

Generalization Properties of Jet Classification

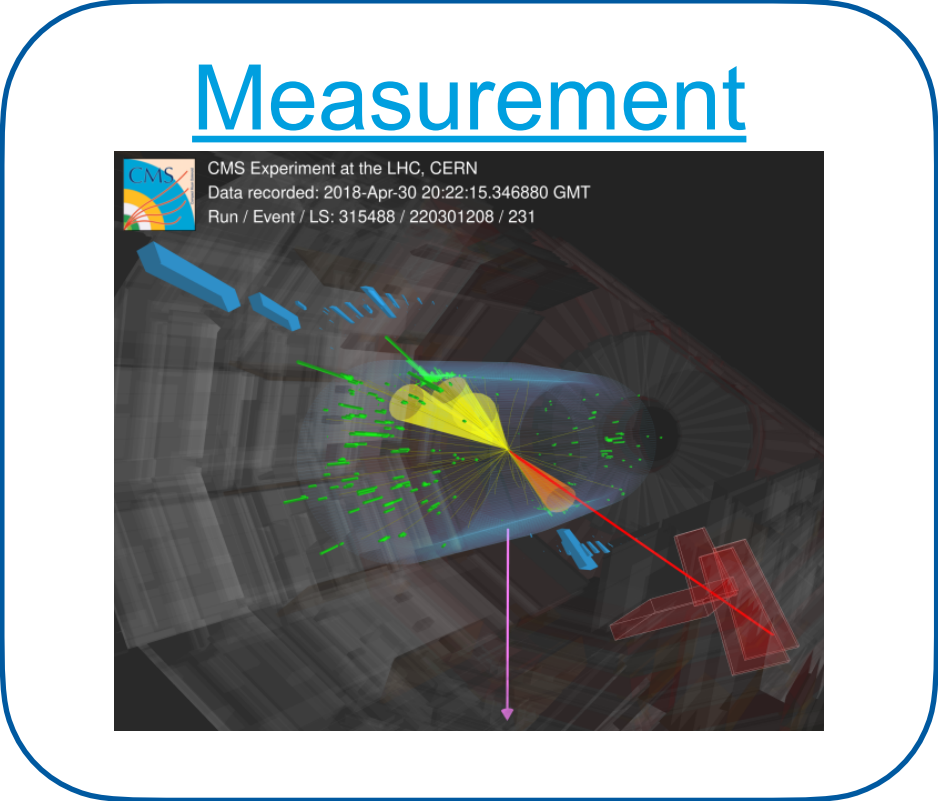
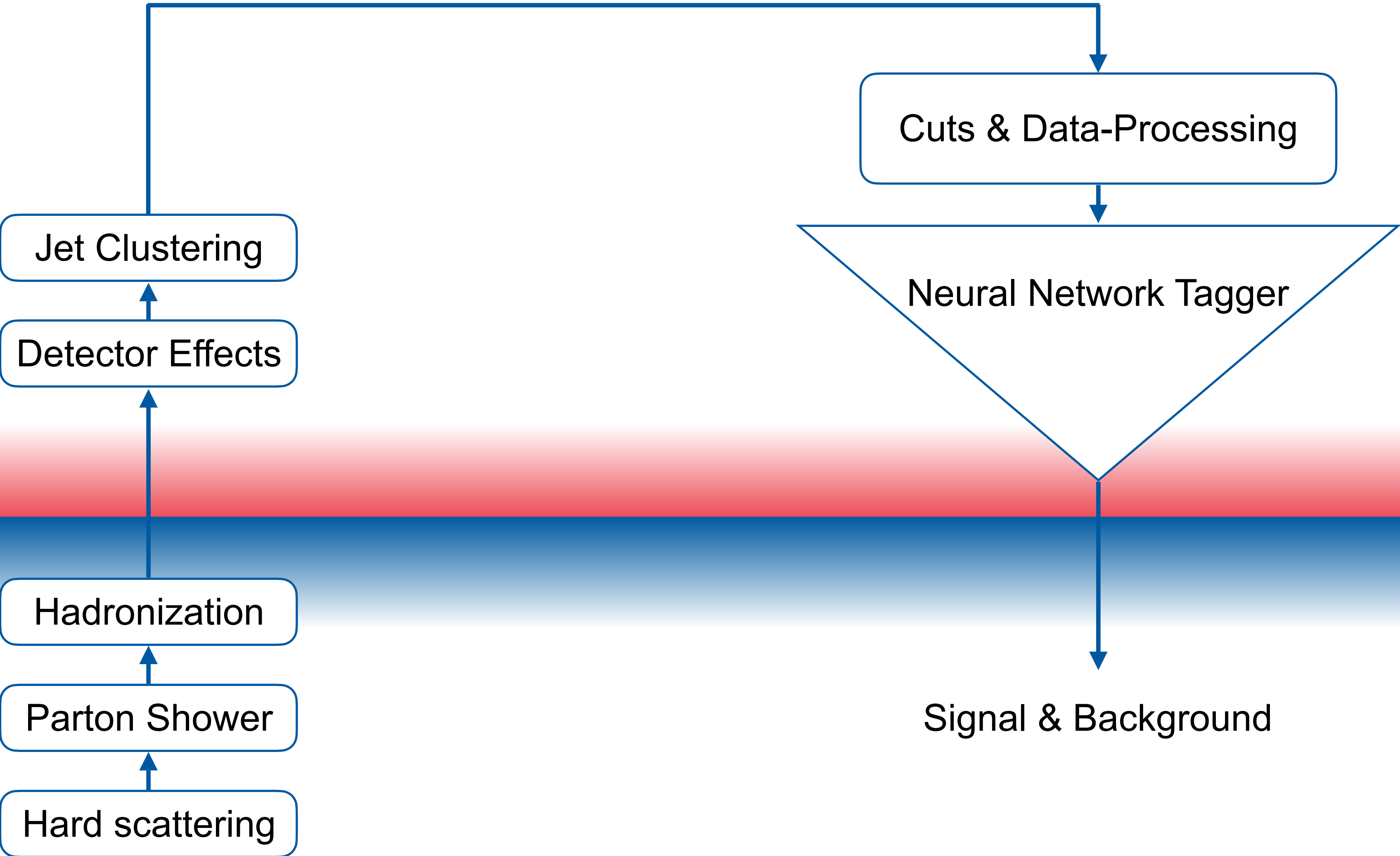
Sebastian Bieringer, Gregor Kasieczka, Jan Kieseler

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sebastian.guido.bieringer@uni-hamburg.de

