GENERATIVE TRANSFORMERS AND HOW TO EVALUATE THEM

Raghav Kansal*, Anni Li, Javier Duarte (UCSD)
Nadya Chernyavskaya, Maurizio Pierini (CERN)
Breno Orzari, Thiago Tomei (SPRACE)

*Also Fermilab

IML Meeting
14/02/2023

ML4PS @ NeurIPS 2020
NeurIPS 2021
2211.10295 2022

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LHC SIMULATIONS

Sources
K. Pedro, HSF 2020
J. Duarte, ANL 2021, Video

LHC SIMULATIONS

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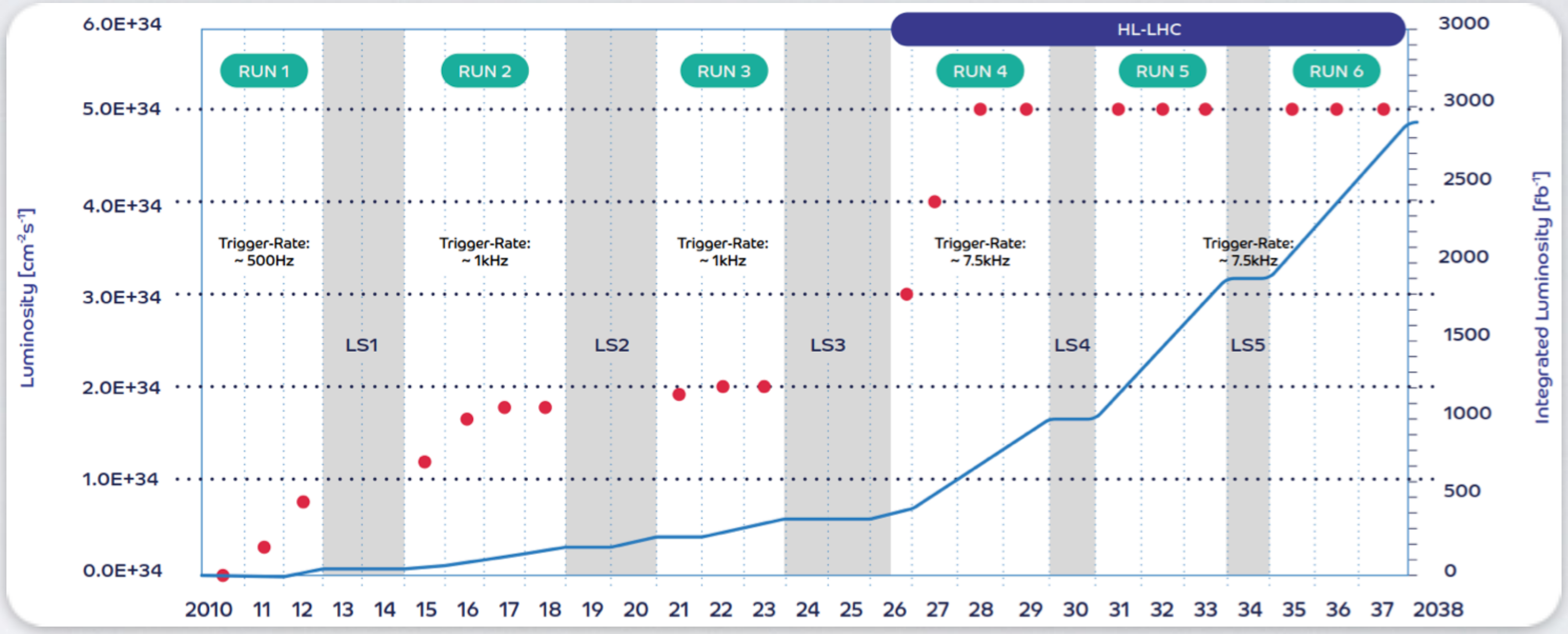

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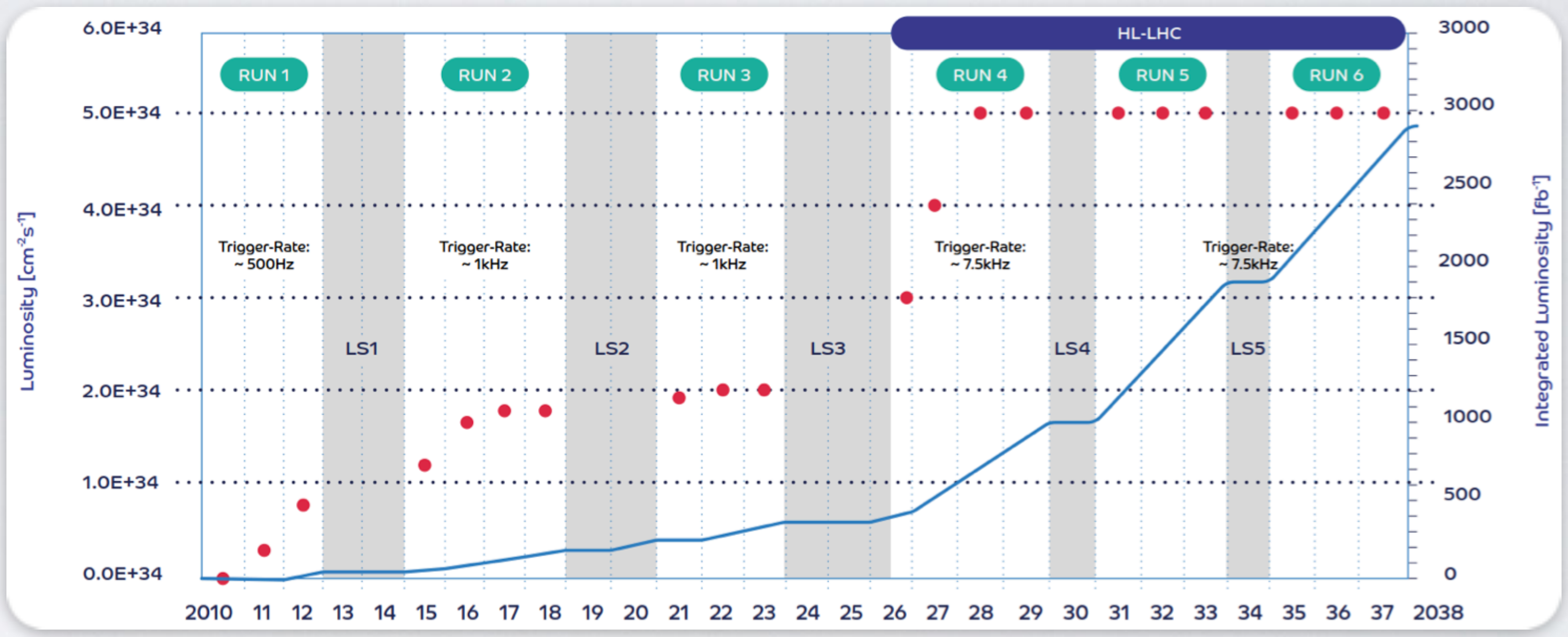

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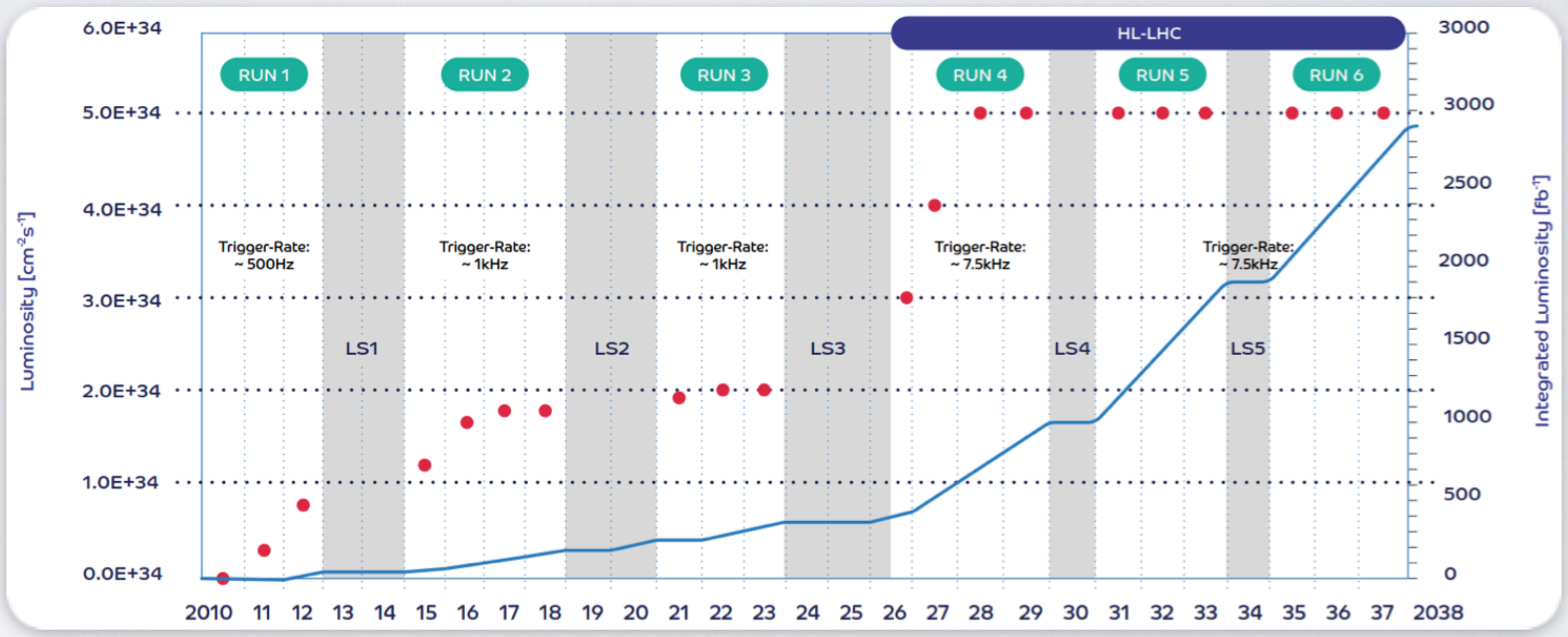

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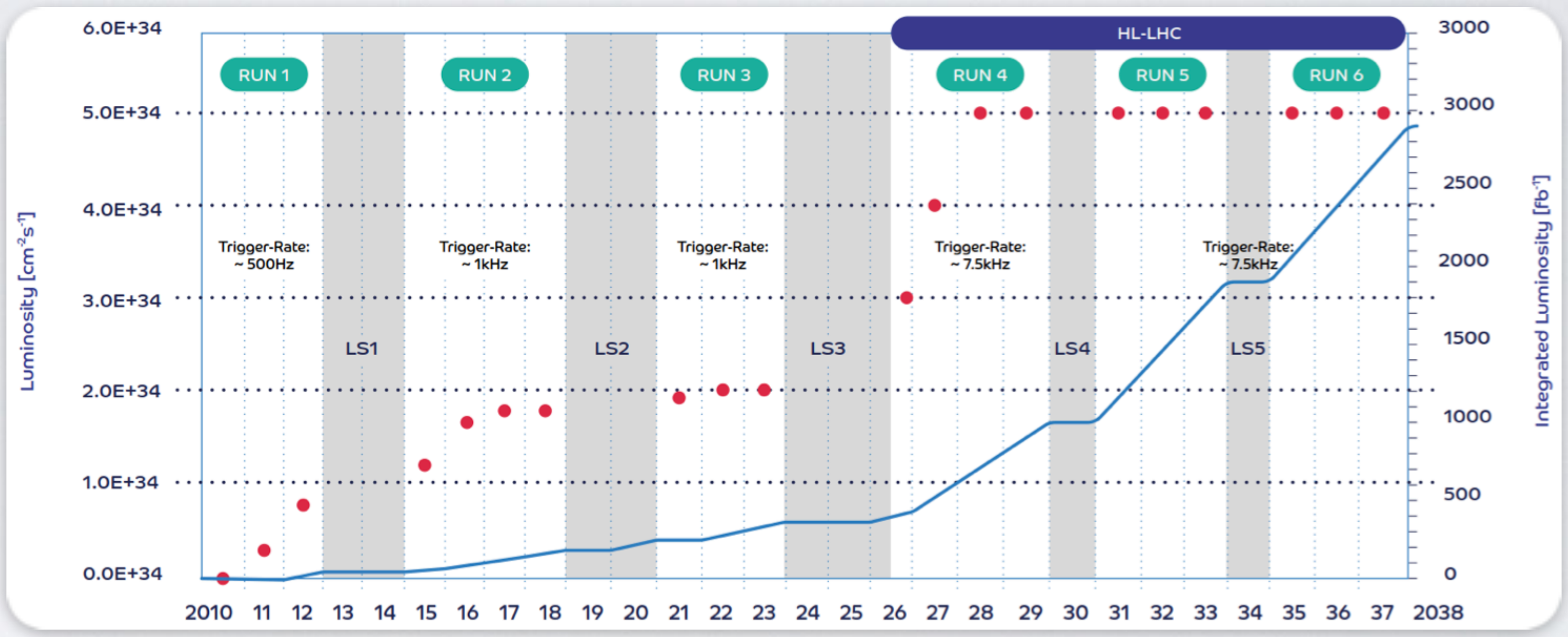

- HL-LHC looming
  - Order-of-magnitude more simulations needed
  - Improved detectors ⇒ higher granularity, increased complexity
  - ML a possible solution?

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*Bias towards CMS

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Hard process
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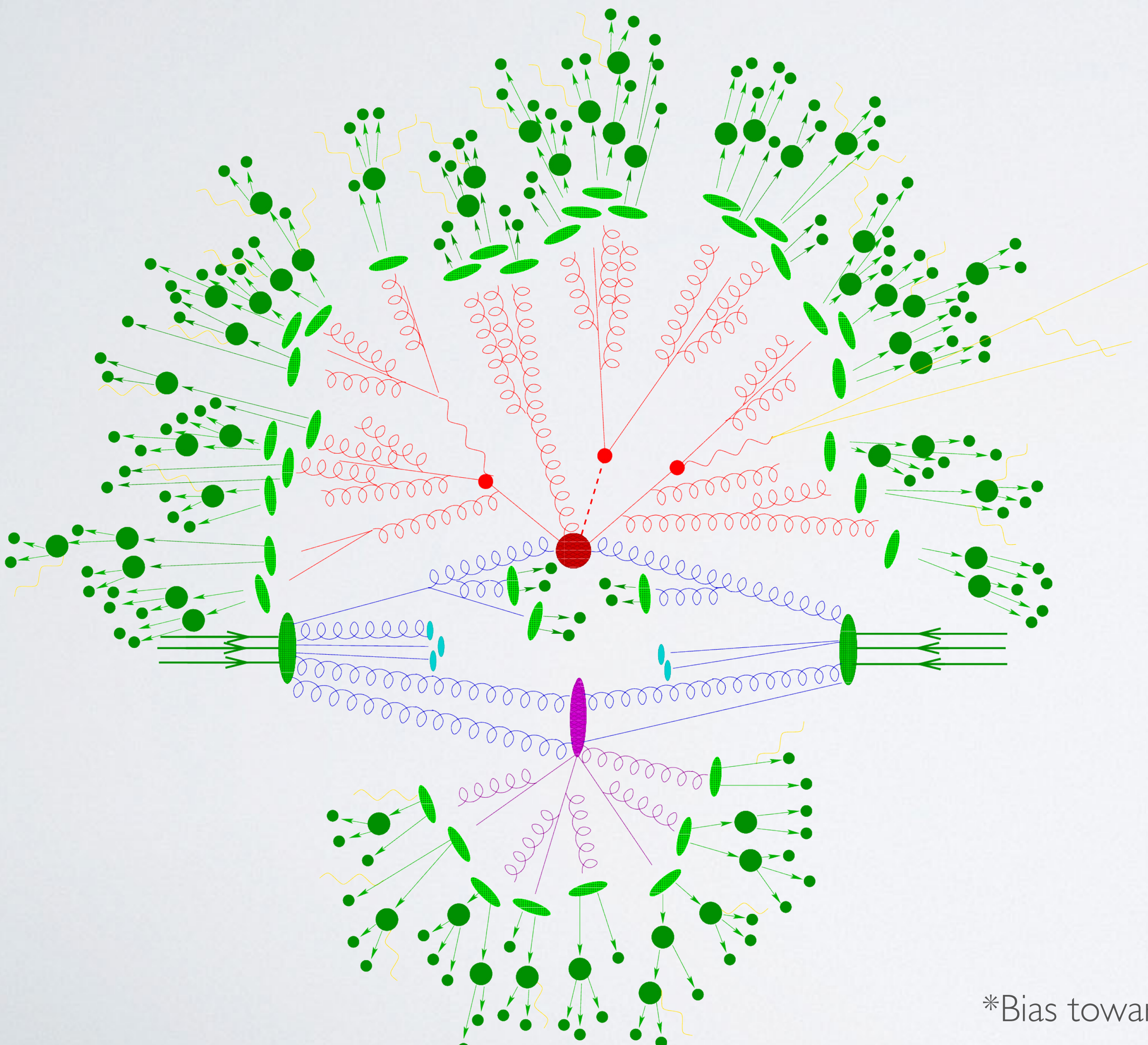

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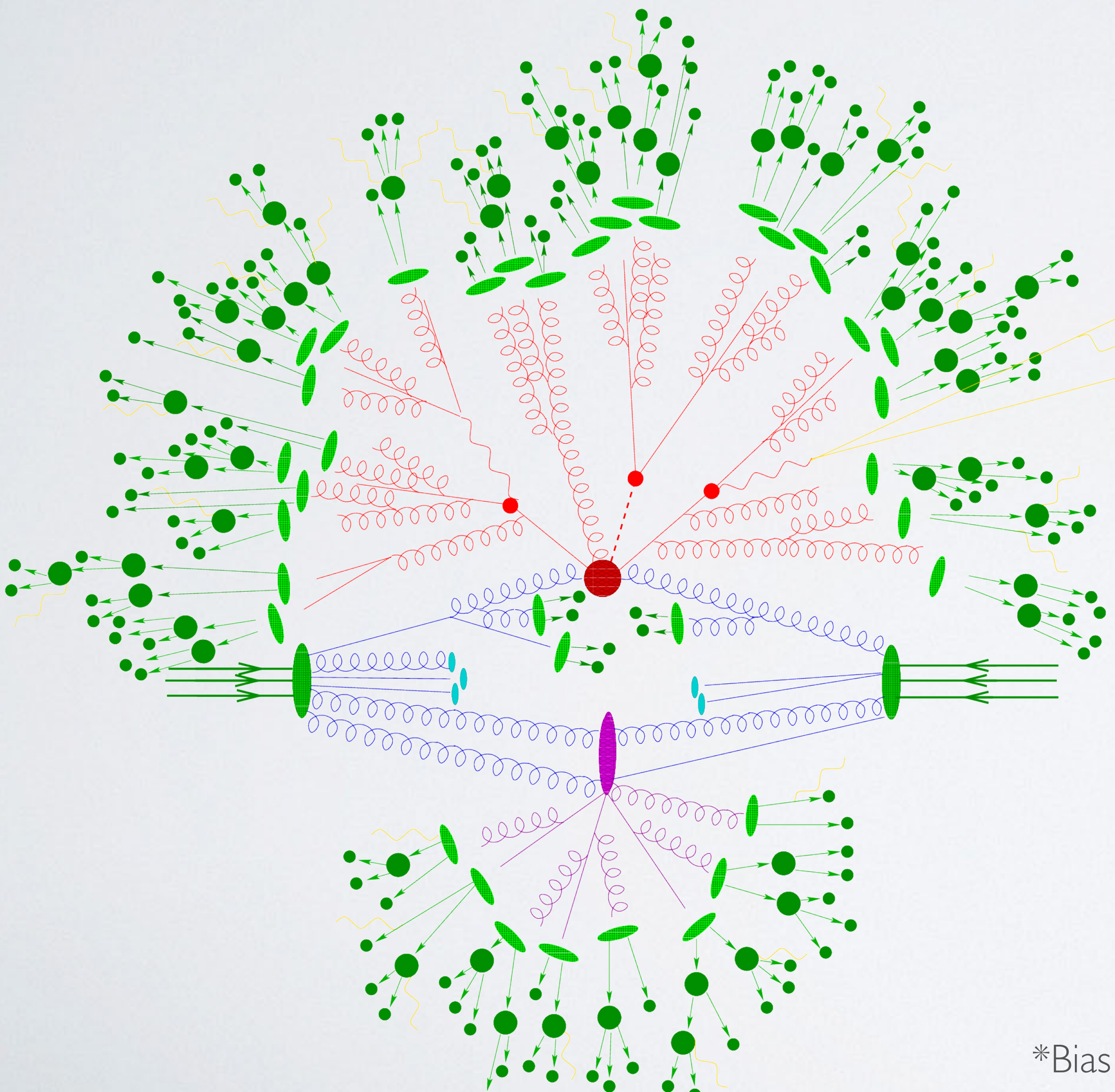

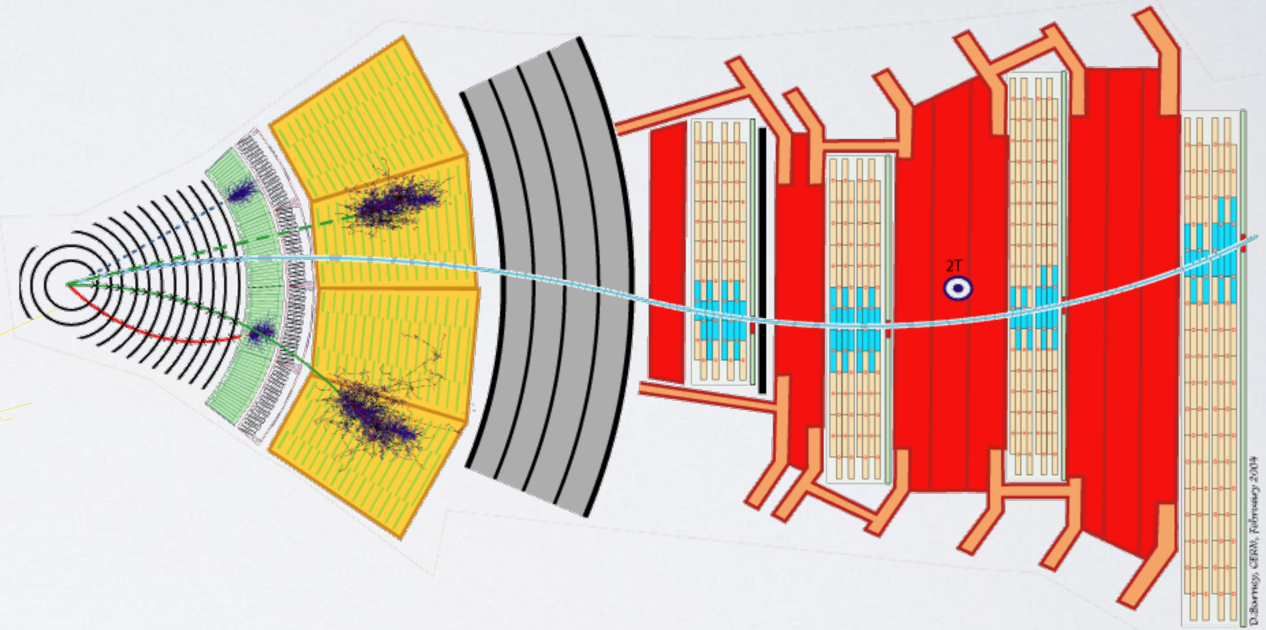

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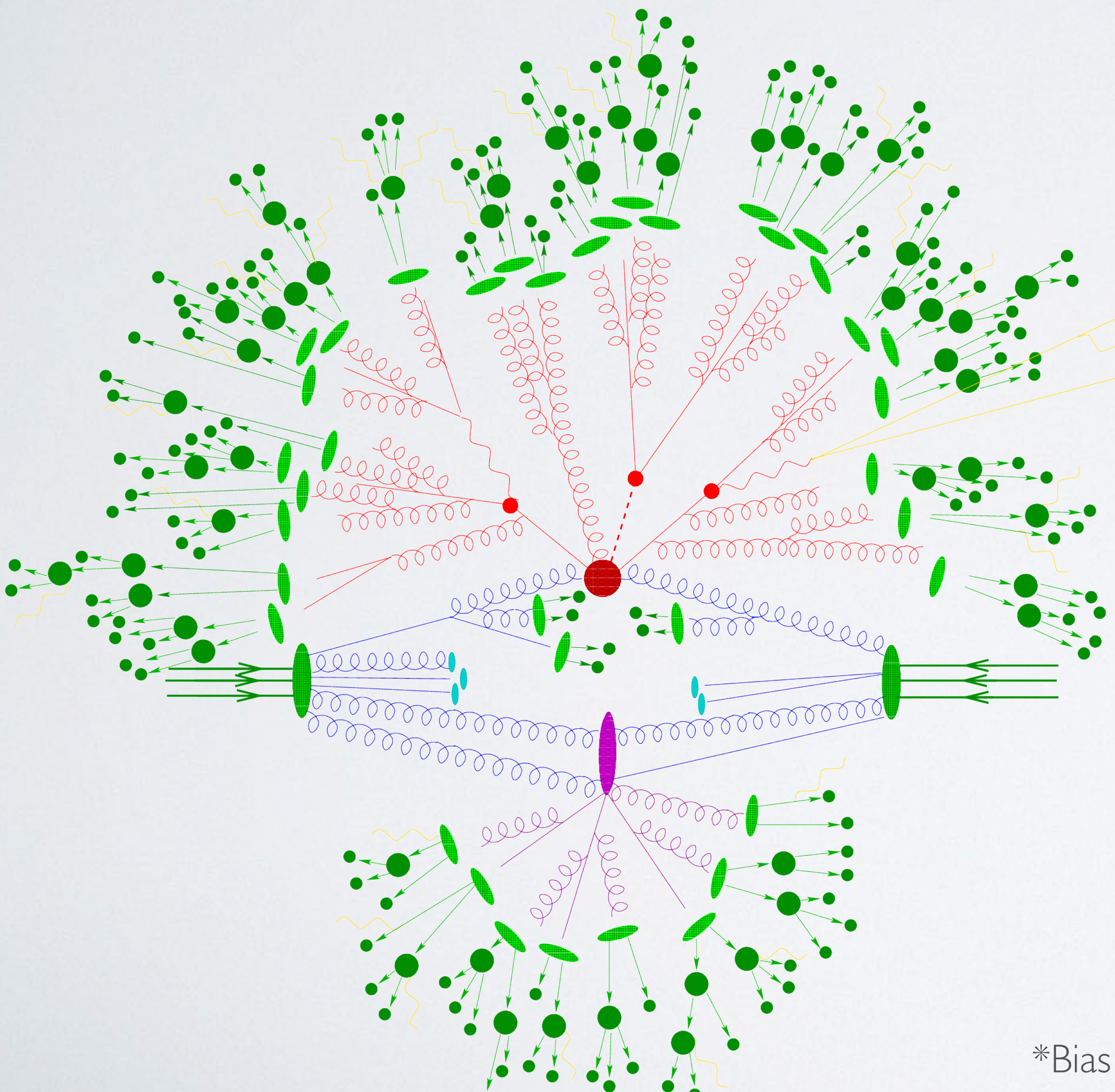

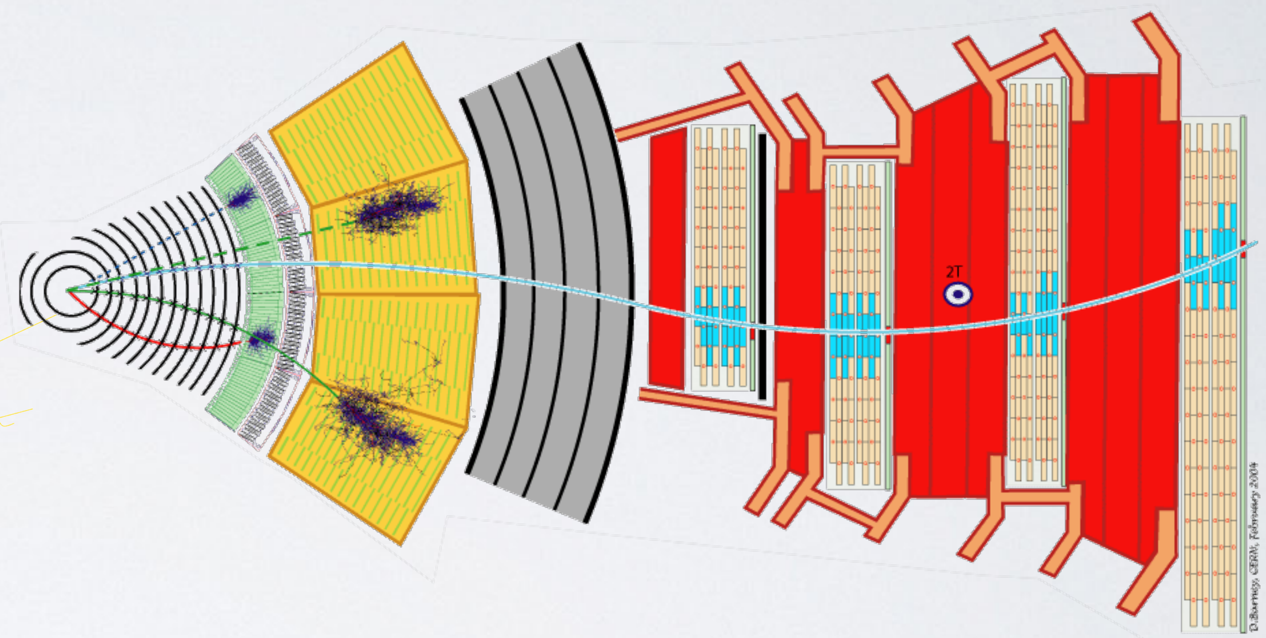

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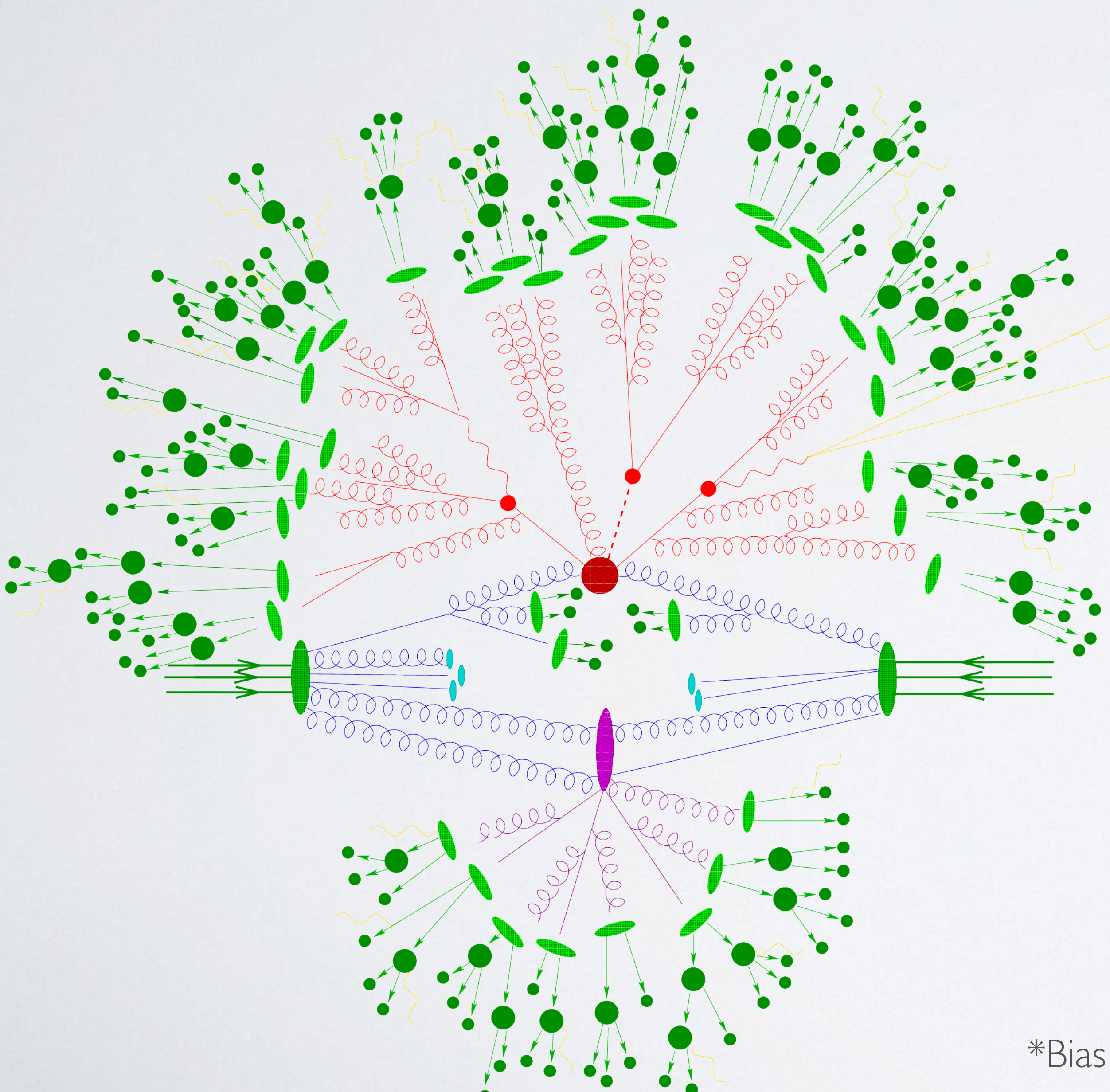

