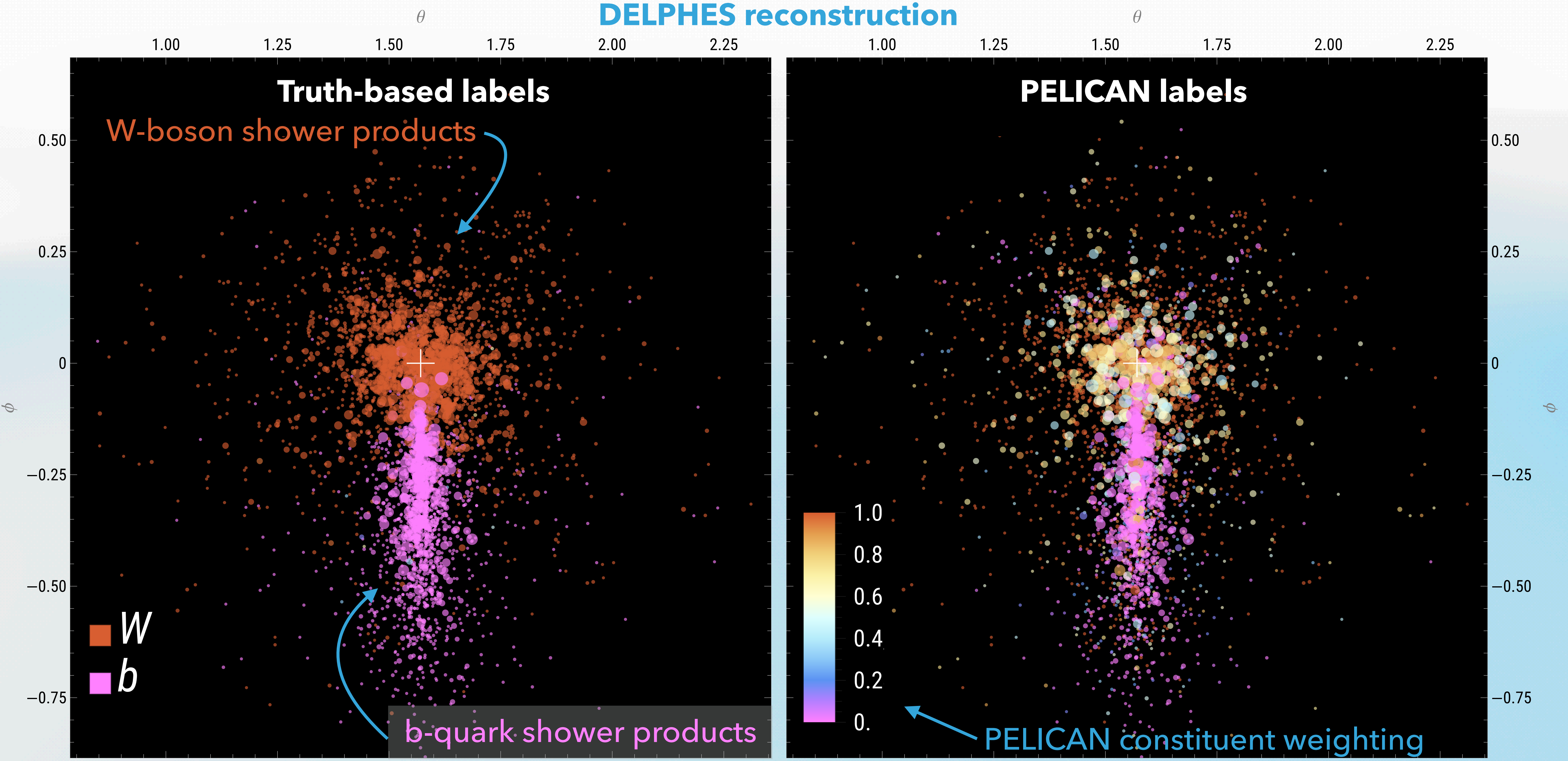
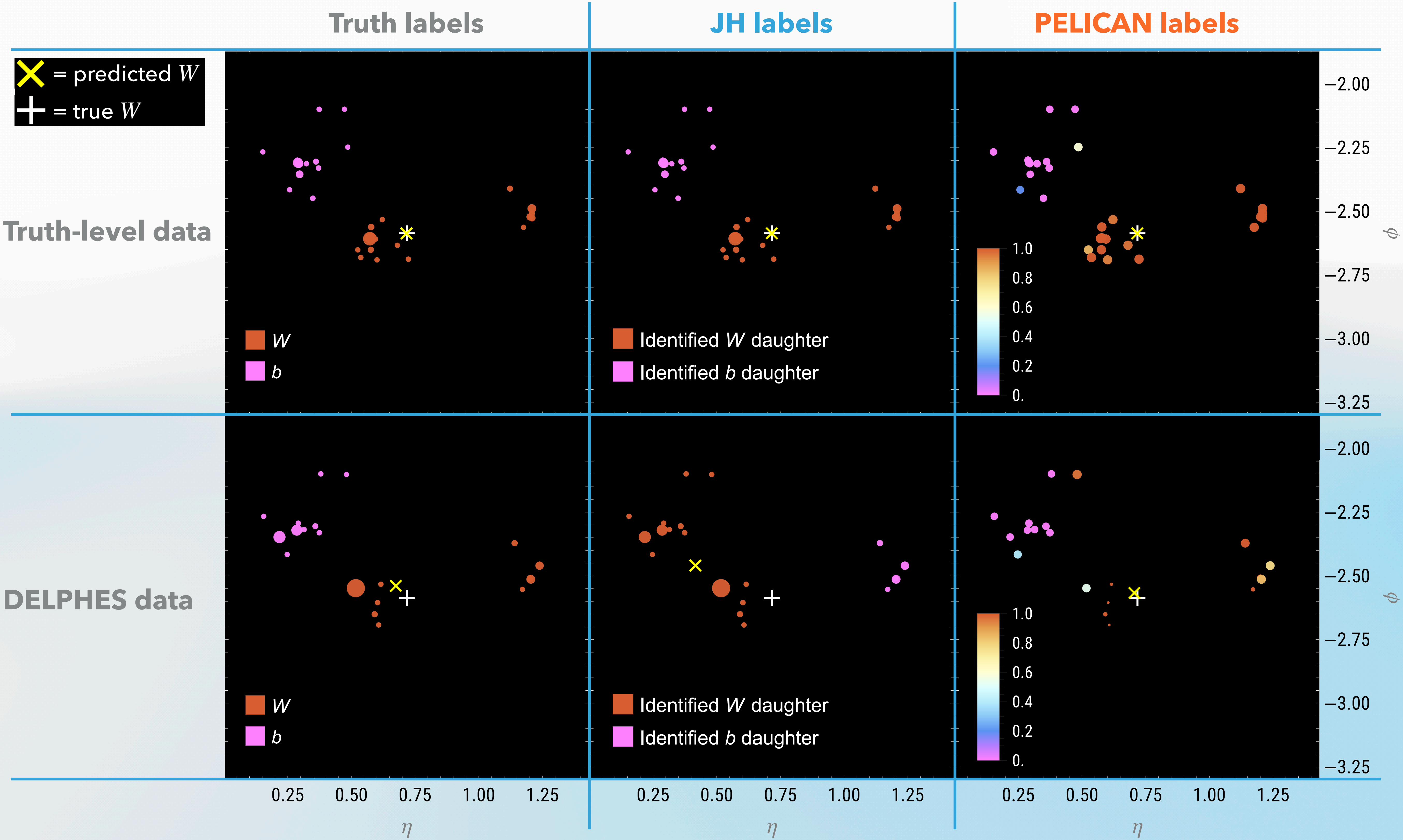
DELPHES reconstruction