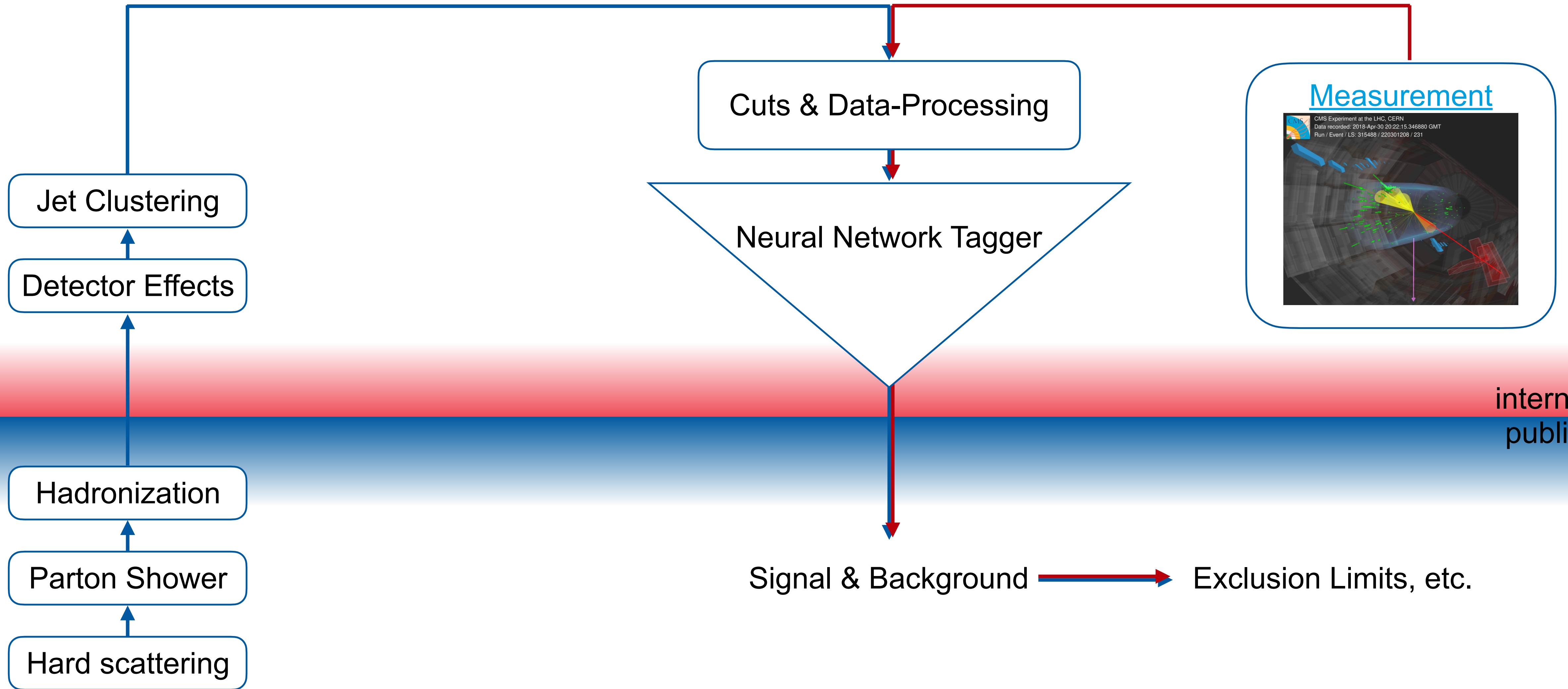
09.11.2023 - ML4jets 2023

Classification Surrogates



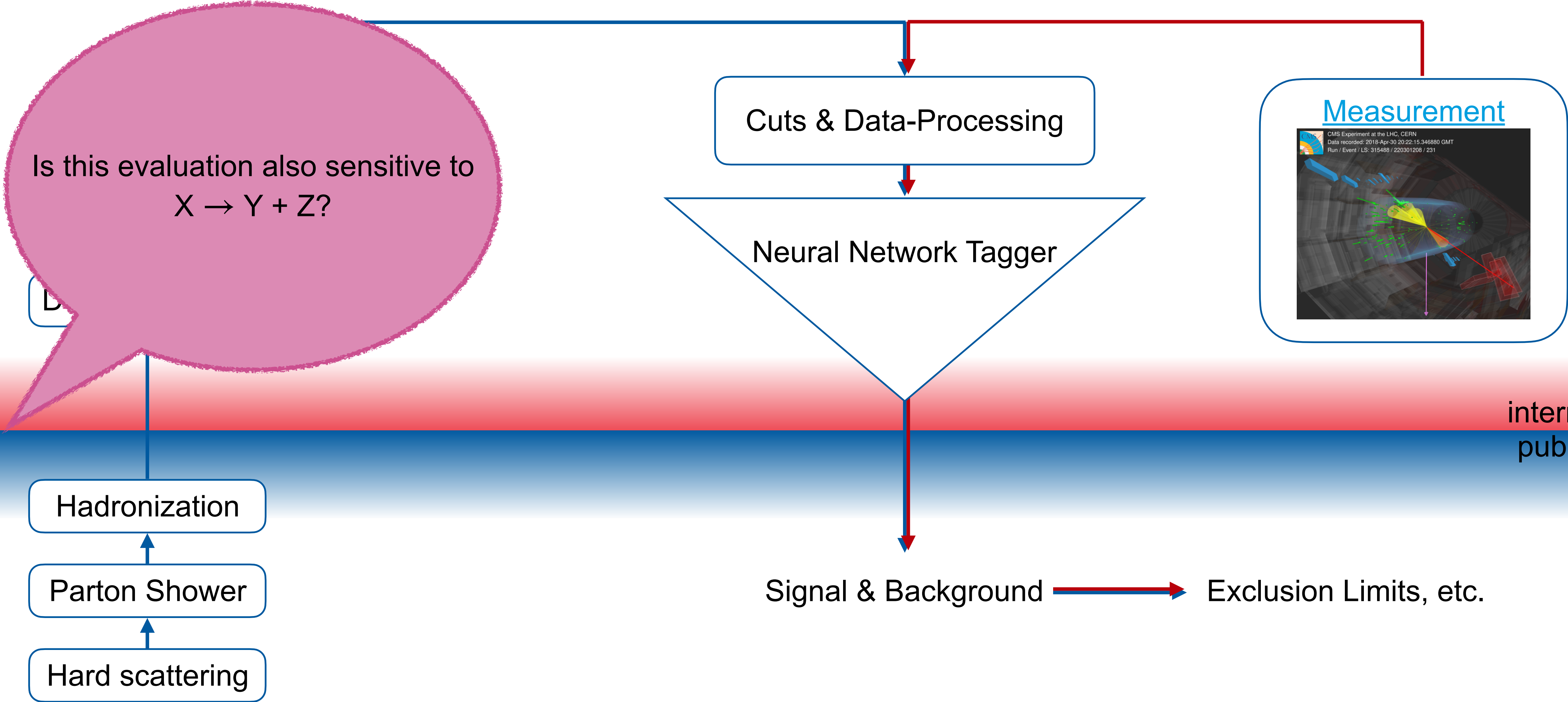
internal
public

Classification Surrogates



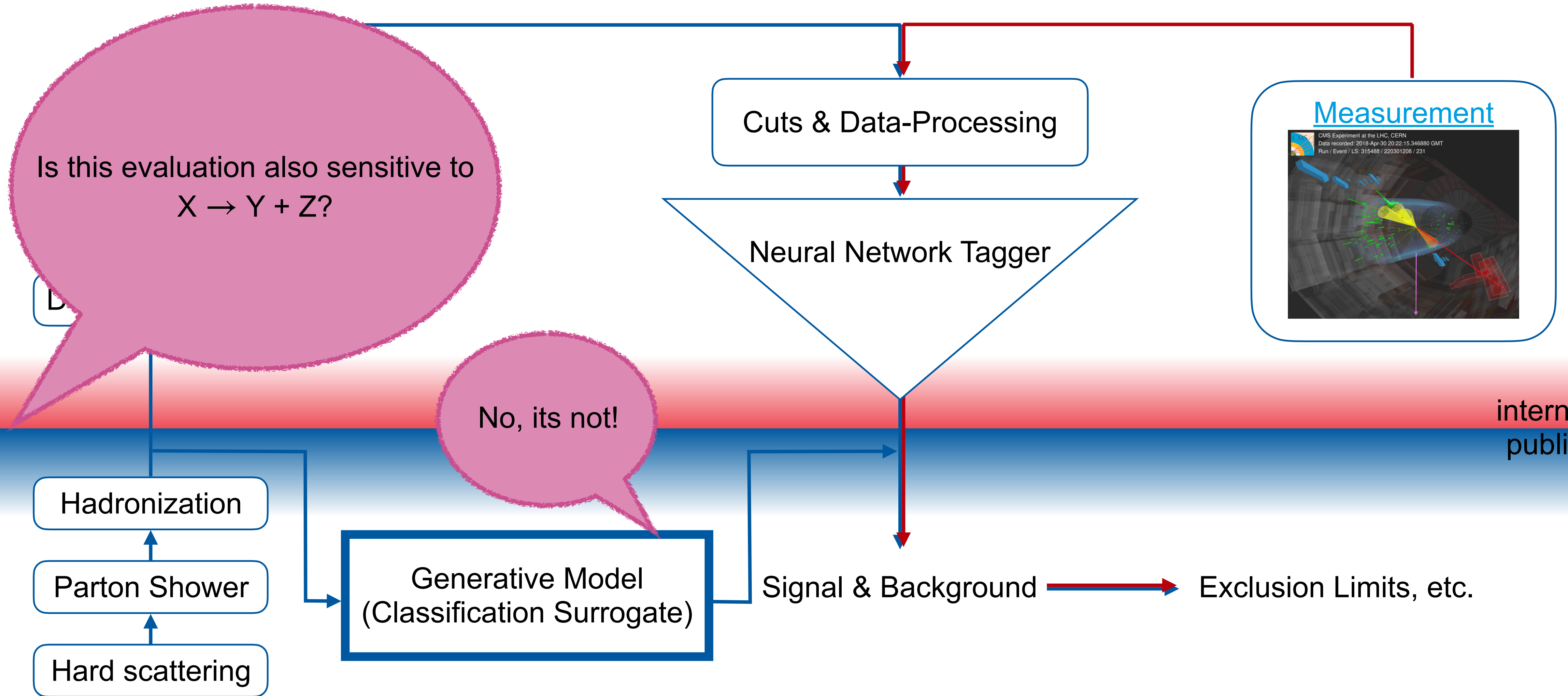
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Classification Surrogates

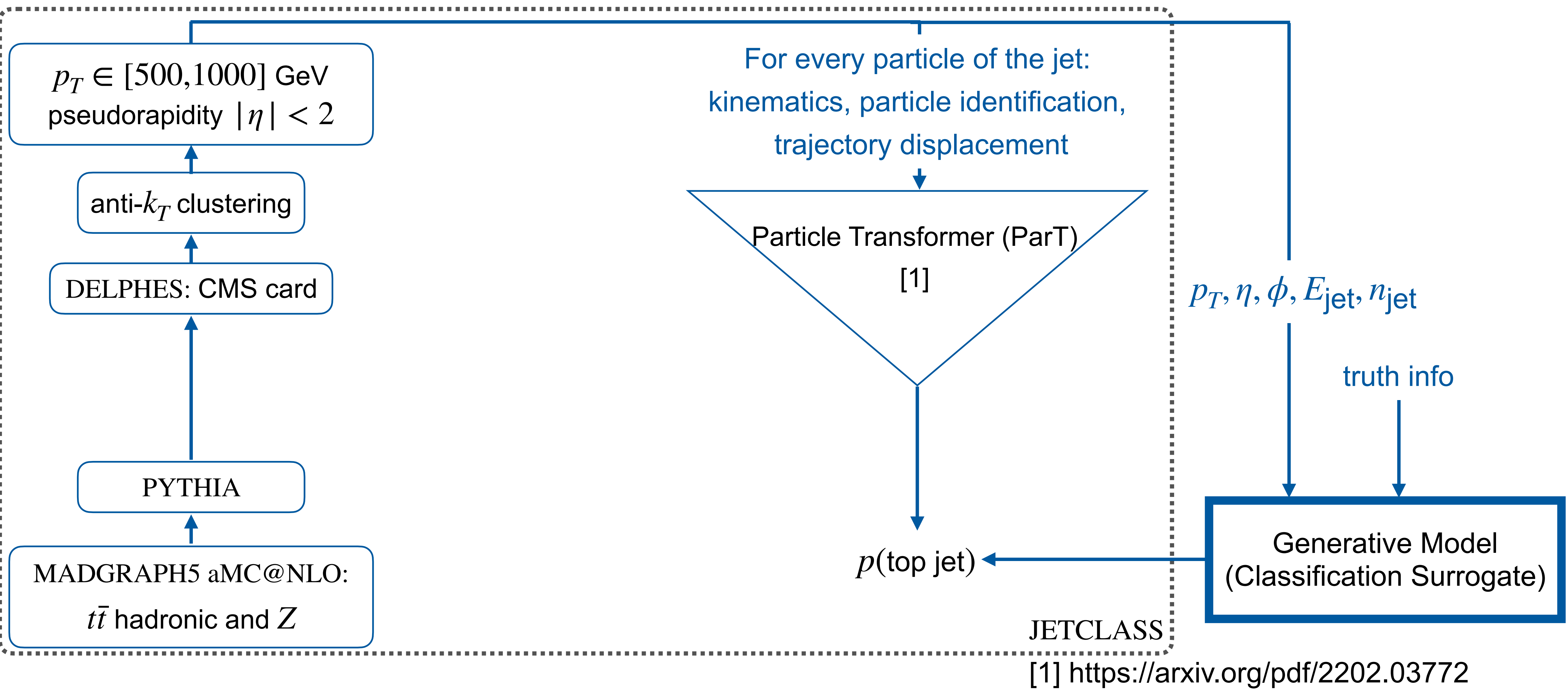


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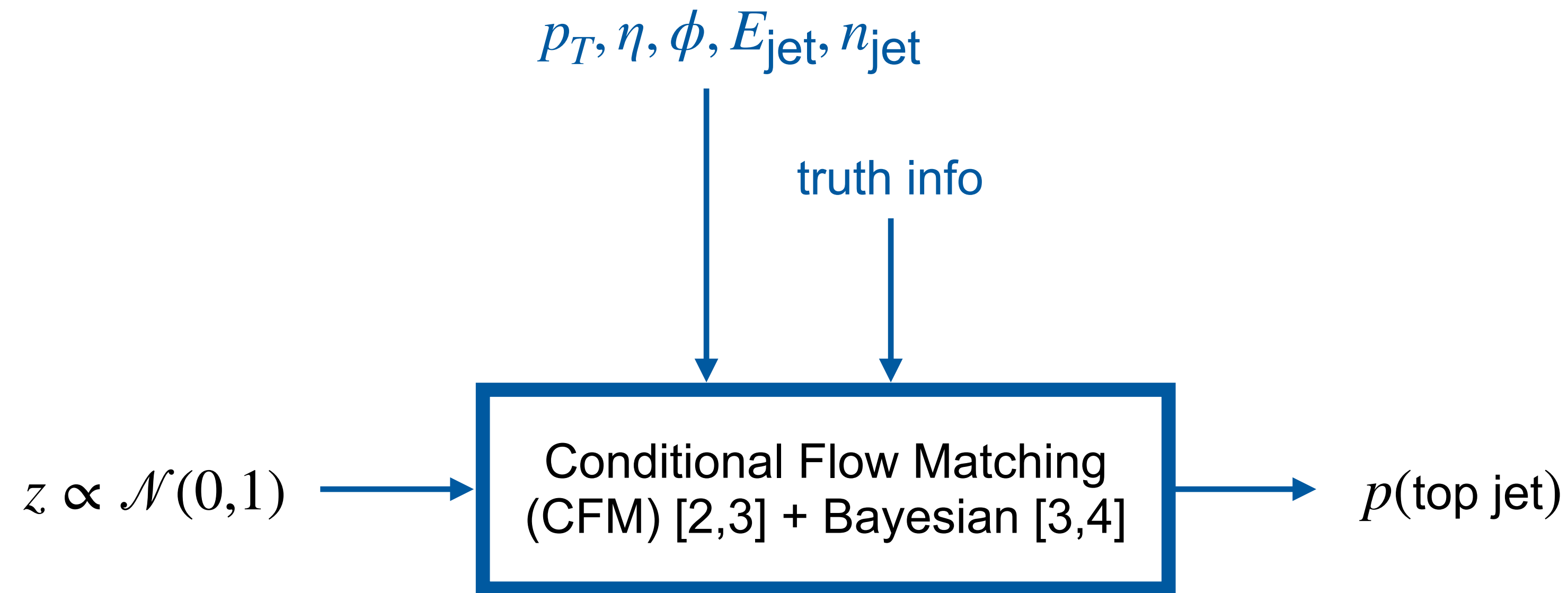
Classification Surrogates



The Toy Setup



The Generative Model



[2] <https://gist.github.com/francois-rozet/fd6a820e052157f8ac6e2aa39e16c1aa>

[3] <https://arxiv.org/pdf/2210.02747>

[4] <https://github.com/IntelLabs/bayesian-torch>

[5] <https://arxiv.org/pdf/2305.10475>

Bayesian CFM

Continuous Normalizing Flow:

- Flow $\phi : [0,1] \times \mathbb{R}^d \rightarrow \mathbb{R}^d$ defined via

$$\frac{d}{dt}\phi_t(x) = v_t(\phi_t(x)) = \tilde{v}_t(x, \theta)$$

- solve the ODE to train and sample
- linear trajectory
- transforms probability distributions

$$p_t(x) = p_0(\phi_t^{-1}(x)) \det \left[\frac{\partial \phi_t^{-1}}{\partial x}(x) \right]$$

Conditional Flow Matching:

- loss that does not ODE solving

$$\mathcal{L}_{\text{FM}}(\theta) = \mathbb{E}_{t,p_t(x)} \left\| v_t(x) - \tilde{v}_t(x, \theta) \right\|^2$$

- by choice of p_t and v_t

$$\mathcal{L}_{\text{CFM}}(\theta) = \mathbb{E}_{t,p_t(x),\epsilon} \left[\tilde{v}_t((1-t)x_0 + t\epsilon, \theta) - (\epsilon - x_0) \right]^2$$

- not a log-Likelihood loss

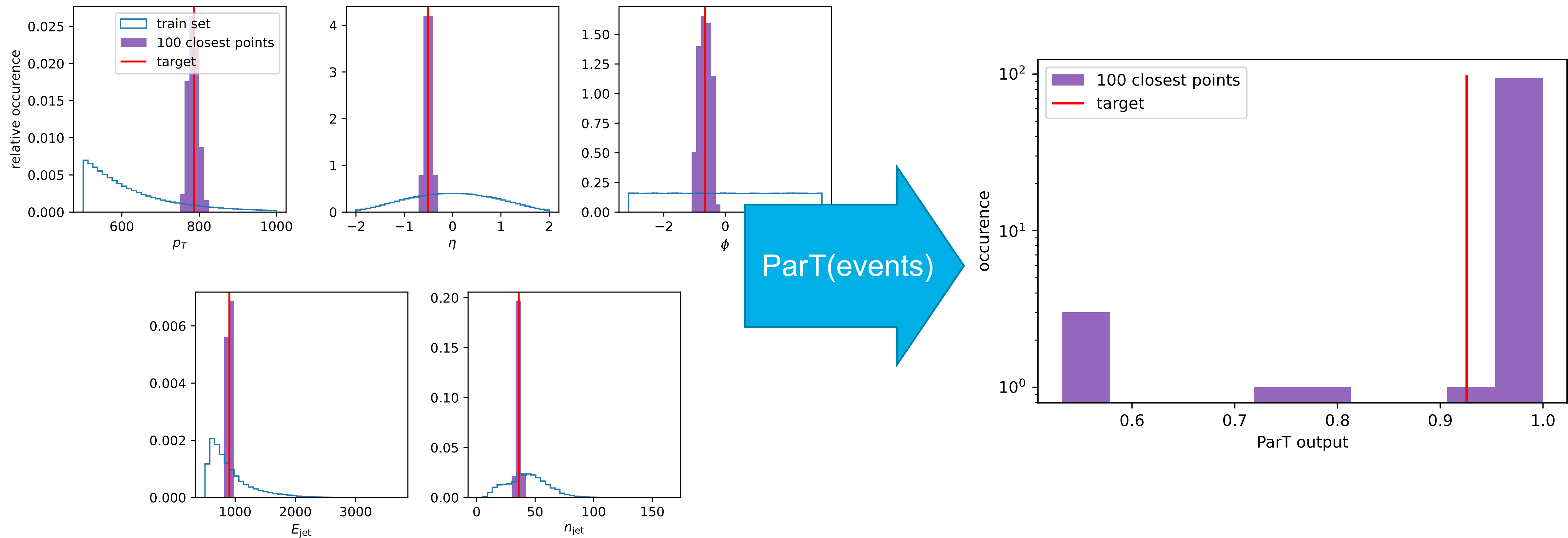
Bayesian Conditional Flow Matching:

- Bayesian loss $\mathcal{L}_{\text{BNN}} = \text{KL} [q(\theta), p(\theta | x)] = - \int d\theta q(\theta) \log p(x | \theta) + \text{KL}[q(\theta), p(\theta)] + \text{const.}$

- connect both $\mathcal{L}_{\text{B-CFM}} = \langle \mathcal{L}_{\text{CFM}} \rangle_{\theta \sim q(\theta)} + c \text{KL}[q(\theta), p(\theta)]$, with $q(\theta)$ uncorrelated Gaussian shape