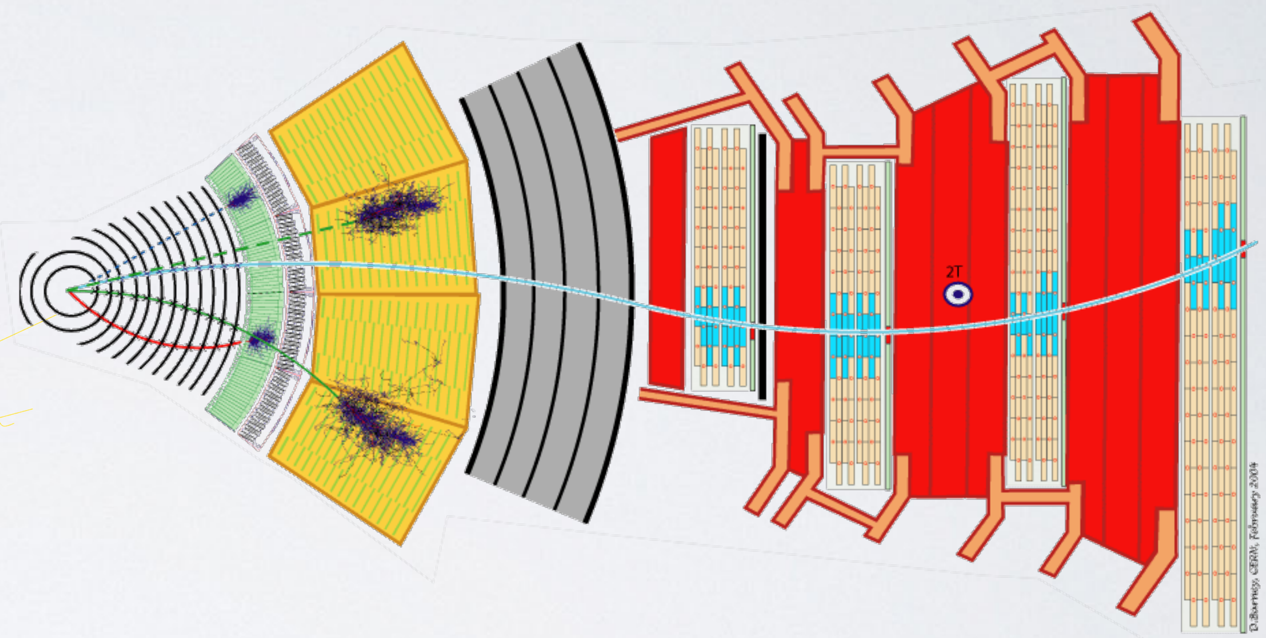

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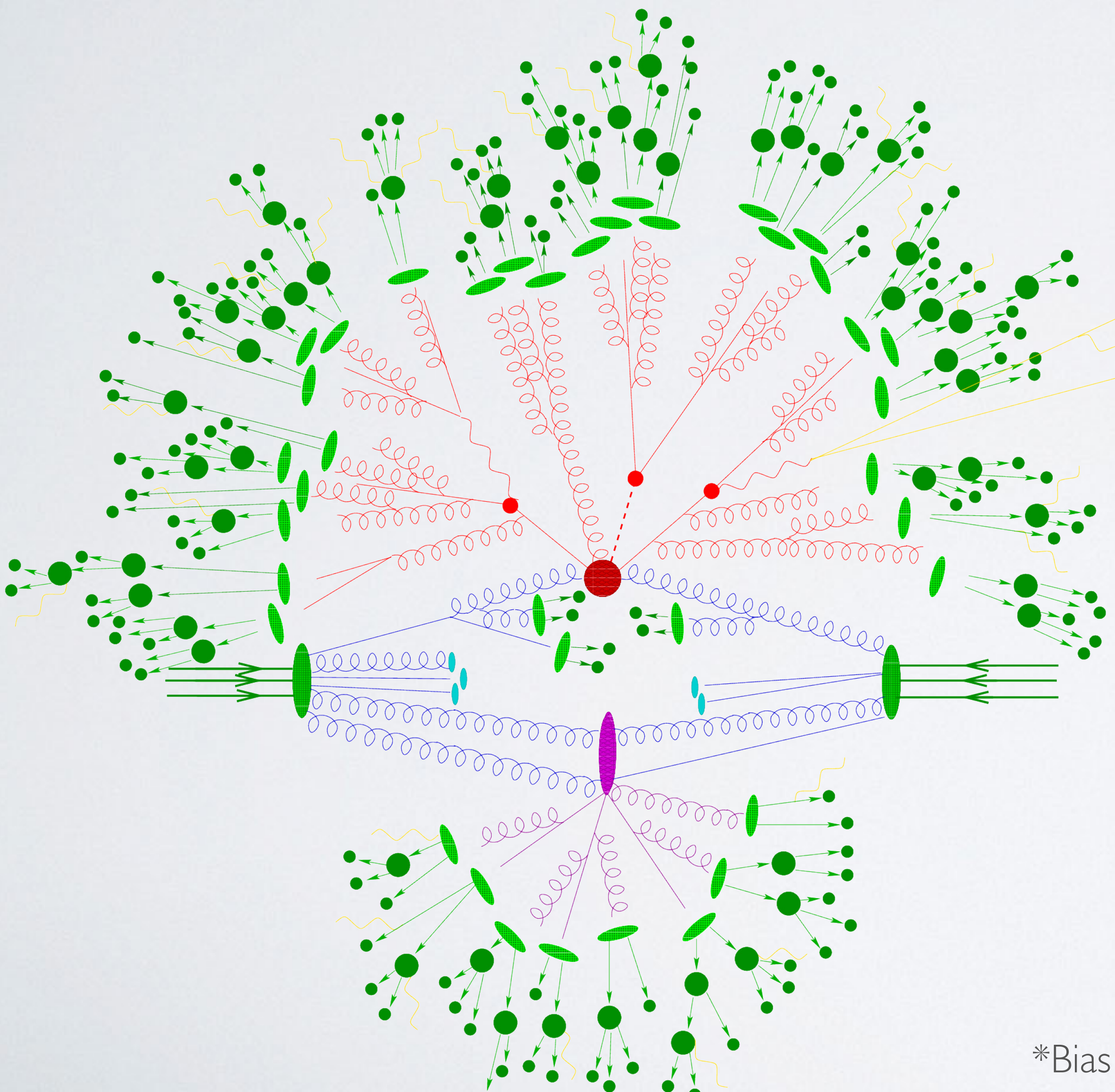

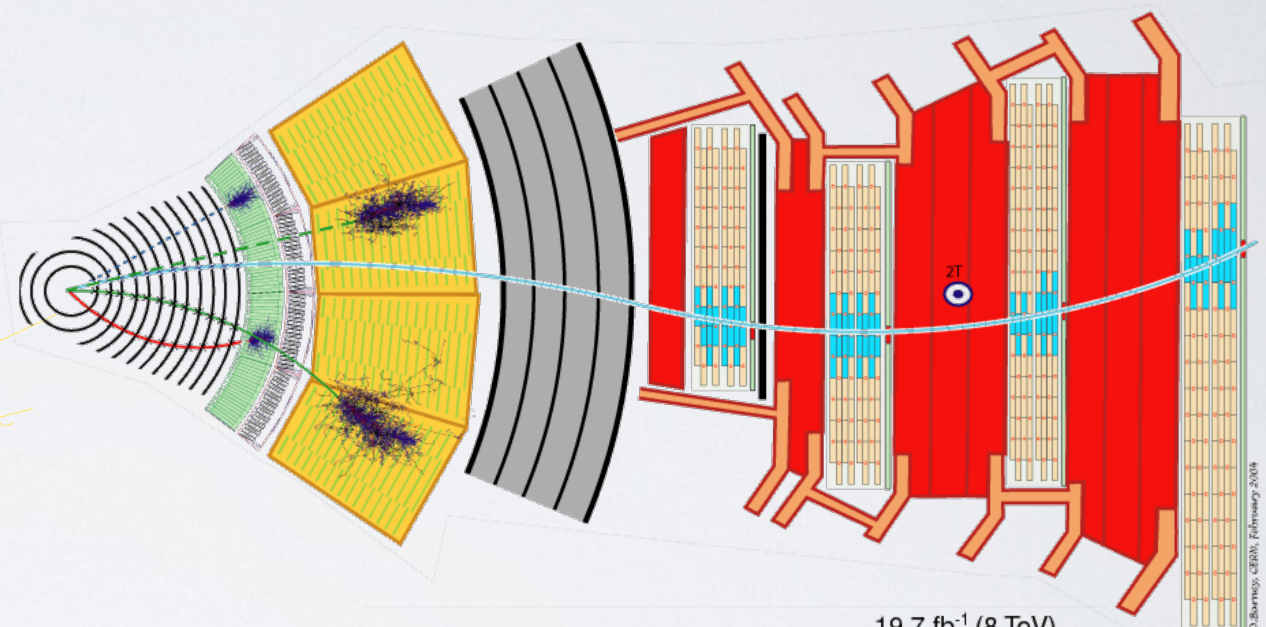

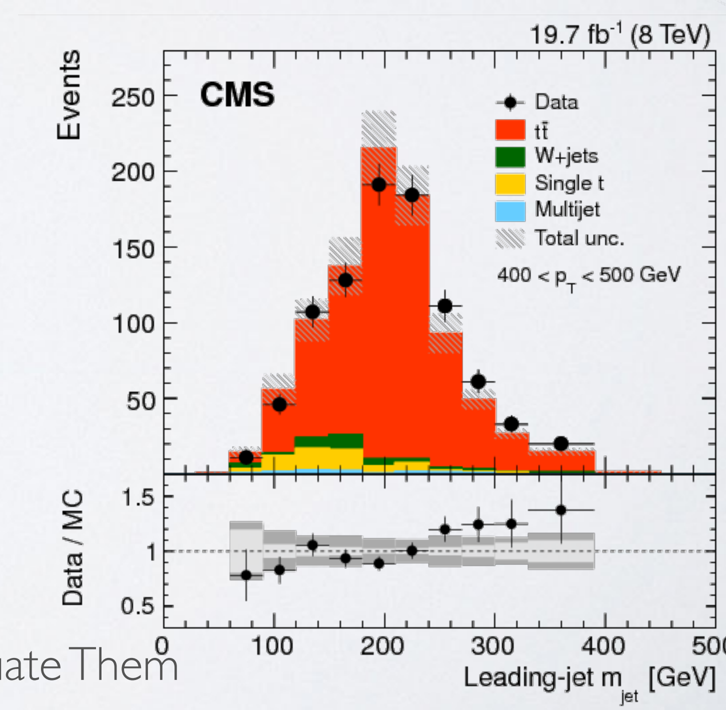

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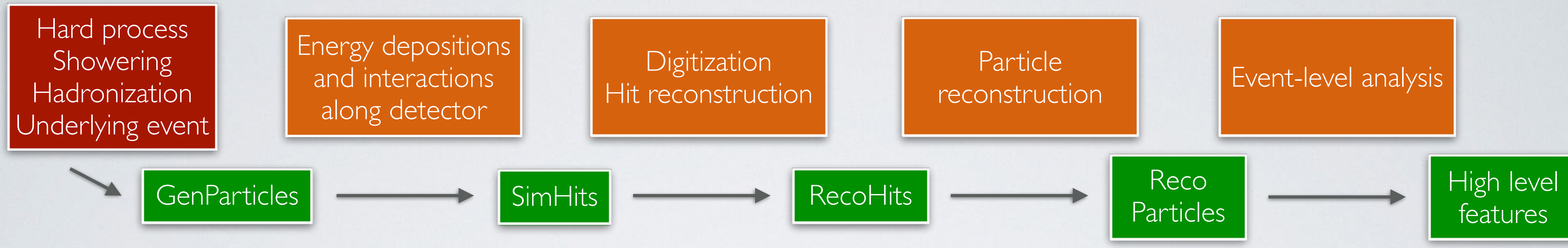

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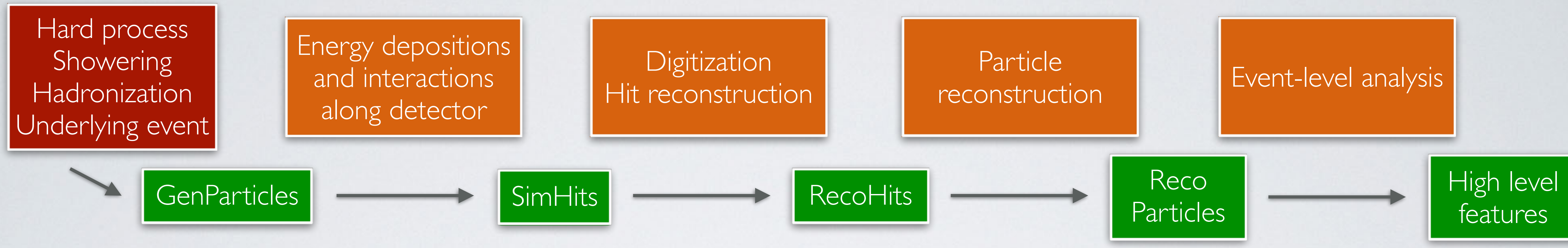

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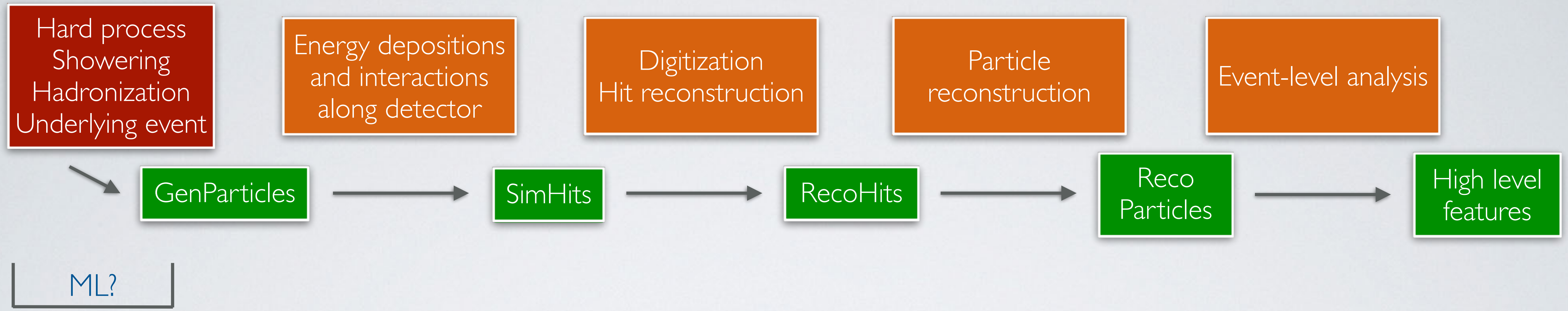

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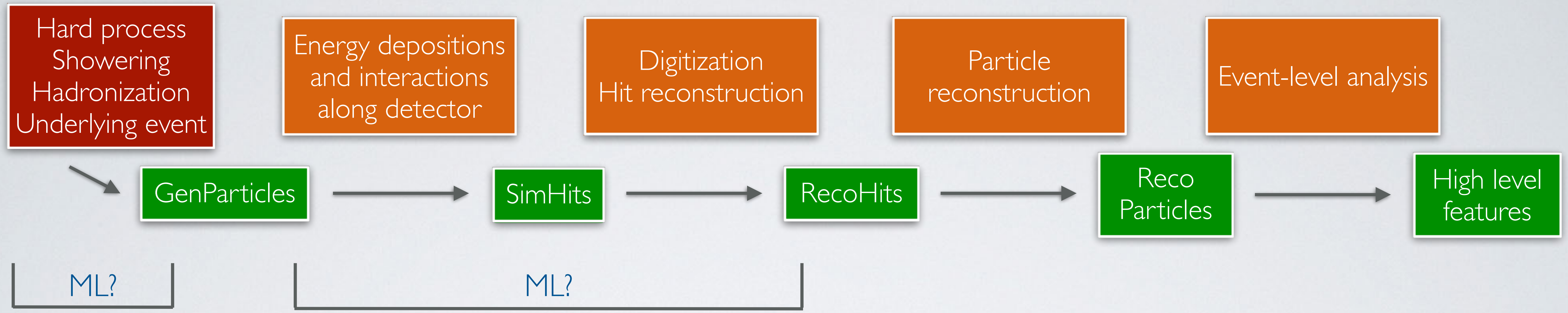

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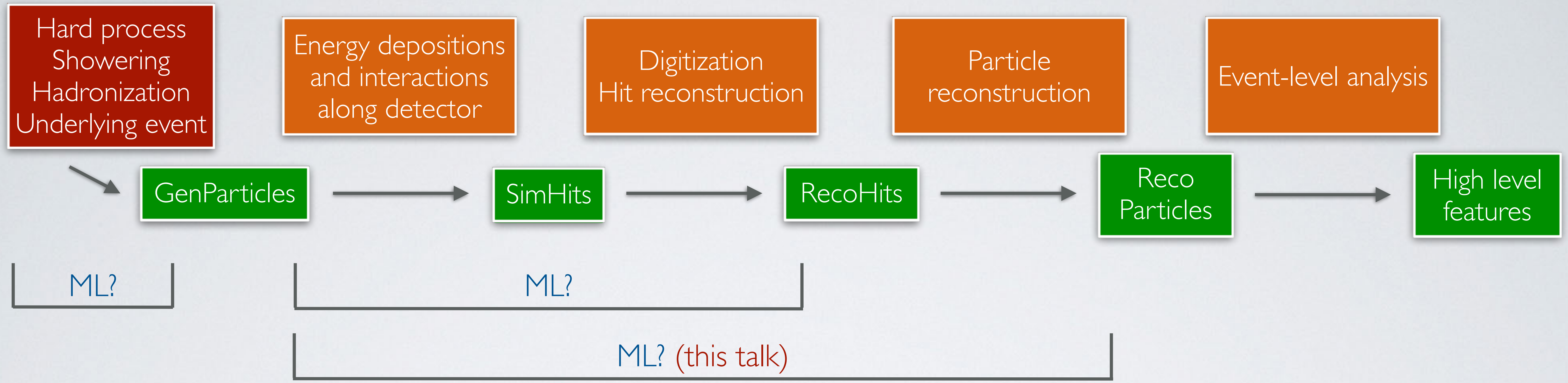

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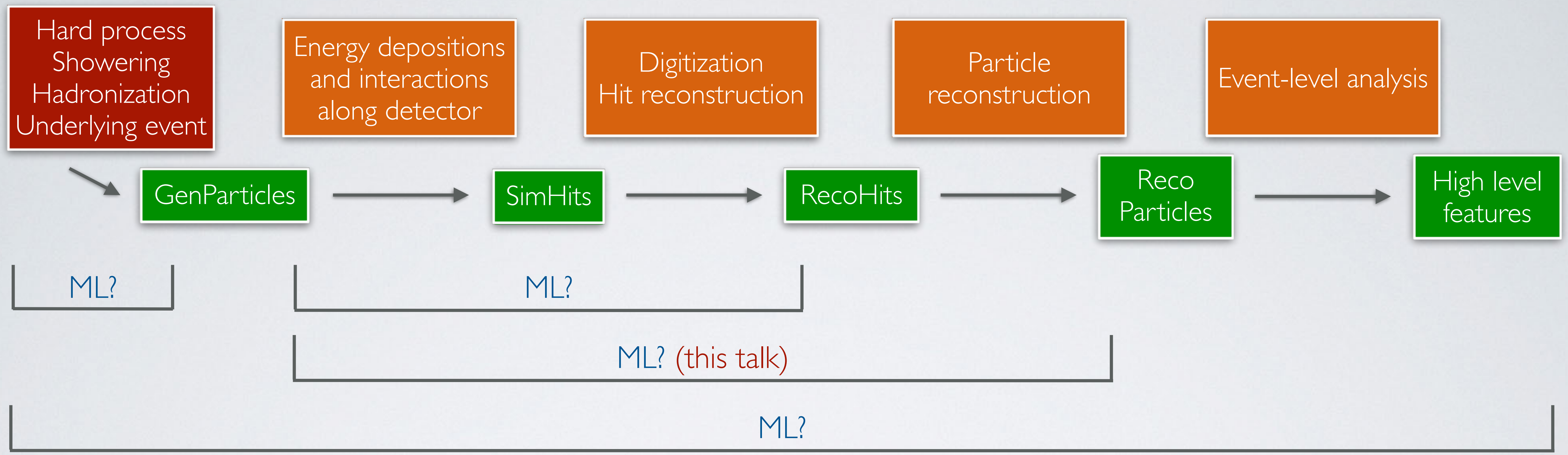

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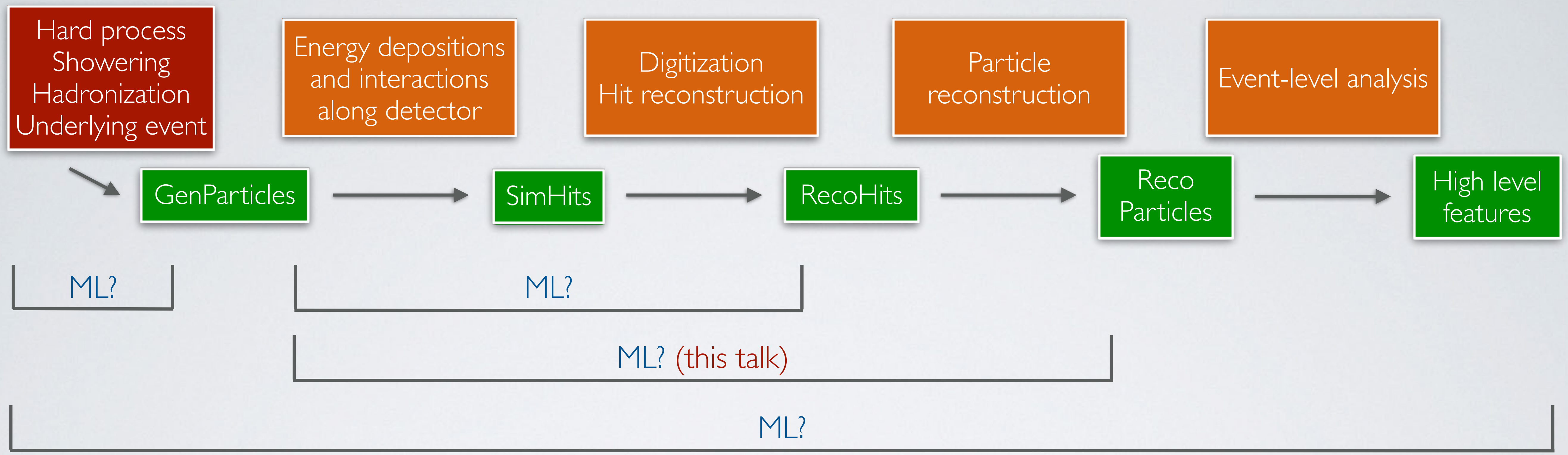

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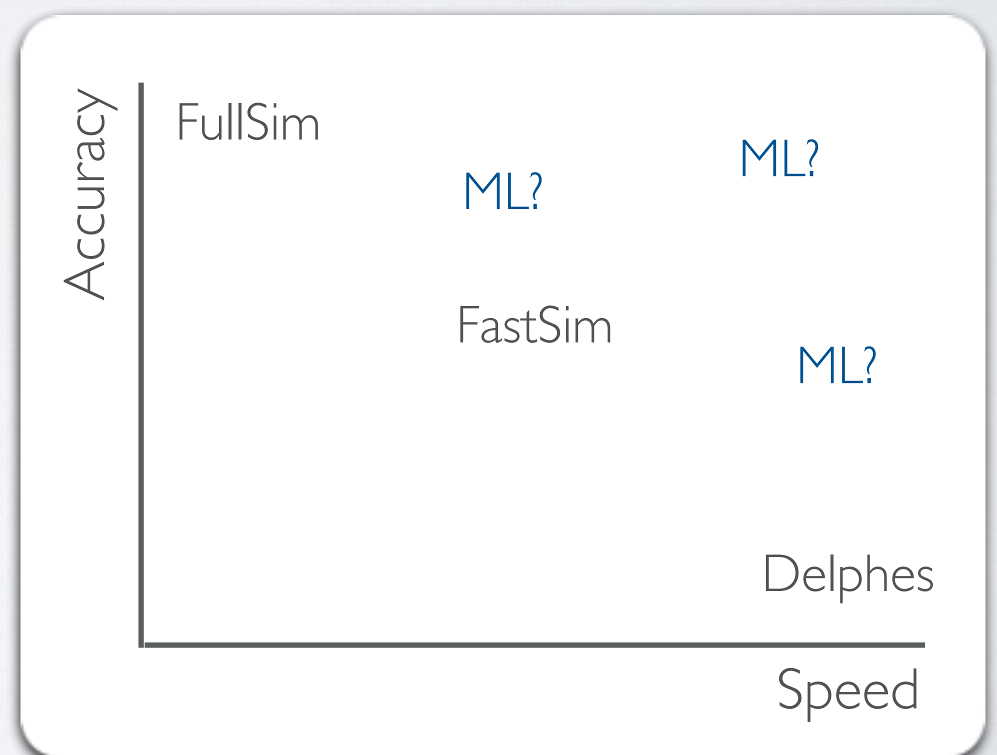
- Trading accuracy of "FullSim" (Geant) for speed



K. Pedro, HSF 2020

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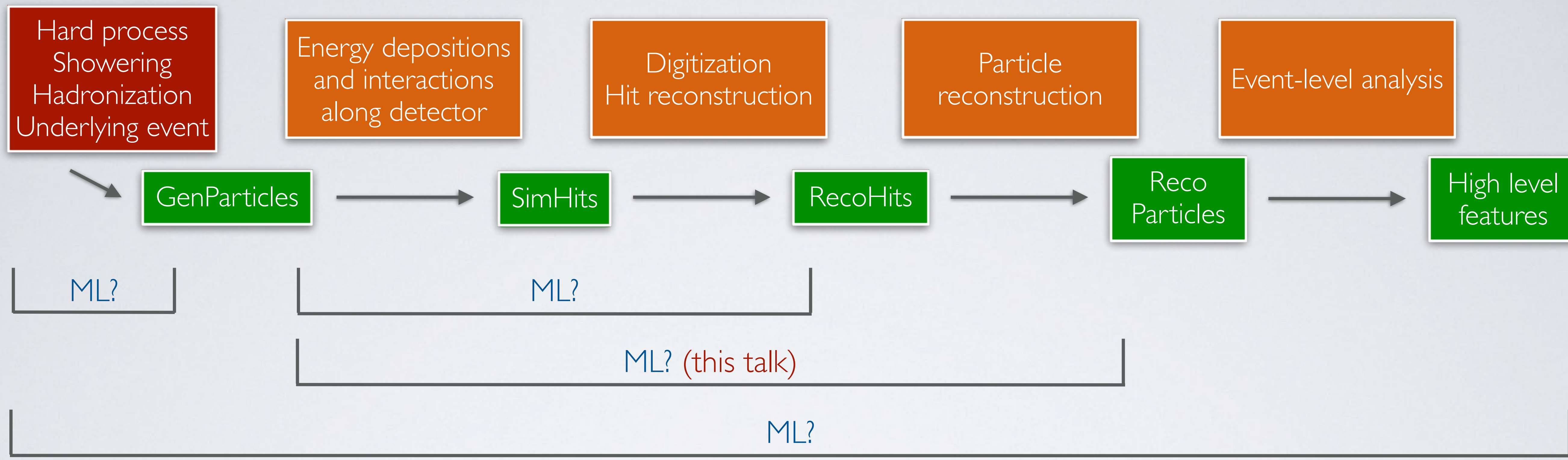
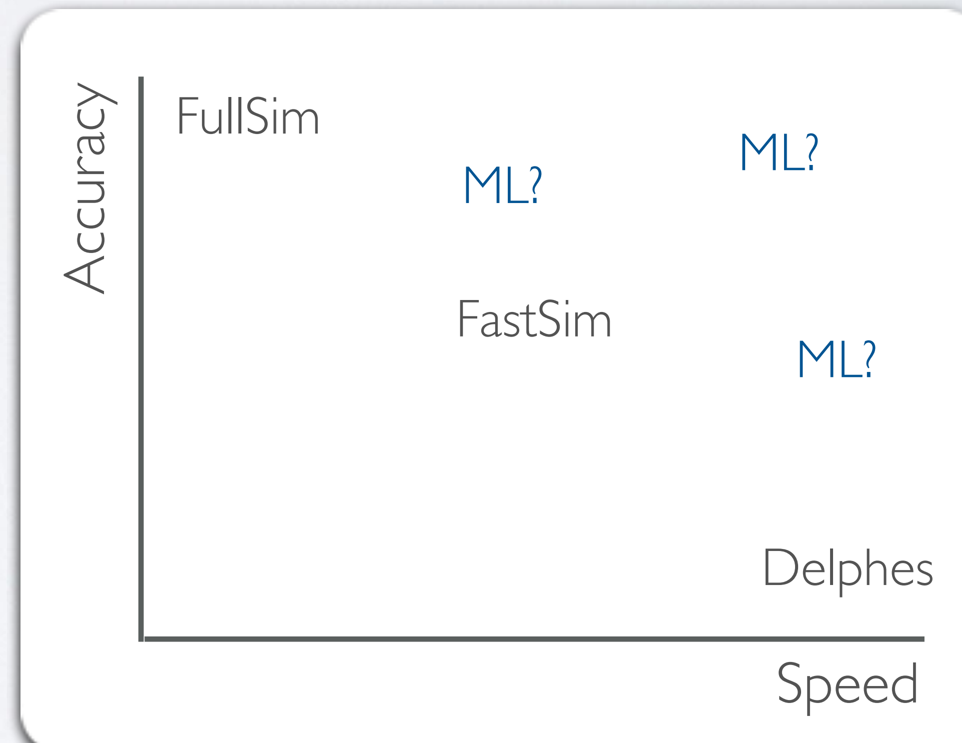


- Opportunity for ML alternatives in many steps
- Trading accuracy of "FullSim" (Geant) for speed
- Trading interpretability/trust for # of steps



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- How do we choose and use these for HL-LHC?

- How do we **trust** generated data?

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- How do we compare generative models?