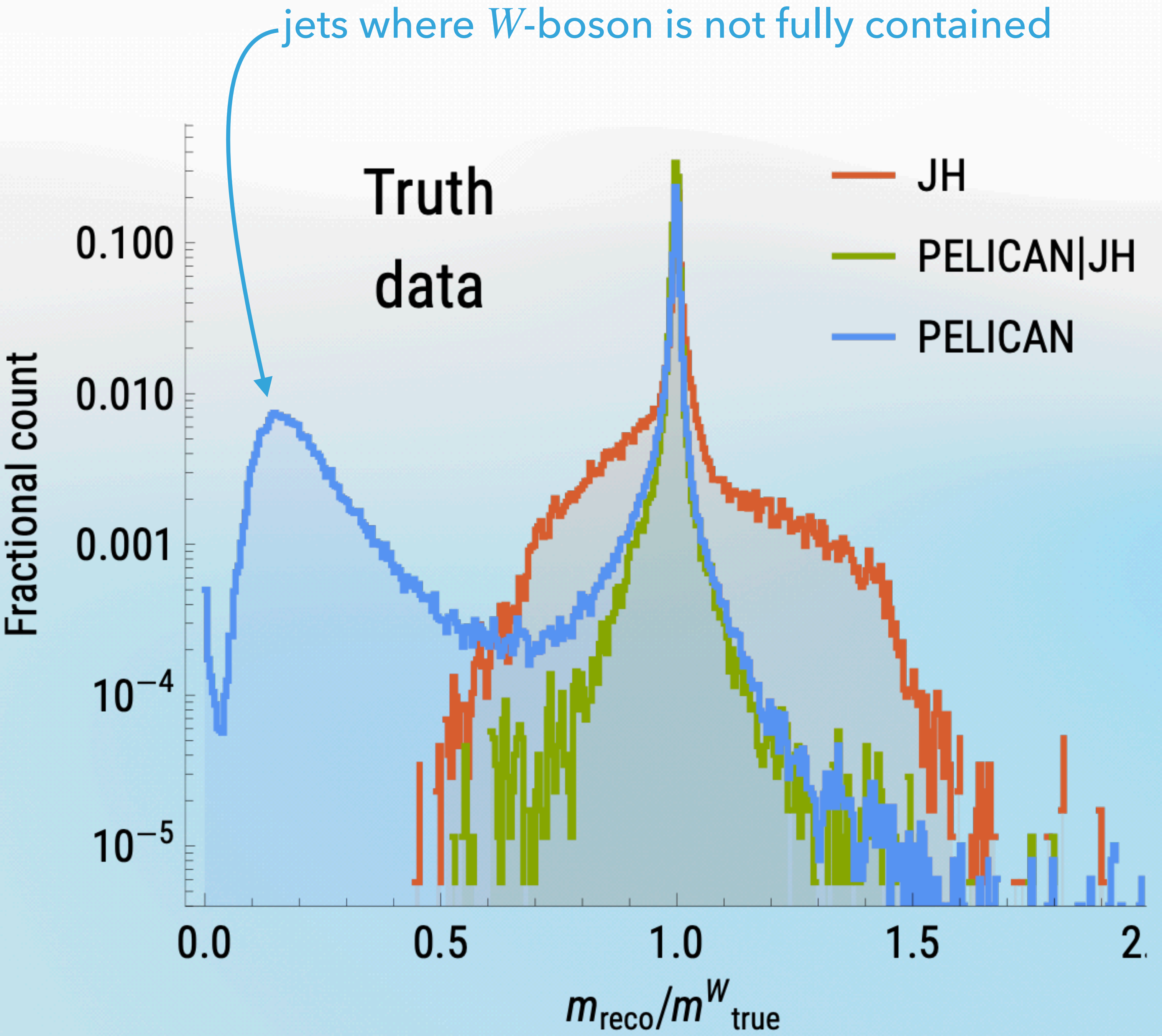


- PELICAN compared with the Johns Hopkins top tagger. [h]



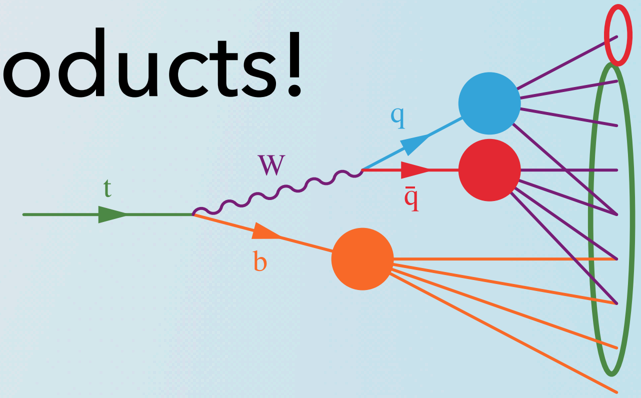
[h] D. E. Kaplan, K. Rehermann, M. D. Schwartz, and B. Tweedie, Top Tagging (2008).

- PELICAN can reconstruct W momentum on *all* jets.
  - JH predicts W momentum *only* on JH-tagged jets.
  - JH-tagged jets account for only ~35% of the dataset.
  - Evaluating PELICAN on tagged jets gives improved mass resolution!
    - What about the untagged jets?