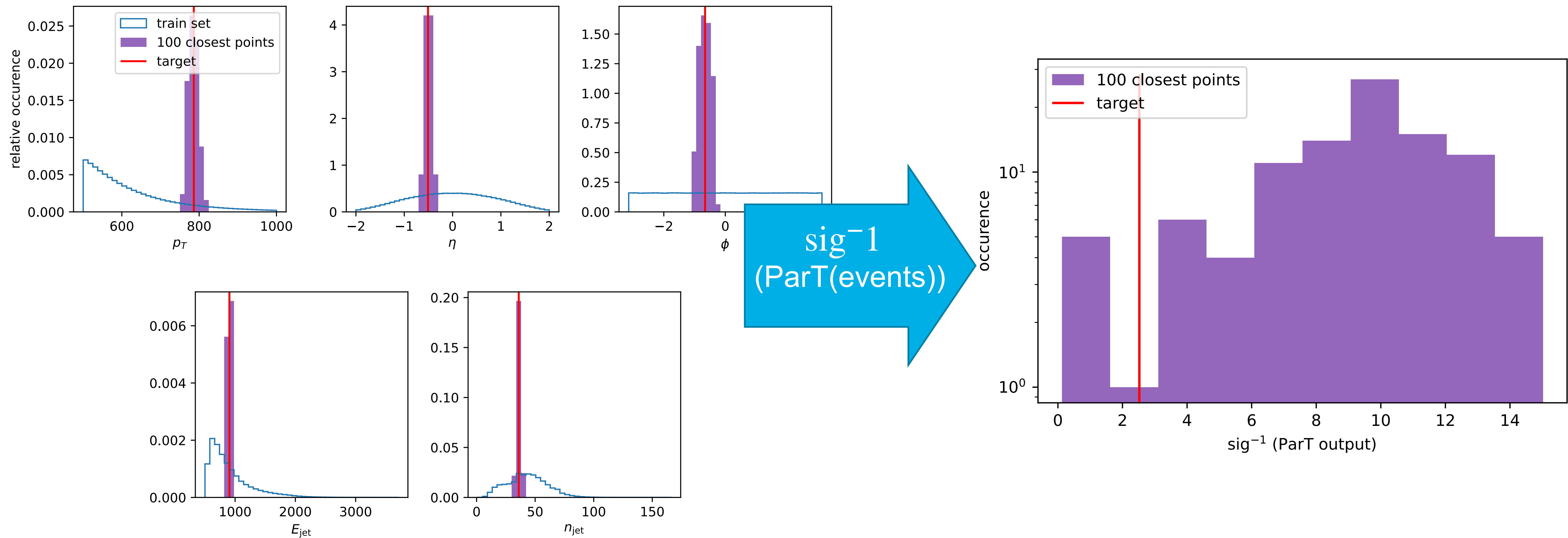
Detector Smearing Distribution

- pick a jet event
- select the 100 events with $p_T, \eta, \phi, E_{\text{jet}}, n_{\text{jet}}$ closest

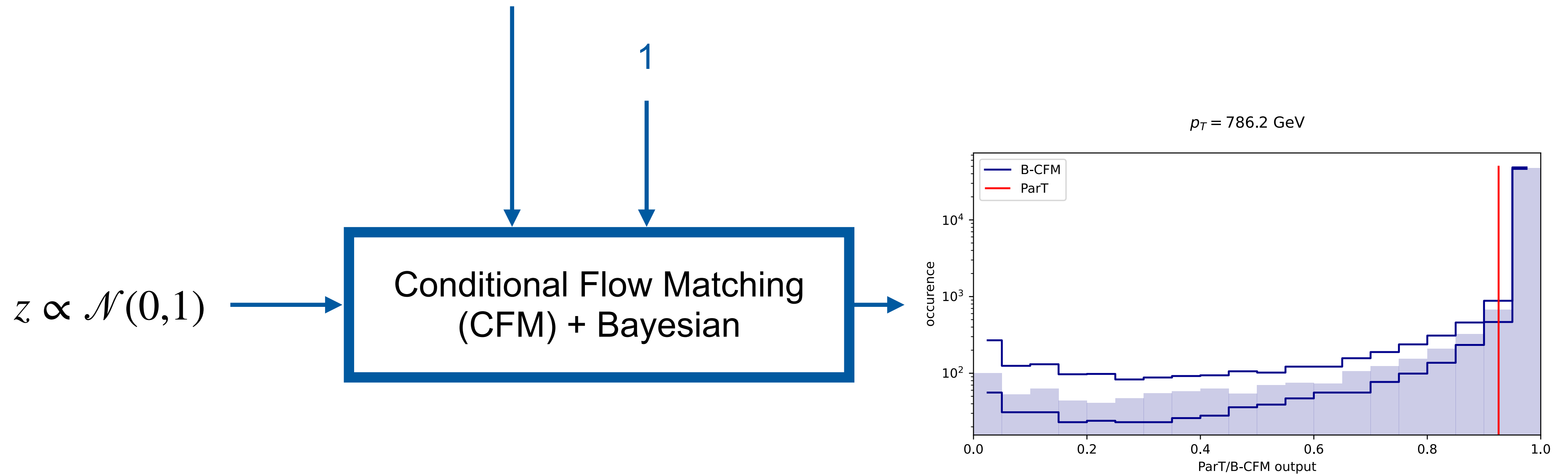
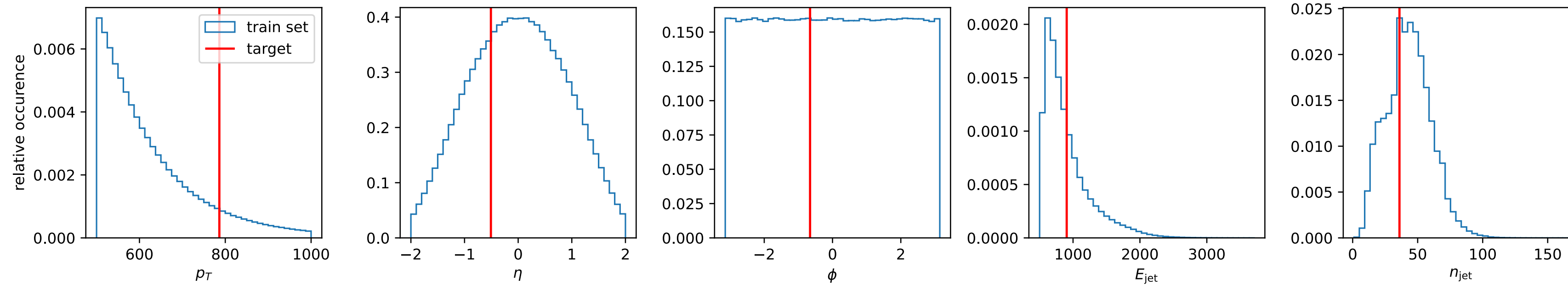


Detector Smearing Distribution

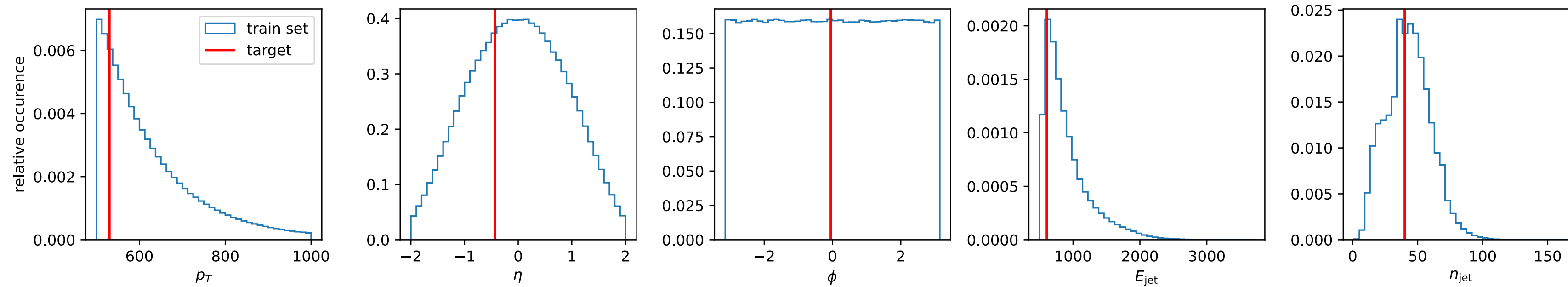
- pick a jet event
- select the 100 events with $p_T, \eta, \phi, E_{\text{jet}}, n_{\text{jet}}$ closest



Learned Detector Smearing Distribution

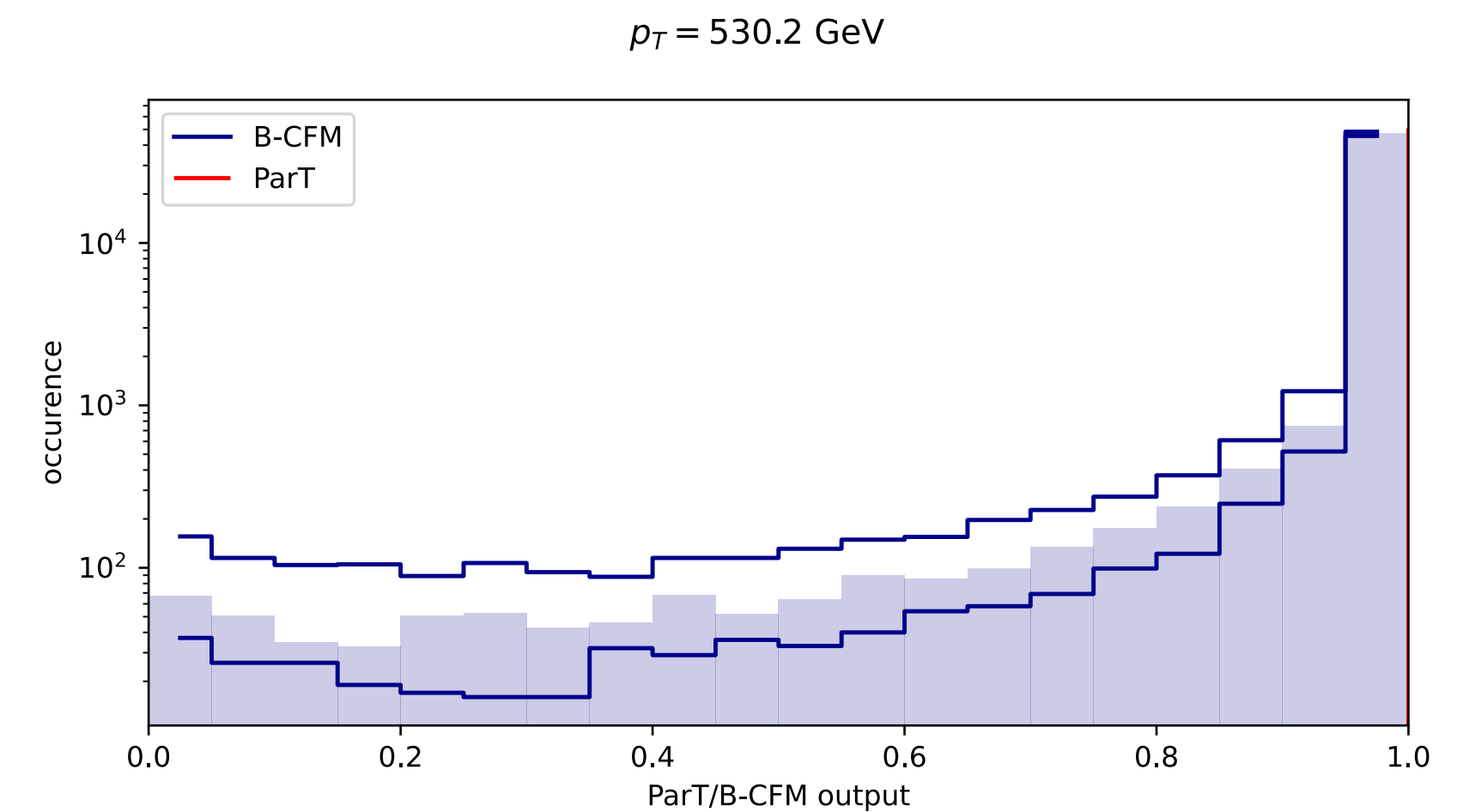


Learned Detector Smearing Distribution

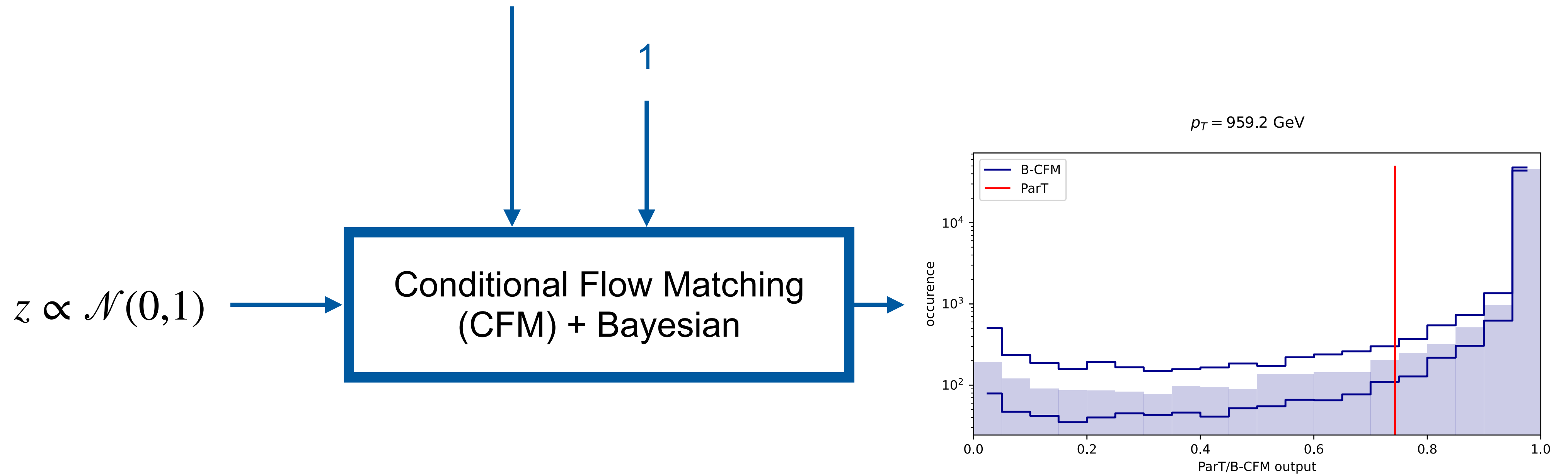
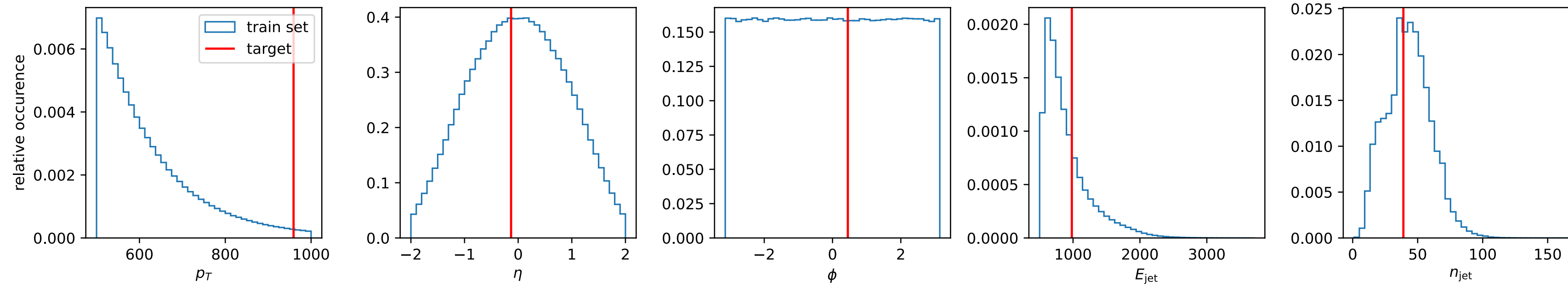