- How do we **trust** generated data? **Evaluation metrics**

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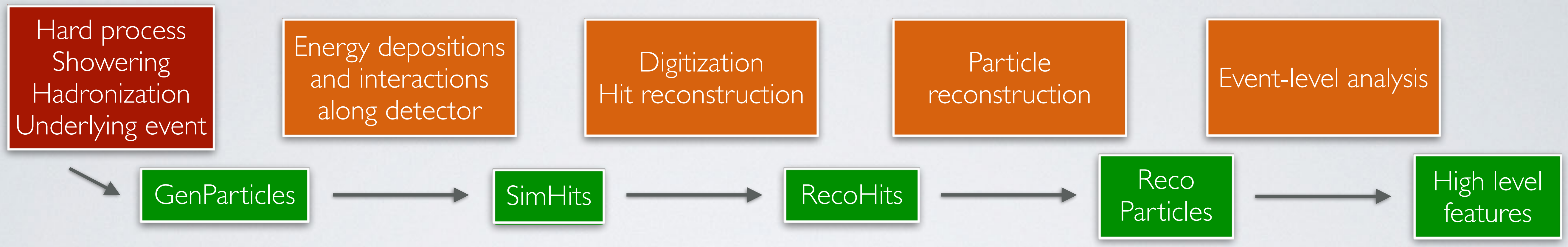

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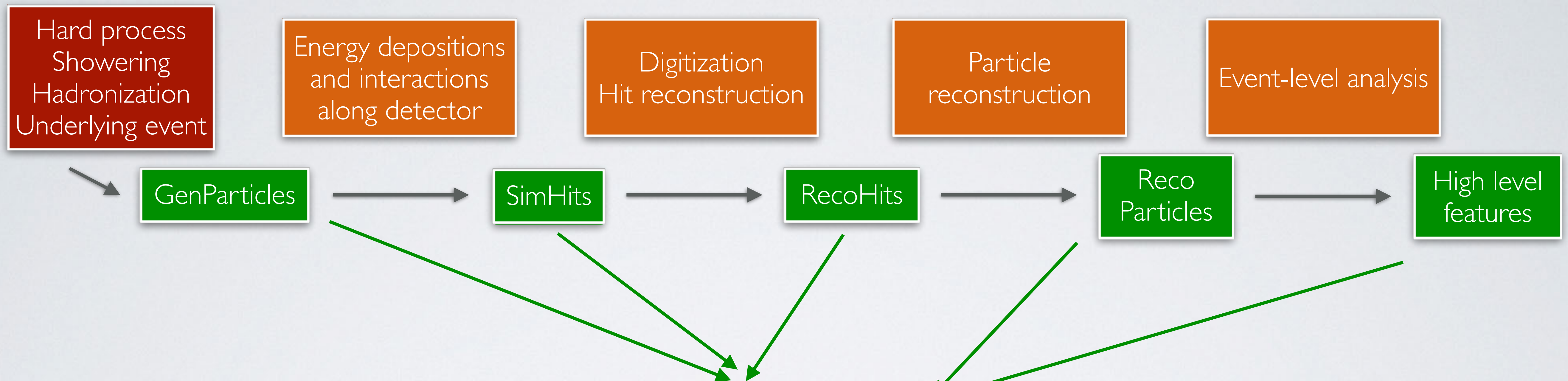

- Want to quantify difference between $p_{\text{real}}(\mathbf{x})$ and $p_{\text{gen}}(\mathbf{x})$ distributions

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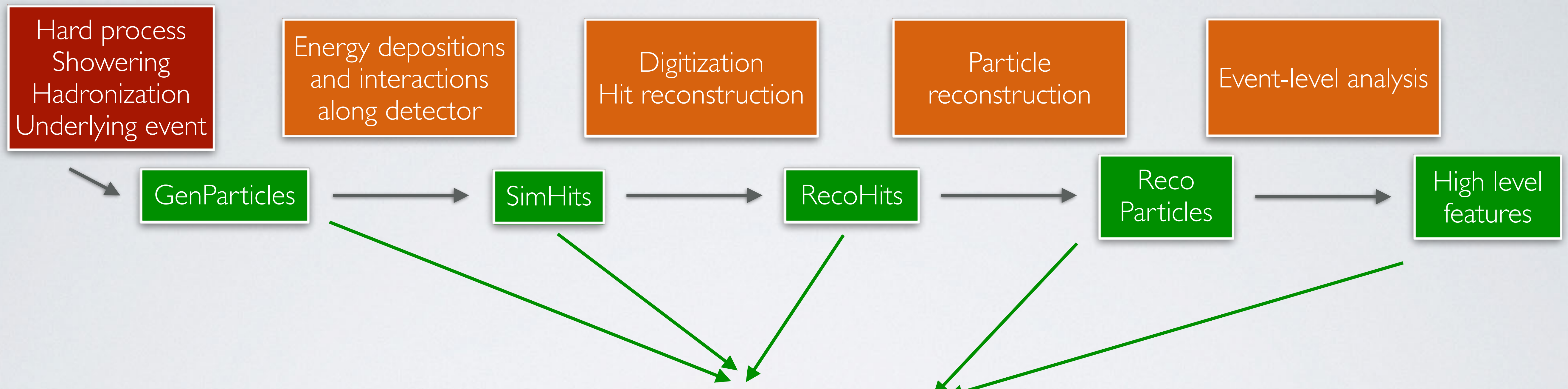

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⇒ Multivariate goodness-of-fit (GOF) / two-sample test

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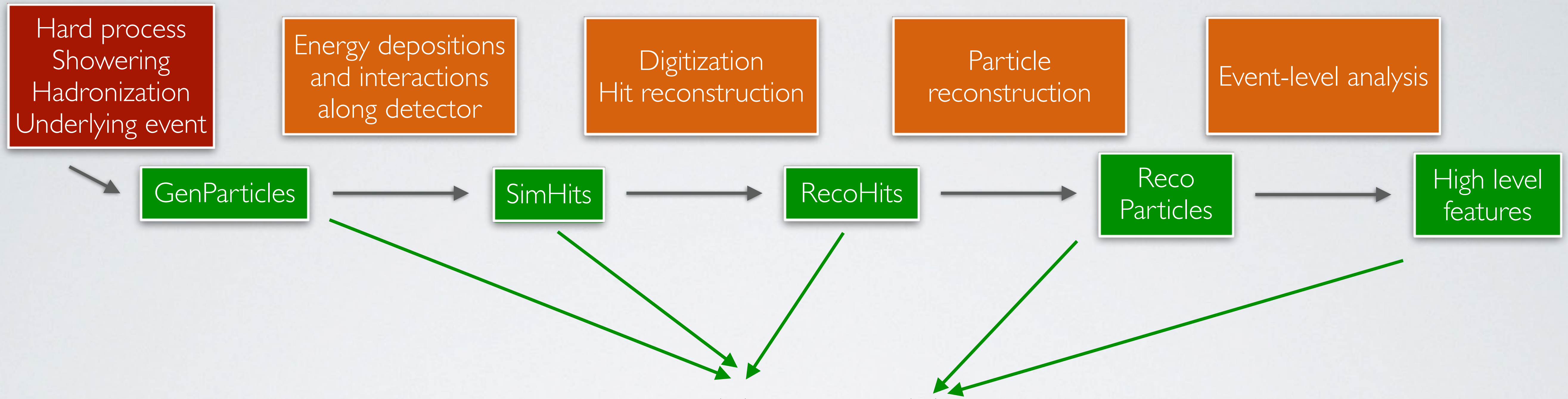

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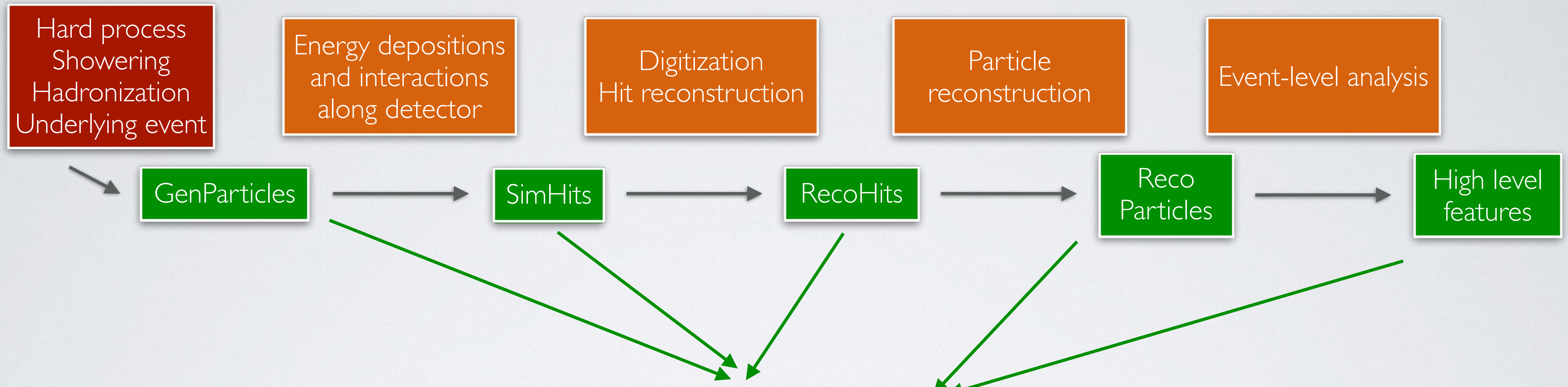

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- Need to choose based on the relevant alternative hypotheses

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METHODS

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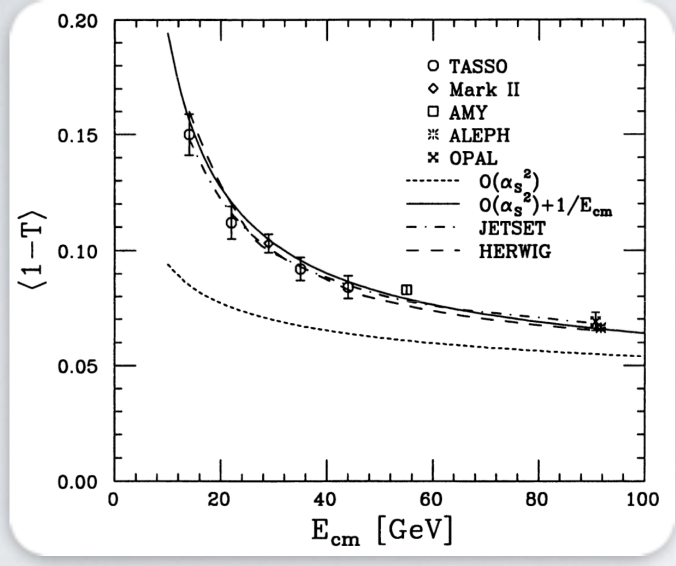
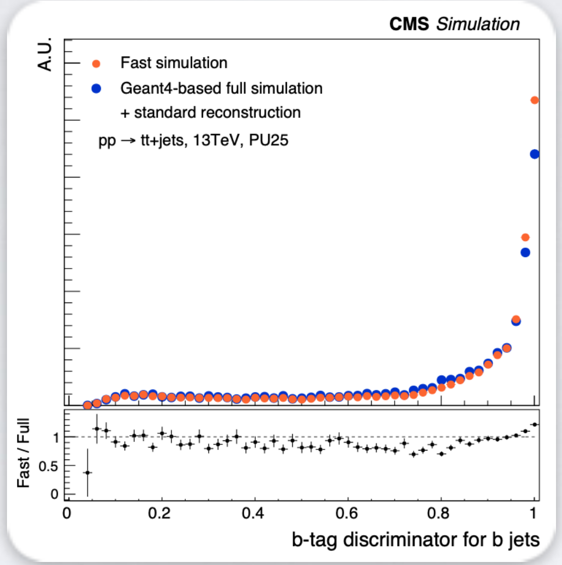
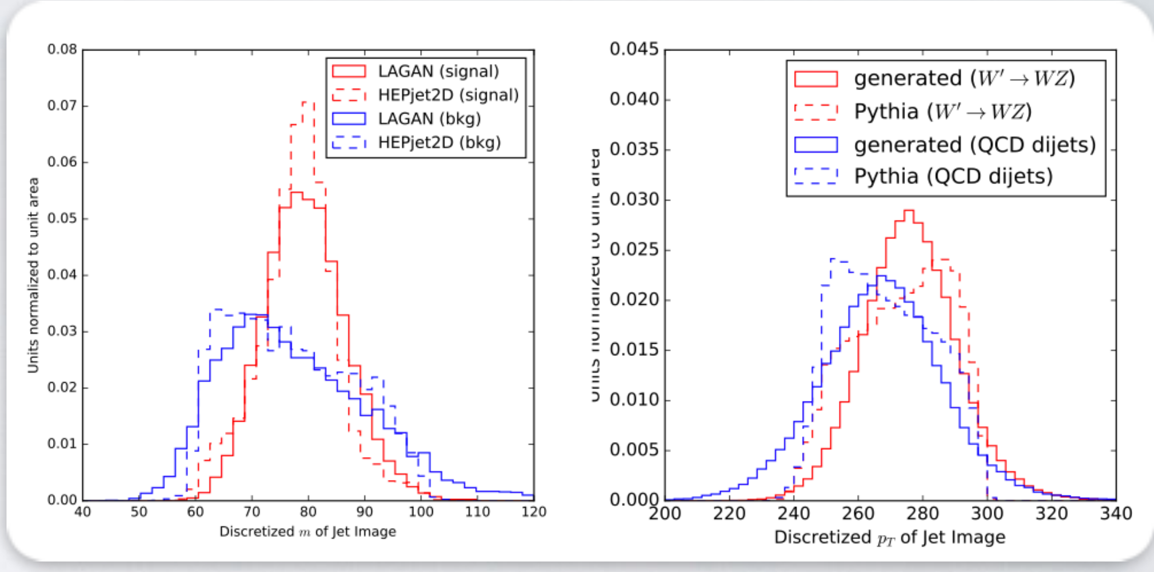
MC generator evaluation (Ellis et al '96)



FastSim (Sekmen '17)



LAGAN (de Oliveira et al '17)



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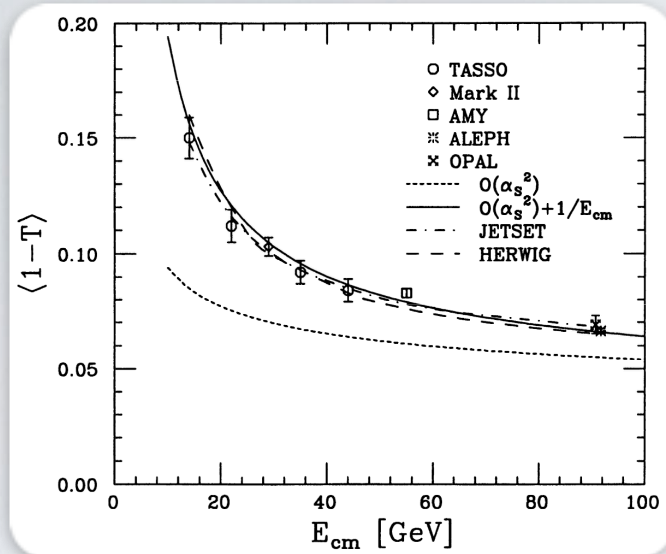

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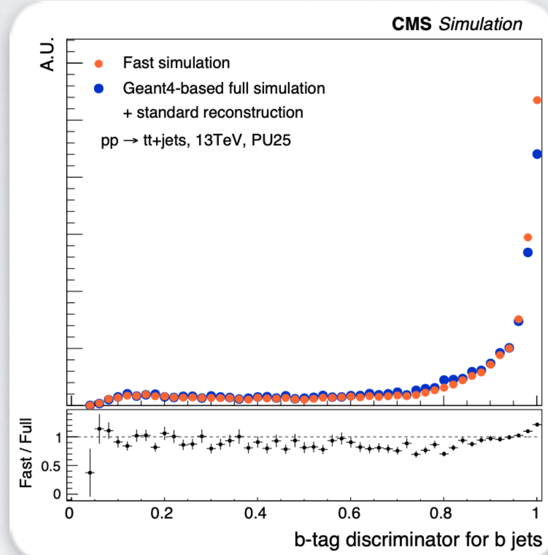

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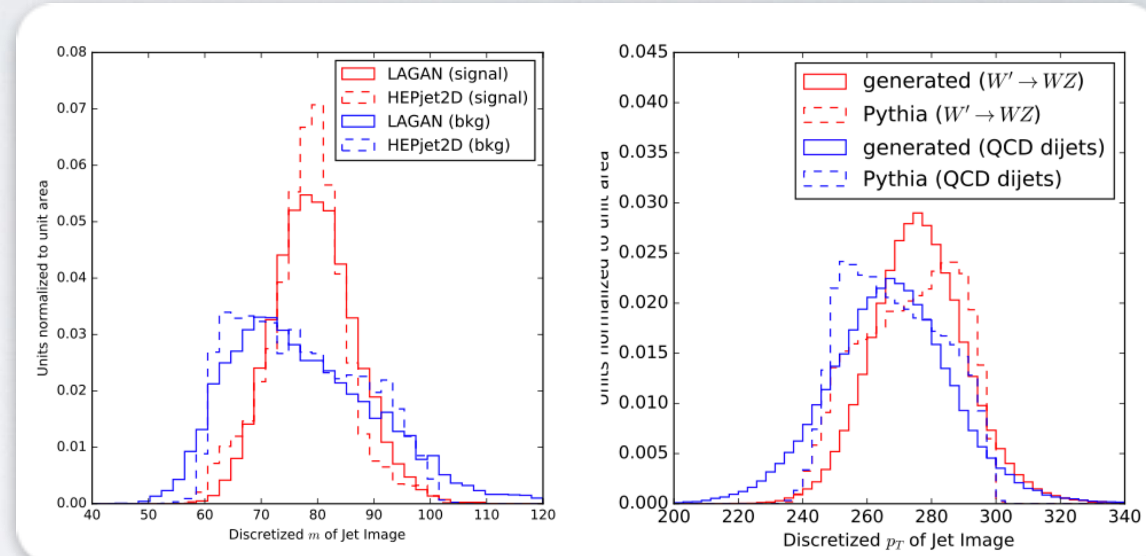

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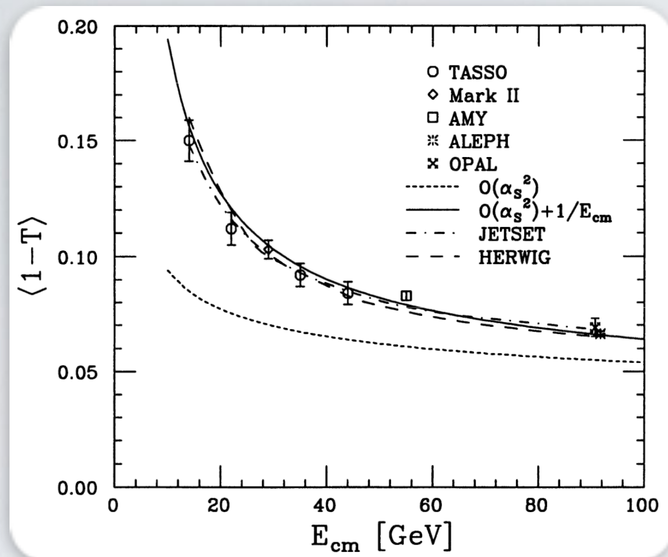

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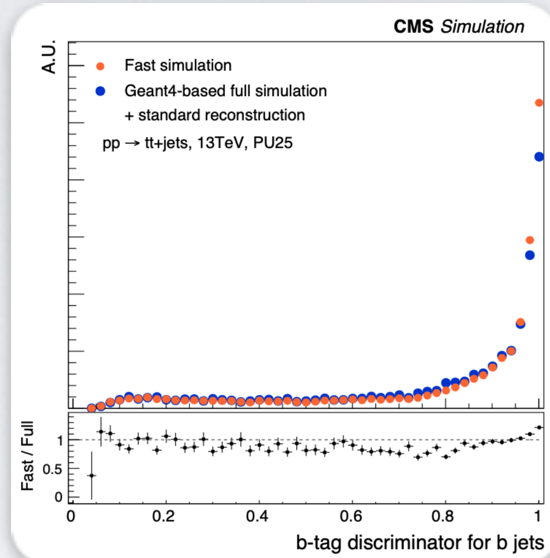

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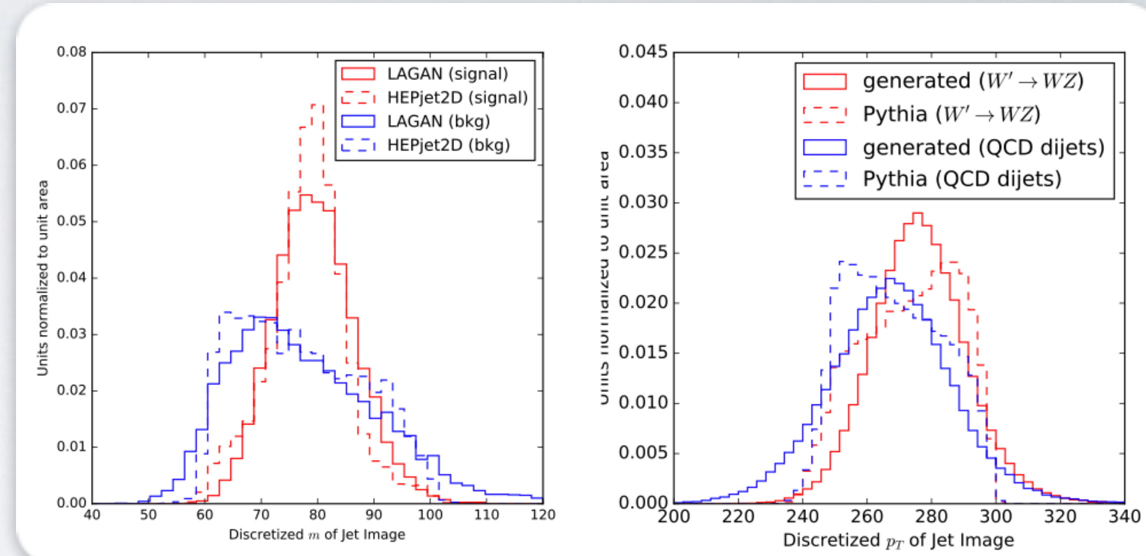

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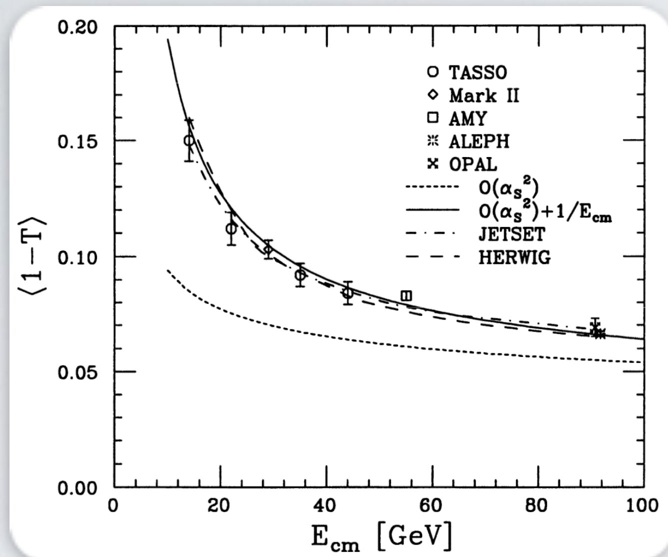

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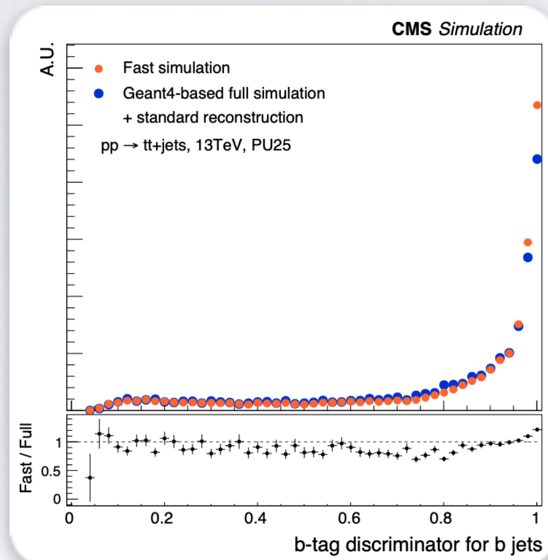

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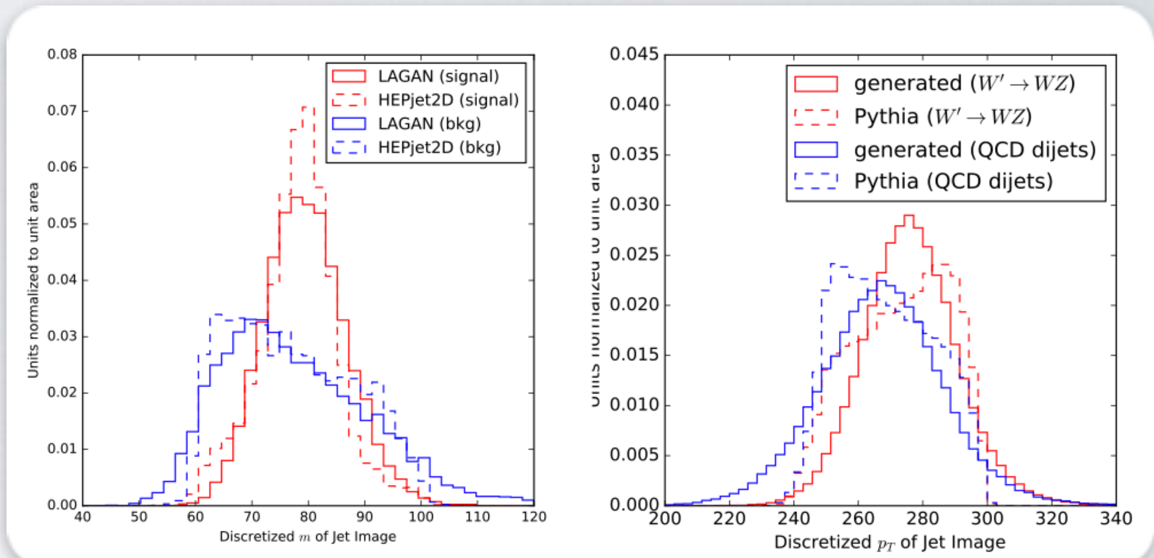

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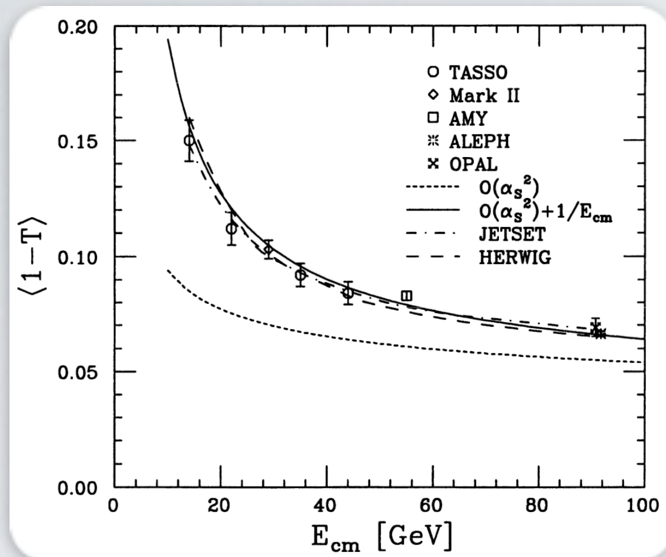

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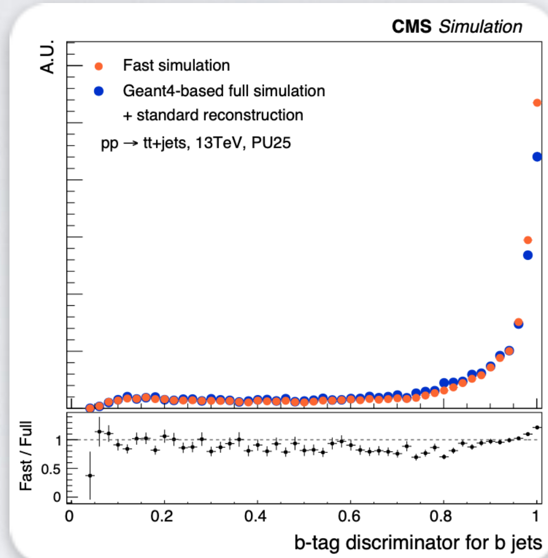

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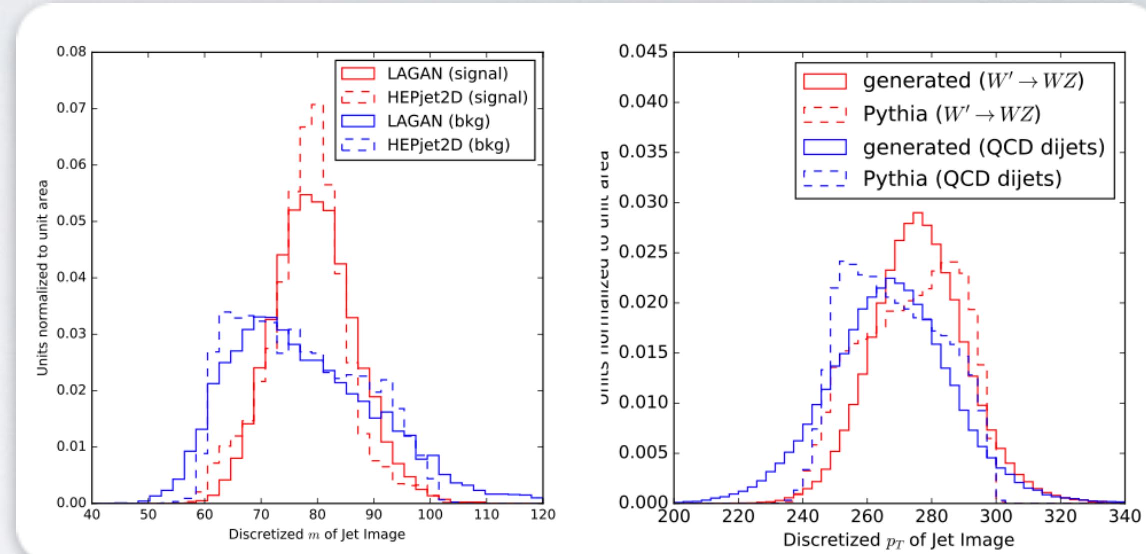

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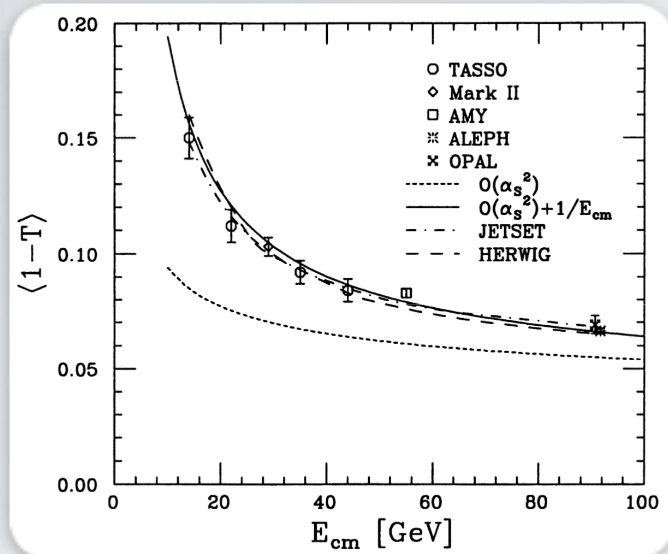

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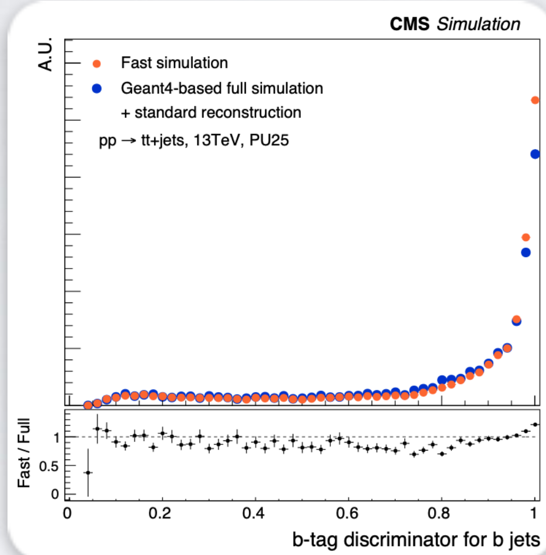