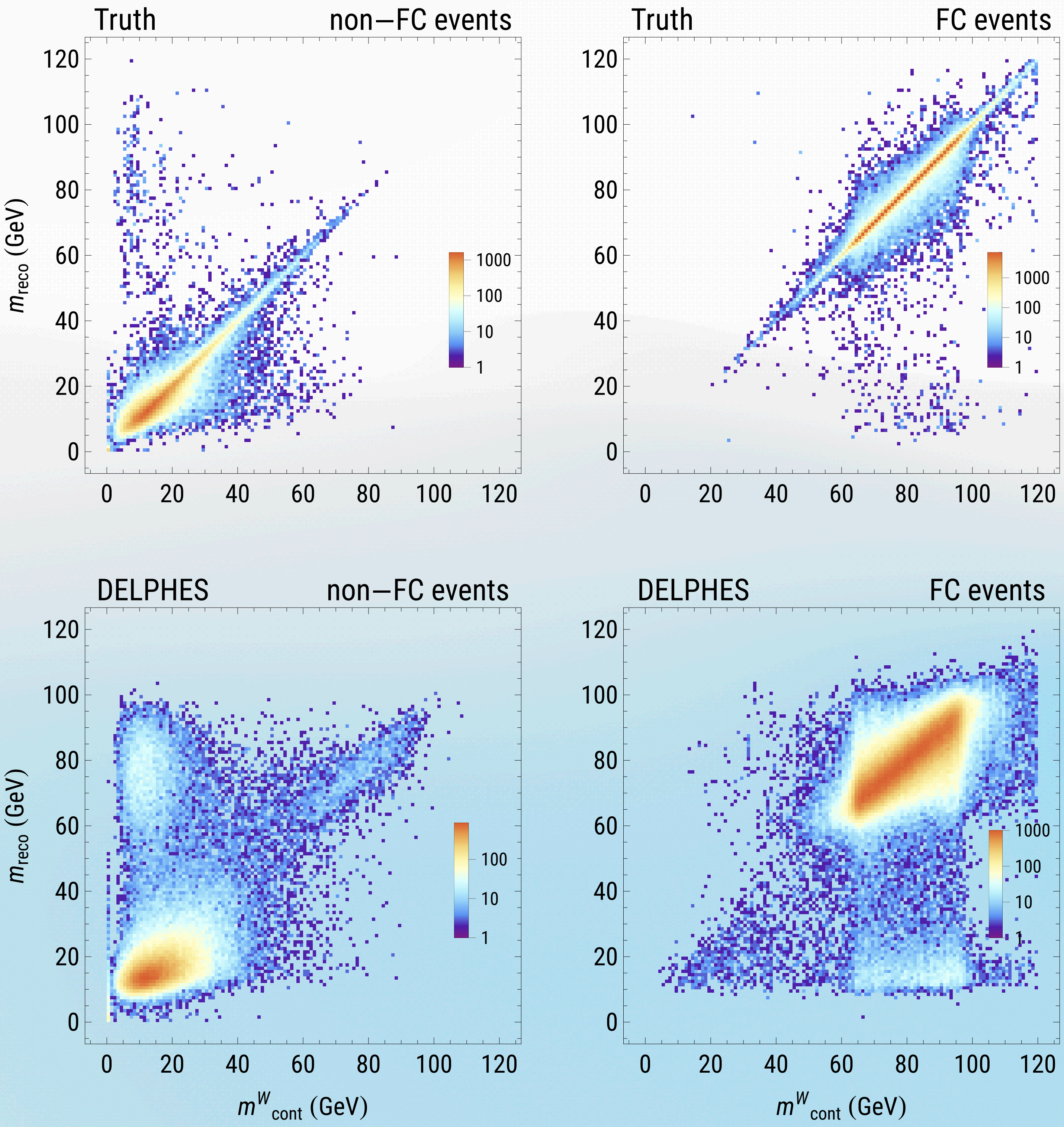

jets where W-boson is not fully contained

PELICAN: MOMENTUM REGRESSION

- Jets may not contain all $W \to qq'$ products.
- Train PELICAN targeting sum momentum of all *contained* W products.
- PELICAN reconstructs the momentum well, and can be used effectively to tag jets containing W decay products!



"FC" = jet contains $\mathrm{W} \to \mathrm{qq}'$



mass of contained W decay/shower products

IR safety

$$\lim_{\epsilon\to 0} f^{(N+1)}\left(p_1, \ldots, p_N, \epsilon p\right) = f^{(N)}\left(p_1, \ldots, p_N\right)$$

C safety

$$C_{12}(p)f = \partial_\lambda f\left(\lambda p, (1-\lambda)p, p_3, \ldots, p_N\right) = 0$$ (where $p^2 = 0$)

- IR- and IRC-safe implementations of PELICAN!
  - IR-safe regressor resolutions $\left(\sigma_{p_T}, \sigma_m, \sigma_{\Delta R}\right)$ worsen 20-35 % (truth-level), 40-50 % (DELPHES reconstruction)
  - IRC-safe regressor resolutions worsen 5-6 × (truth-level).

- PELICAN performs well in top-quark tagging, and W-boson momentum regression, and provides constituent-level information!
- Plenty of other problems where PELICAN can be used!
  - Top quark helicity measurement (in hadronic W channel)
  - Reconstructing resonant decays, complex decay chains
  - Charged particle tracking (add charge info!)
  - Full event reconstruction…

CONCLUSION & ACKNOWLEDGEMENTS

- PELICAN repo: https://github.com/abogatskiy/PELICAN
- New paper: https://arxiv.org/abs/2307.16506

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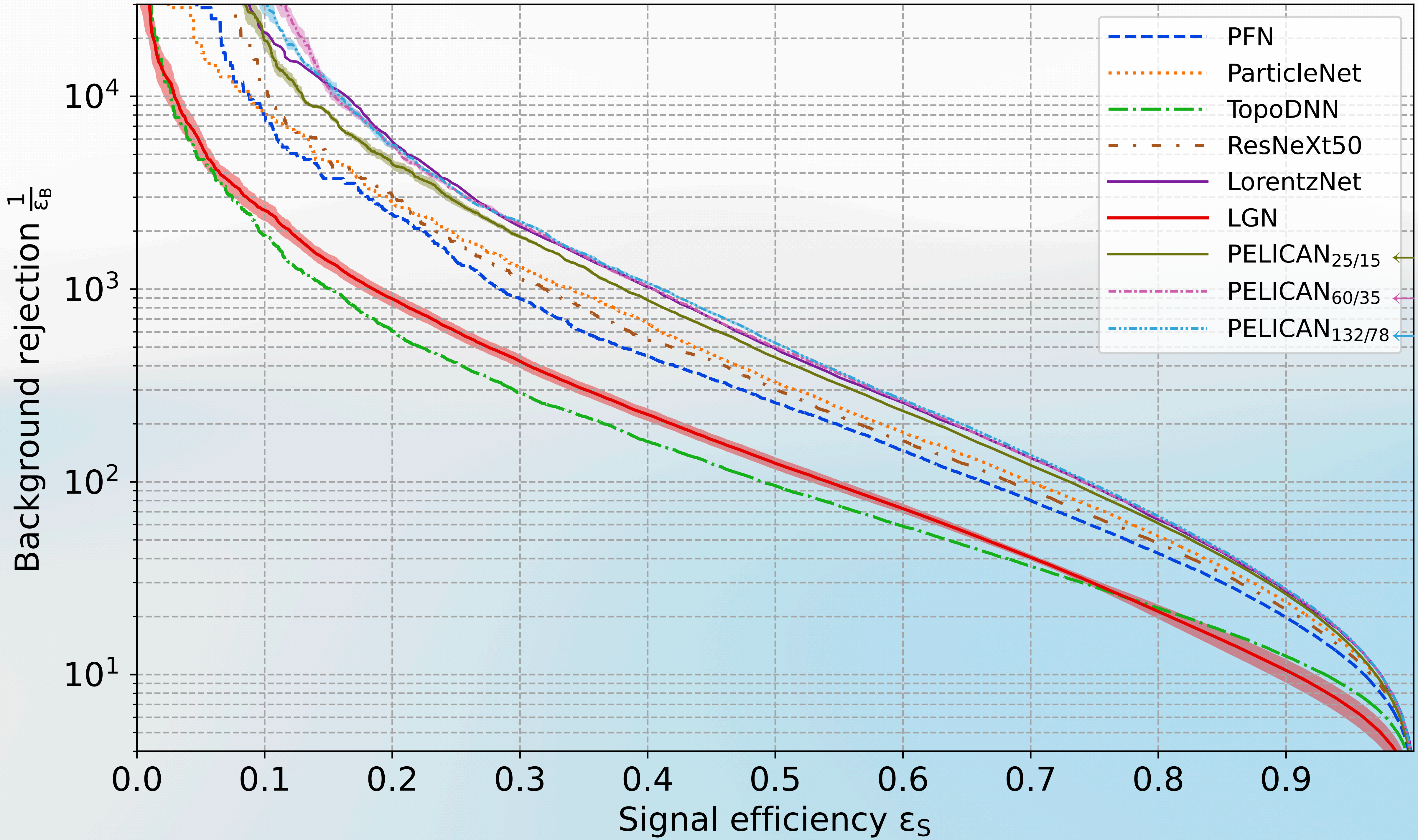
QUESTIONS?

BACKUP

- Latest top-tagging results show that performance saturates quickly w.r.t. number of parameters. [i]



← 11k params
← 48k params
← 208k params

[i] A. Bogatskiy, T. Hoffman, D. W. Miller, J. T. Offermann, X. Liu, Explainable Equivariant Networks: PELICAN (2023).