$$z \propto \mathcal{N}(0,1)$$

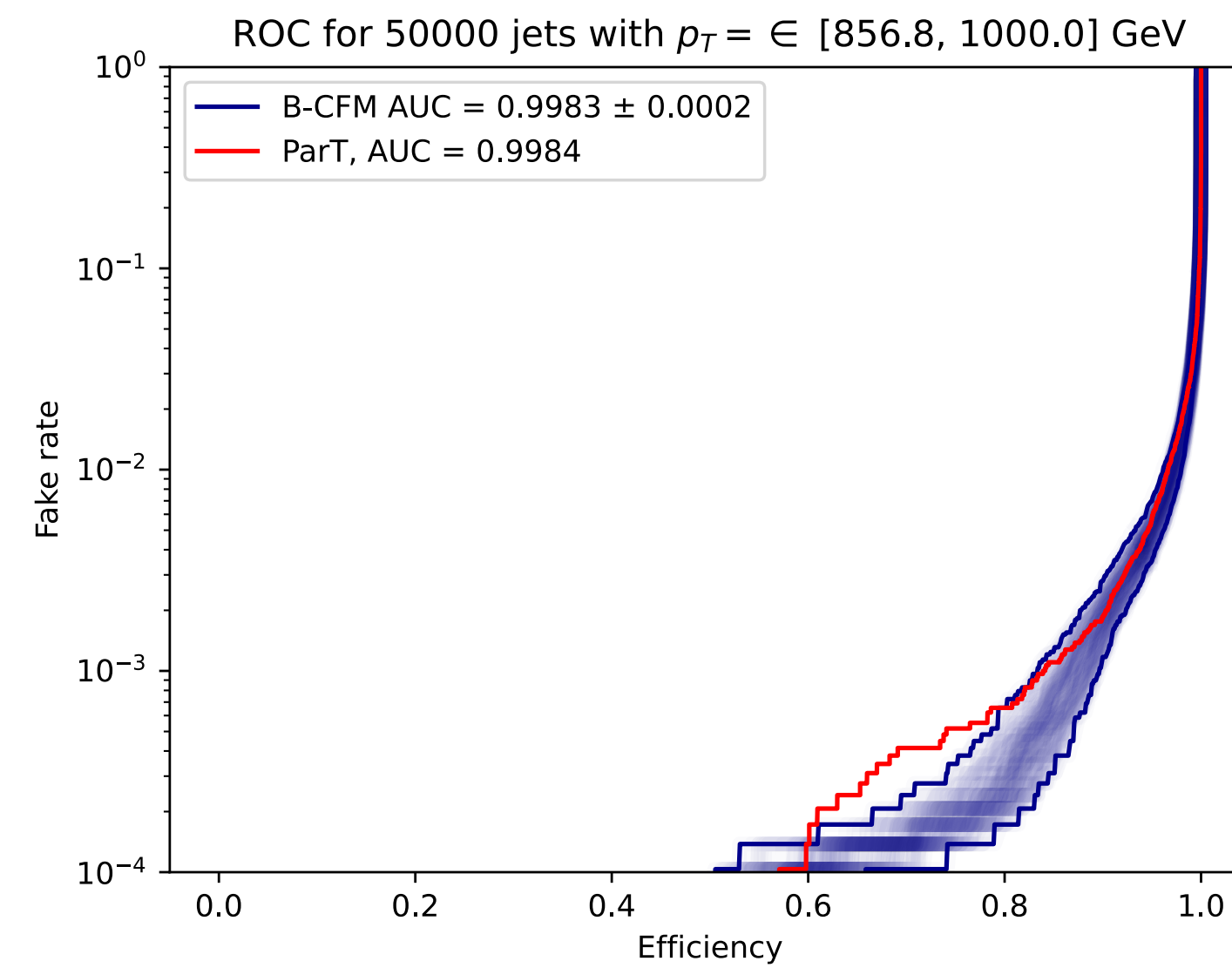
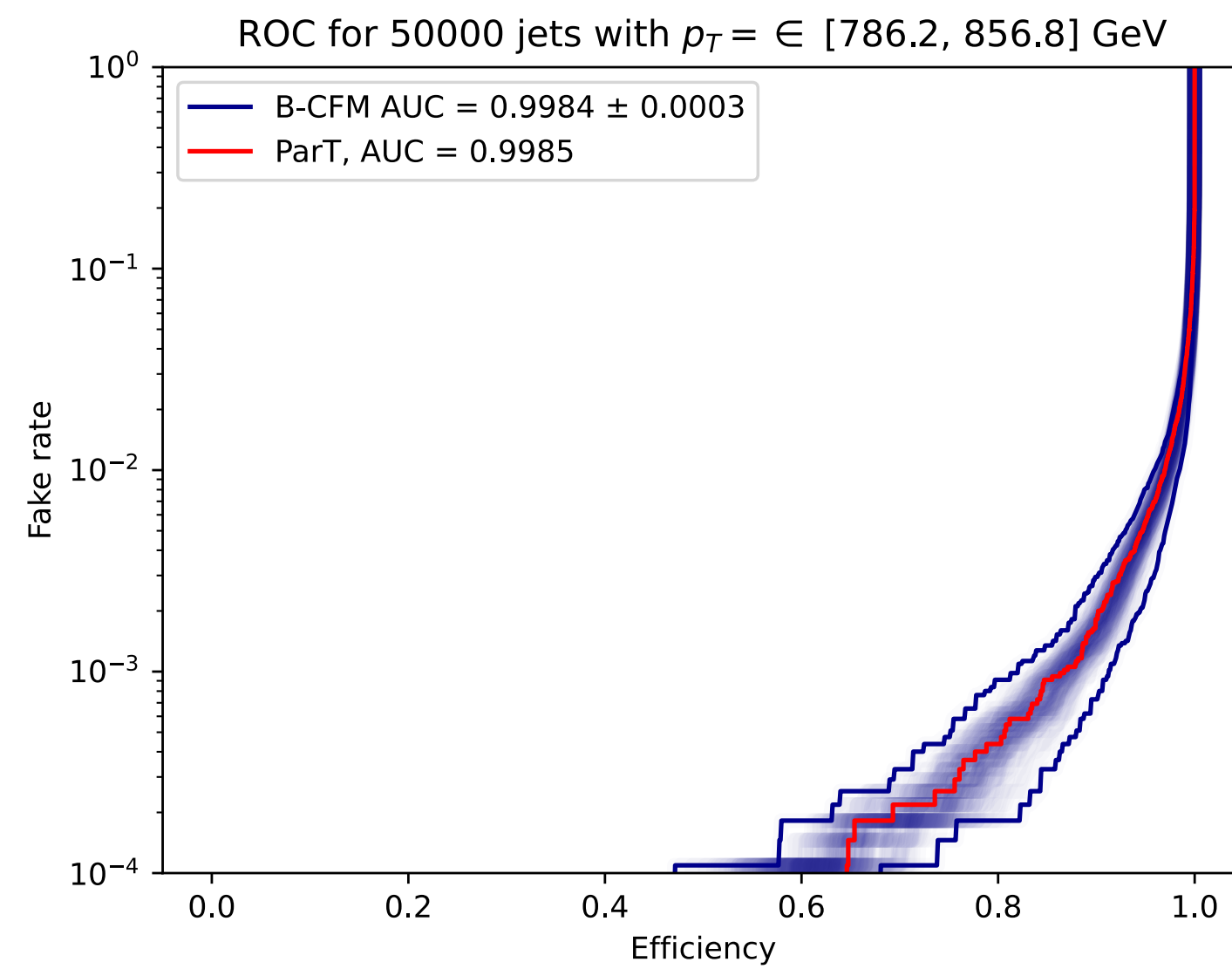
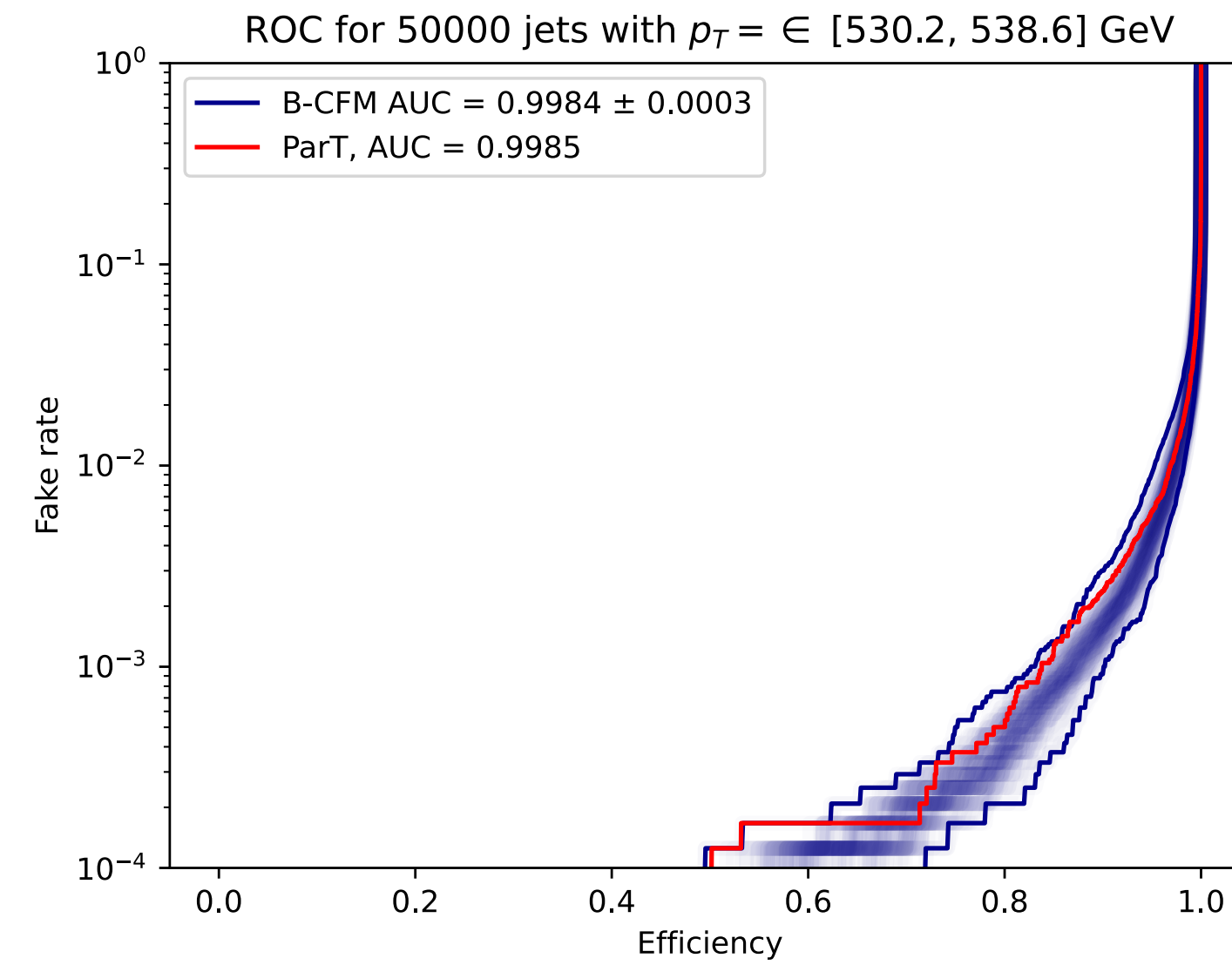
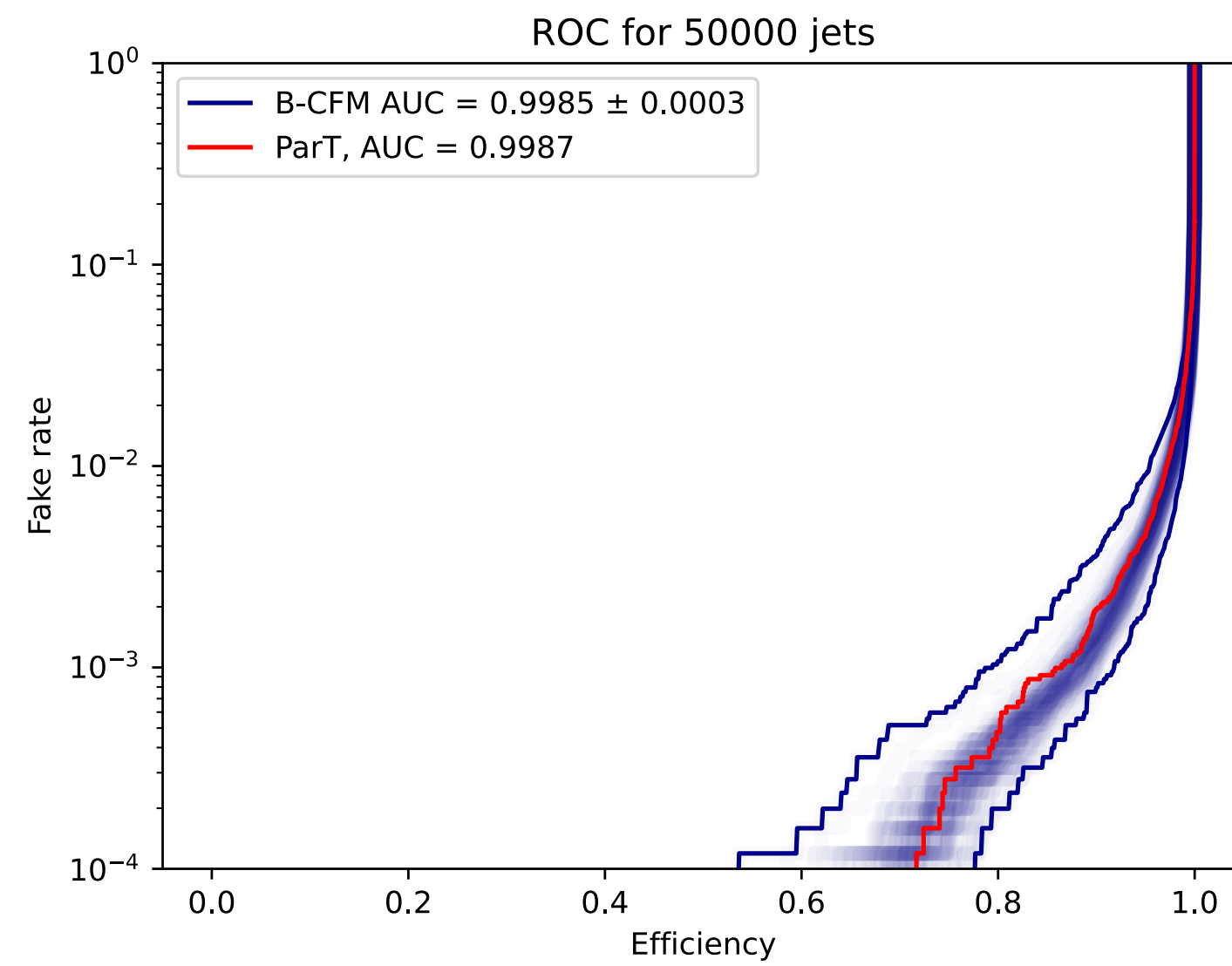
Conditional Flow Matching
(CFM) + Bayesian