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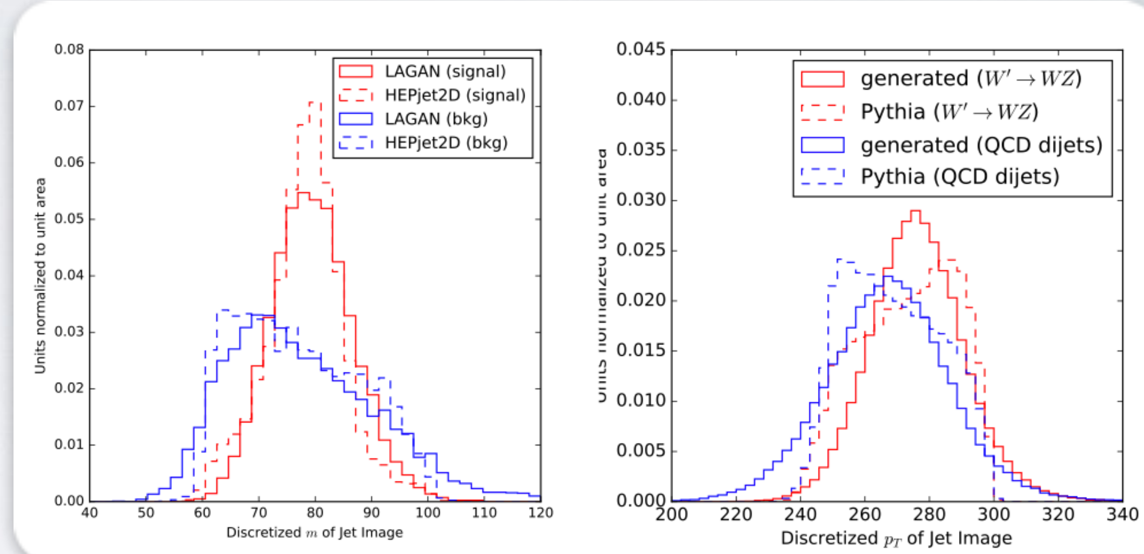

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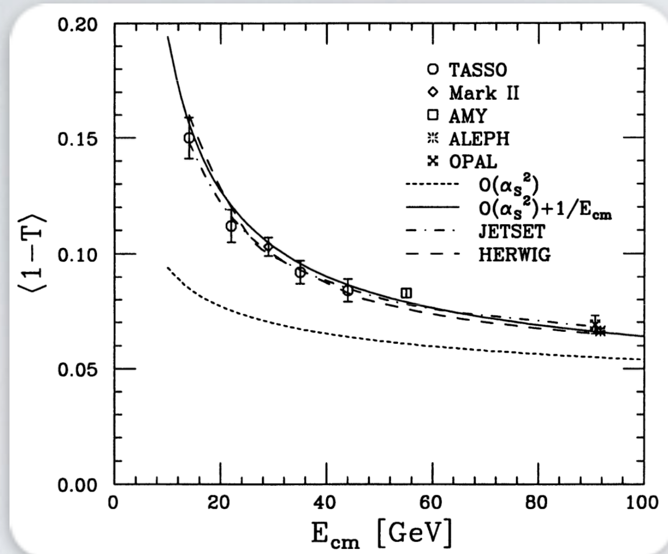

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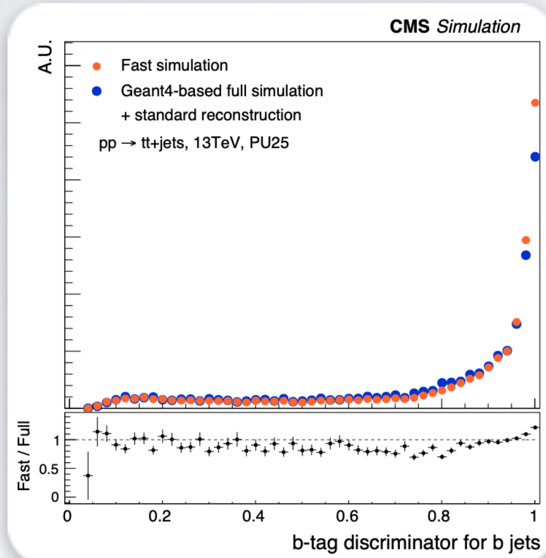

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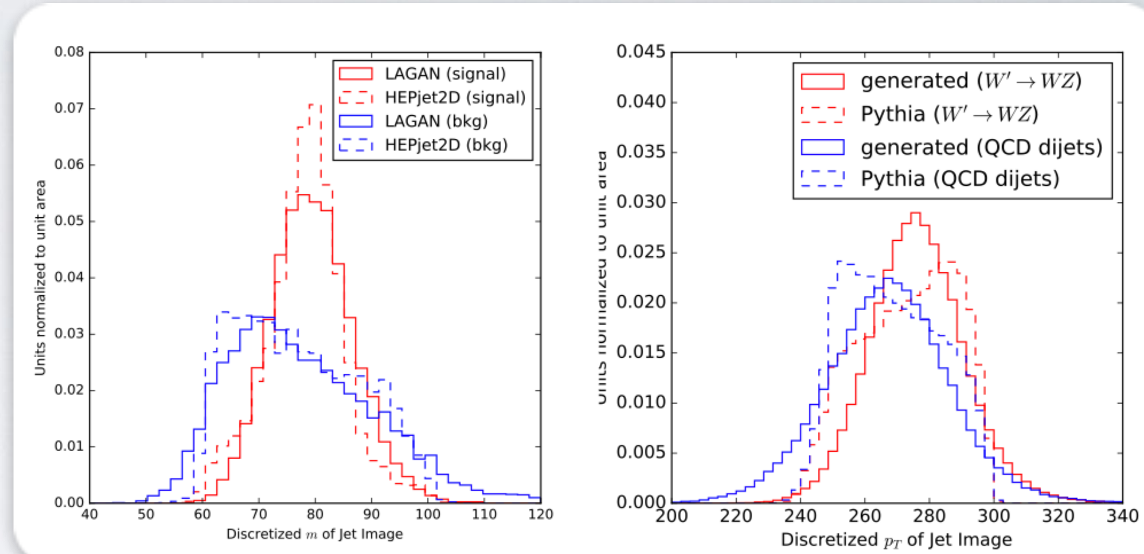

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- Cons:
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  - No well-defined way to aggregate scores across multiple distributions

$p_{\text{real}}(\mathbf{x})$ vs $p_{\text{gen}}(\mathbf{x})$

Sources 1, 2

$p_{\text{real}}(\mathbf{x})$ vs $p_{\text{gen}}(\mathbf{x})$

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Integral Probability Metrics $D_{\mathscr{F}}(p_{\text{real}}, p_{\text{gen}})$

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Integral Probability Metrics $D_{\mathcal{F}}(p_{\text{real}}, p_{\text{gen}})$

Wasserstein 1-distance (W_1)

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maximum mean discrepancy (MMD)

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f-Divergences $D_f(p_{\text{real}}, p_{\text{gen}})$

$$\int p_{\text{real}}(x)\, f\left(\frac{p_{\text{real}}(x)}{p_{\text{gen}}(x)} \right) dx$$

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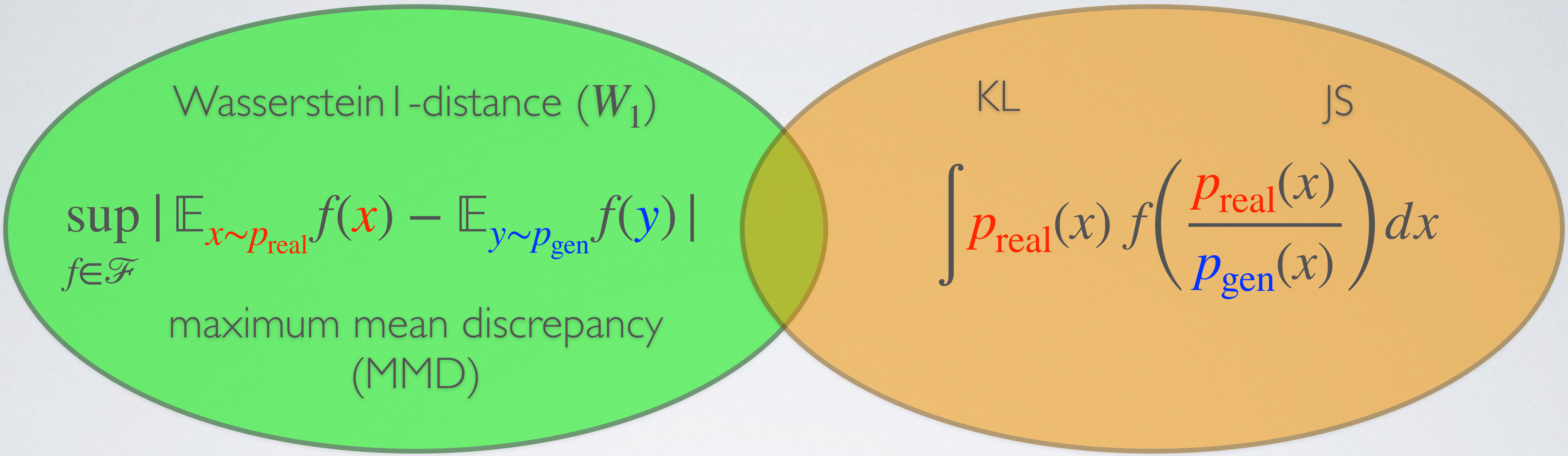

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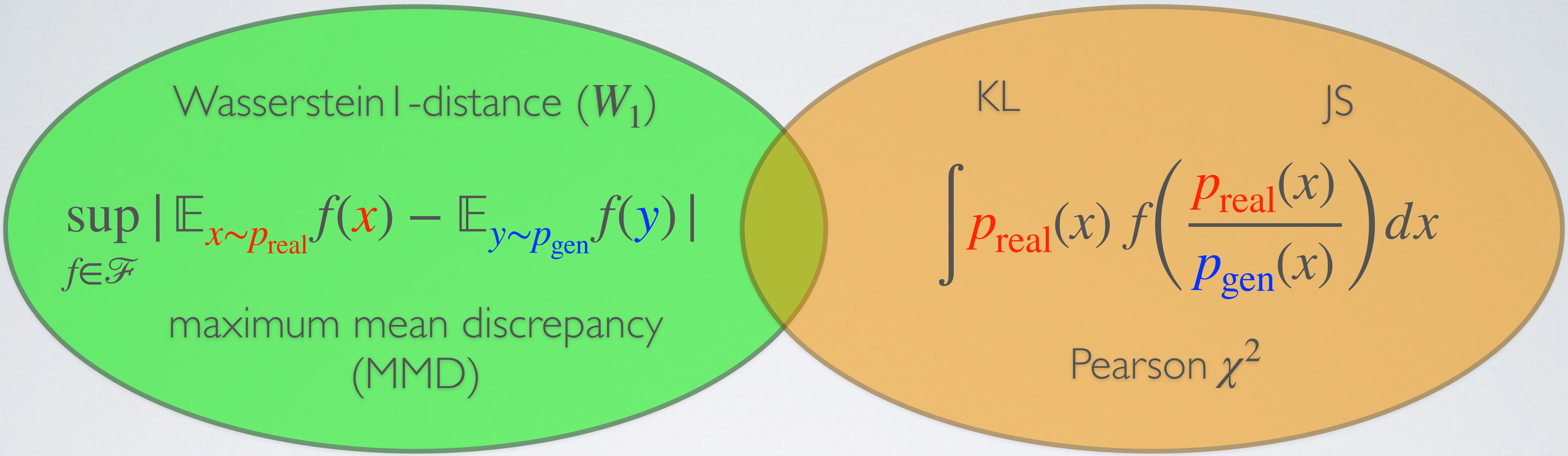

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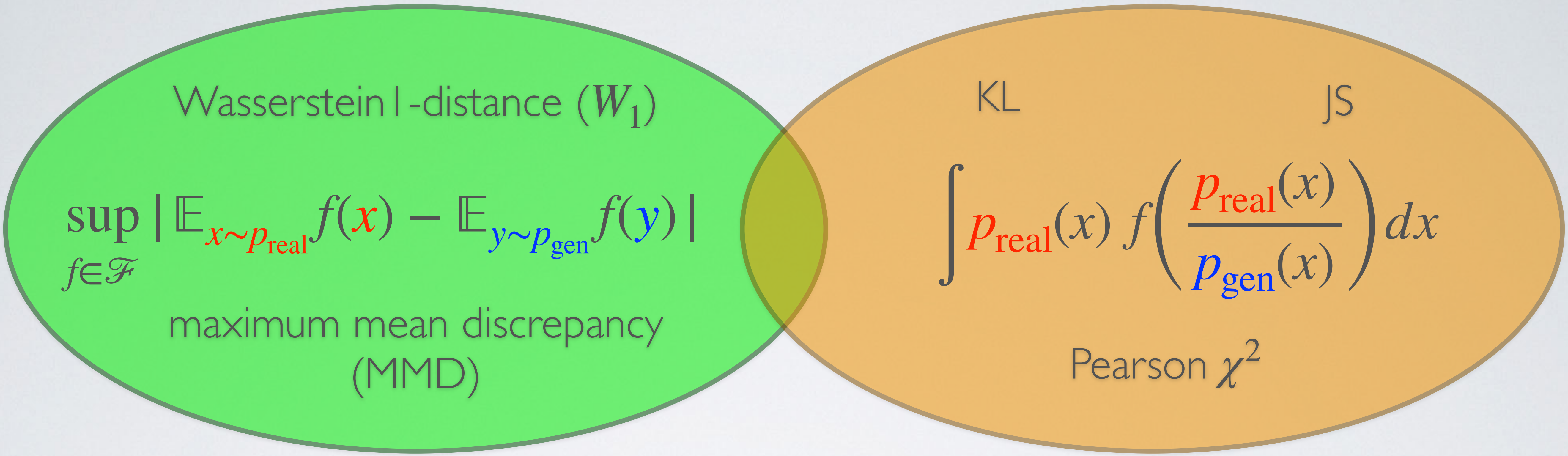

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Pearson χ^2

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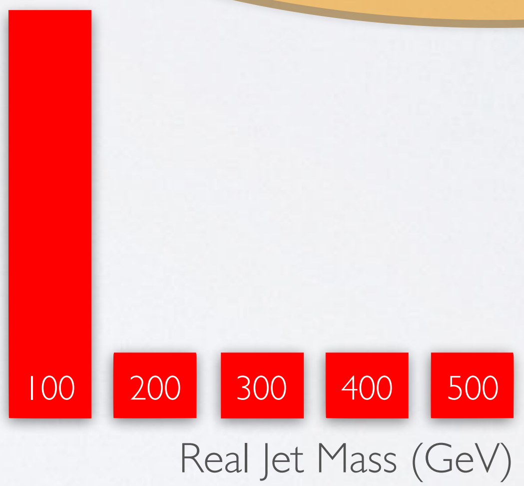

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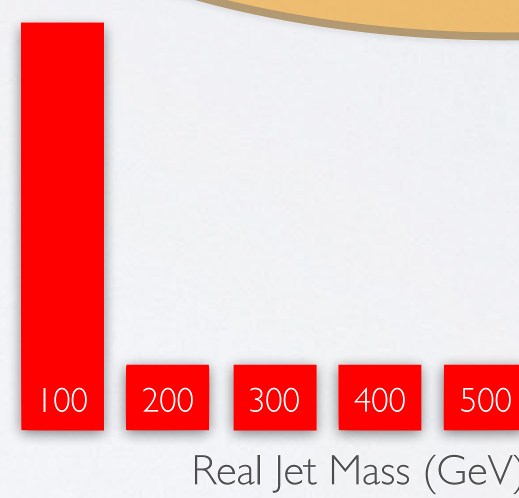

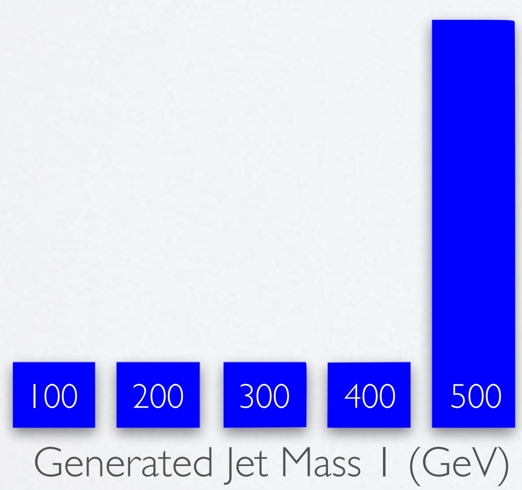

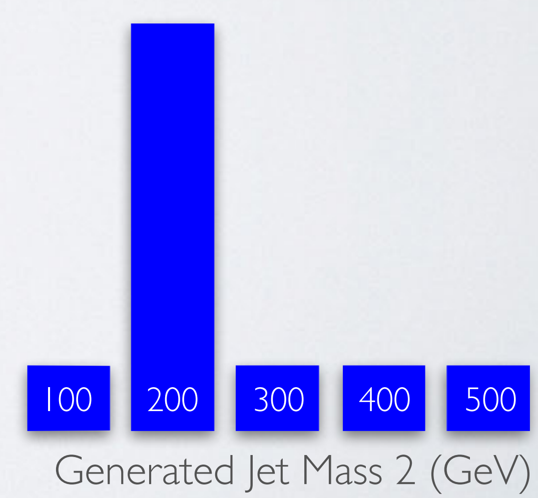

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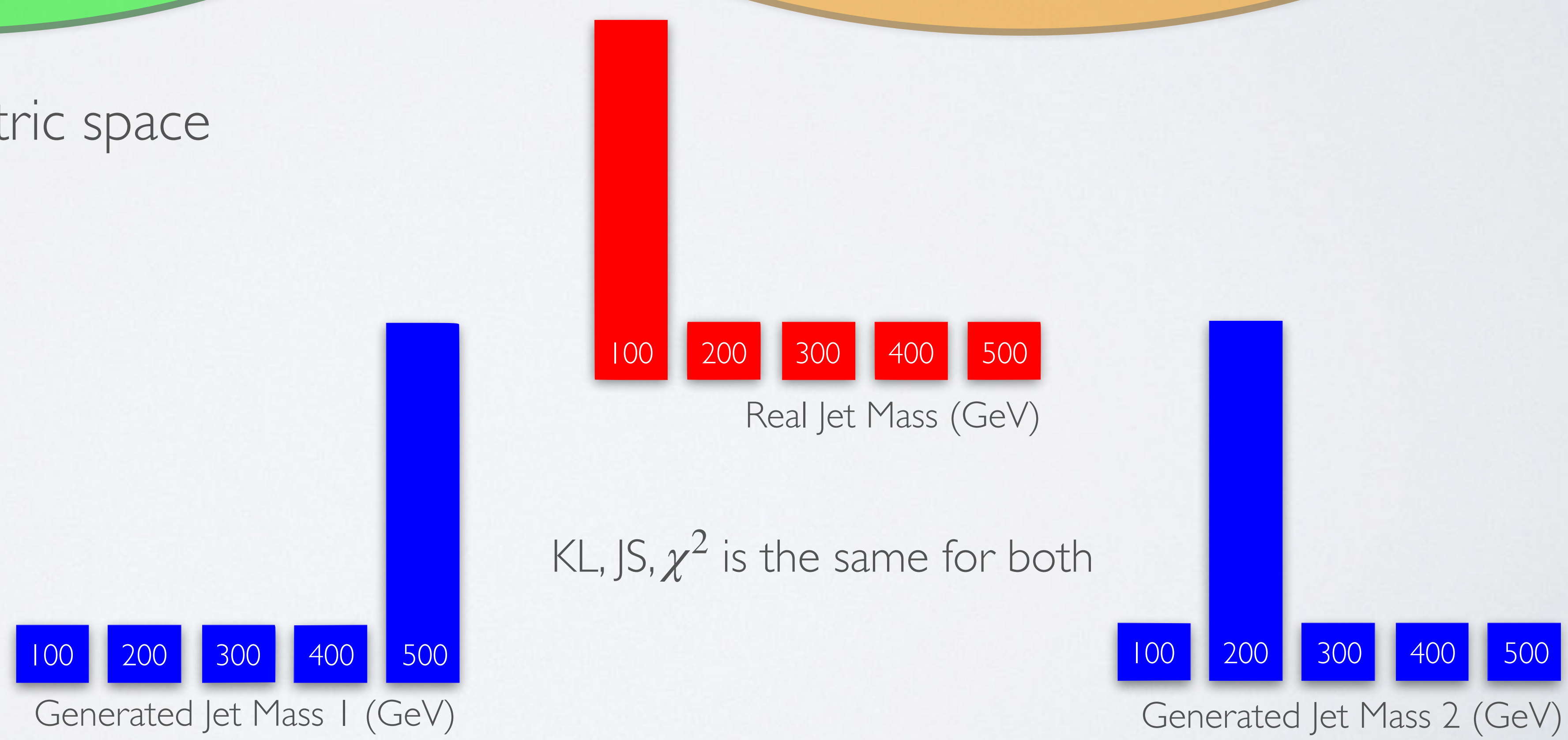

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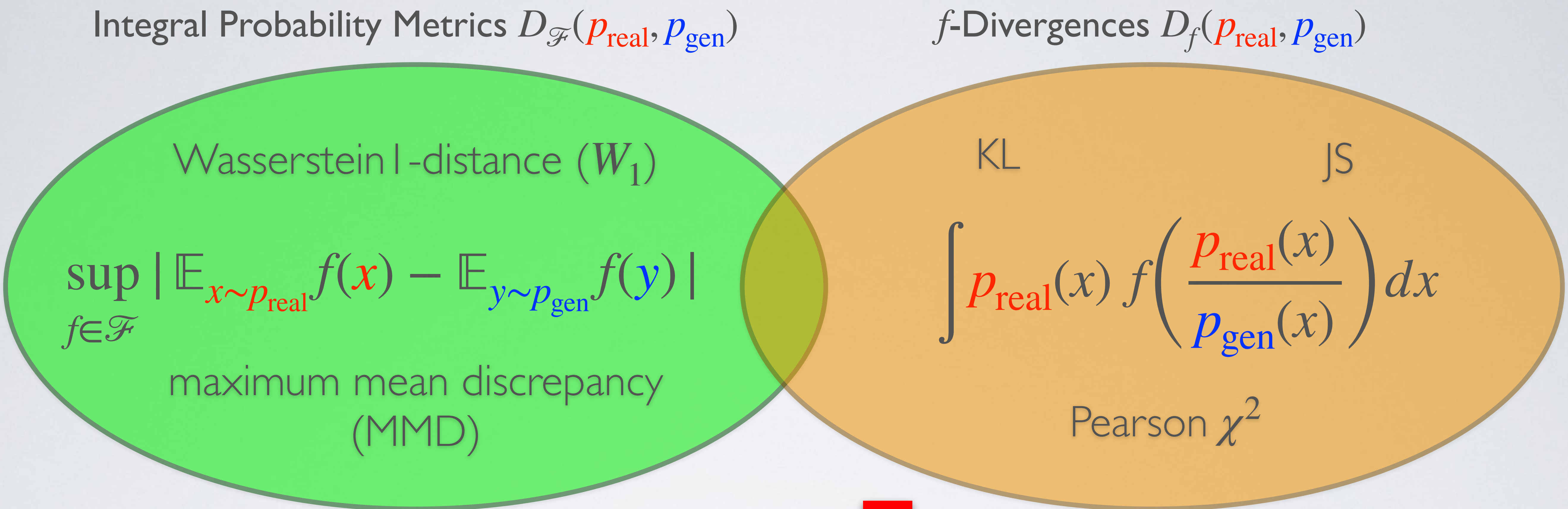

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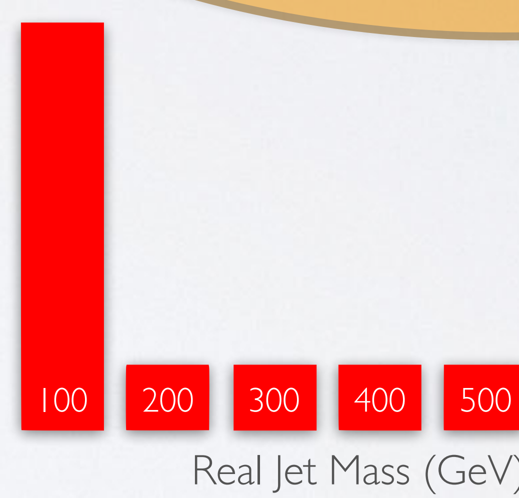
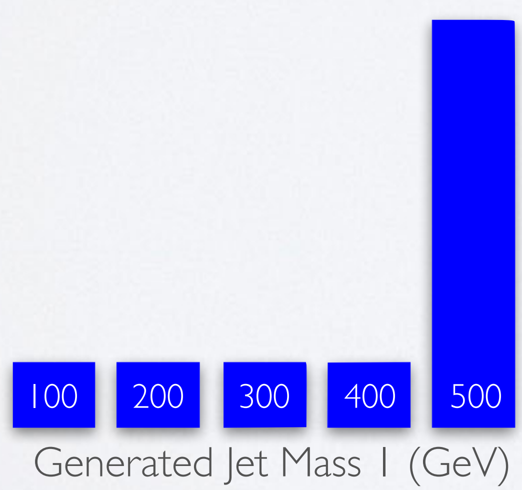
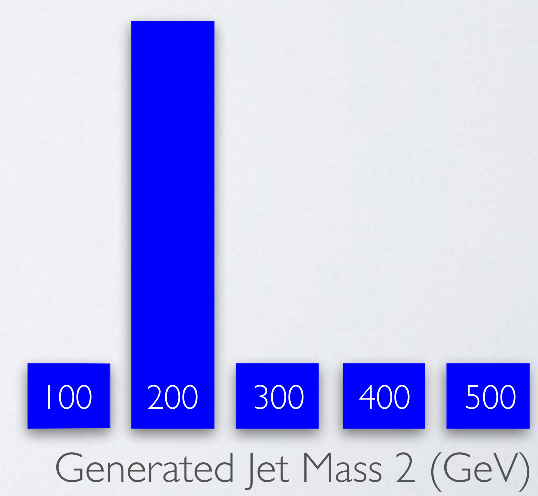
- More useful for comparing generative models





KL, JS, χ^2 is the same for both



$p_{\mathrm{real}}(\mathbf{x})$ vs $p_{\mathrm{gen}}(\mathbf{x})$

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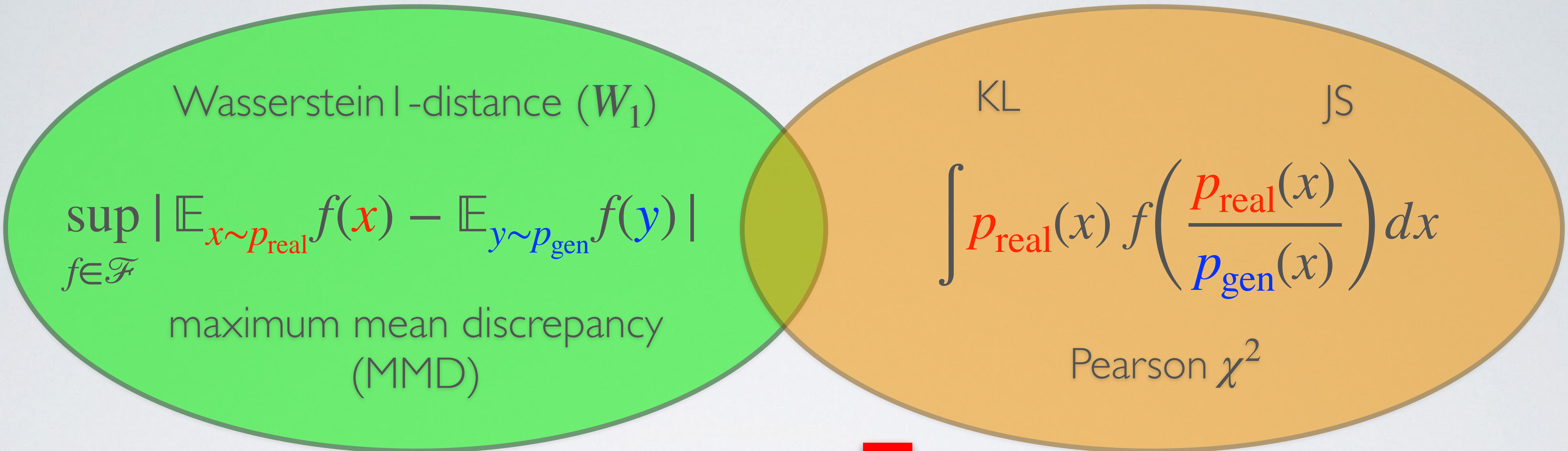
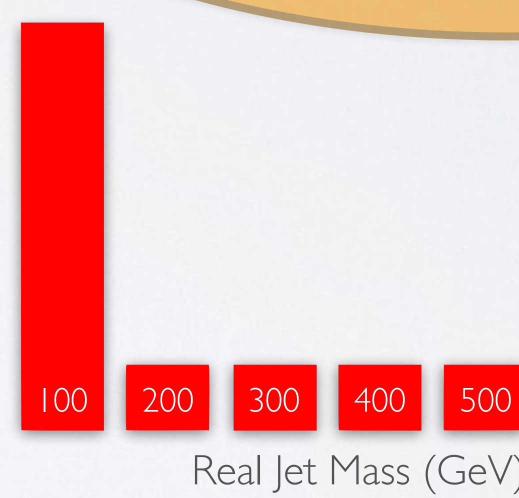


- IPMs take into account metric space
- More useful for comparing generative models
- And more efficient to calculate in high dimensions



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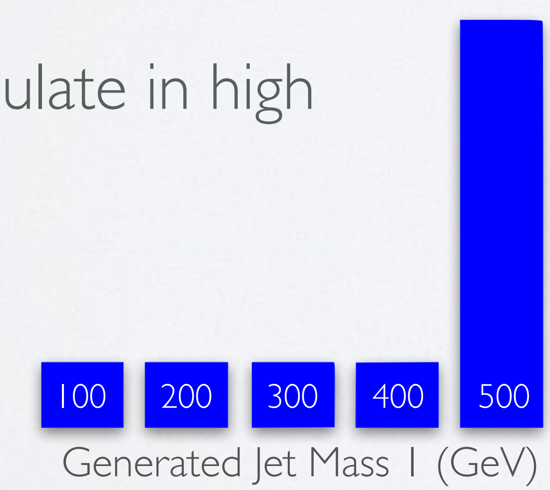

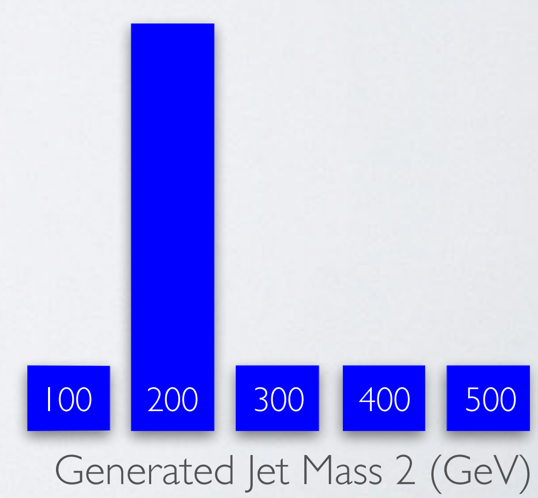

MORE ON IPMS

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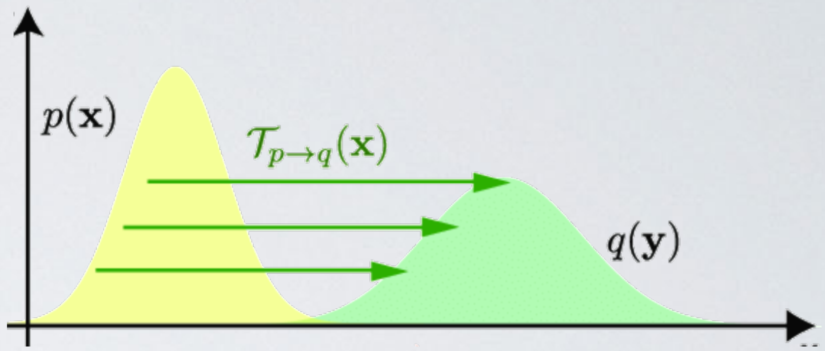