PELICAN: TOP-TAGGING

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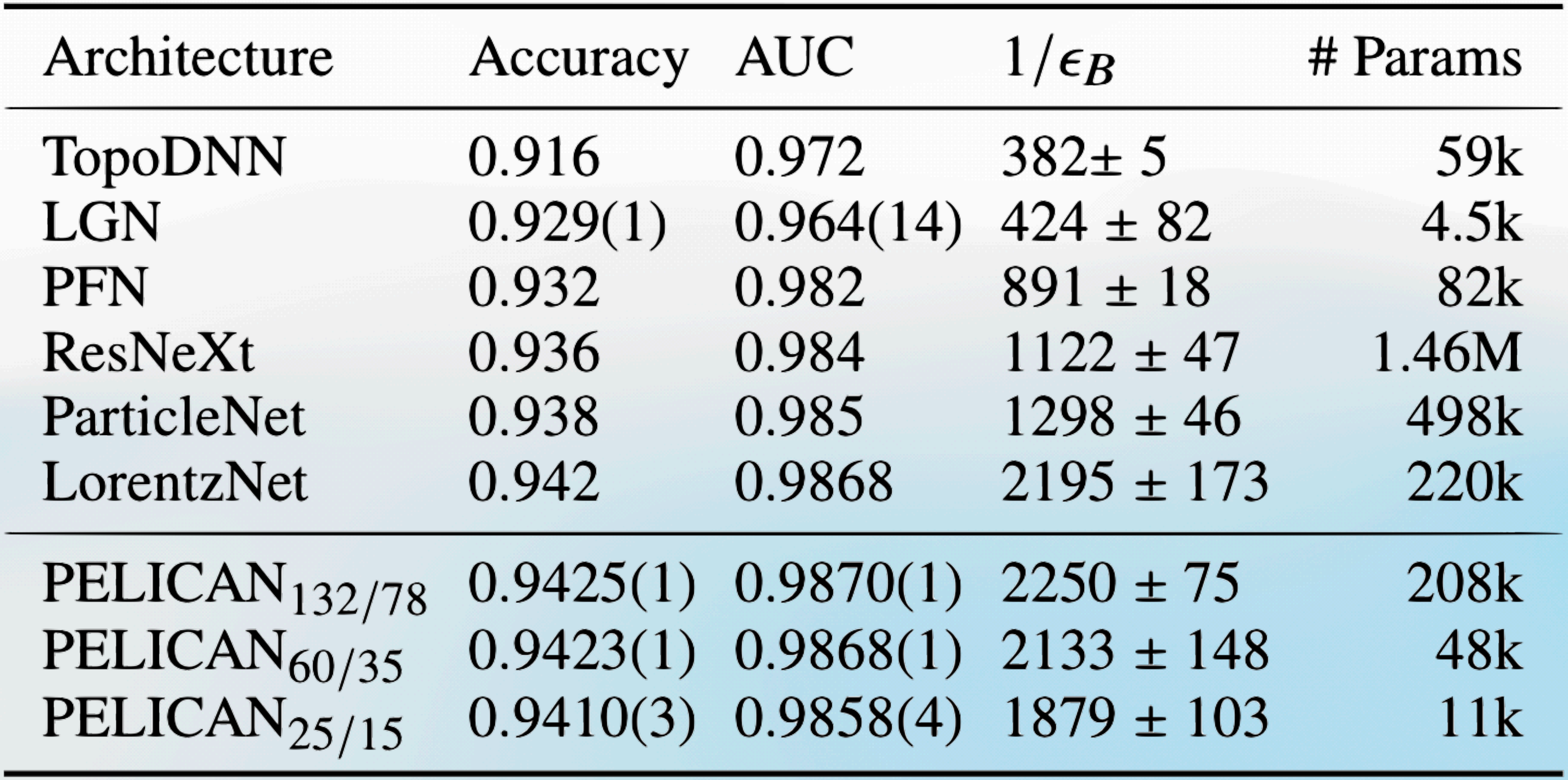


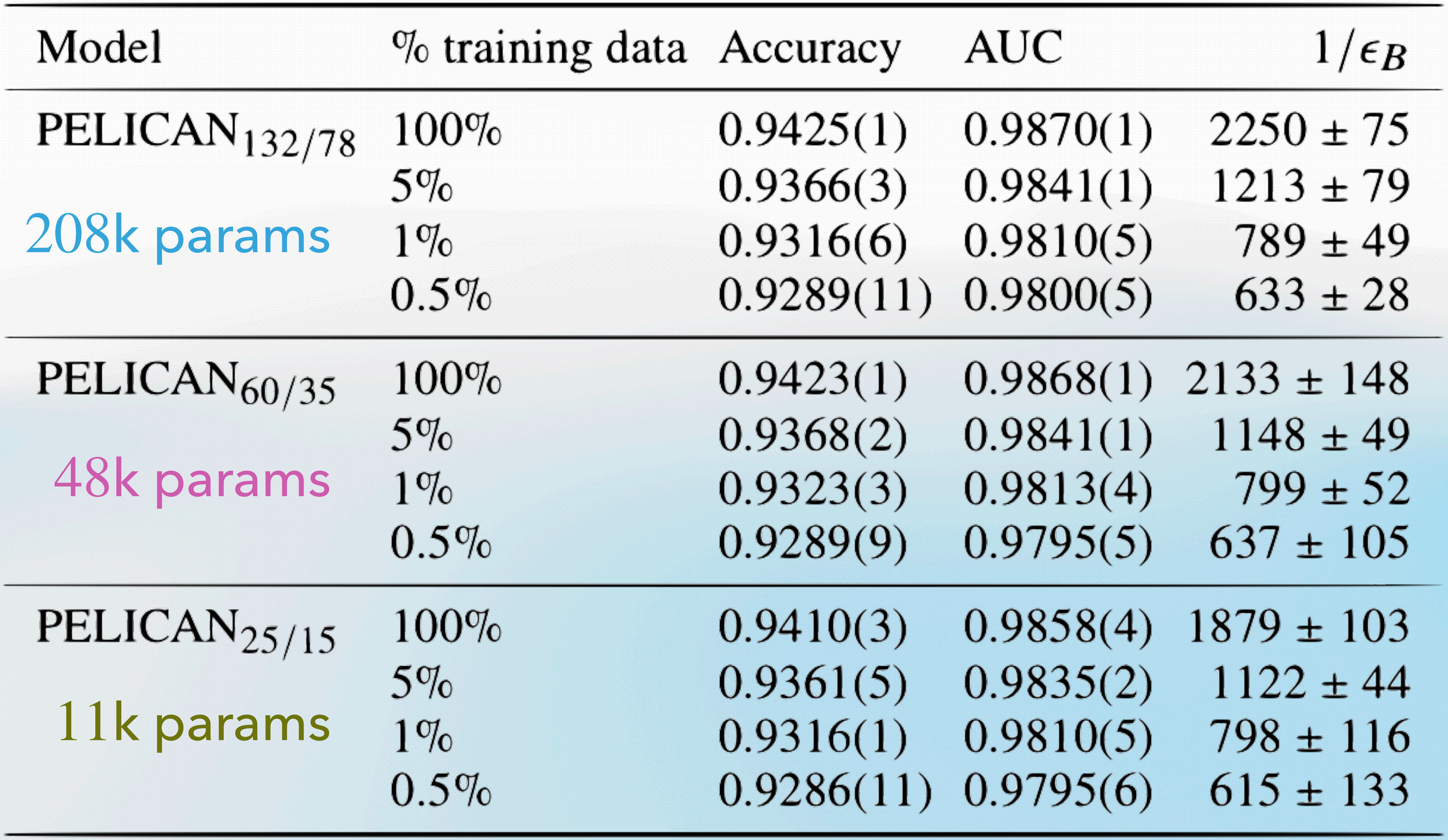
Architecture	Accuracy	AUC	$1/\epsilon_B$	# Params
TopoDNN	0.916	0.972	382± 5	59k
LGN	0.929(1)	0.964(14)	424 ± 82	4.5k
PFN	0.932	0.982	891 ± 18	82k
ResNeXt	0.936	0.984	1122 ± 47	1.46M
ParticleNet	0.938	0.985	1298 ± 46	498k
LorentzNet	0.942	0.9868	2195 ± 173	220k
$\text{PELICAN}_{132/78}$	0.9425(1)	0.9870(1)	2250 ± 75	208k
$\text{PELICAN}_{60/35}$	0.9423(1)	0.9868(1)	2133 ± 148	48k
$\text{PELICAN}_{25/15}$	0.9410(3)	0.9858(4)	1879 ± 103	11k

$\text{PELICAN}_{X/Y}$ = MSG has X input channels, Y output channels

[i] A. Bogatskiy, T. Hoffman, D. W. Miller, J. T. Offermann, X. Liu, Explainable Equivariant Networks: PELICAN (2023).