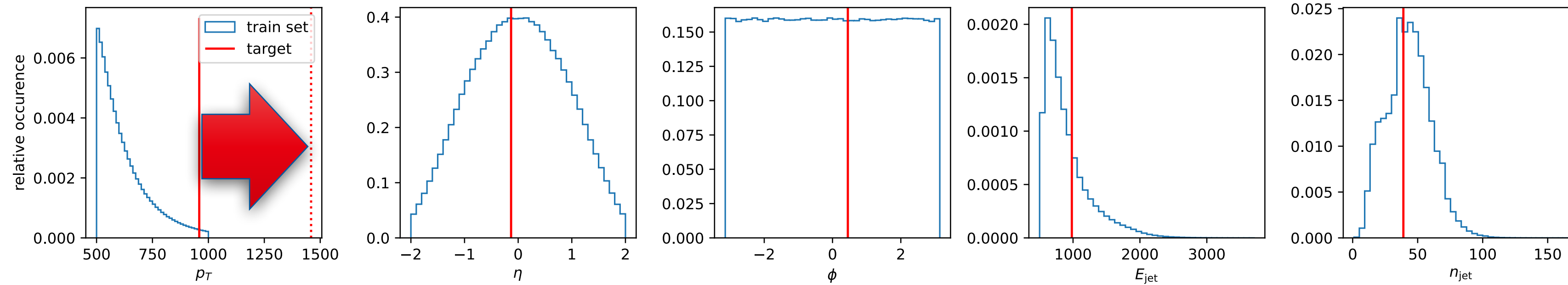
Learned Detector Smearing Distribution



Predicted ROC

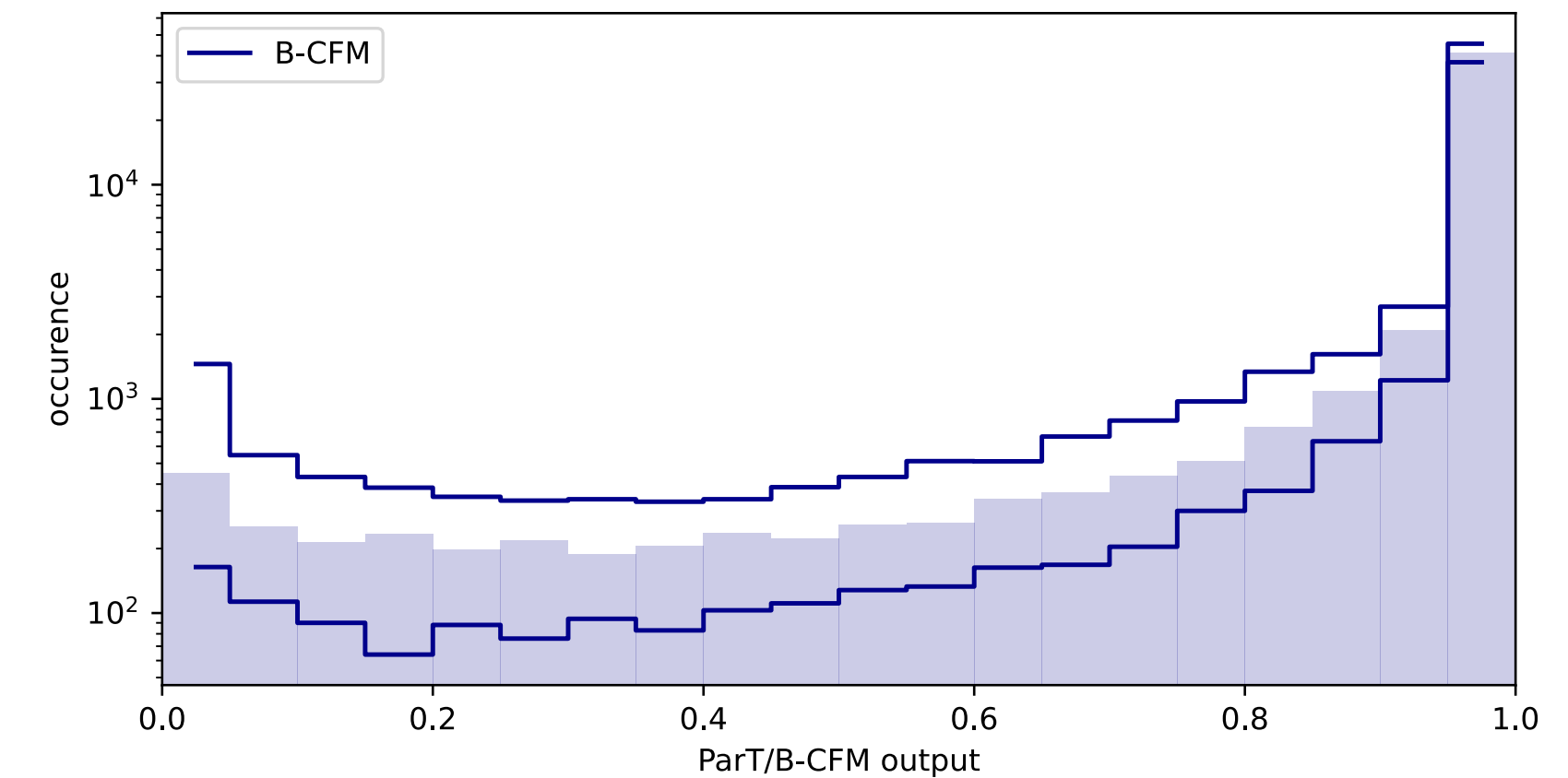


Unphysical Inputs

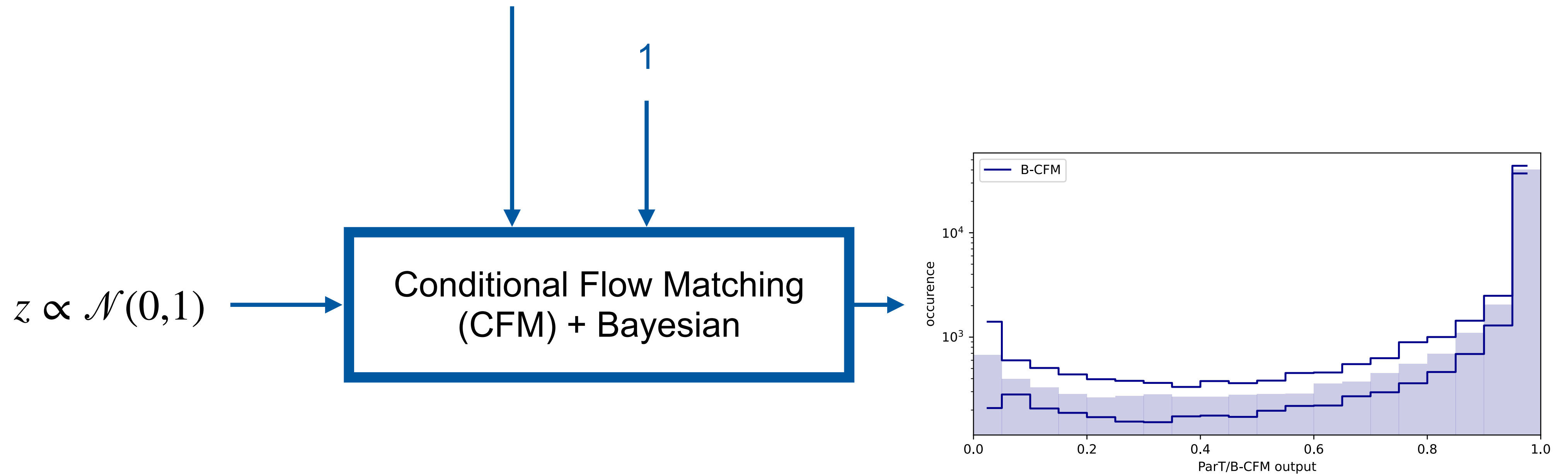
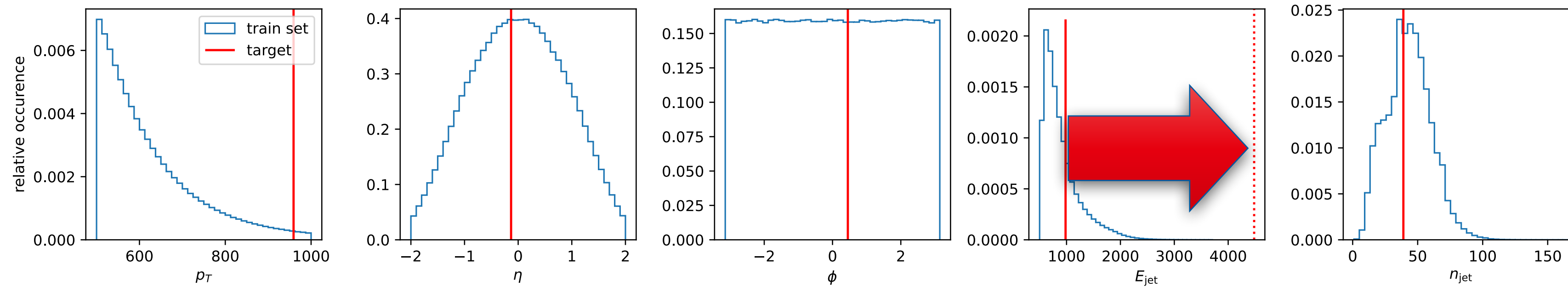