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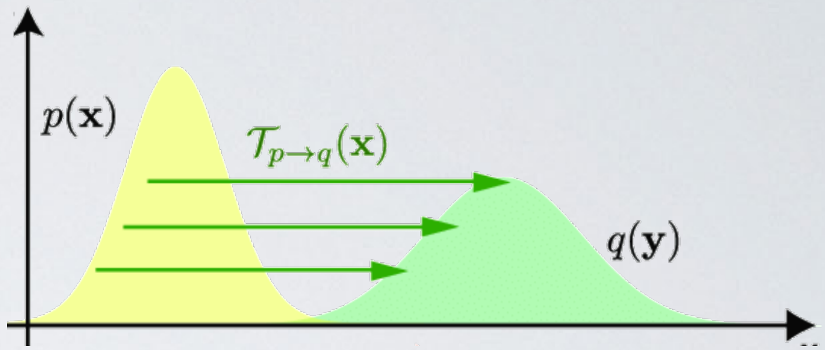

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    - Sensitive to quality, diversity; but biased and slow convergence

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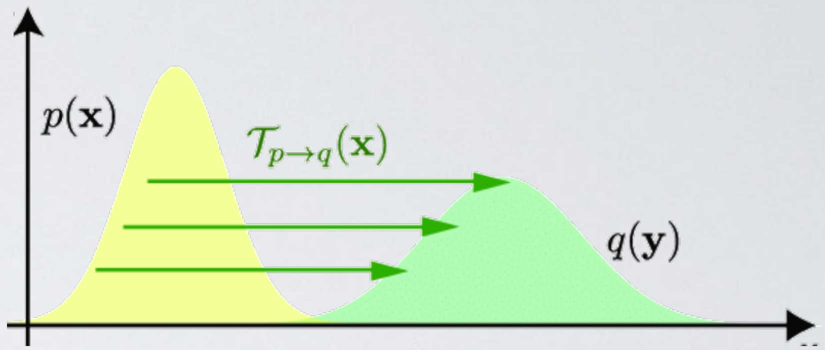

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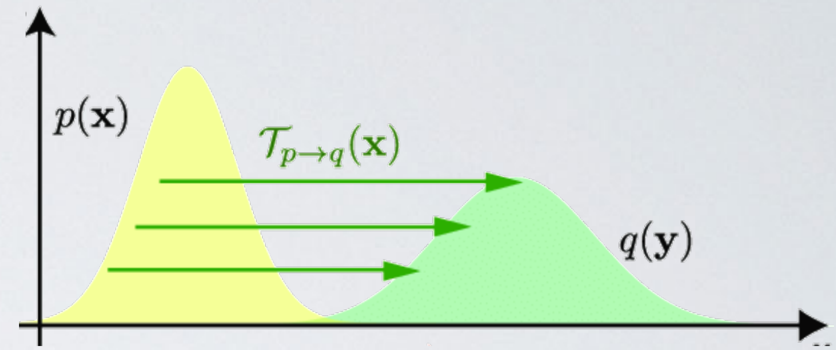

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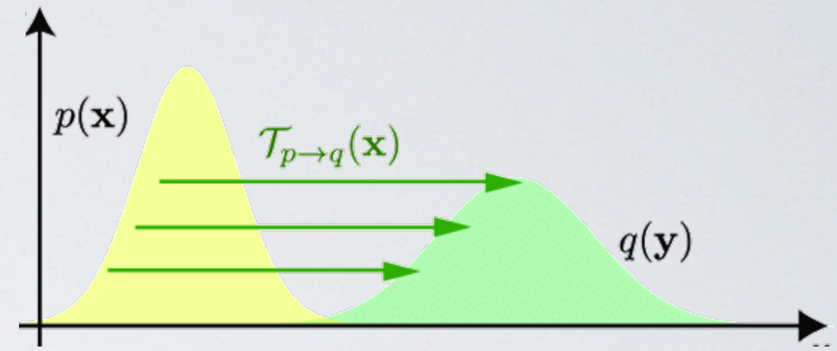

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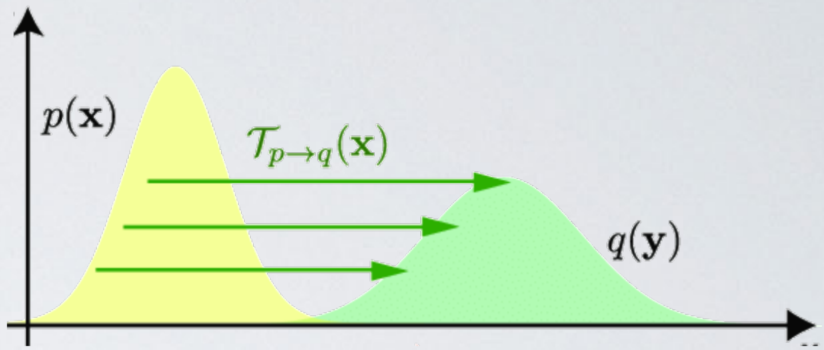

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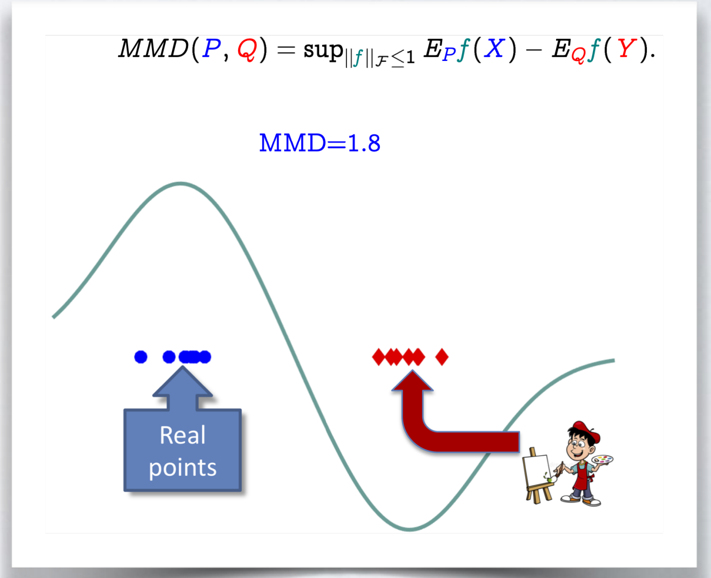
Gretton 2020



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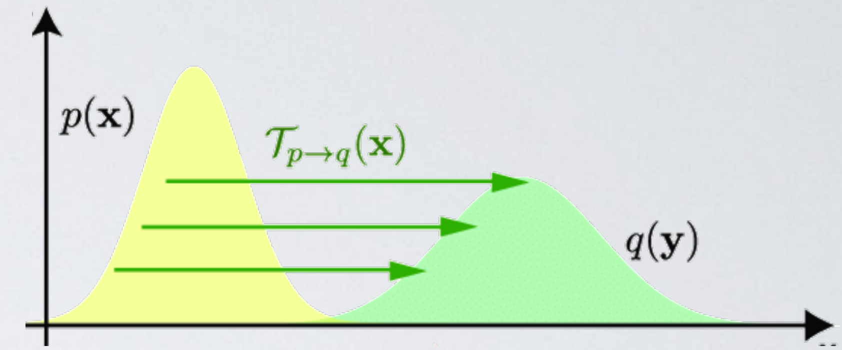

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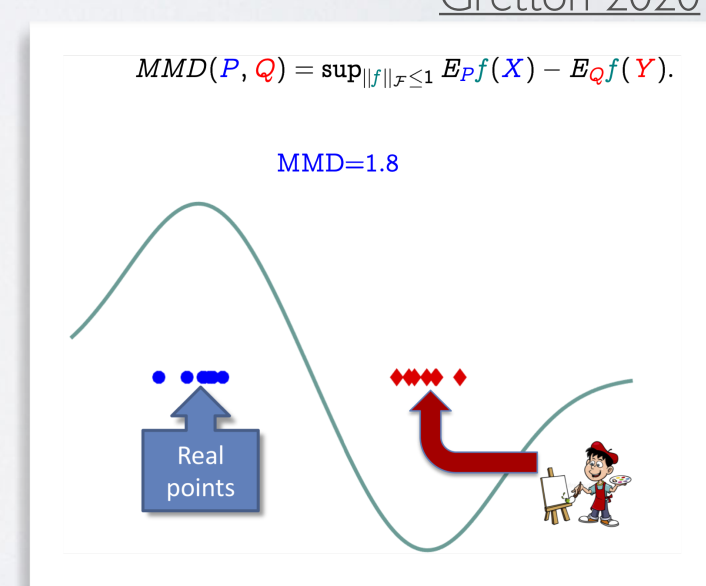

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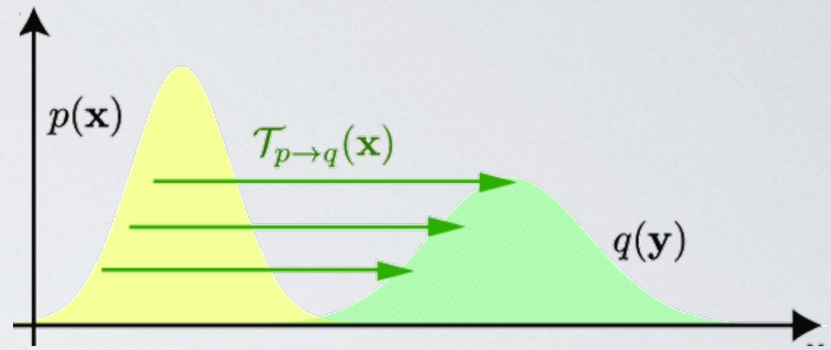

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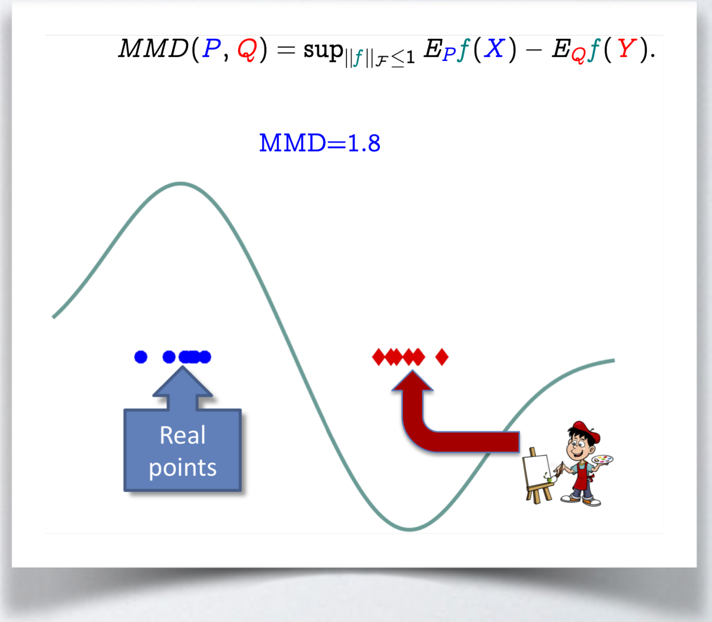
  - Fast, unbiased estimators, used in computer vision (KID) but depends on kernel

Gretton 2020



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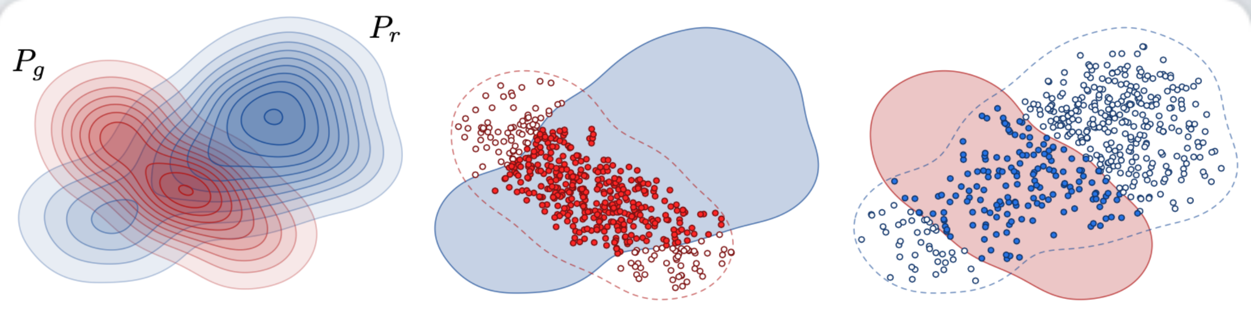

(a) Example distributions (b) Precision (c) Recall

MORE METRICS

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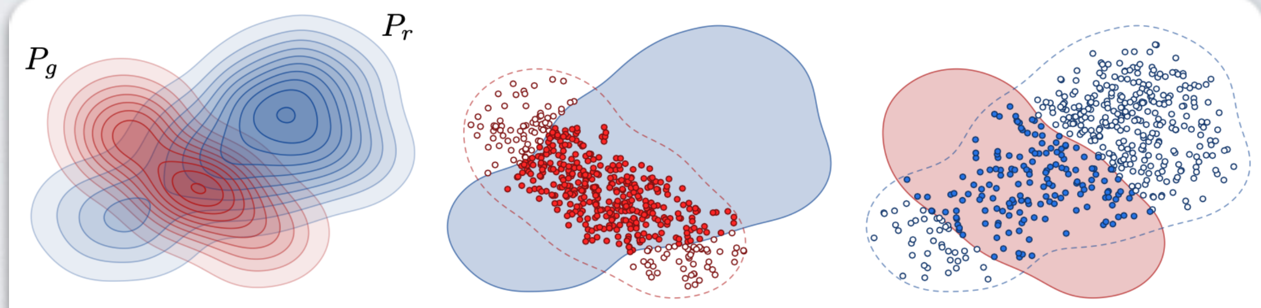

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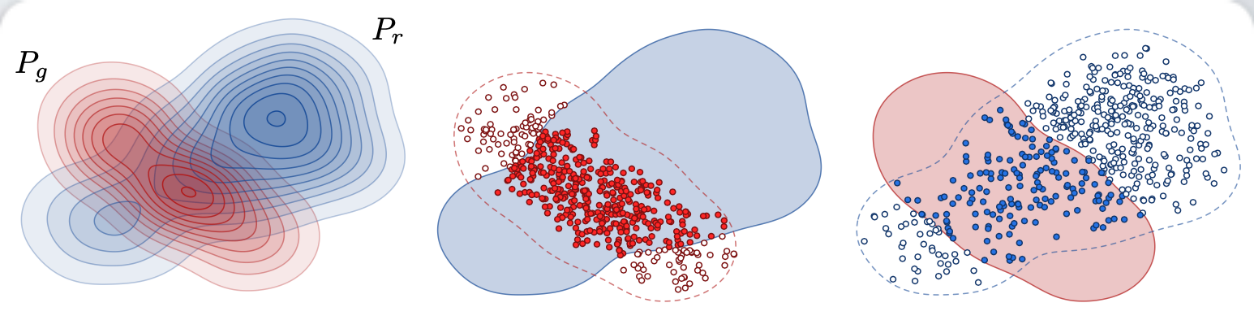

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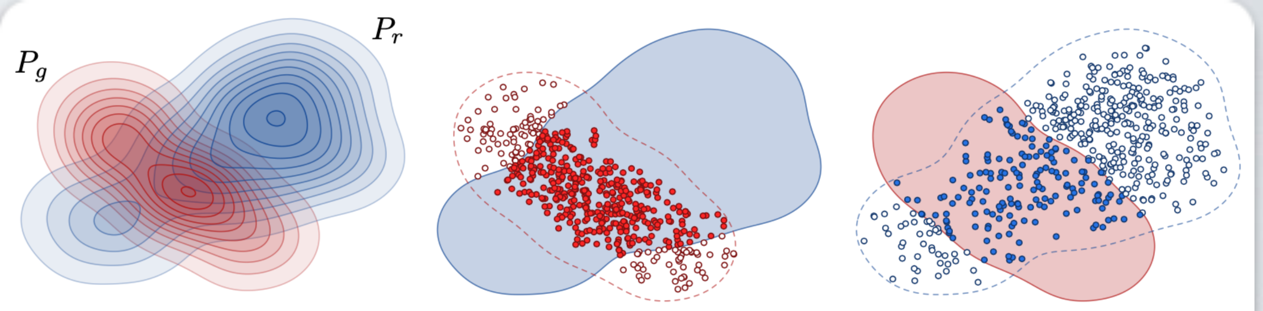

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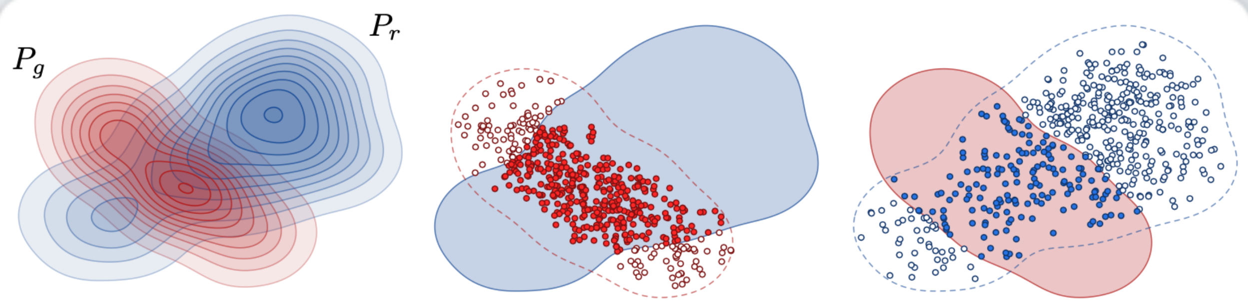

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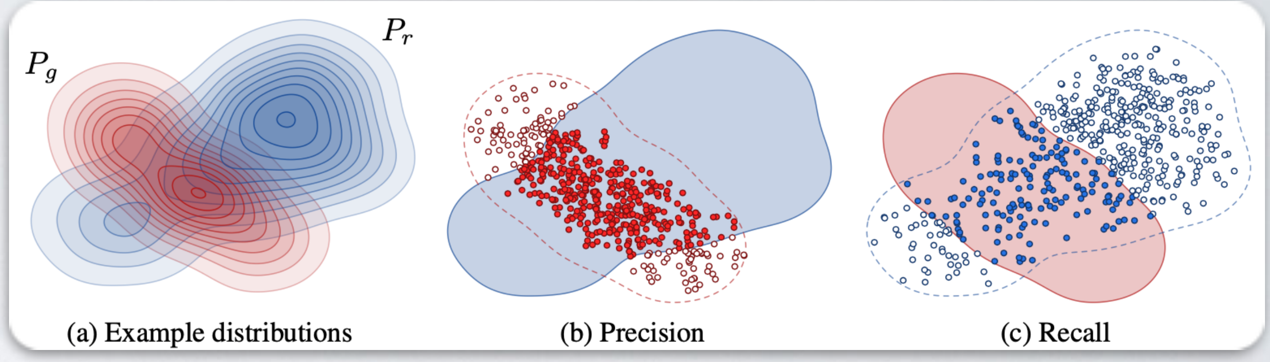

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  - In terms of GOF testing: comparing different test statistics for different models

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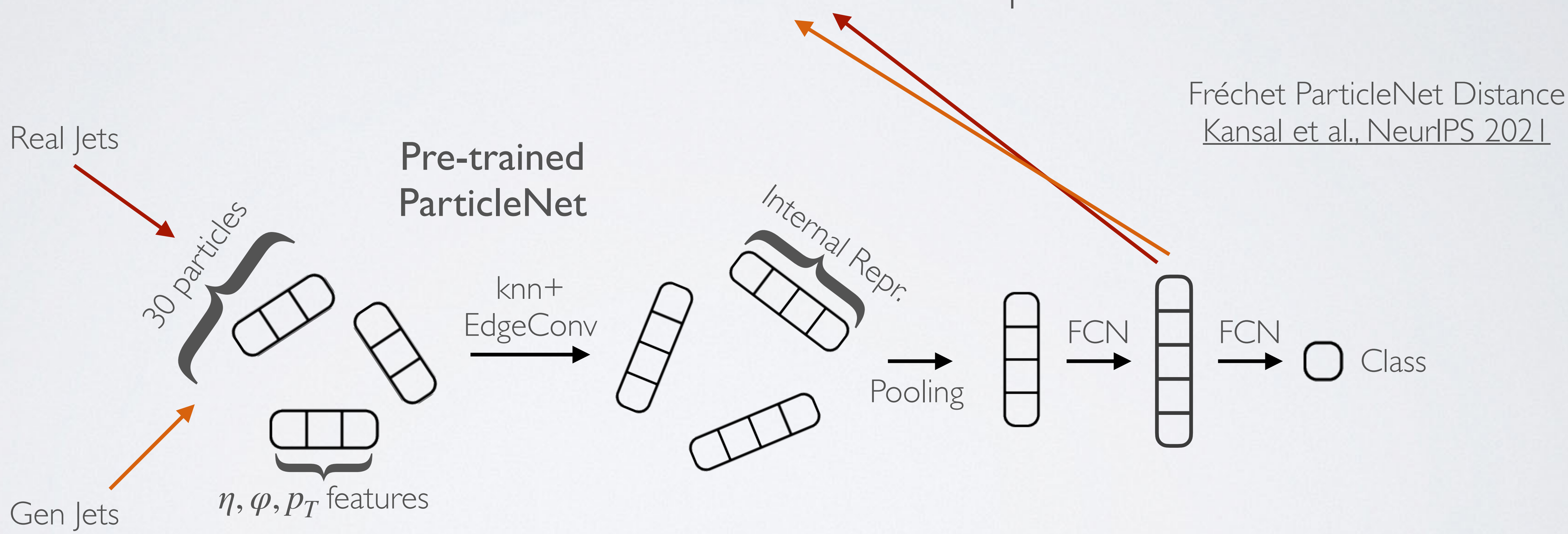

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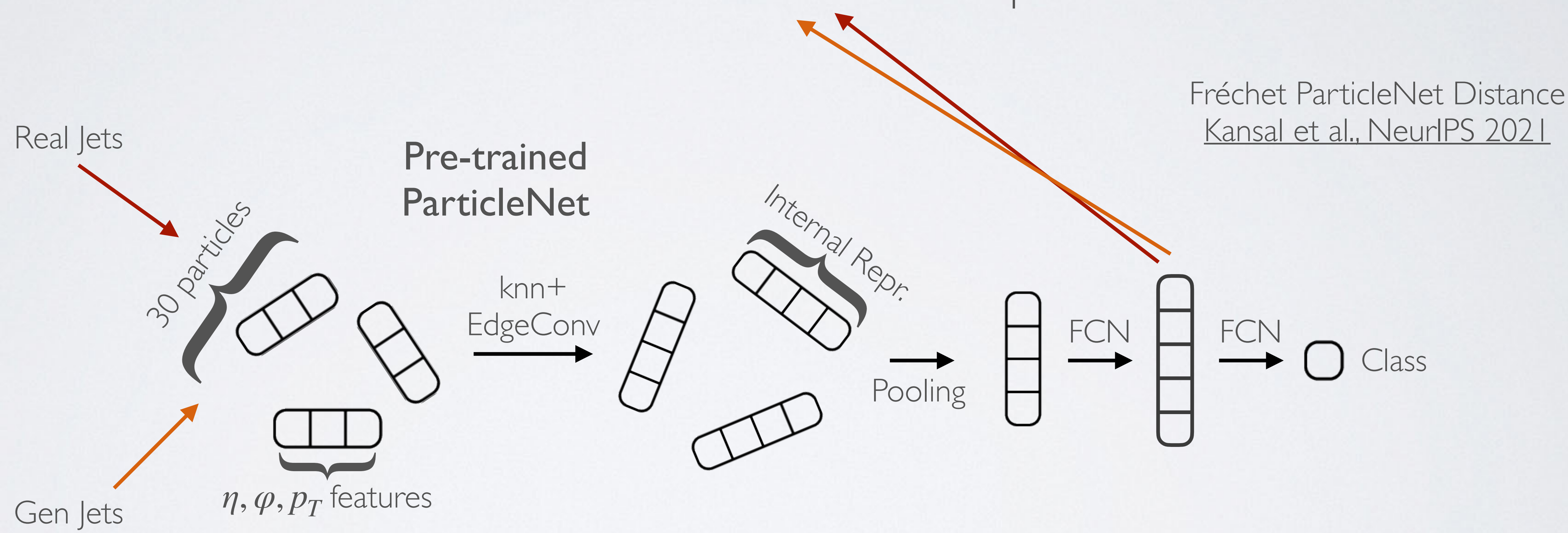

- Alternative? Use physicists' hand-engineered features: jet observables, shower-shape variables

TESTS

JET DISTRIBUTIONS

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- Sample of gluon jets to test sensitivity of metrics

RK et al. 2022

JET DISTRIBUTIONS

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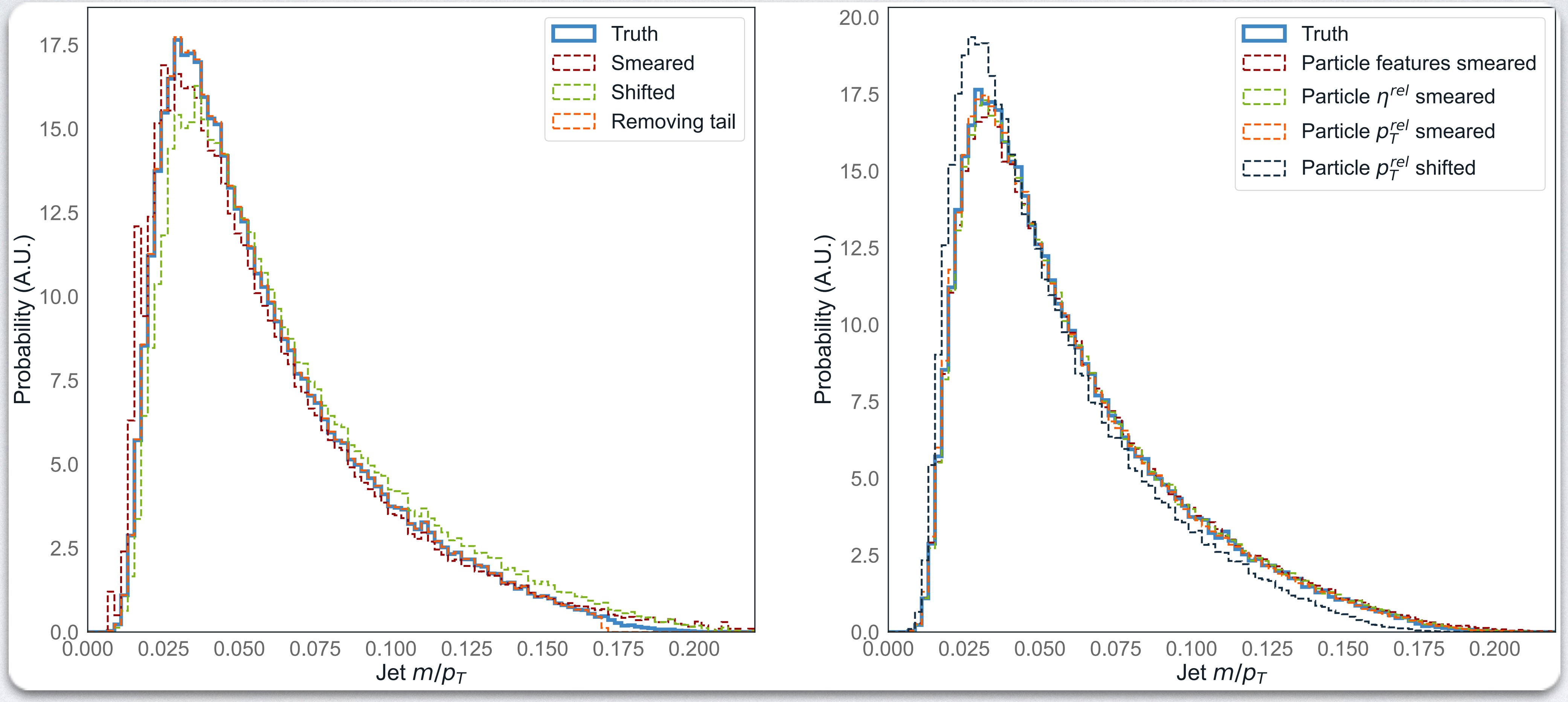
- We distort true distribution by: 1) Re-weighting in mass + 2) Smearing/shifting particle feature



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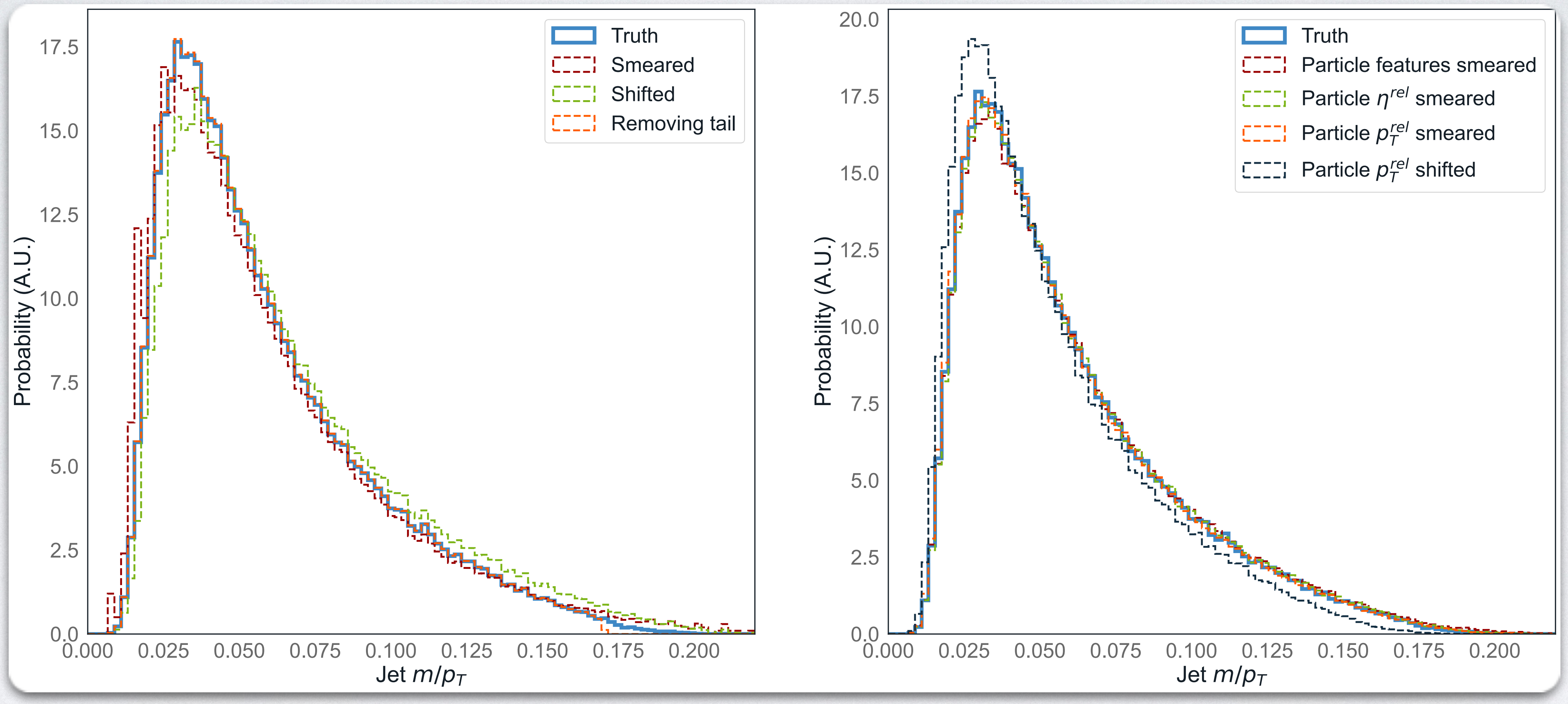