PELICAN: TOP-TAGGING

- PELICAN is very efficient with training data. [i]

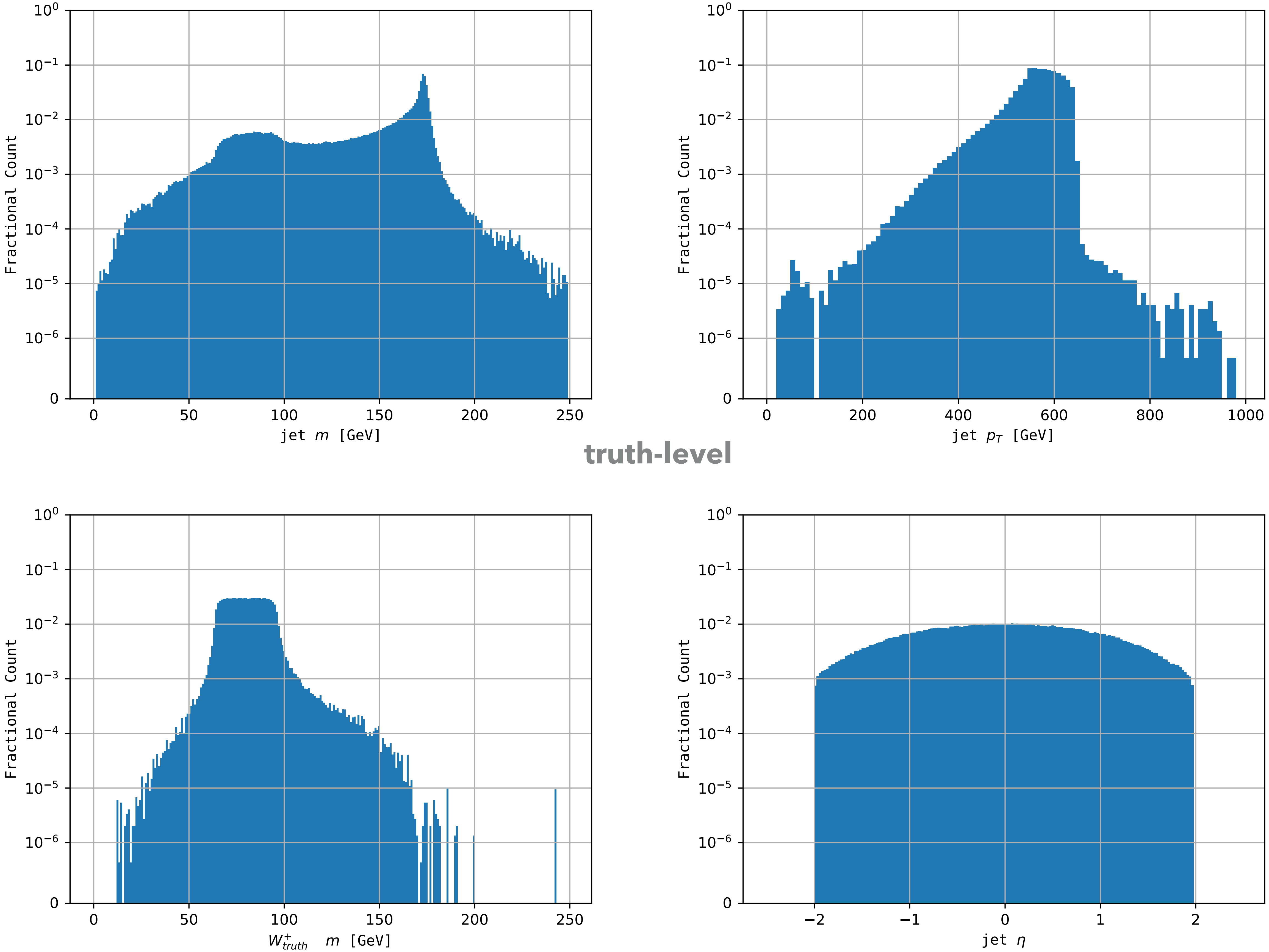


Model	% training data	Accuracy	AUC	$1/\epsilon_B$
$\text{PELICAN}_{132/78}$	100%	0.9425(1)	0.9870(1)	2250 ± 75
	5%	0.9366(3)	0.9841(1)	1213 ± 79
208k params	1%	0.9316(6)	0.9810(5)	789 ± 49
	0.5%	0.9289(11)	0.9800(5)	633 ± 28
$\text{PELICAN}_{60/35}$	100%	0.9423(1)	0.9868(1)	2133 ± 148
	5%	0.9368(2)	0.9841(1)	1148 ± 49
48k params	1%	0.9323(3)	0.9813(4)	799 ± 52
	0.5%	0.9289(9)	0.9795(5)	637 ± 105
$\text{PELICAN}_{25/15}$	100%	0.9410(3)	0.9858(4)	1879 ± 103
	5%	0.9361(5)	0.9835(2)	1122 ± 44
11k params	1%	0.9316(1)	0.9810(5)	798 ± 116
	0.5%	0.9286(11)	0.9795(6)	615 ± 133

[i] A. Bogatskiy, T. Hoffman, D. W. Miller, J. T. Offermann, X. Liu, Explainable Equivariant Networks: PELICAN (2023).