$$z \propto \mathcal{N}(0,1)$$

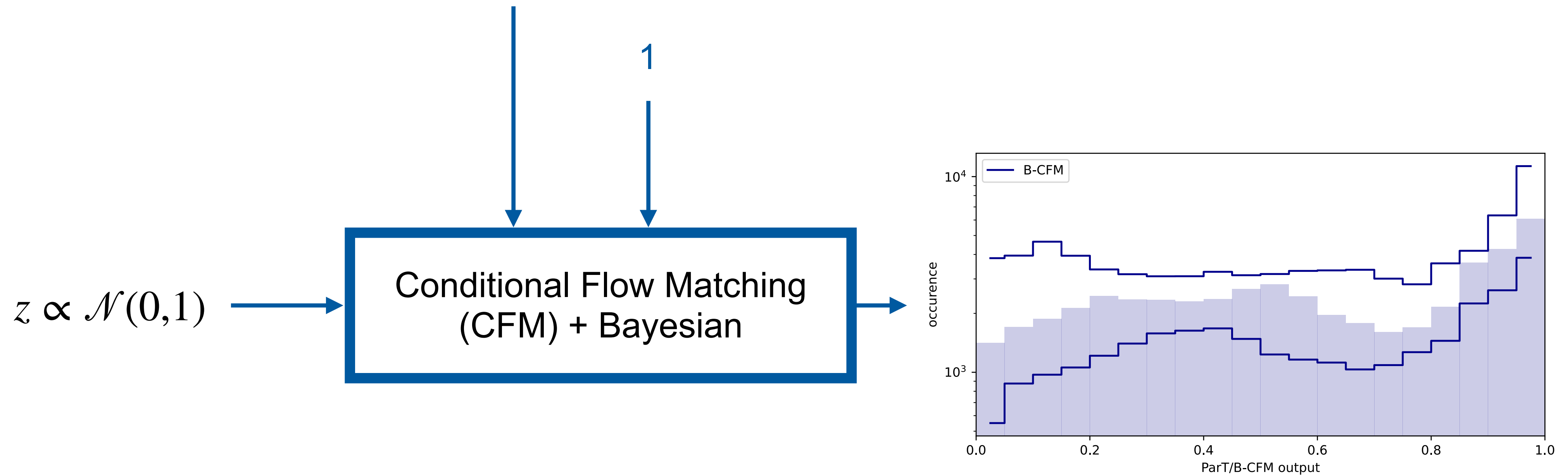
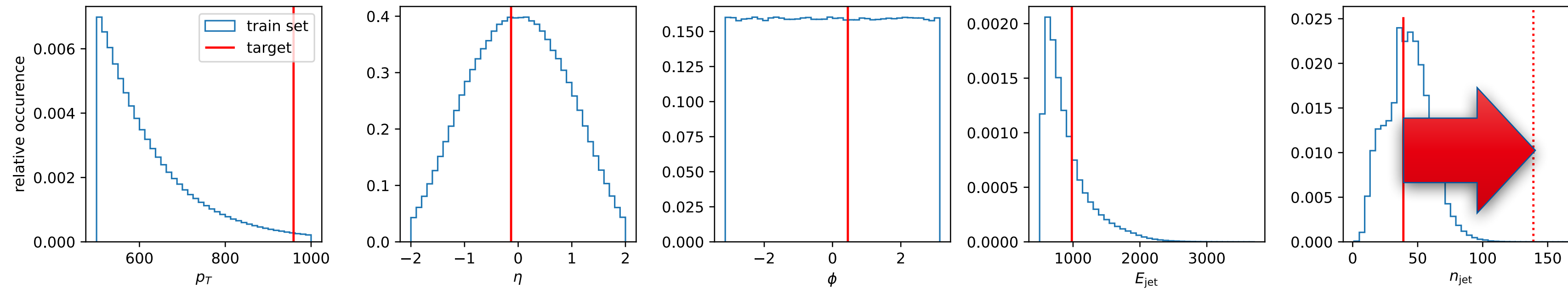
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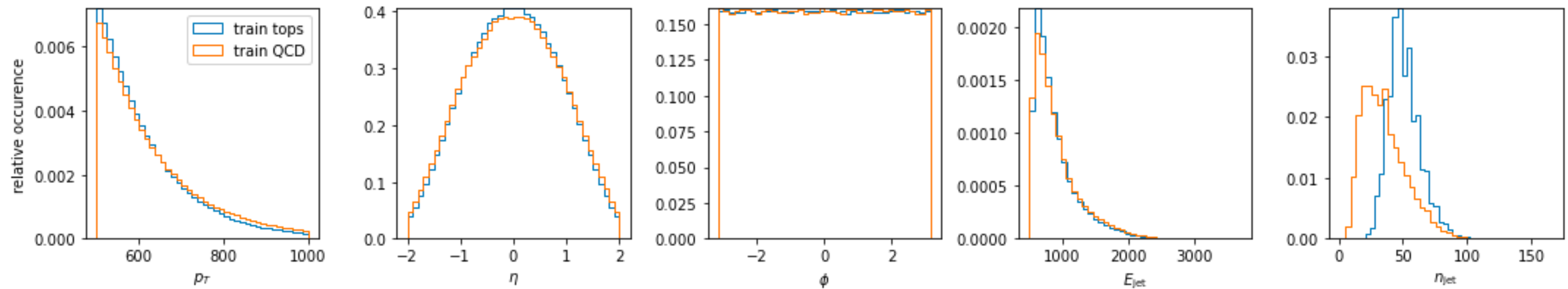
Unphysical Inputs



Unphysical Inputs

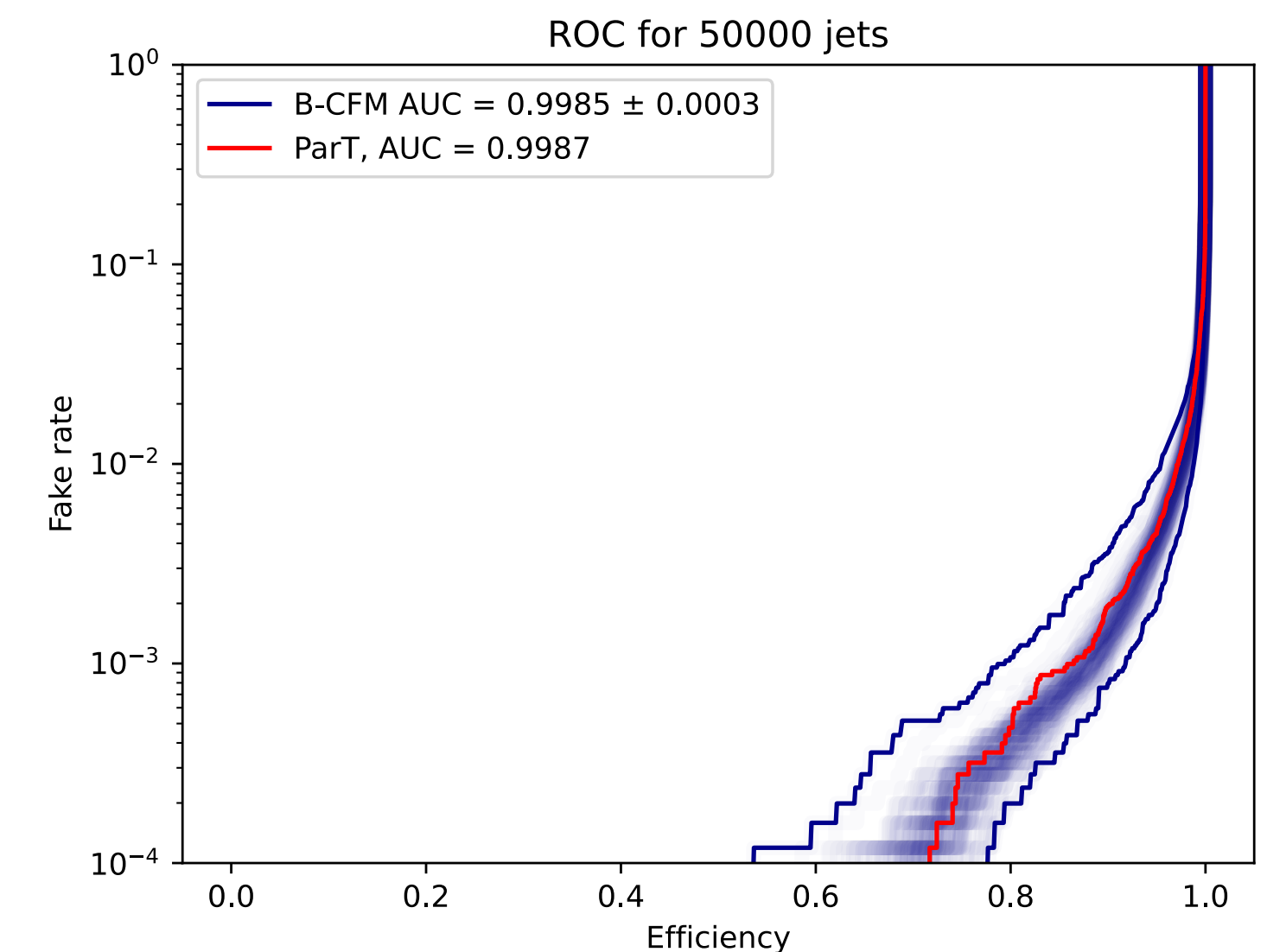
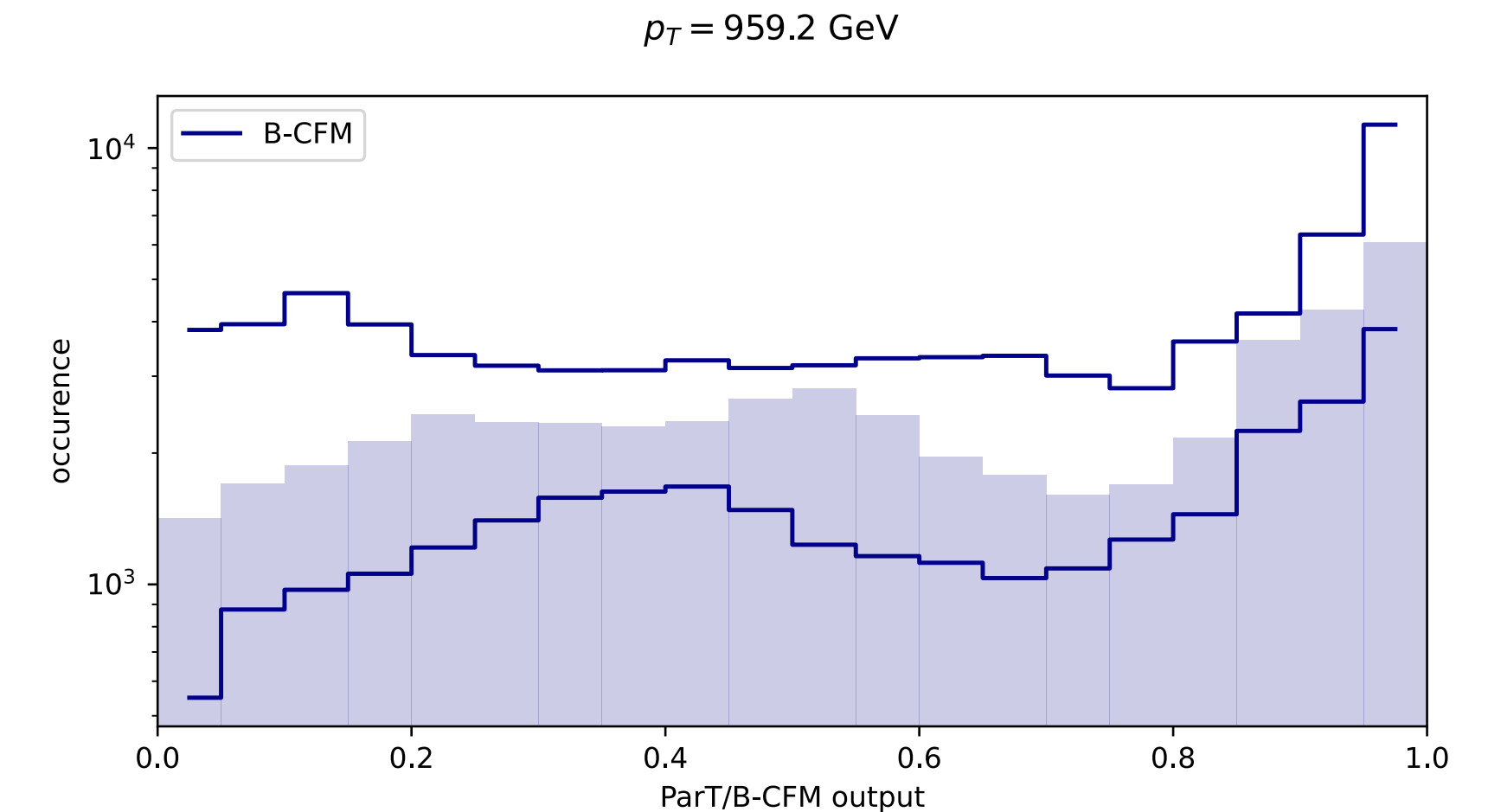


Top vs. QCD jets



Conclusion

- CFM model can predict the in-distribution behavior of a large classifier well
 - Independent of detector-level data
 - Can be shared with in analysis
- Further investigation of Bayesian methods to fix out-of-distribution predictions for all dimensions