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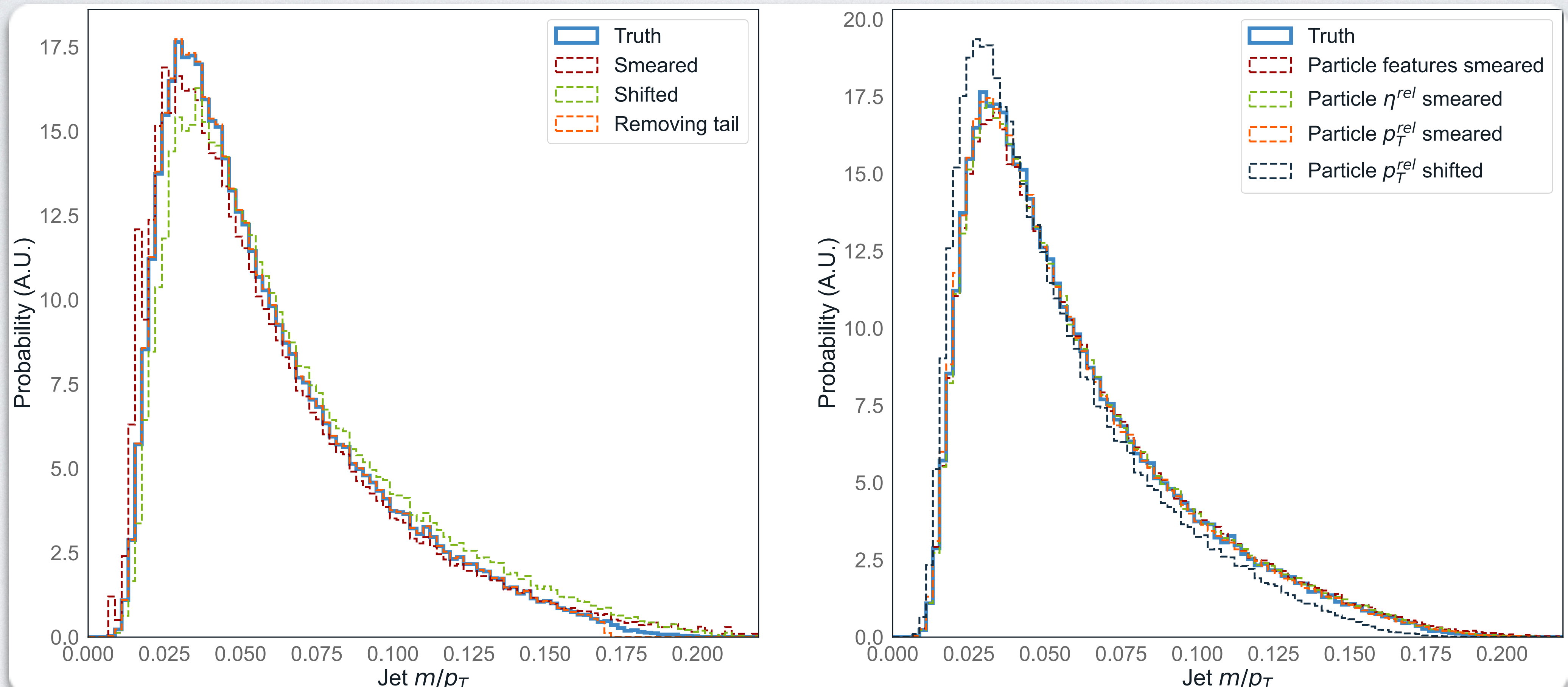

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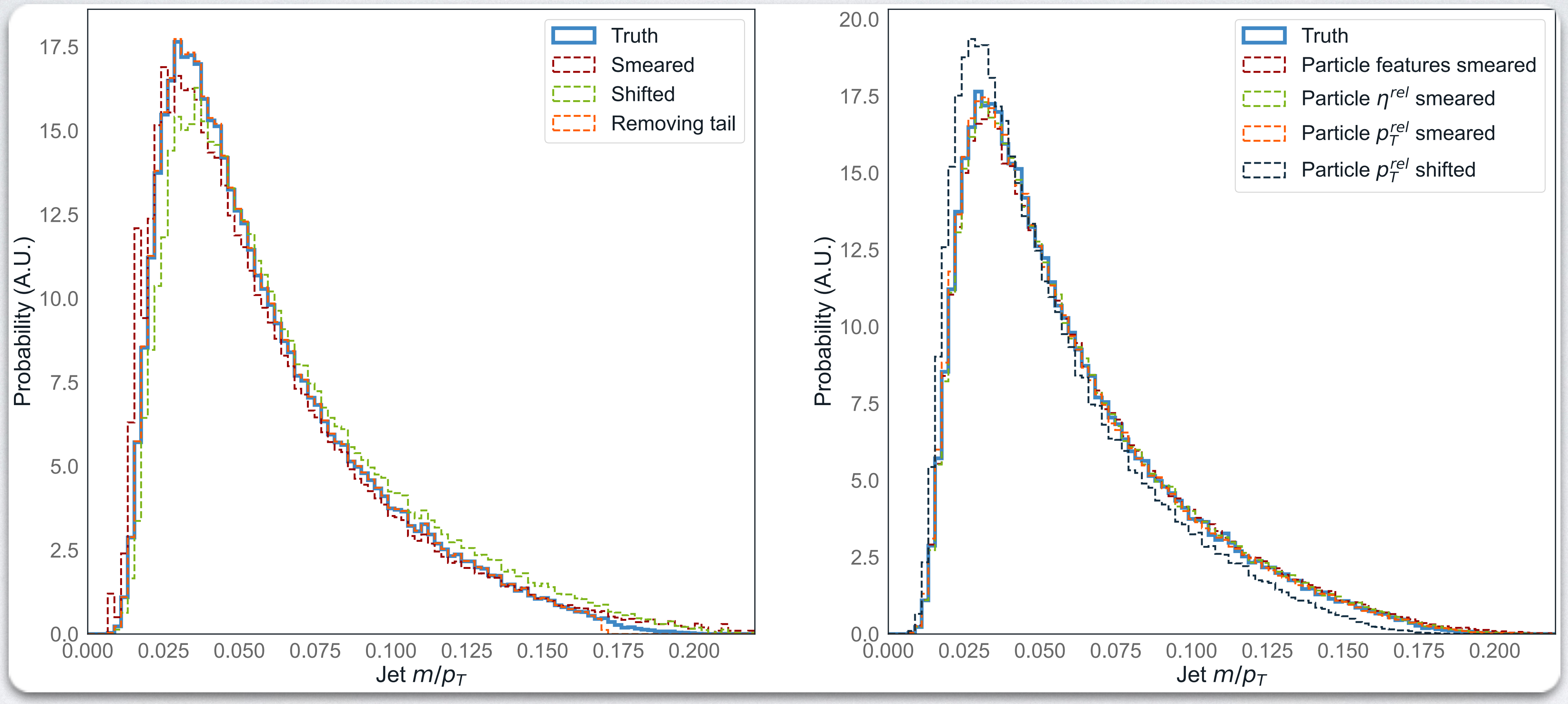

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1. Energy Flow Polynomials (EFPs) ($d \leq 4$)
2. ParticleNet activations

RESULTS

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Metric	Truth	Smeared	Shifted	Removing tail	Particle features smeared	Particle η^{rel} smeared	Particle $p_{\mathrm{T}}^{\mathrm{rel}}$ smeared	Particle $p_{\mathrm{T}}^{\mathrm{rel}}$ shifted
$W_1^M \times 10^3$								
Sign.								
Wasserstein EFP								
Sign.								
FGD_∞ EFP $\times 10^3$								
Sign.								
MMD EFP $\times 10^3$								
Sign.								
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Sign.								
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$W_1^M \times 10^3$	0.28 ± 0.05	2.1 ± 0.2	6.0 ± 0.3	0.6 ± 0.2	1.7 ± 0.2	0.9 ± 0.3	0.5 ± 0.2	5.8 ± 0.2
Sign.	—	37 ± 3	114 ± 6	7 ± 2	28 ± 3	12 ± 4	4 ± 1	111 ± 3
Wasserstein EFP	0.02 ± 0.01	0.09 ± 0.05	0.10 ± 0.02	0.016 ± 0.007	0.19 ± 0.08	0.03 ± 0.01	0.03 ± 0.02	0.06 ± 0.02
Sign.	—	6 ± 4	7 ± 1	0.06 ± 0.02	14 ± 6	0.8 ± 0.4	0.9 ± 0.6	4 ± 1
FGD_∞ EFP $\times 10^3$	0.08 ± 0.03	$\mathbf{20 \pm 1}$	$\mathbf{26.6 \pm 0.9}$	$\mathbf{2.4 \pm 0.1}$	21 ± 2	$\mathbf{3.6 \pm 0.3}$	2.3 ± 0.2	29.1 ± 0.4
Sign.	—	$\mathbf{580 \pm 30}$	$\mathbf{760 \pm 20}$	$\mathbf{66 \pm 4}$	610 ± 40	$\mathbf{103 \pm 8}$	64 ± 4	830 ± 10
MMD EFP $\times 10^3$	-0.006 ± 0.005	0.17 ± 0.06	0.9 ± 0.1	0.03 ± 0.02	0.35 ± 0.09	0.08 ± 0.05	0.01 ± 0.02	1.8 ± 0.1
Sign.	—	30 ± 10	170 ± 20	6 ± 4	70 ± 10	10 ± 10	3 ± 5	360 ± 20
Precision EFP	0.9 ± 0.1	0.94 ± 0.04	0.978 ± 0.005	0.88 ± 0.08	0.7 ± 0.1	0.94 ± 0.06	0.7 ± 0.1	0.79 ± 0.09
Sign.	—	0	0	0.109 ± 0.009	1.9 ± 0.3	0	2.0 ± 0.3	0.9 ± 0.1
Recall EFP	0.9 ± 0.1	0.88 ± 0.07	0.97 ± 0.01	0.92 ± 0.06	0.83 ± 0.05	0.92 ± 0.07	0.8 ± 0.1	0.8 ± 0.1
Sign.	—	0.16 ± 0.01	0	0	0.58 ± 0.04	0	0.8 ± 0.1	1.1 ± 0.2
Wasserstein PN	1.65 ± 0.06	1.7 ± 0.1	2.4 ± 0.4	1.71 ± 0.08	4.5 ± 0.1	1.79 ± 0.05	4.0 ± 0.4	7.6 ± 0.2
Sign.	—	0.84 ± 0.05	12 ± 2	0.97 ± 0.05	45 ± 1	2.26 ± 0.06	37 ± 3	95 ± 3
FGD_∞ PN $\times 10^3$	0.6 ± 0.4	37 ± 2	202 ± 4	4.3 ± 0.4	$\mathbf{1220 \pm 10}$	20 ± 1	$\mathbf{1230 \pm 10}$	$\mathbf{3630 \pm 10}$
Sign.	—	98 ± 4	540 ± 0	9.8 ± 0.9	$\mathbf{3320 \pm 20}$	51 ± 3	$\mathbf{3340 \pm 30}$	$\mathbf{9870 \pm 30}$
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Sign.	—	0.57 ± 0.04	0	0	8 ± 4	0	8 ± 5	4.0 ± 0.8
Recall PN	0.70 ± 0.05	0.61 ± 0.04	0.61 ± 0.08	0.73 ± 0.06	0.014 ± 0.009	0.7 ± 0.1	0.01 ± 0.01	0.57 ± 0.09
Sign.	—	1.8 ± 0.1	1.8 ± 0.2	0	14 ± 9	0	10 ± 10	2.6 ± 0.4
Classifier LLF AUC	0.50	0.52	0.54	0.50	0.97	0.81	0.93	0.99
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RK et al. 2022

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$W_1^M \times 10^3$	0.28 ± 0.05	2.1 ± 0.2	6.0 ± 0.3	0.6 ± 0.2	1.7 ± 0.2	0.9 ± 0.3	0.5 ± 0.2	5.8 ± 0.2
Sign.	—	37 ± 3	114 ± 6	7 ± 2	28 ± 3	12 ± 4	4 ± 1	111 ± 3
Wasserstein EFP	0.02 ± 0.01	0.09 ± 0.05	0.10 ± 0.02	0.016 ± 0.007	0.19 ± 0.08	0.03 ± 0.01	0.03 ± 0.02	0.06 ± 0.02
Sign.	—	6 ± 4	7 ± 1	0.06 ± 0.02	14 ± 6	0.8 ± 0.4	0.9 ± 0.6	4 ± 1
FGD_∞ EFP $\times 10^3$	0.08 ± 0.03	$\mathbf{20 \pm 1}$	$\mathbf{26.6 \pm 0.9}$	$\mathbf{2.4 \pm 0.1}$	21 ± 2	$\mathbf{3.6 \pm 0.3}$	2.3 ± 0.2	29.1 ± 0.4
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MMD EFP $\times 10^3$	-0.006 ± 0.005	0.17 ± 0.06	0.9 ± 0.1	0.03 ± 0.02	0.35 ± 0.09	0.08 ± 0.05	0.01 ± 0.02	1.8 ± 0.1
Sign.	—	30 ± 10	170 ± 20	6 ± 4	70 ± 10	10 ± 10	3 ± 5	360 ± 20
Precision EFP	0.9 ± 0.1	0.94 ± 0.04	0.978 ± 0.005	0.88 ± 0.08	0.7 ± 0.1	0.94 ± 0.06	0.7 ± 0.1	0.79 ± 0.09
Sign.	—	0	0	0.109 ± 0.009	1.9 ± 0.3	0	2.0 ± 0.3	0.9 ± 0.1
Recall EFP	0.9 ± 0.1	0.88 ± 0.07	0.97 ± 0.01	0.92 ± 0.06	0.83 ± 0.05	0.92 ± 0.07	0.8 ± 0.1	0.8 ± 0.1
Sign.	—	0.16 ± 0.01	0	0	0.58 ± 0.04	0	0.8 ± 0.1	1.1 ± 0.2
Wasserstein PN	1.65 ± 0.06	1.7 ± 0.1	2.4 ± 0.4	1.71 ± 0.08	4.5 ± 0.1	1.79 ± 0.05	4.0 ± 0.4	7.6 ± 0.2
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Sign.	—	0.57 ± 0.04	0	0	8 ± 4	0	8 ± 5	4.0 ± 0.8
Recall PN	0.70 ± 0.05	0.61 ± 0.04	0.61 ± 0.08	0.73 ± 0.06	0.014 ± 0.009	0.7 ± 0.1	0.01 ± 0.01	0.57 ± 0.09
Sign.	—	1.8 ± 0.1	1.8 ± 0.2	0	14 ± 9	0	10 ± 10	2.6 ± 0.4
Classifier LLF AUC	0.50	0.52	0.54	0.50	0.97	0.81	0.93	0.99
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JET SIMULATION

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DATASET

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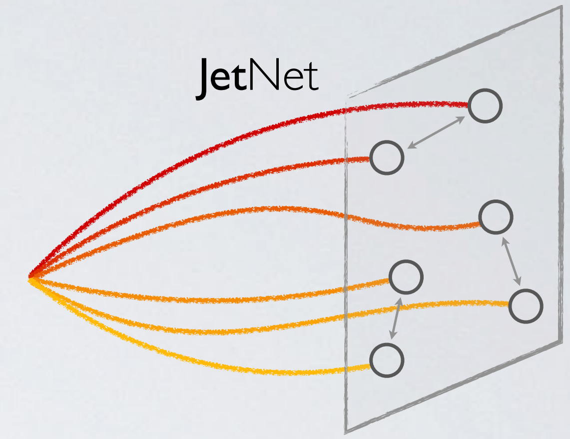

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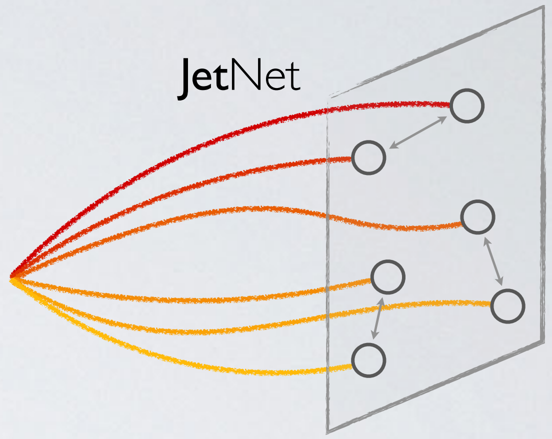

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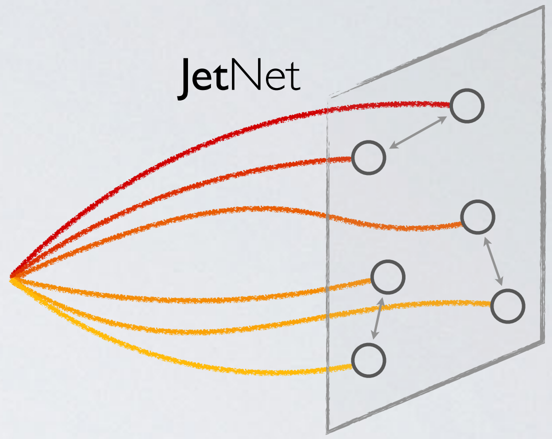

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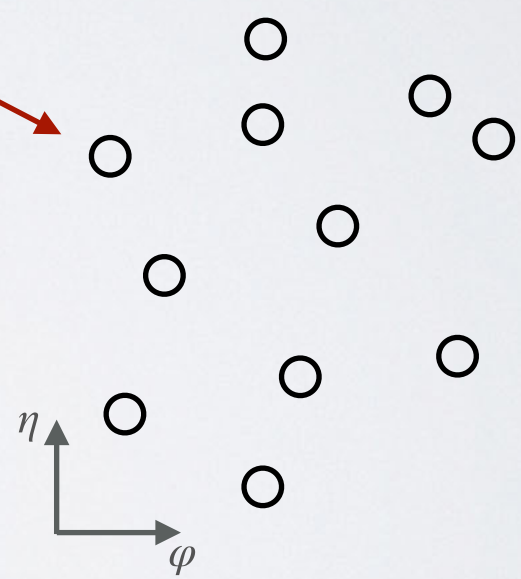

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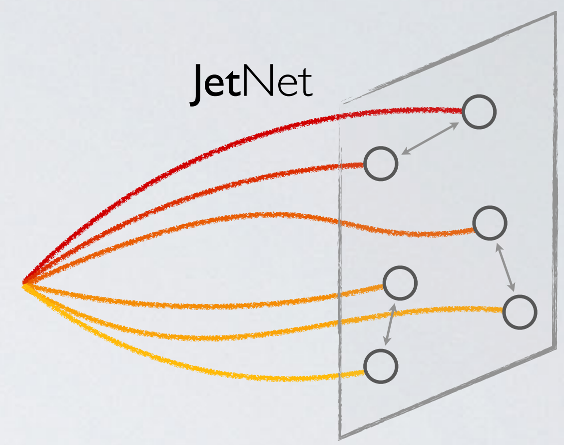

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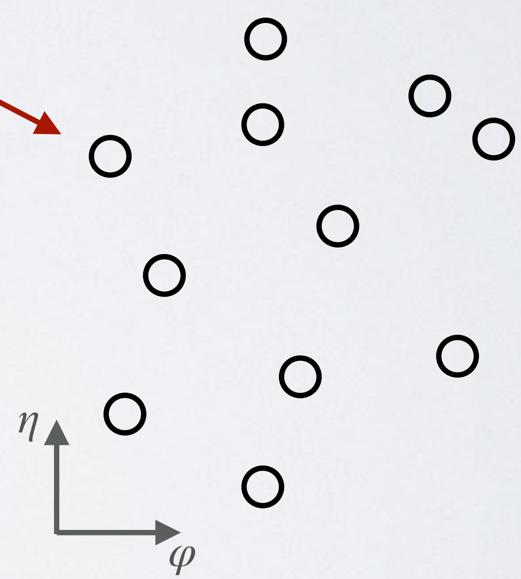

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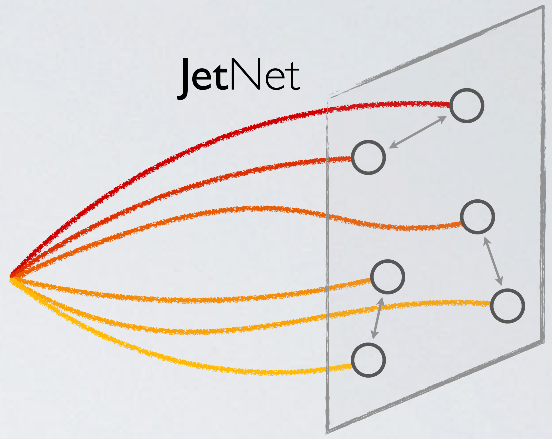

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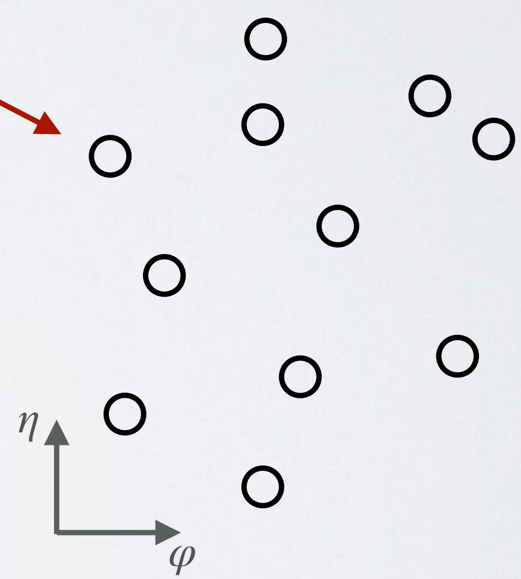

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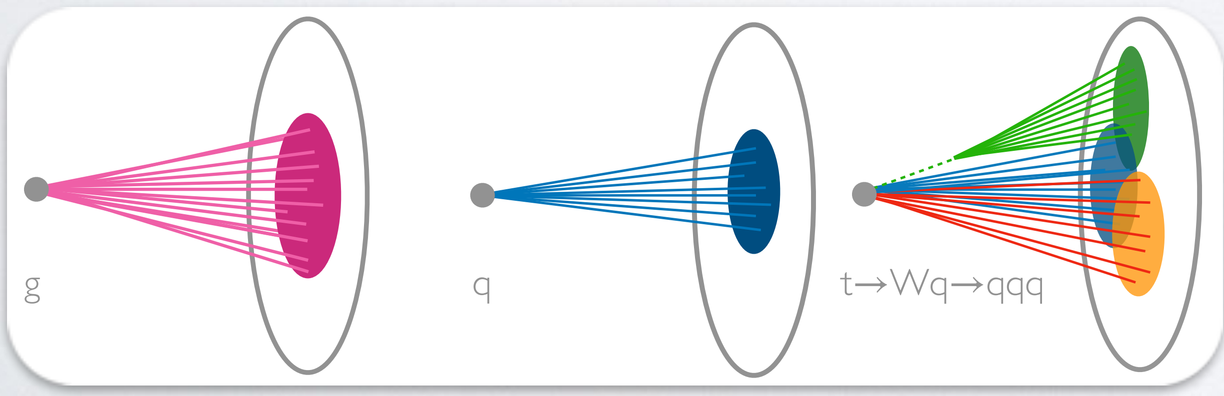

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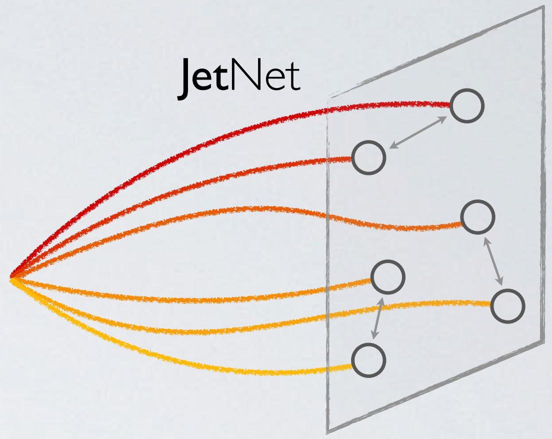

JetNet Library:
25k downloads, [1, 2, 3]

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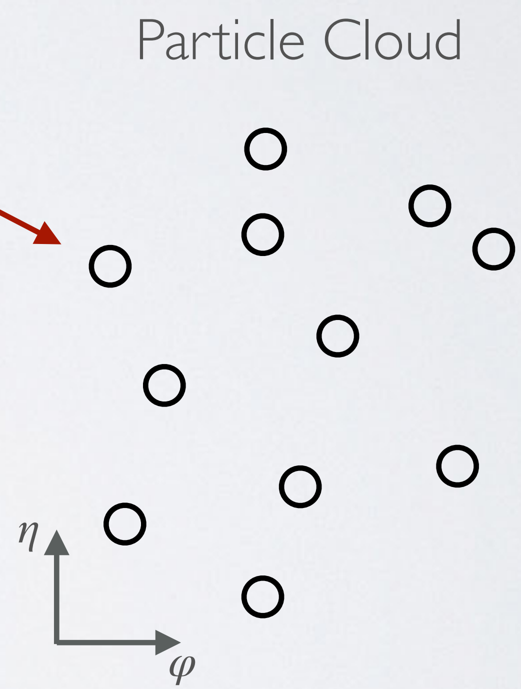

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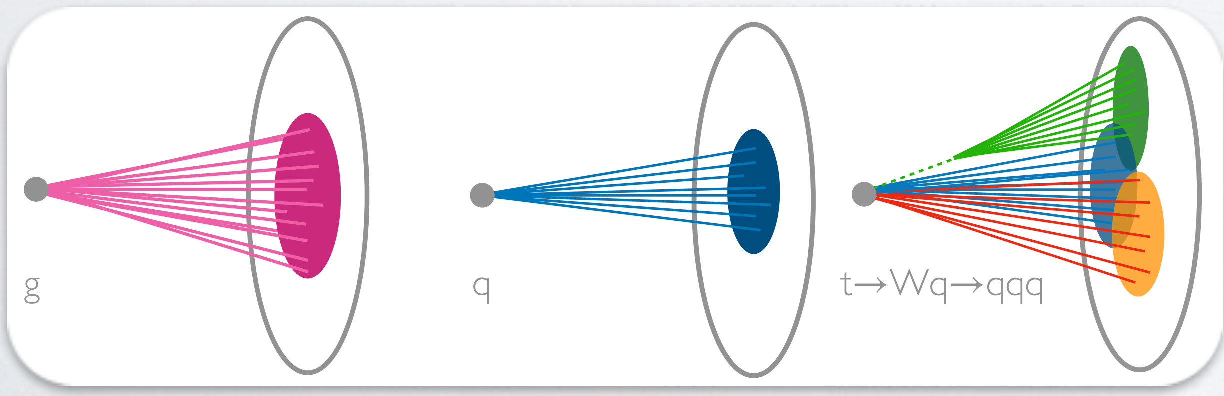

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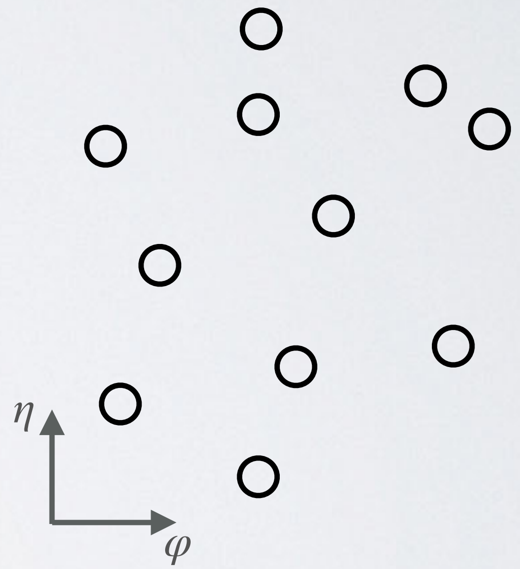

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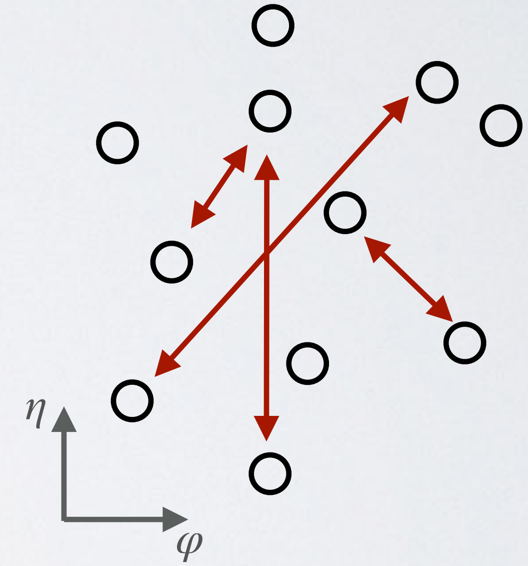

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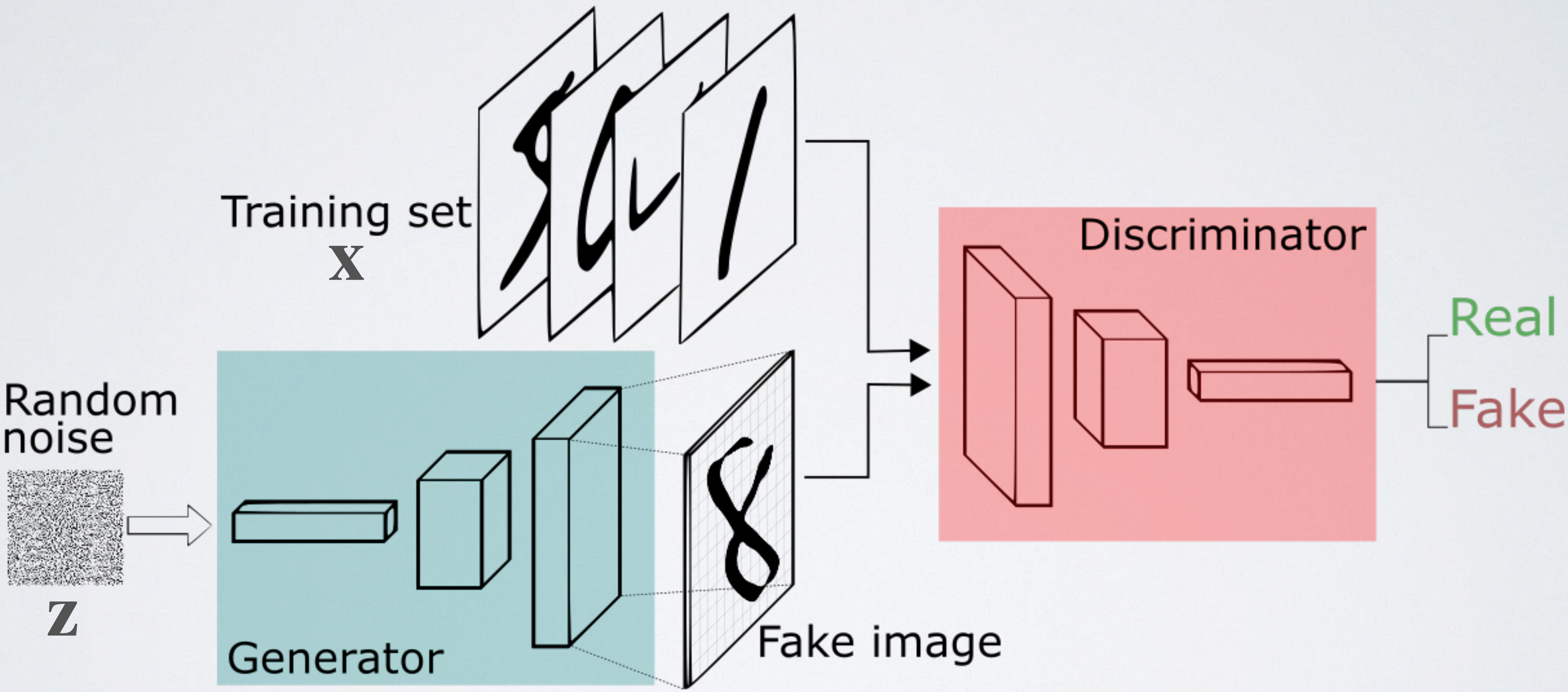
GENERATIVE ADVERSARIAL NETWORKS



MPGAN

RK et al., NeurIPS 2021

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- We develop a GAN with a fully-connected message-passing (MP) generator and discriminator