W-BOSON MOMENTUM REGRESSION: DATASET

HEPData4ML tool: https://github.com/janTOffermann/HEPData4ML



truth-level

W-BOSON MOMENTUM REGRESSION: DATASET

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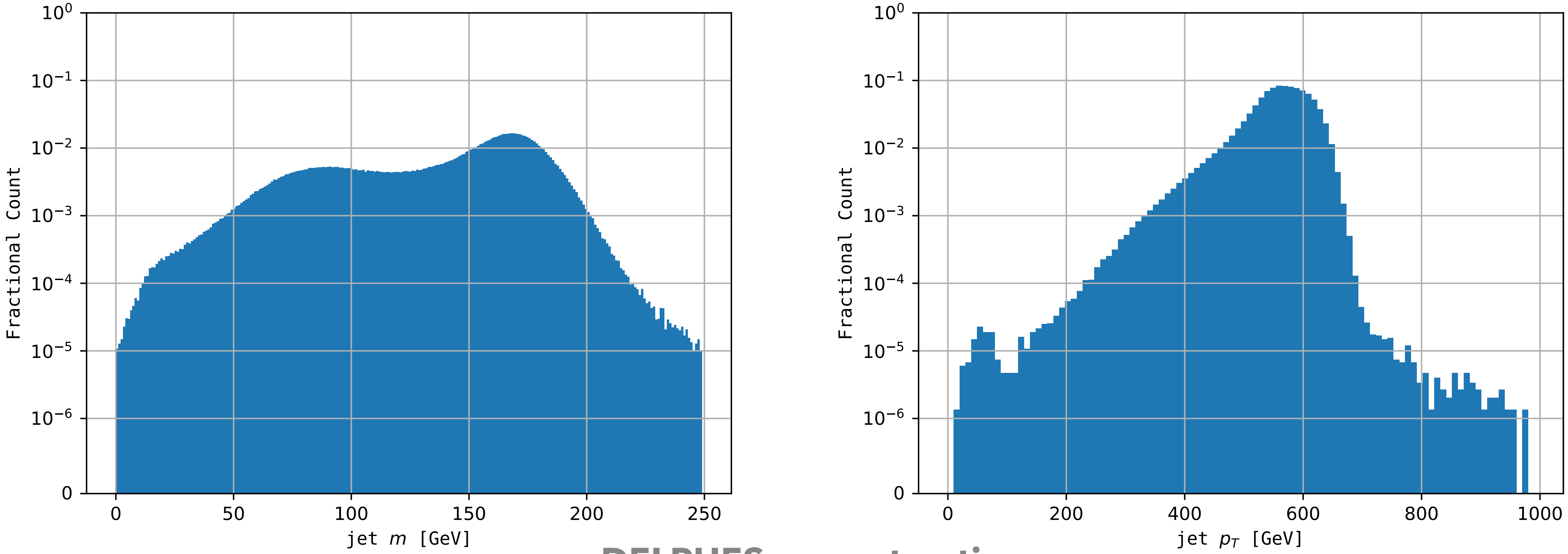
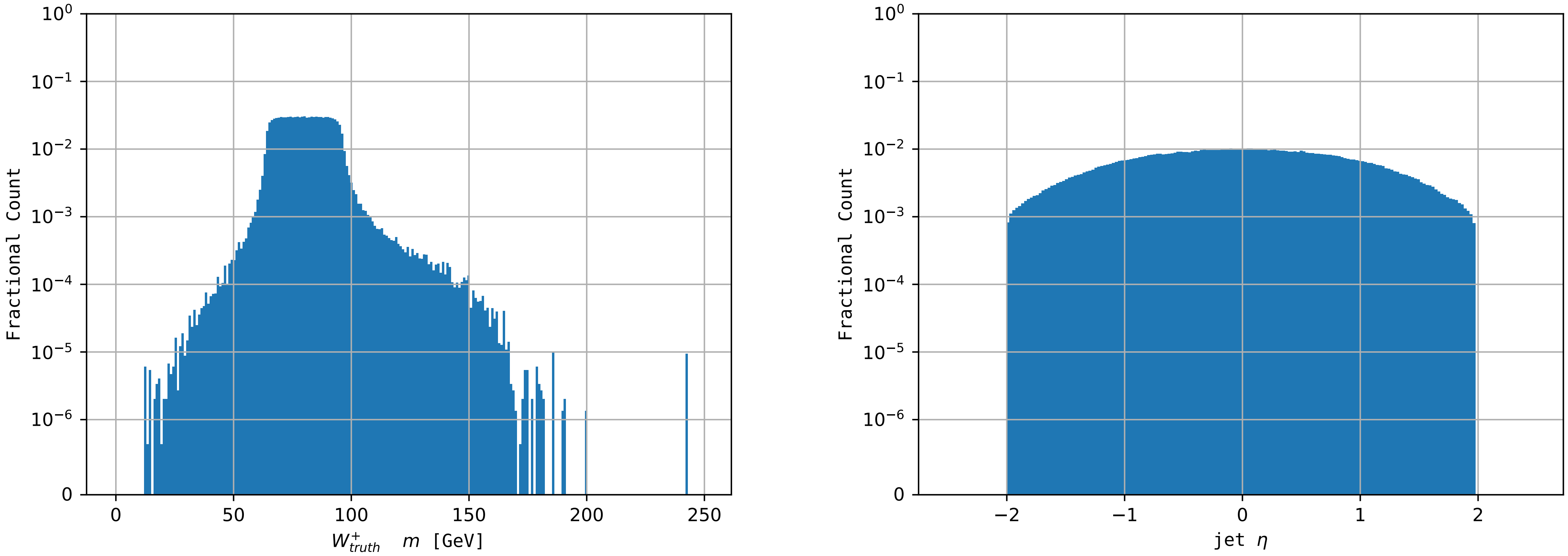
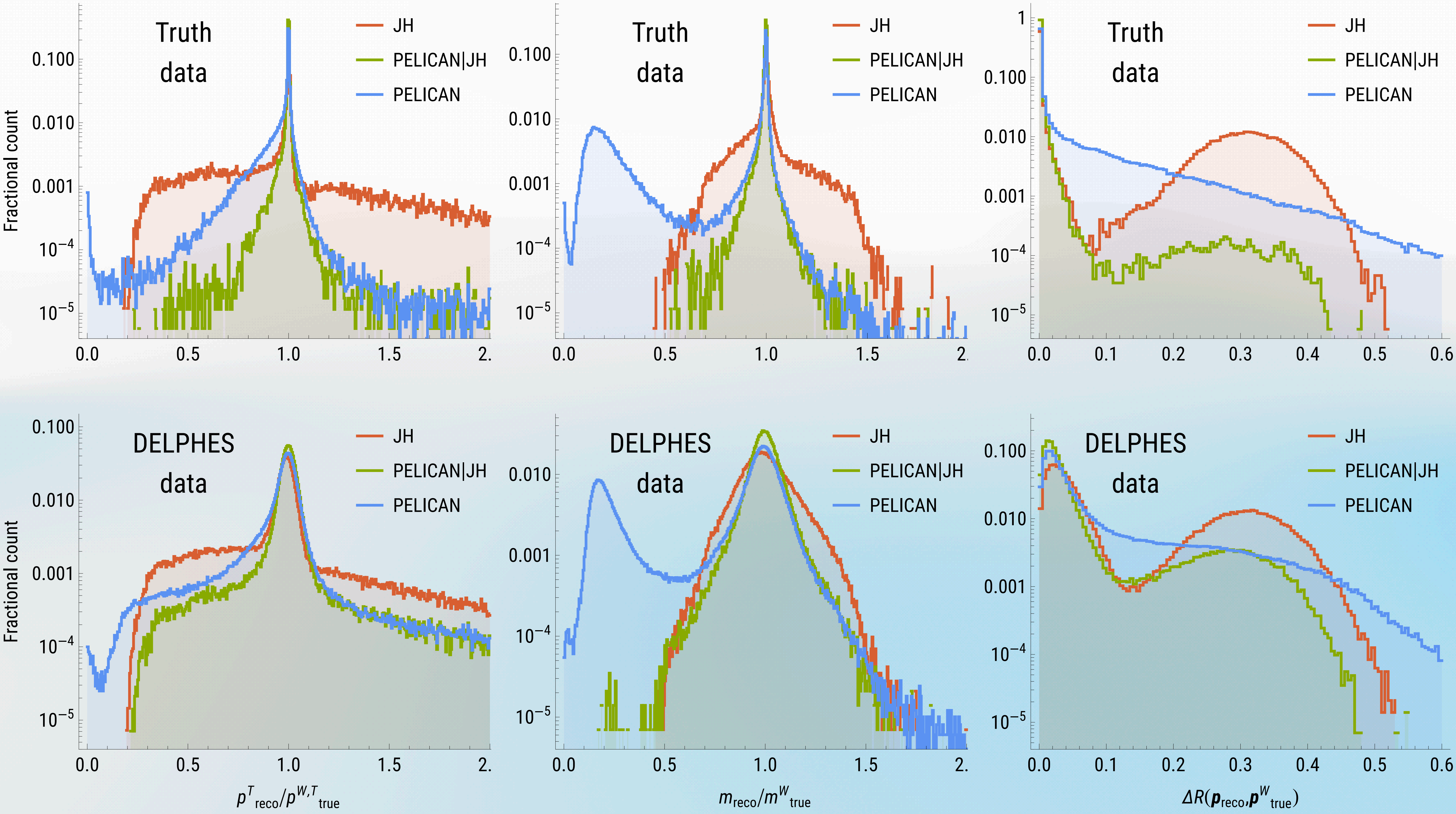