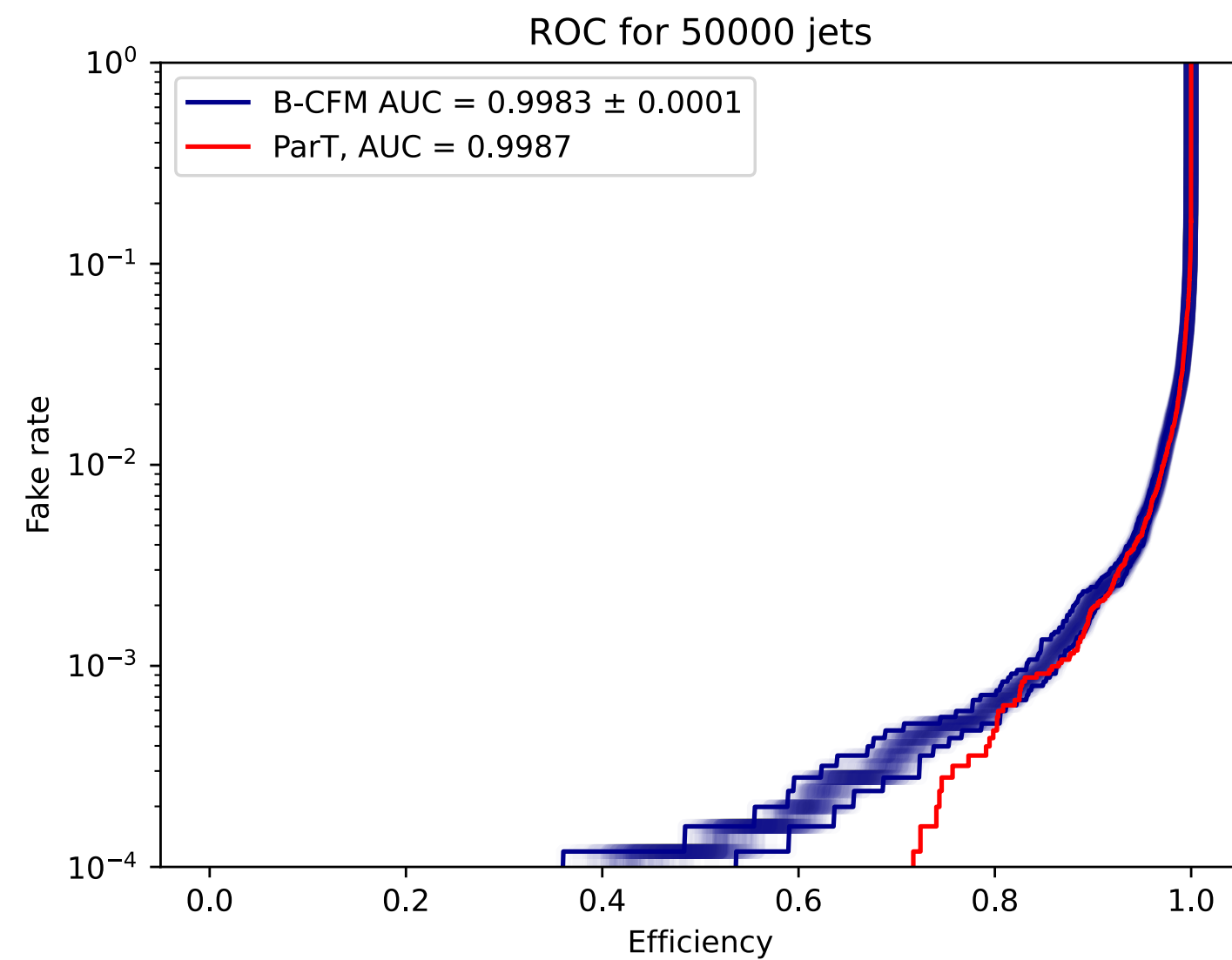


Effects of the Prior Parameter c

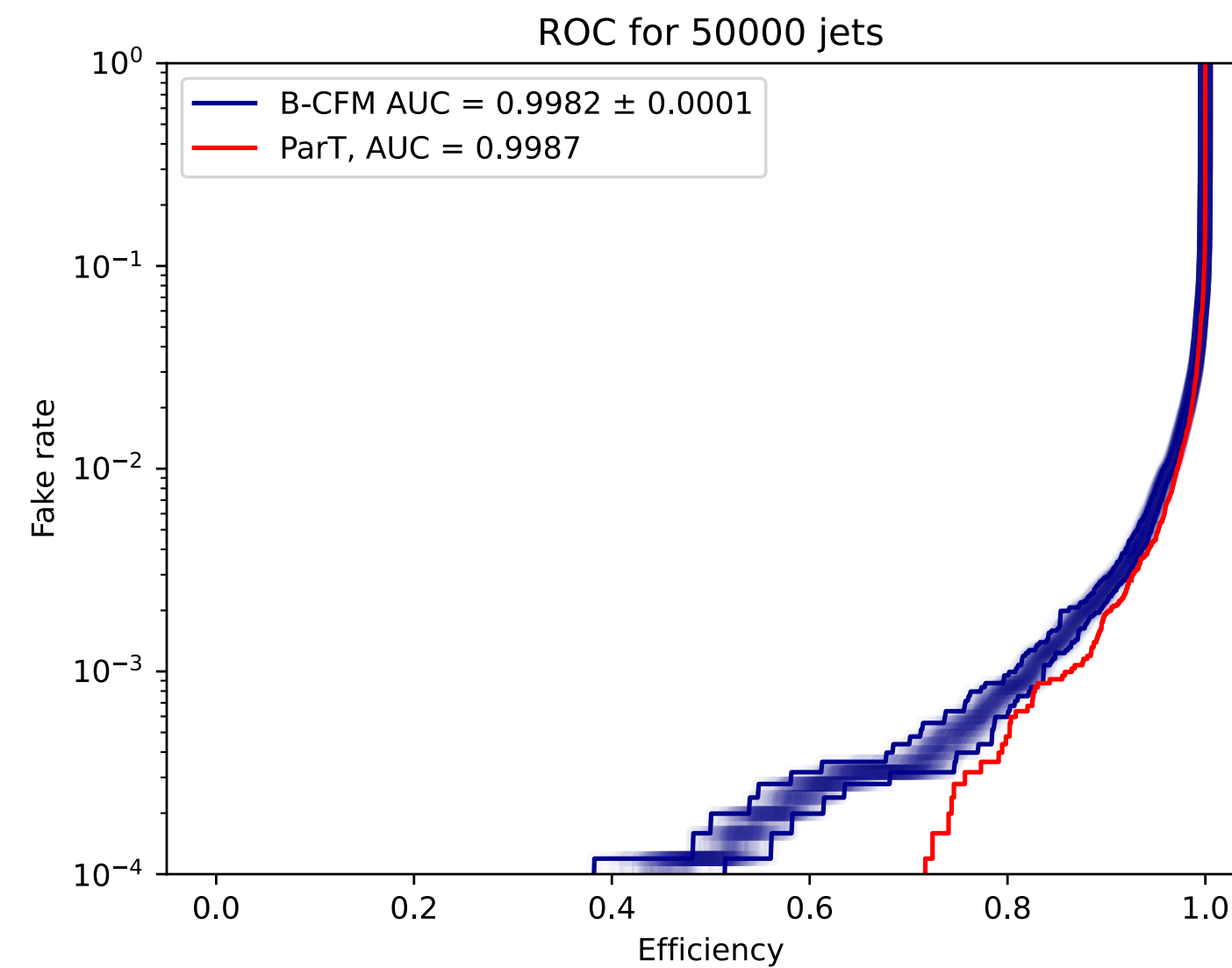
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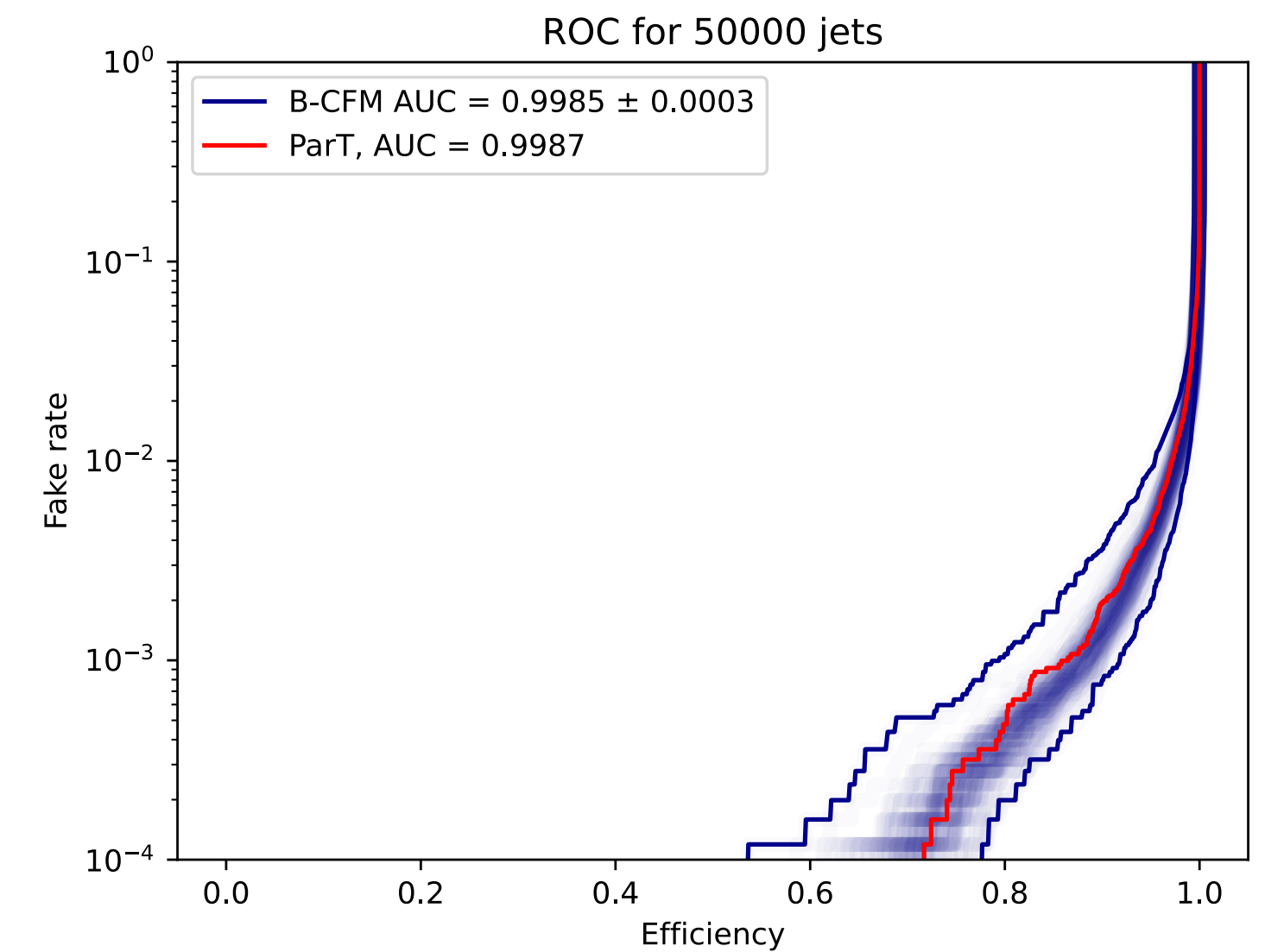
$c = 0.01$



$c = 1$



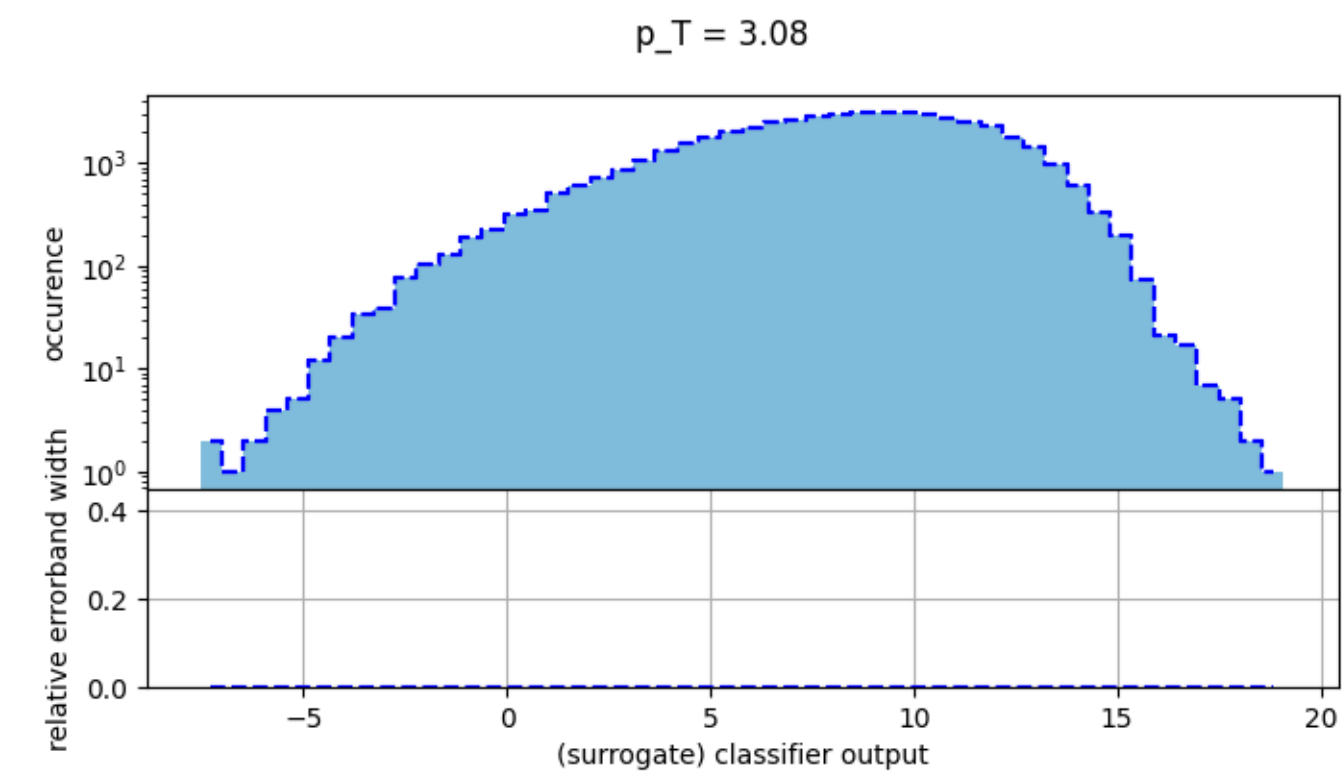
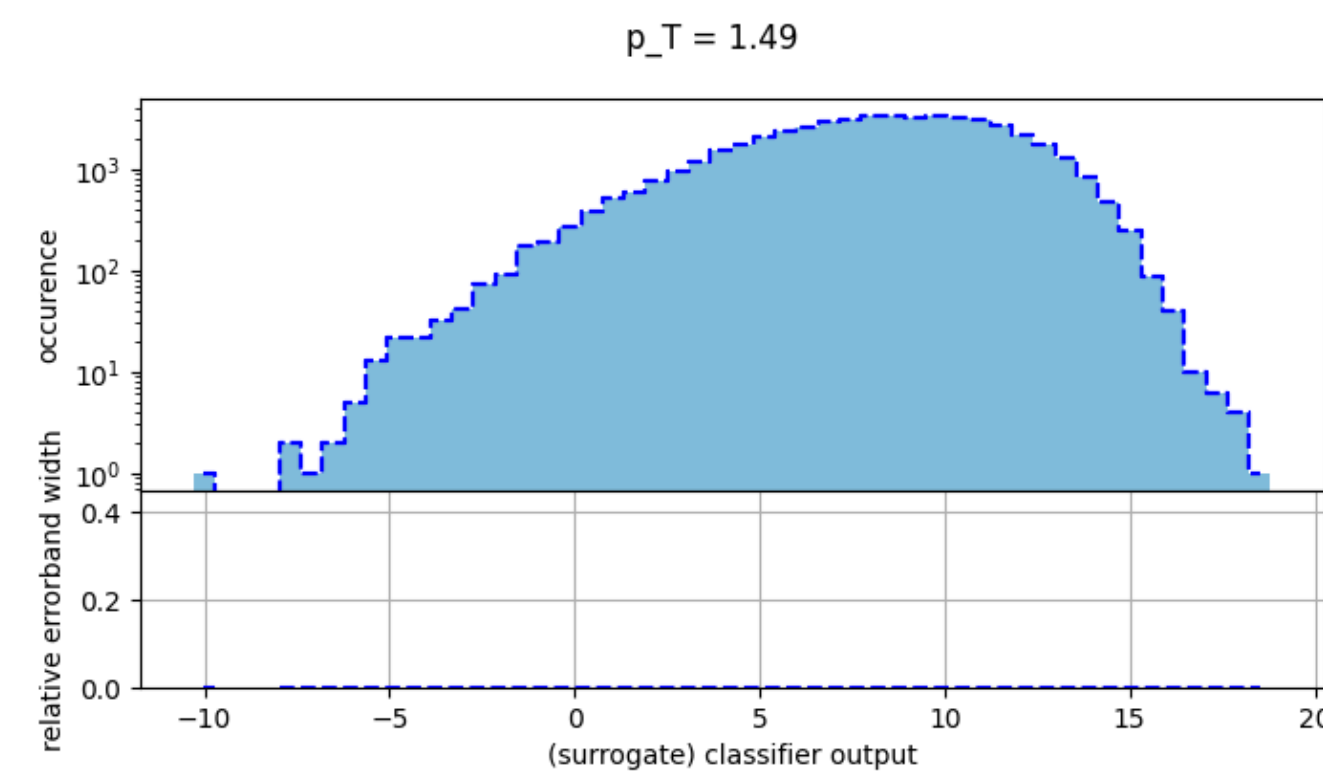
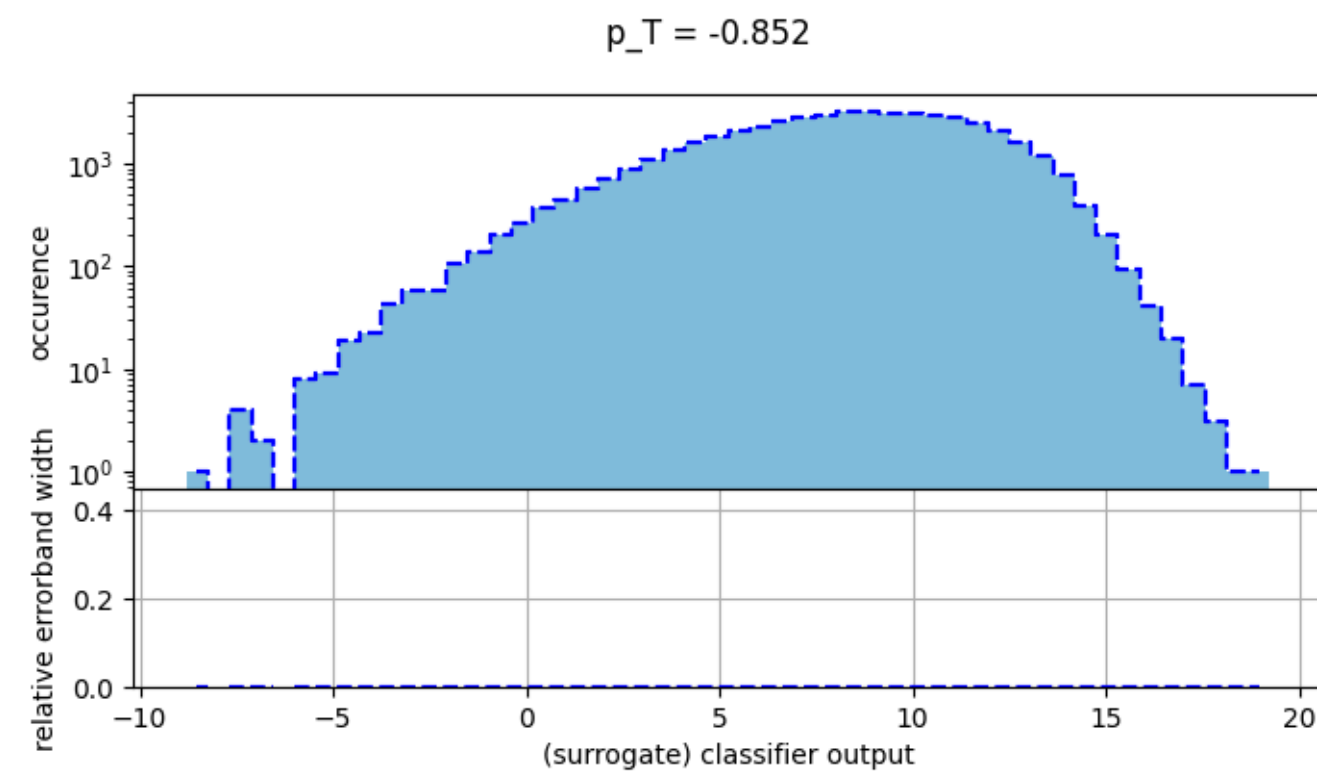
$c = 100$