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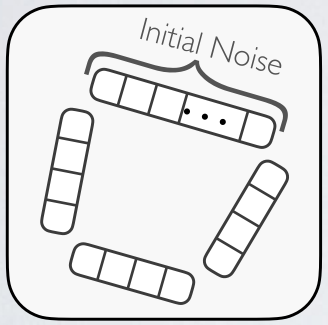

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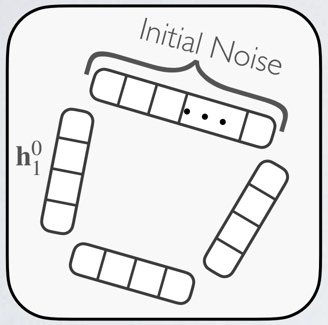

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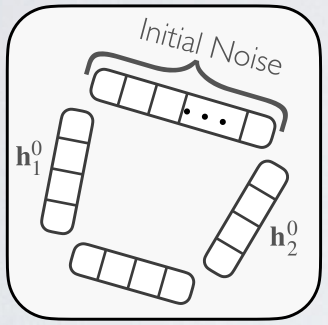

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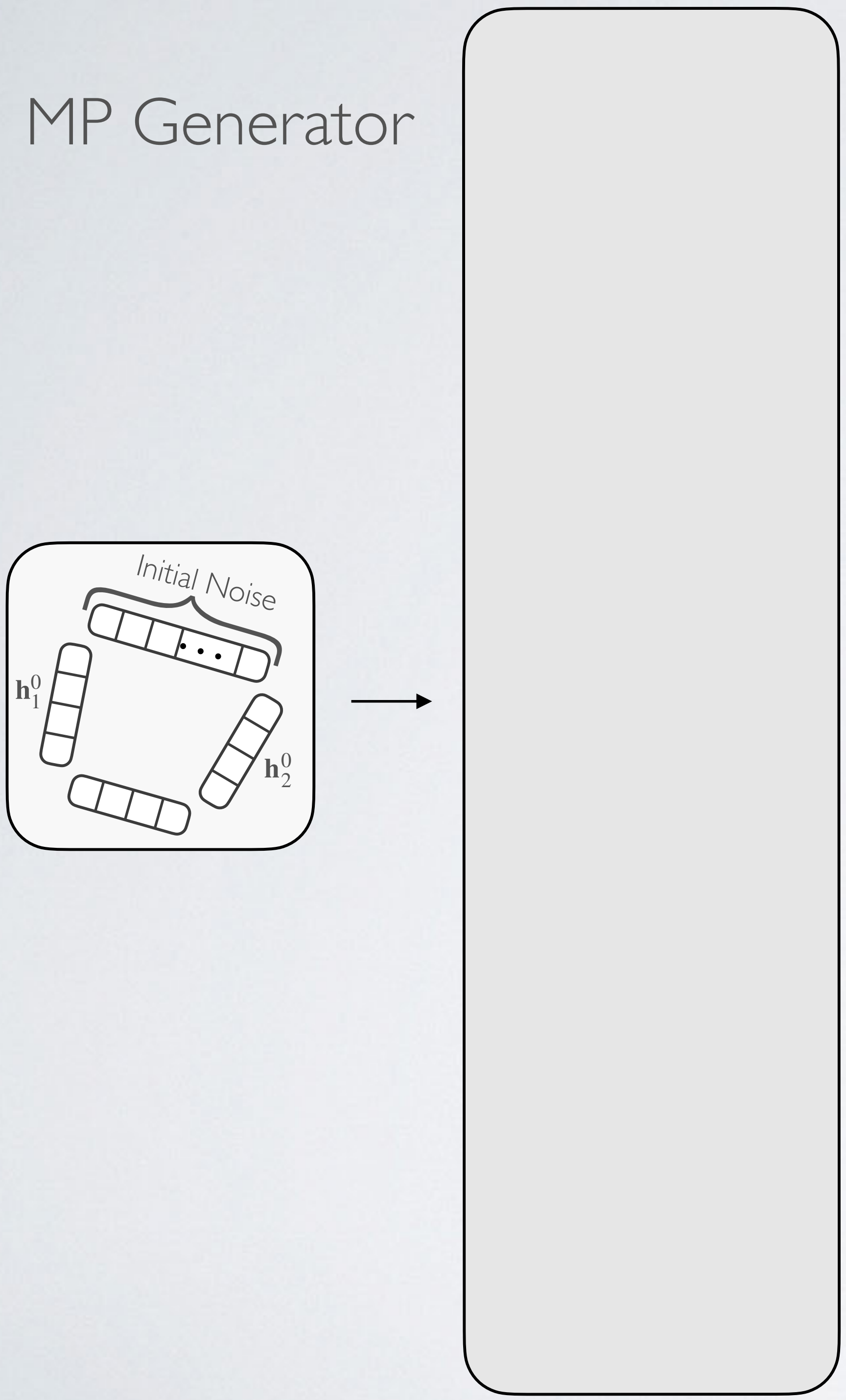

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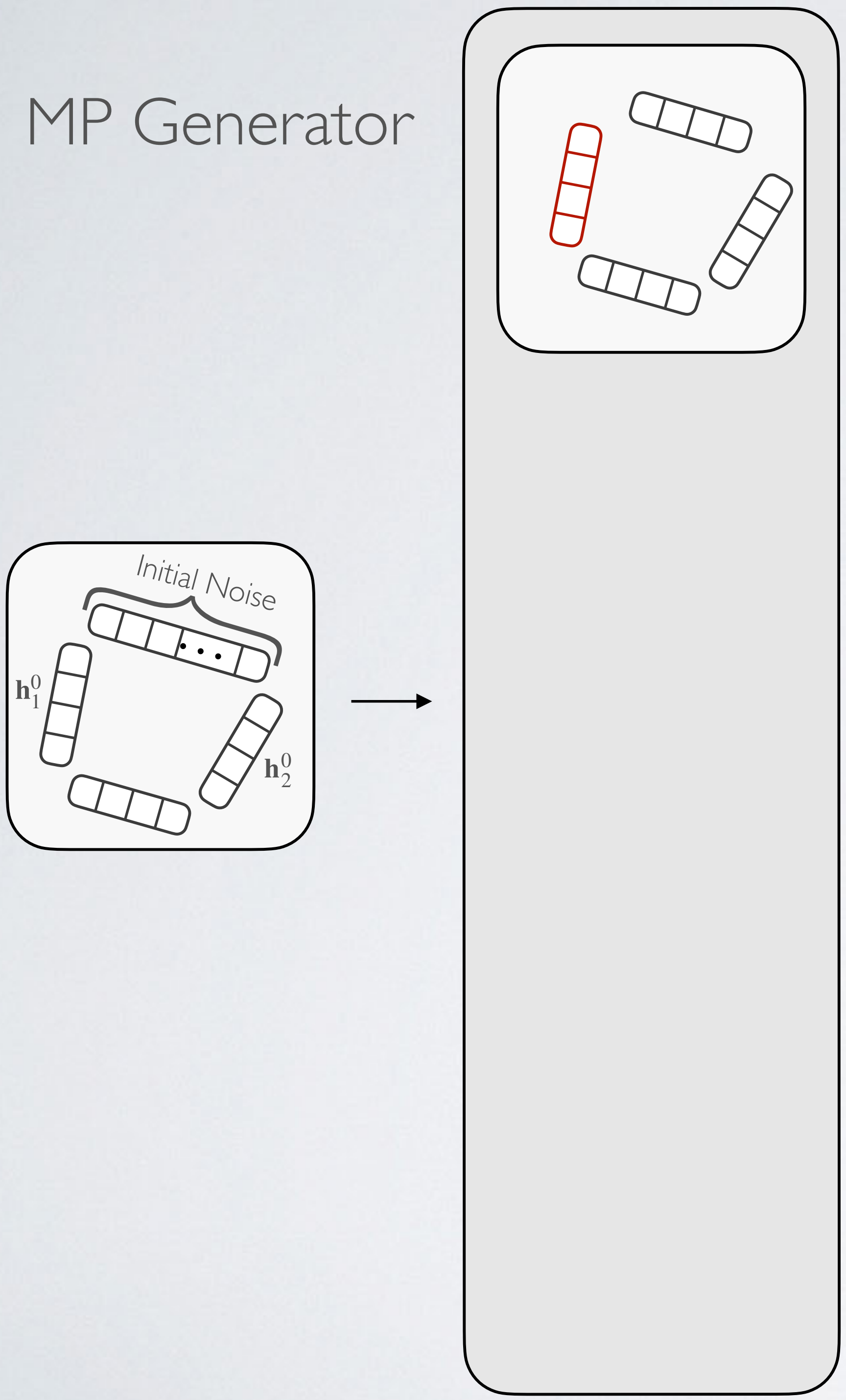

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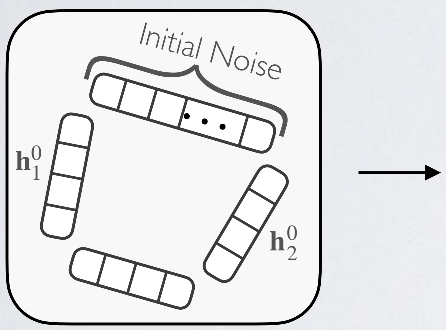

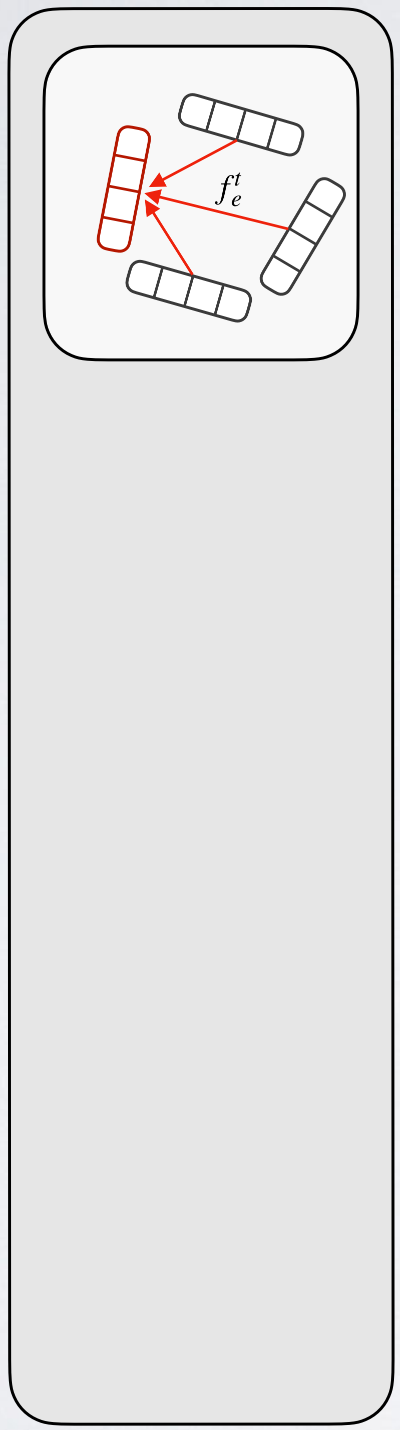

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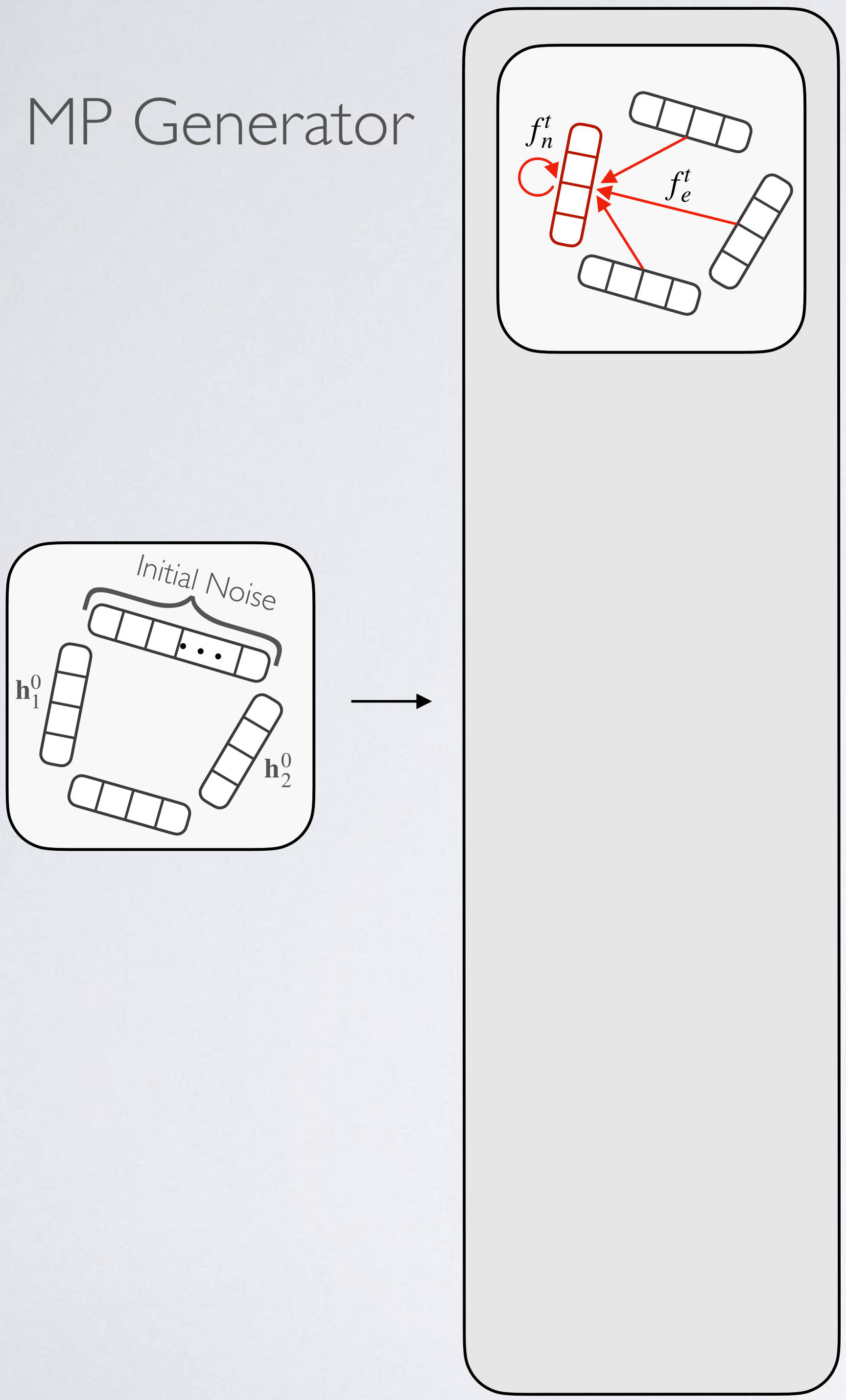

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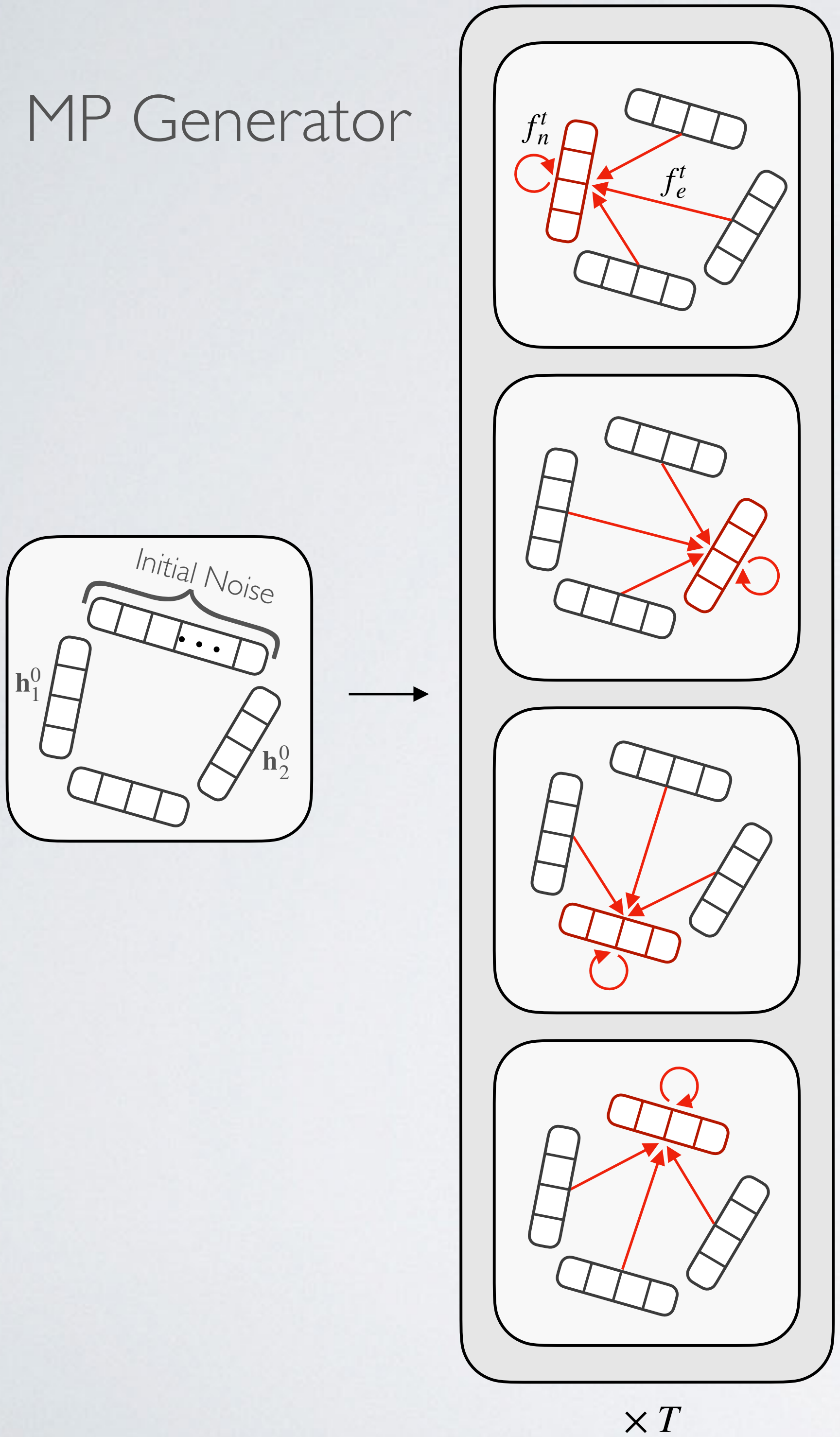

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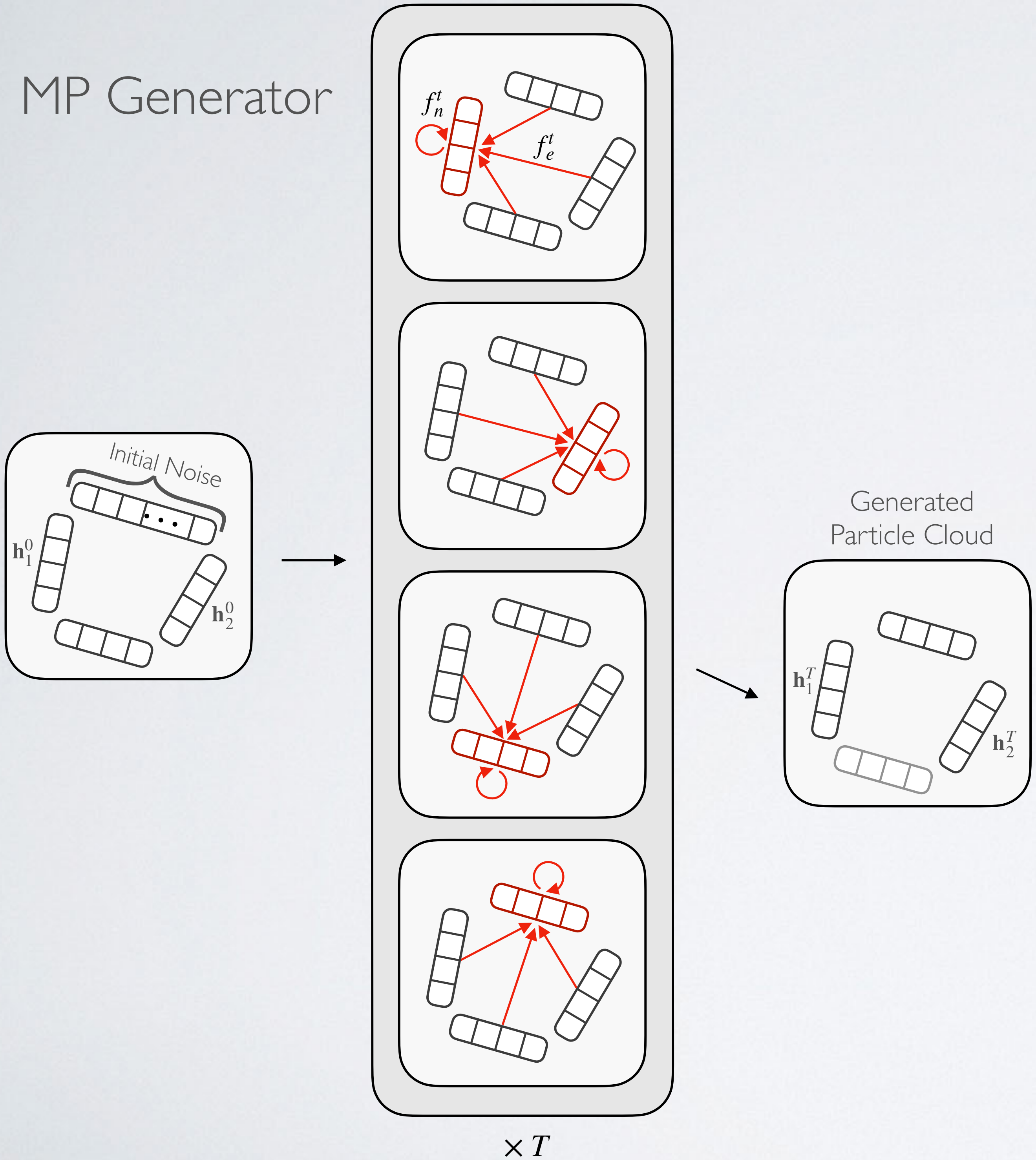

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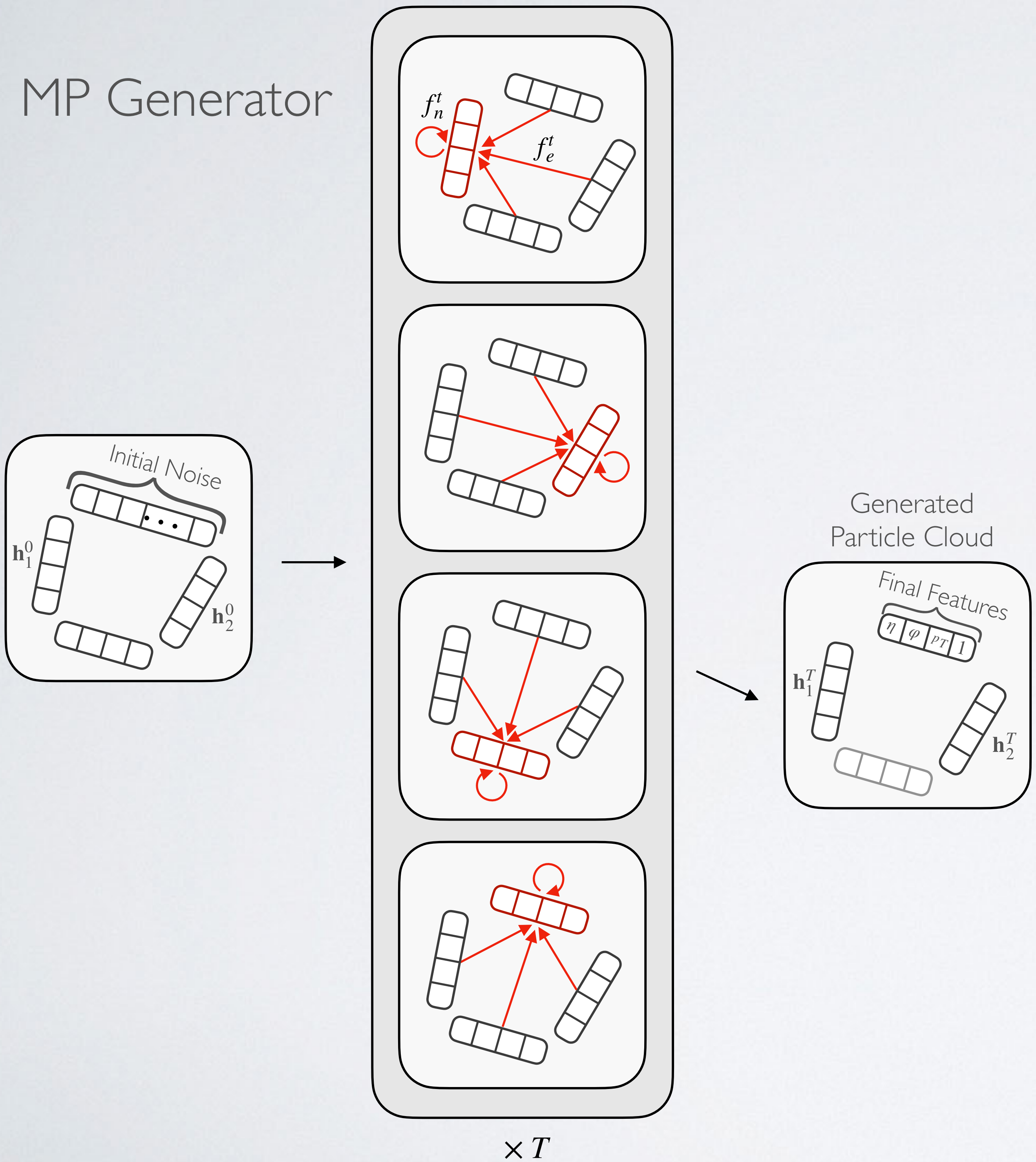

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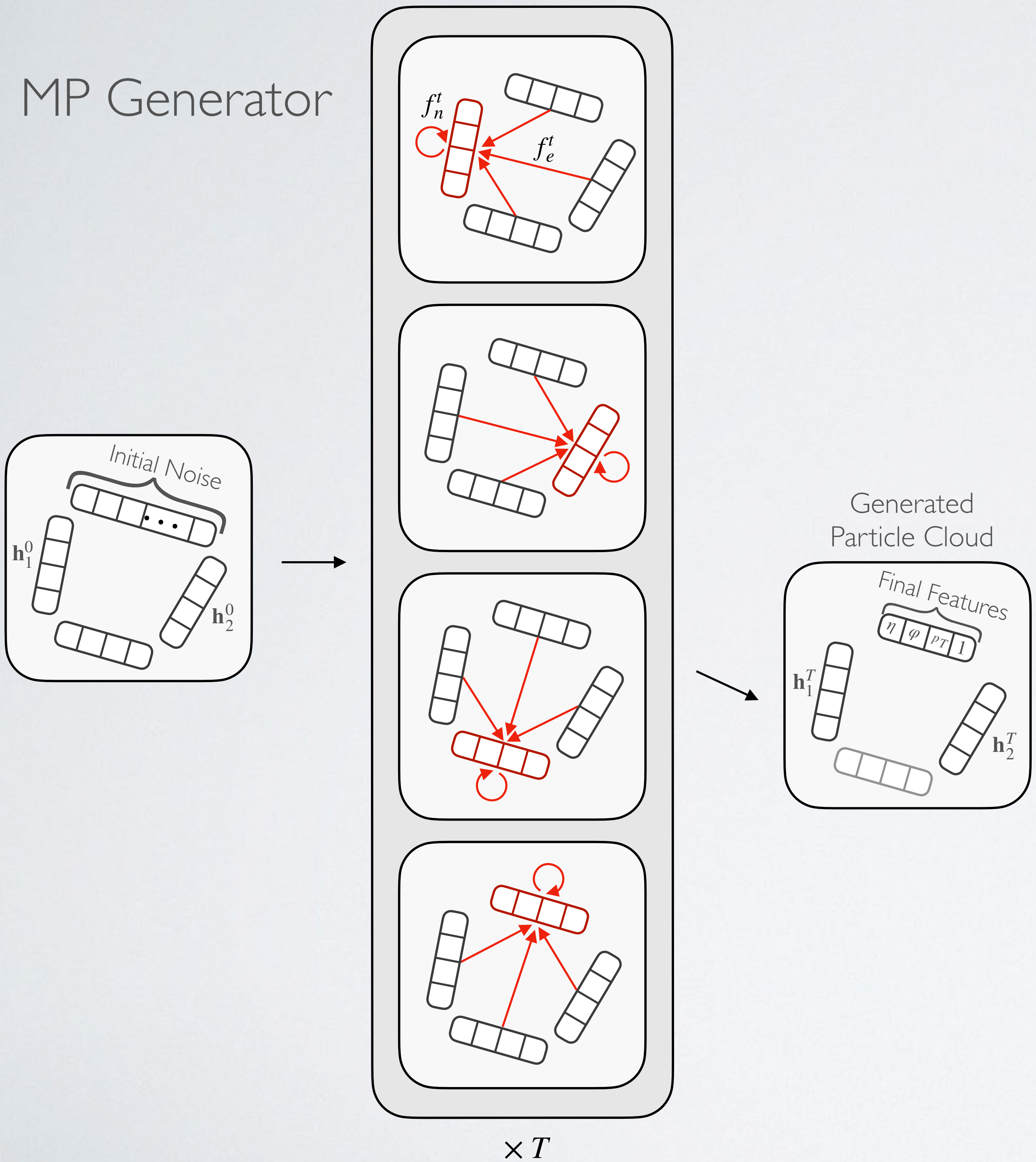

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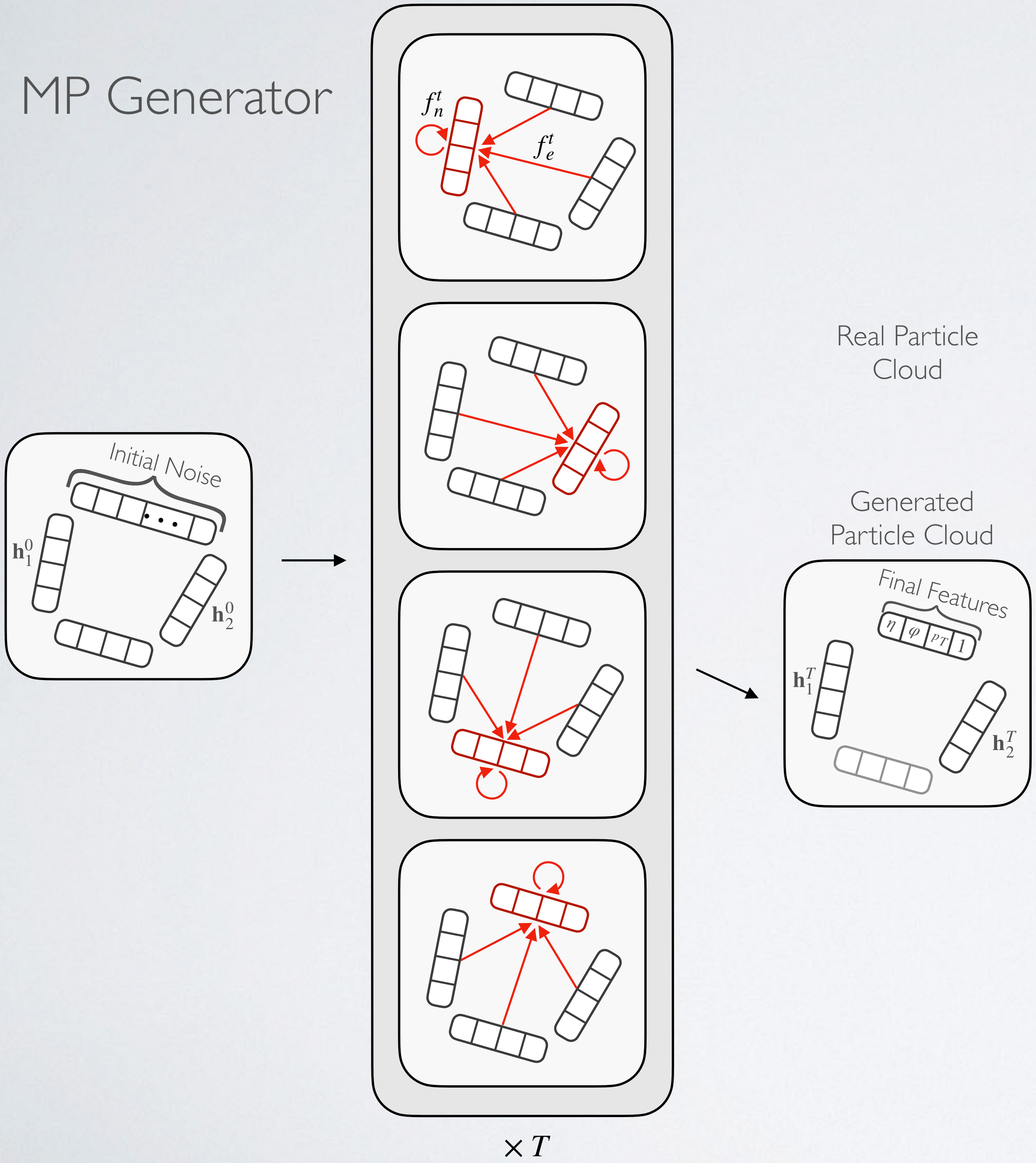