DELPHES reconstruction

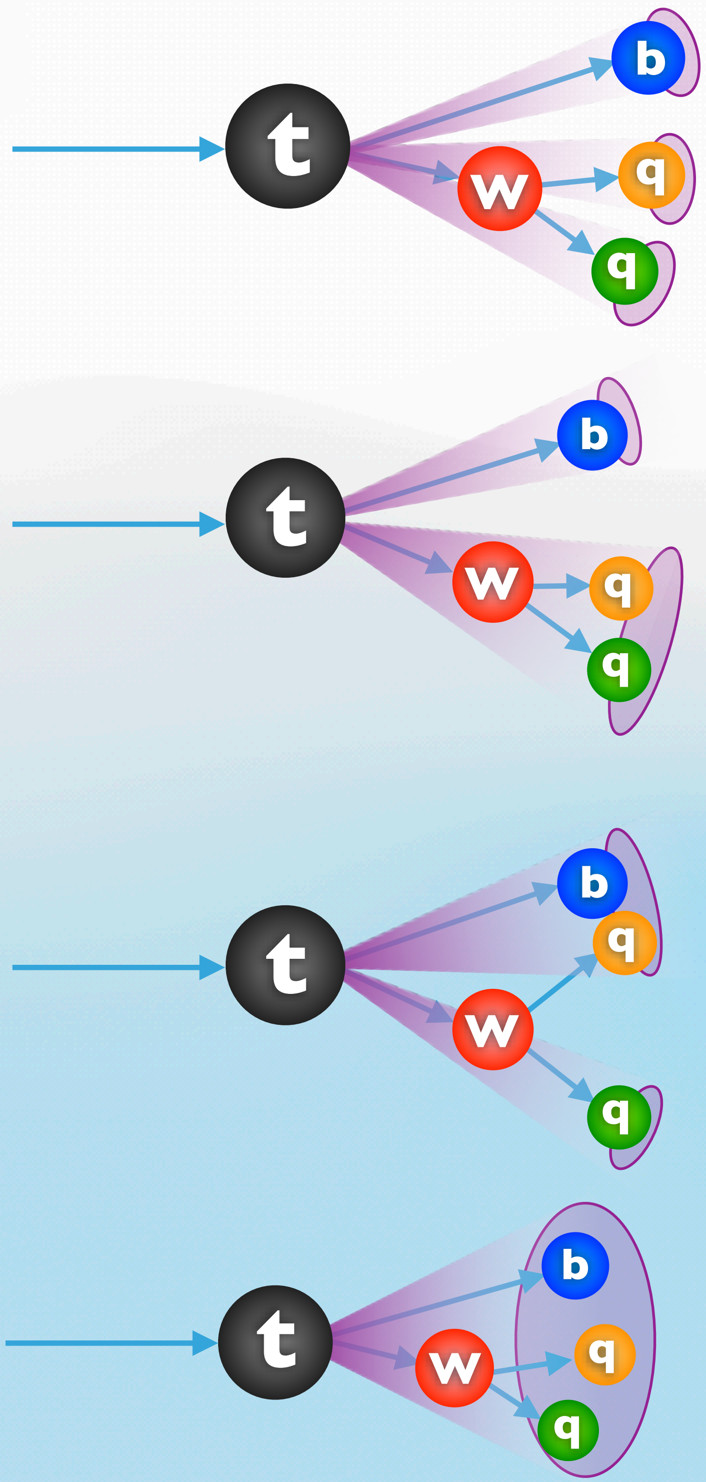


W-BOSON MOMENTUM REGRESSION: RESOLUTIONS



W-BOSON MOMENTUM REGRESSION: CONTAINMENT

- Top quark jets might not contain all the decay products.
- Cannot reconstruct W-boson from jets that do not contain $W \to qq'$ (not enough info!).
- Can train regressor to construct sum of W decay products within the jet.



Unmerged
(q jet + q jet + b jet)

Partially merged
(qq jet + b jet)

Partially merged
(bq jet + q jet)

Fully merged
(bqq jet)

Image Source: Jet Substructure HATS@LPC (June 18-19, 2014) (modified)

W-BOSON MOMENTUM REGRESSION: JOHNS HOPKINS TOP TAGGER

- Re-cluster jet with Cambridge-Aachen algorithm.
- Iteratively de-cluster the CA jet, producing 2 subjets.
- Throw out softer jet if $p_{T,2} / p_T < \delta_p$.
- Continue until:
  - Both objects harder than δ_p. ← both objects are subjets, repeat process on them
  - Both objects softer than δ_p.
  - Two objects are too close, $|\Delta\eta| + |\Delta\phi| < \delta_r$.
  - Only one calorimeter cell is left.