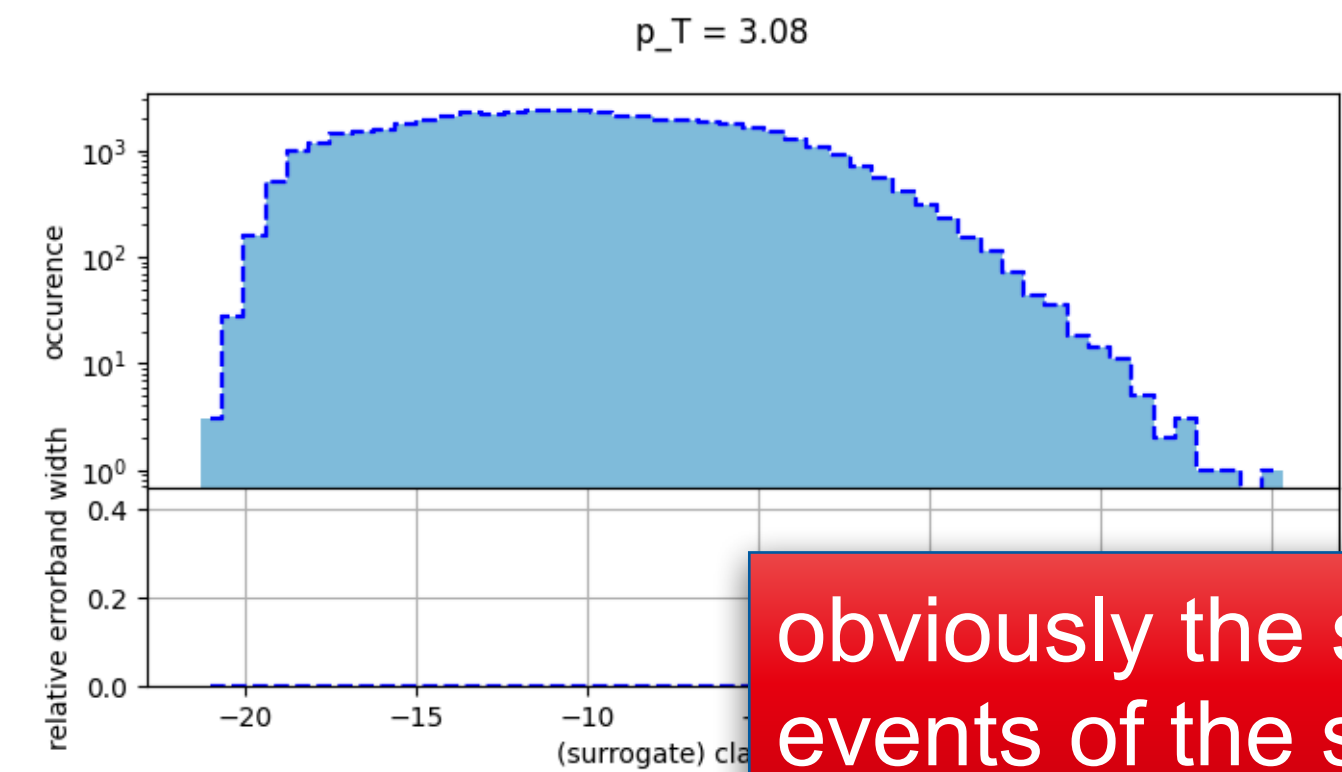
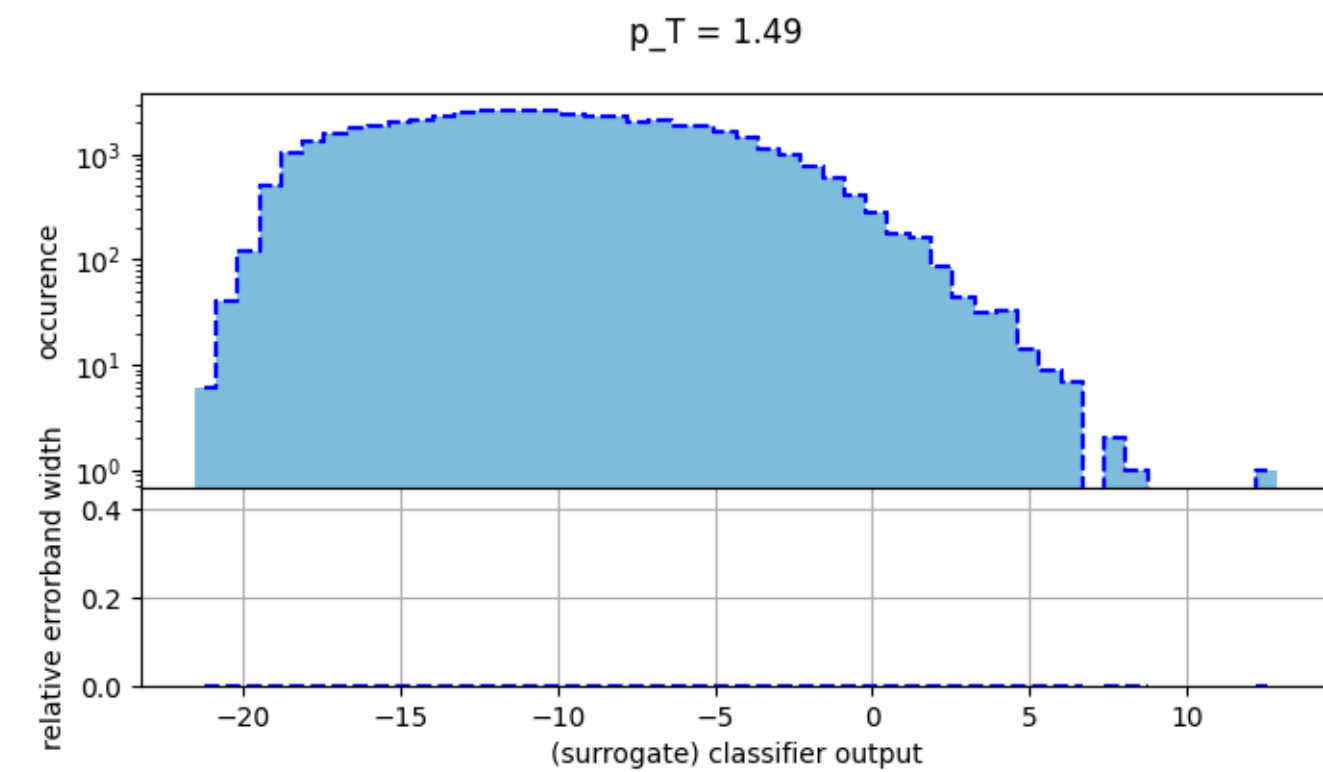
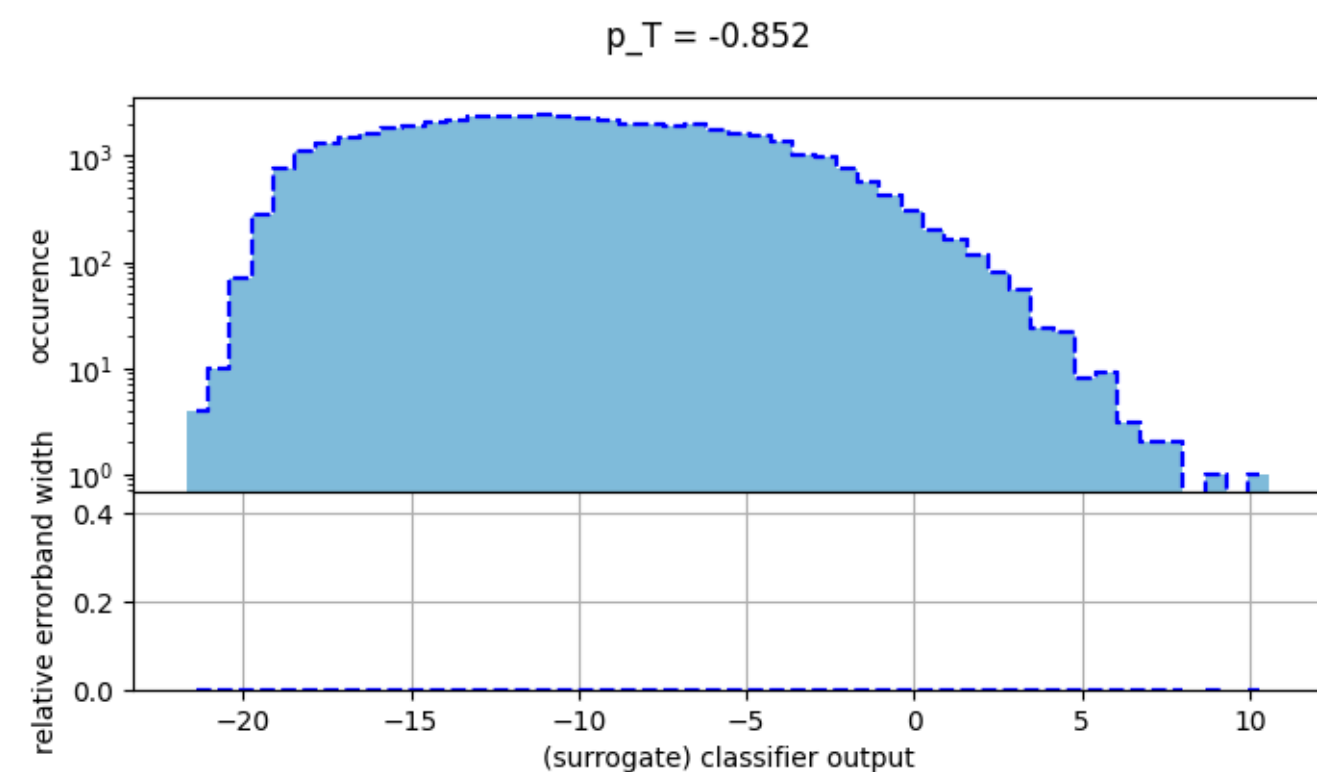
What if only trained on truth?



top jets



not top jets



obviously the same for events of the same class