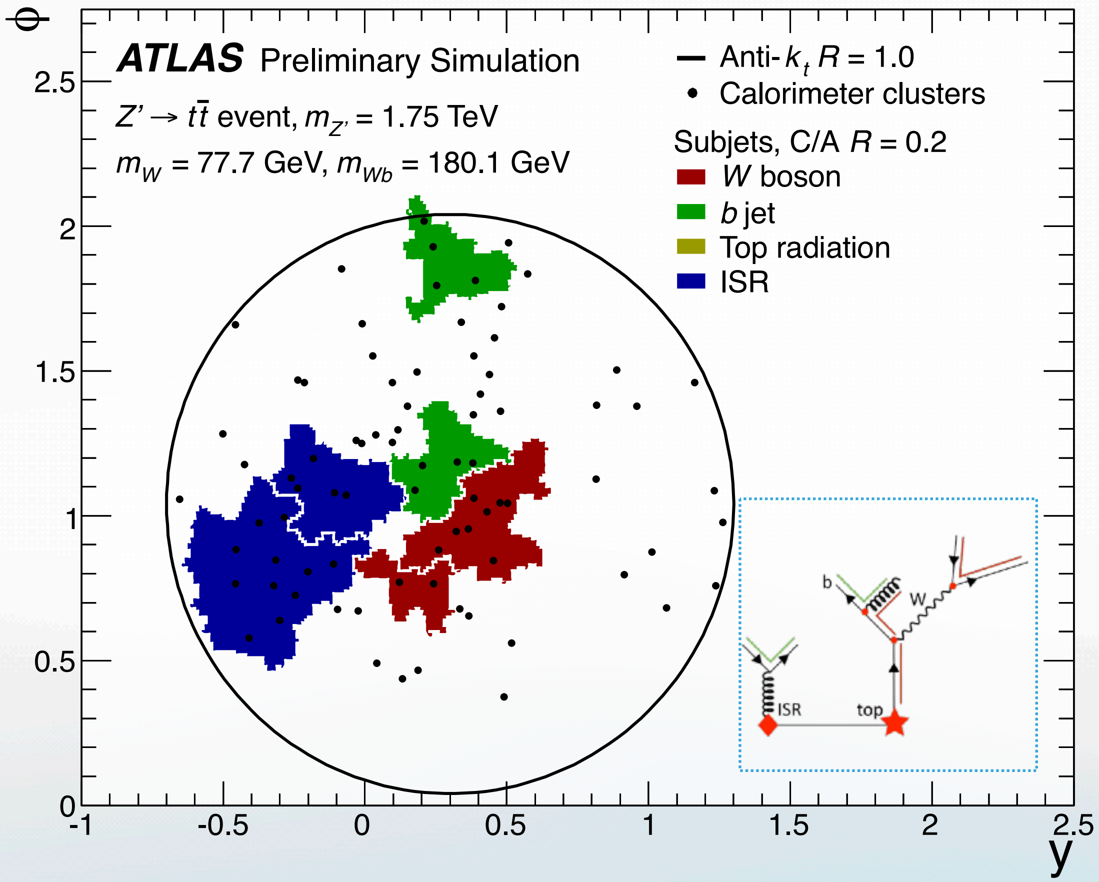
objects are irreducible

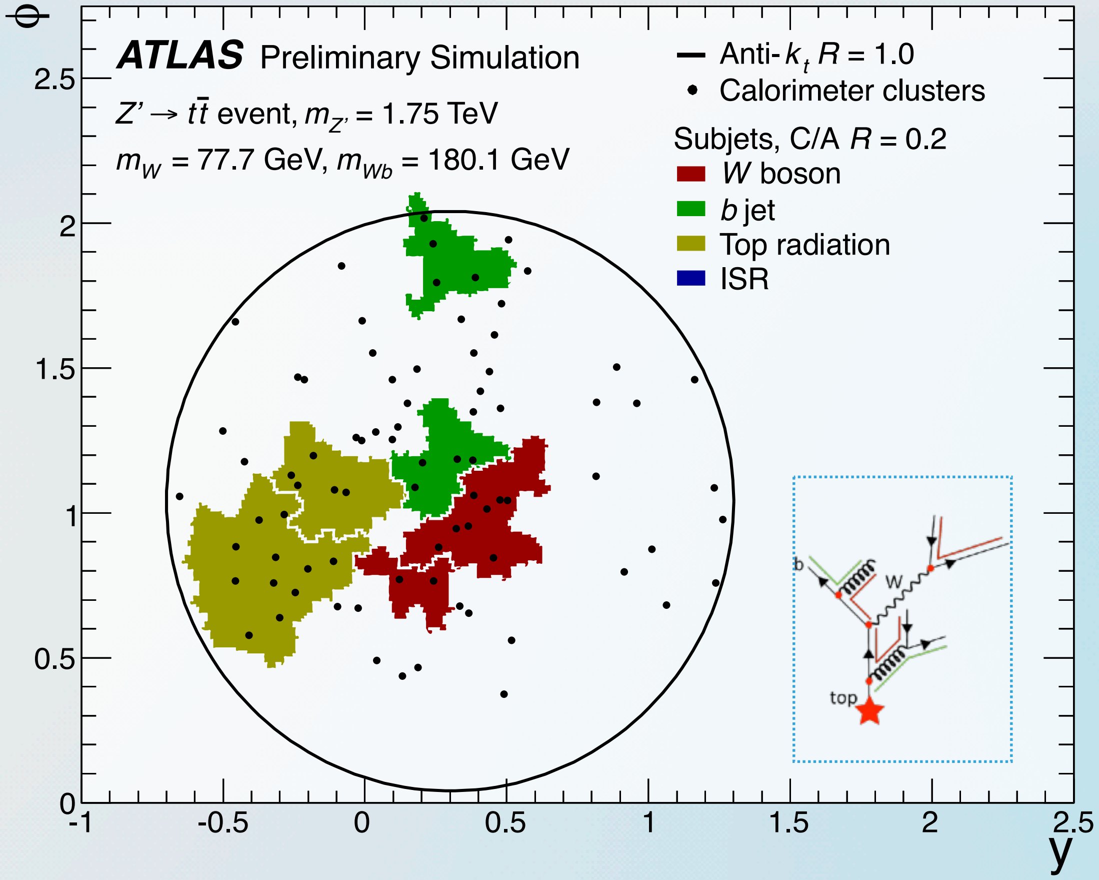
W-BOSON MOMENTUM REGRESSION: JOHNS HOPKINS TOP TAGGER

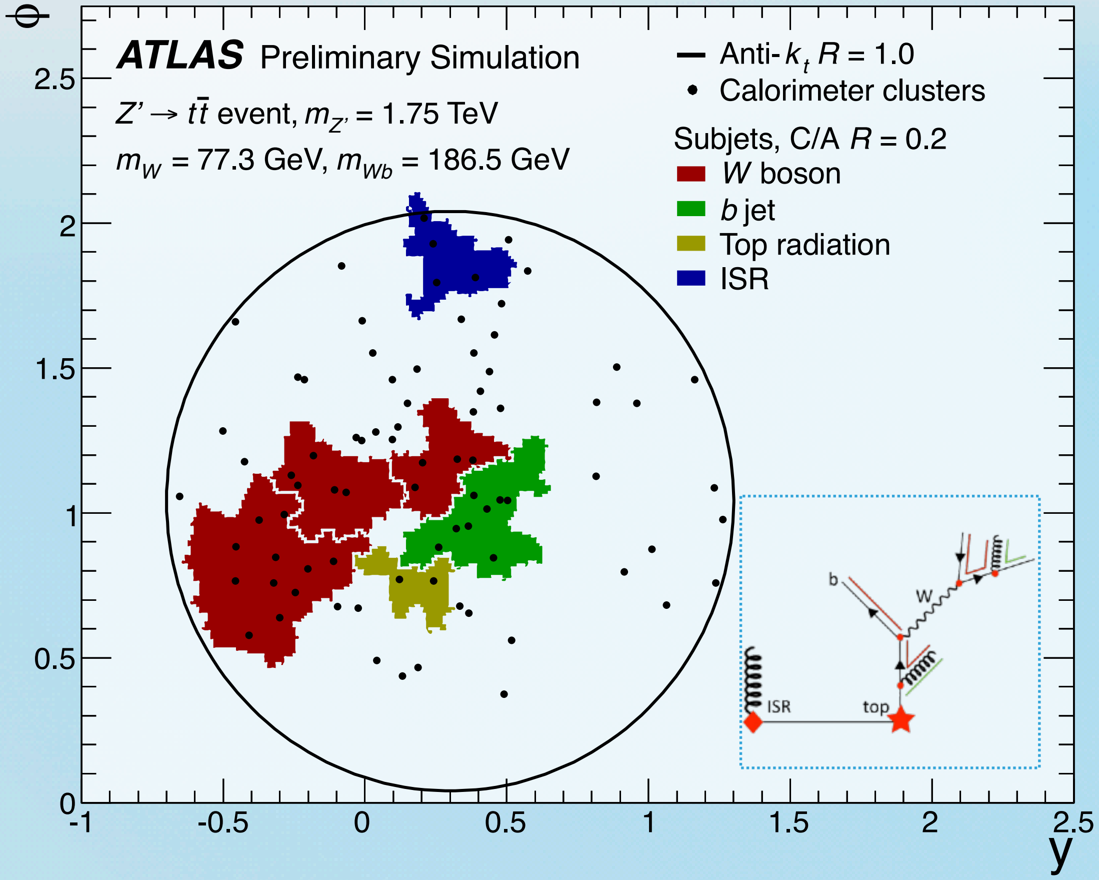
- Reject jets which only yield 2 subjets.
- For jets with 3+ subjets, W candidate will be constructed from the 2 subjets whose mass is closest to m_W.
- Implemented with (default) values and cuts:
  - $\delta_p = 0.1, \delta_r = 0.19$
  - Cuts:
    - $m_t^{\text{reco}} \in \{150{,}200\}$ GeV, $m_W^{\text{reco}} \in \{65{,}95\}$ GeV
    - $\cos\left(\theta_W\right) < 0.7$

W-BOSON MOMENTUM REGRESSION: SHOWER DECONSTRUCTION

- Shower deconstruction is a method for determining the likeliest showering history of a given jet.
- Identification done at the *subjet* level.







PELICAN: ACHIEVING IRC SAFETY

- Achieving IR safety = remove dependence on multiplicity.
  - Remove scaling functions based on # of particles.
  - Set bias to zero in all linear layers.
  - Input embedding maps $0 \to 0$, activation has a fixed point at zero. *(PELICAN already satisfies these)*
  - *Soft masking*: *Last 12 aggregators* followed by multiplication by $J \cdot p_i$, with $J = \sum_{i=1}^{N} p_i$ scaled and clipped to be within $\left[-1,1\right]$.

- Achieving C-safety = output depends on massless inputs only through their sum.
  - Soft mask applied after input layer, multiplication by m_i^2 instead of by $J \cdot p_i$.
  - This *also* gives IR safety → applied C-safety modification gives a fully IRC-safe PELICAN.
- More significant negative effect on performance than just using the IR-safe modifications.