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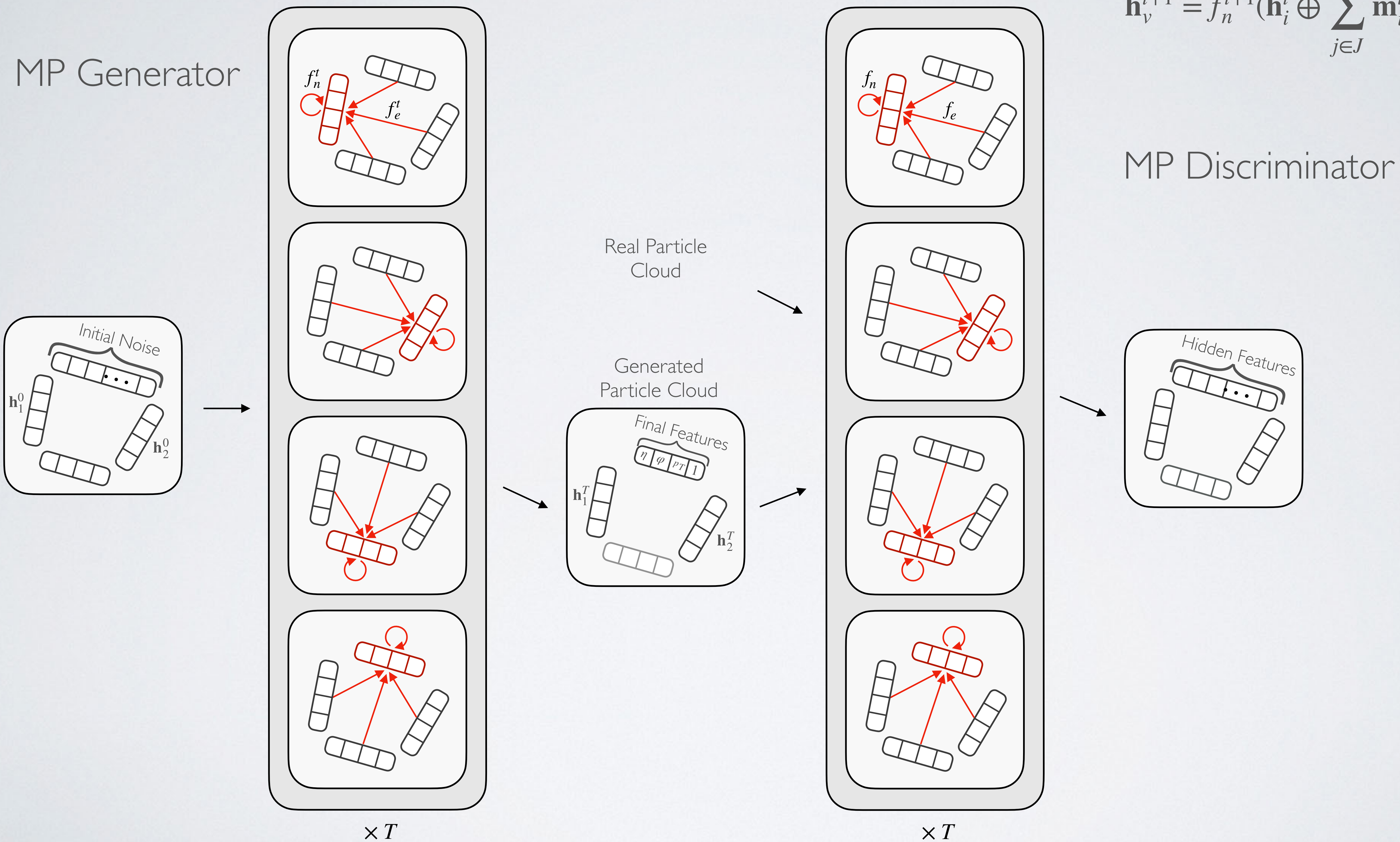

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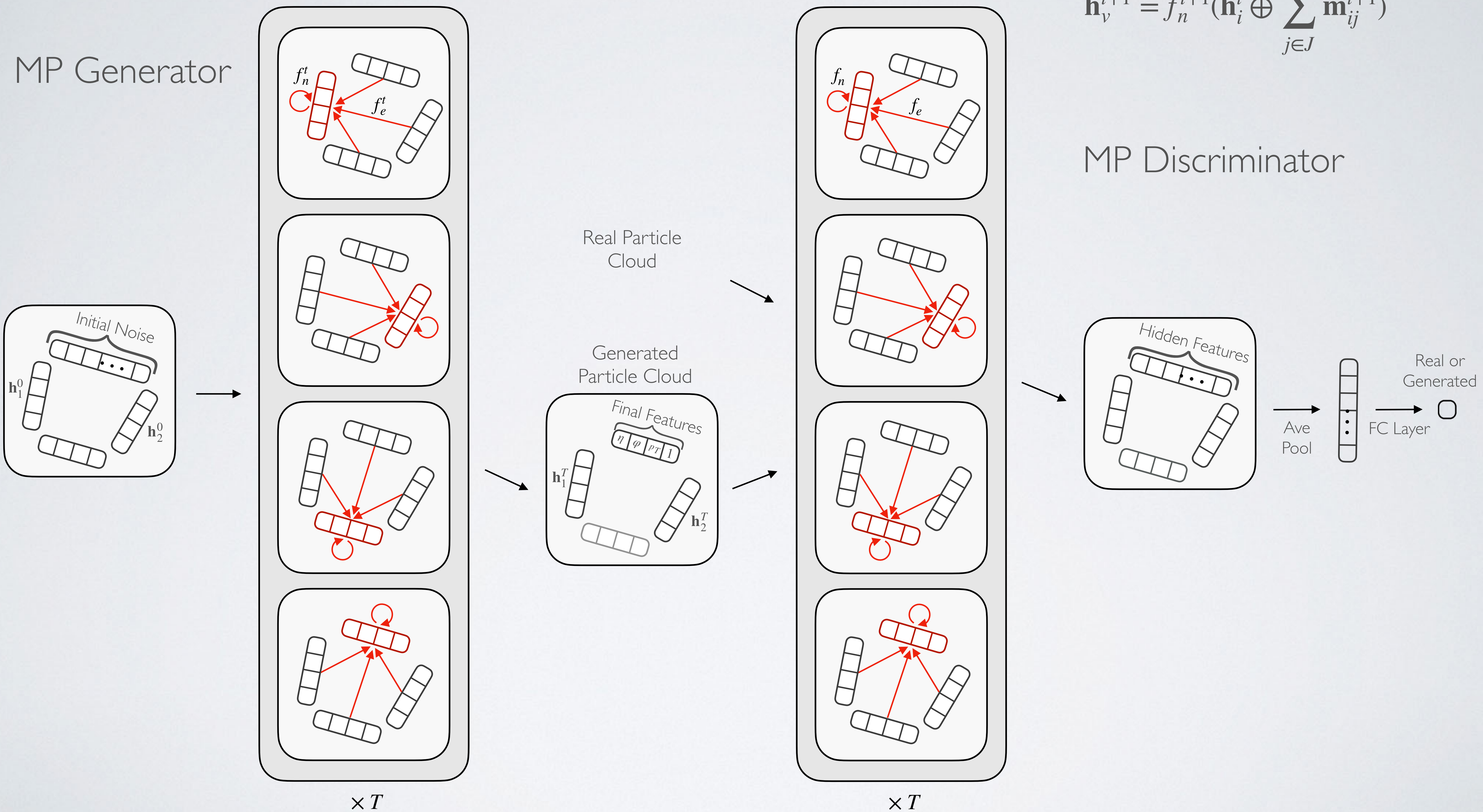

MPGAN: RESULTS

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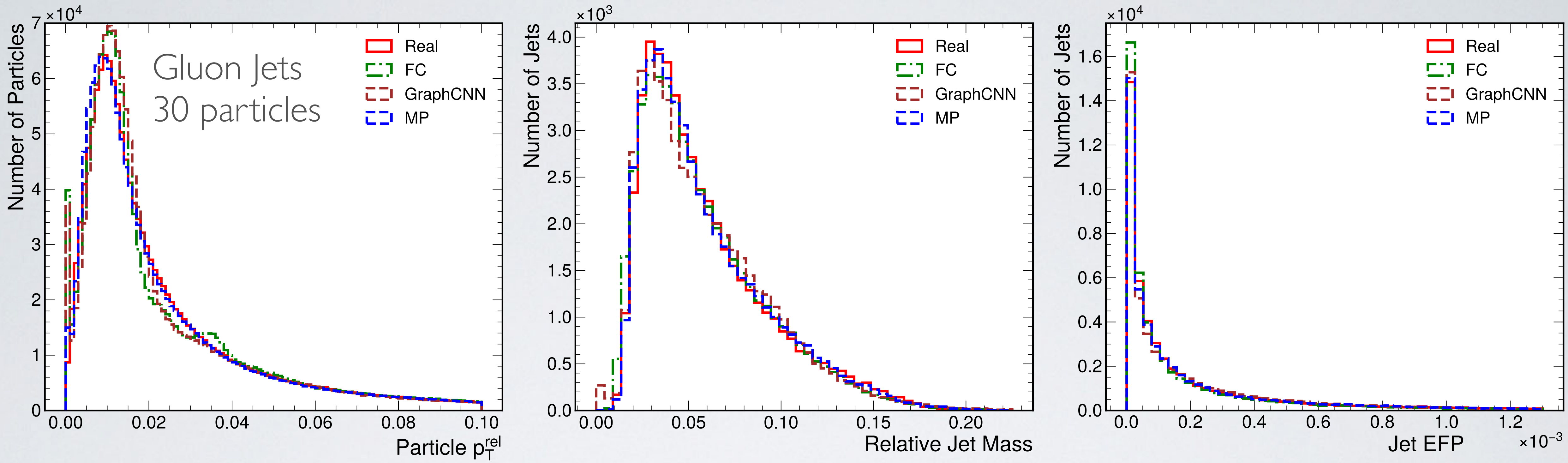

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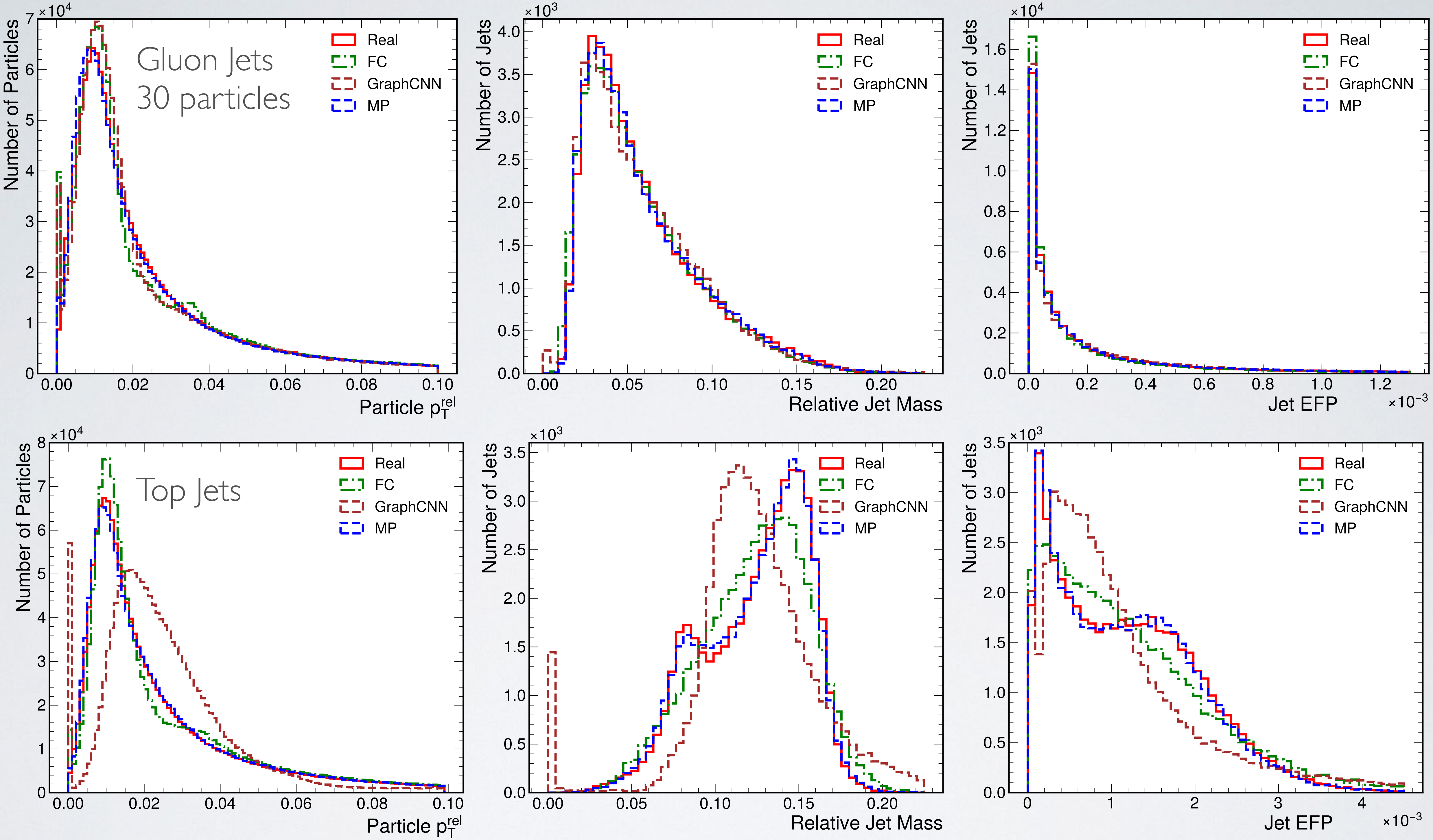

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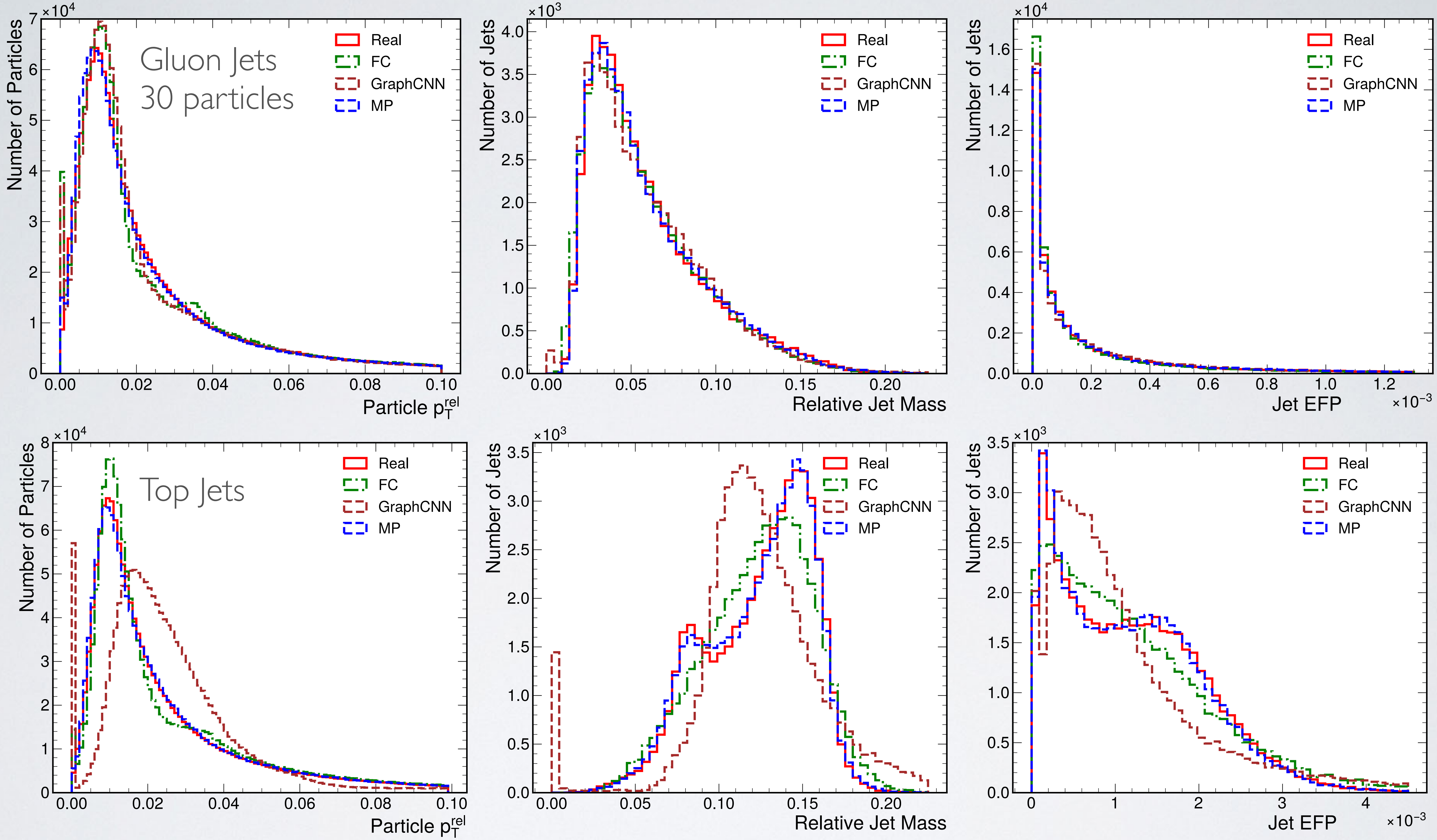

- MPGAN (blue) learns real (red) distributions well

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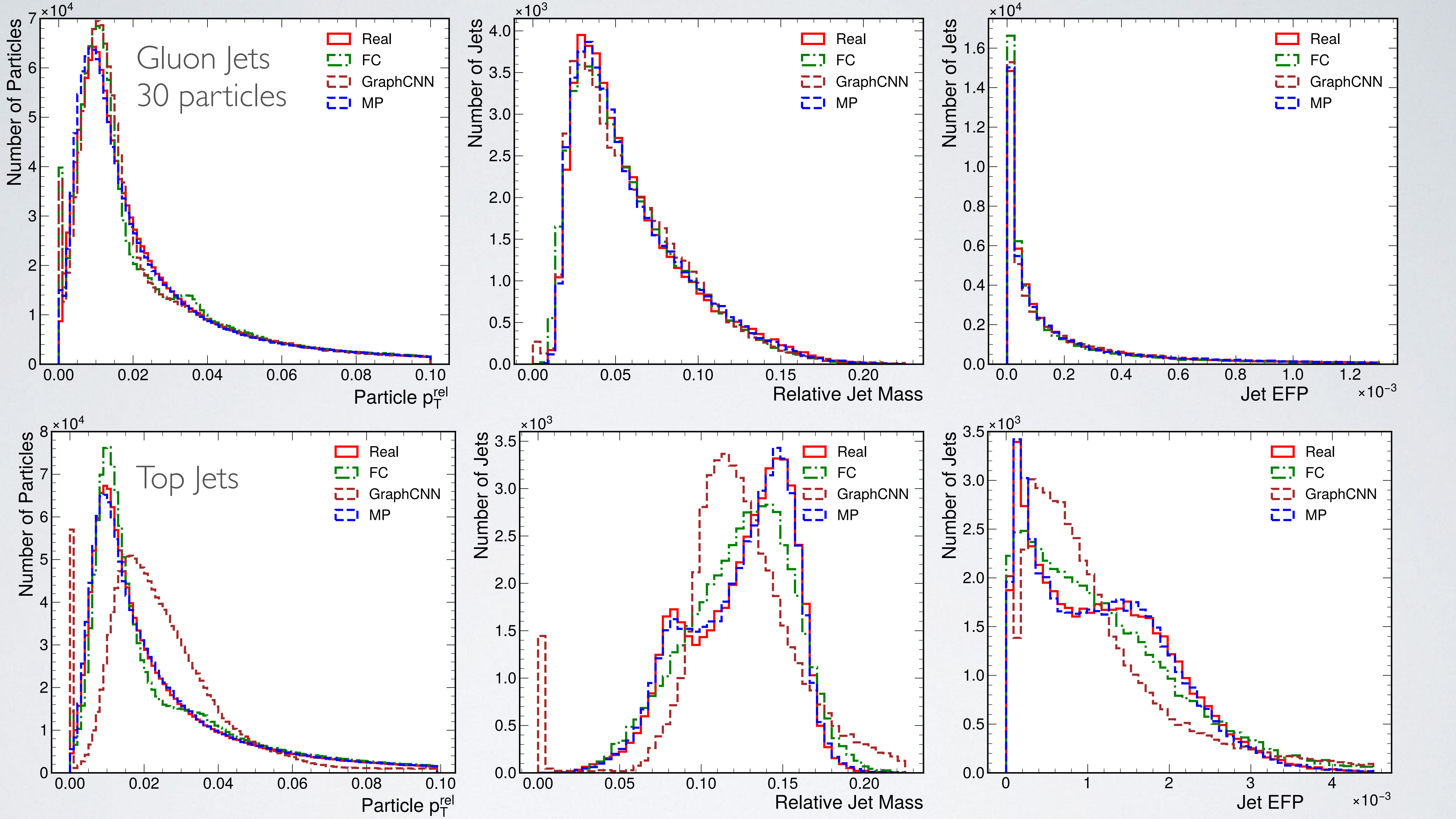

- MPGAN (blue) learns real (red) distributions well
- Outperforms all existing point cloud GANs (metrics in backup)

APPROACH 2: GAPT

RK et al., 2022

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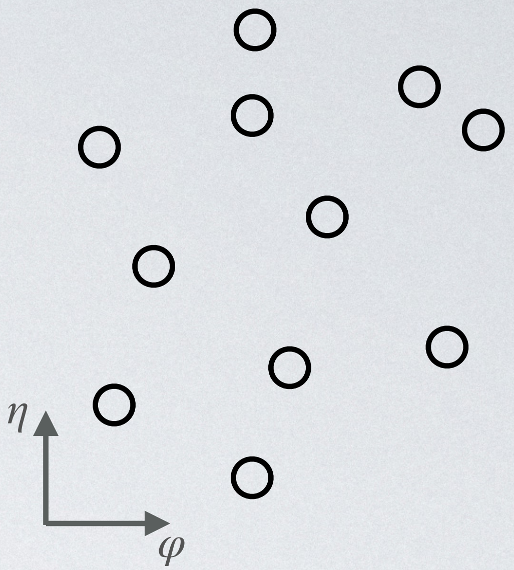

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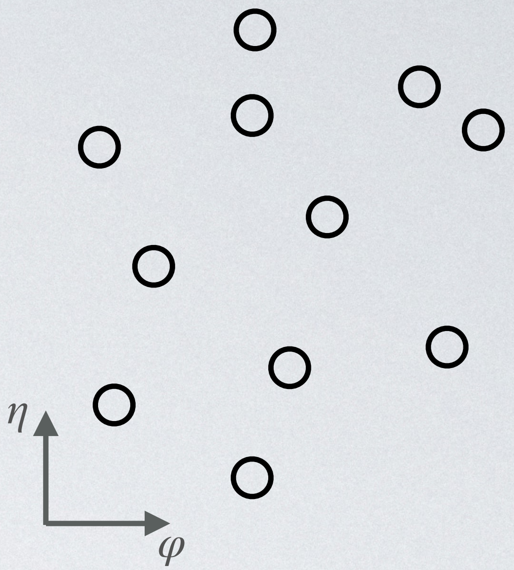
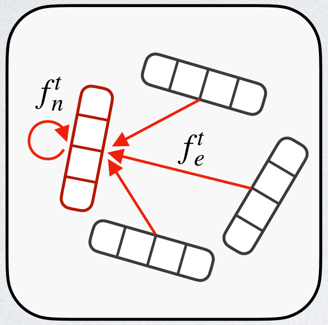


Message passing



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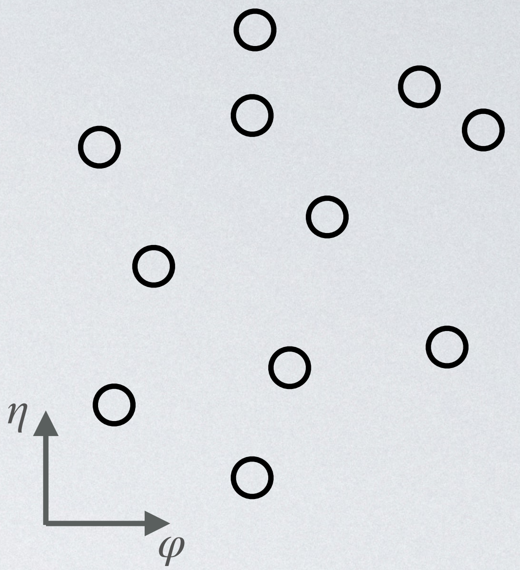

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Self-attention (set transformers, Lee et al. ICML 2019)

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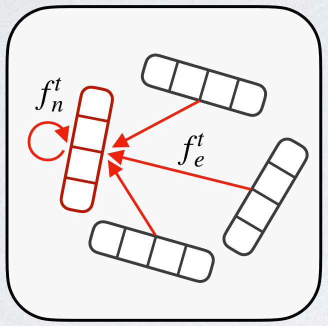

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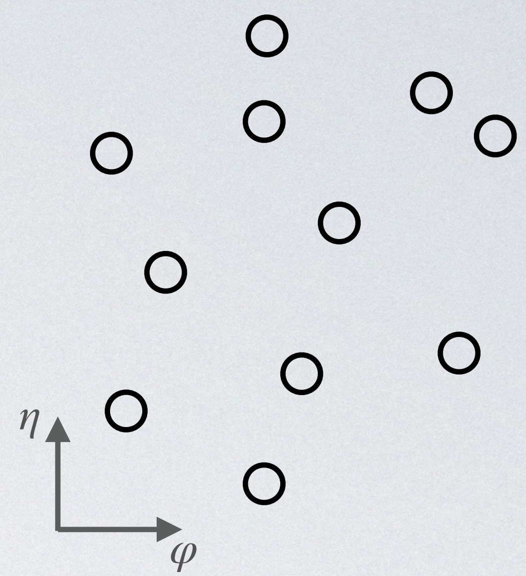

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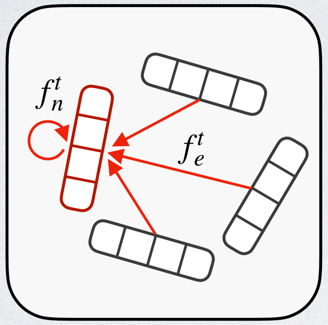

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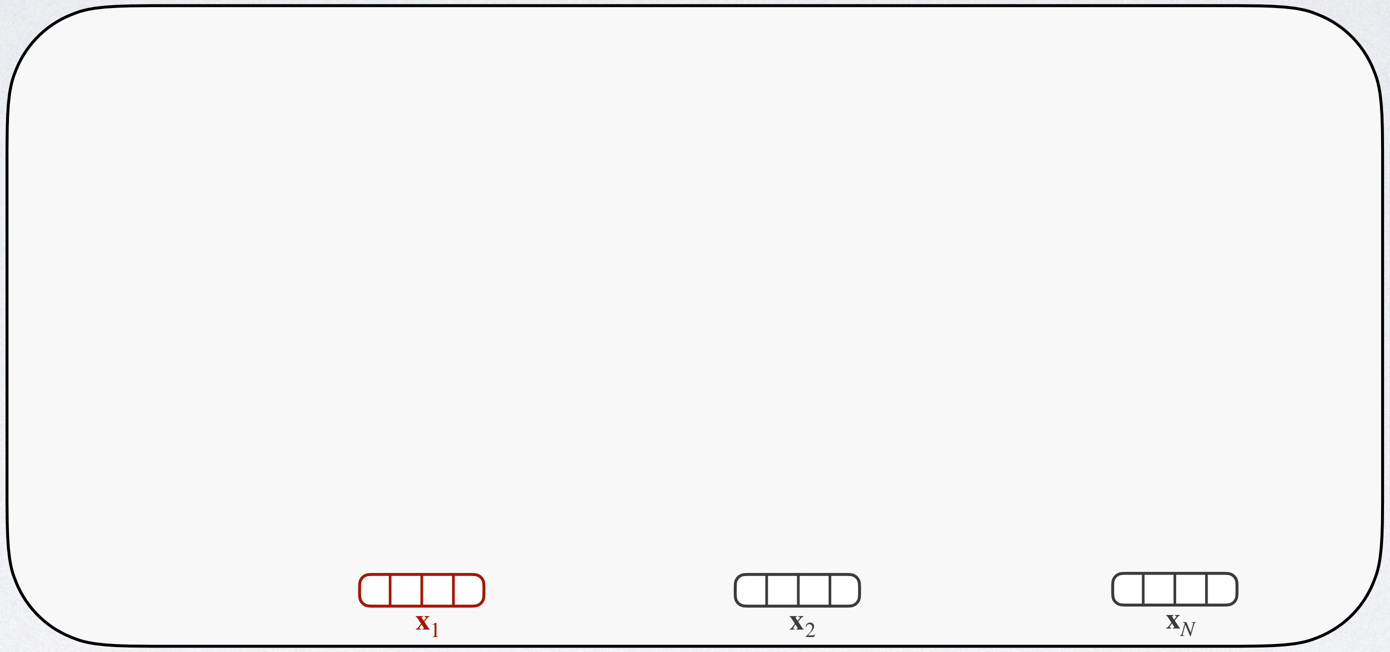

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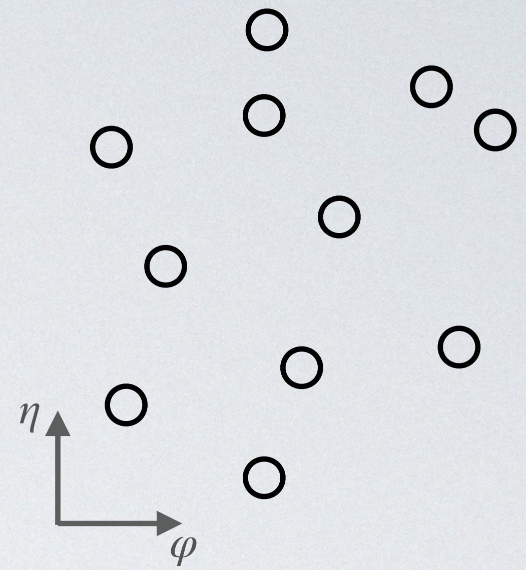

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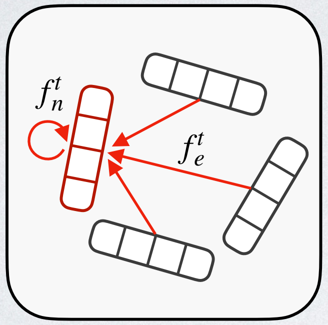

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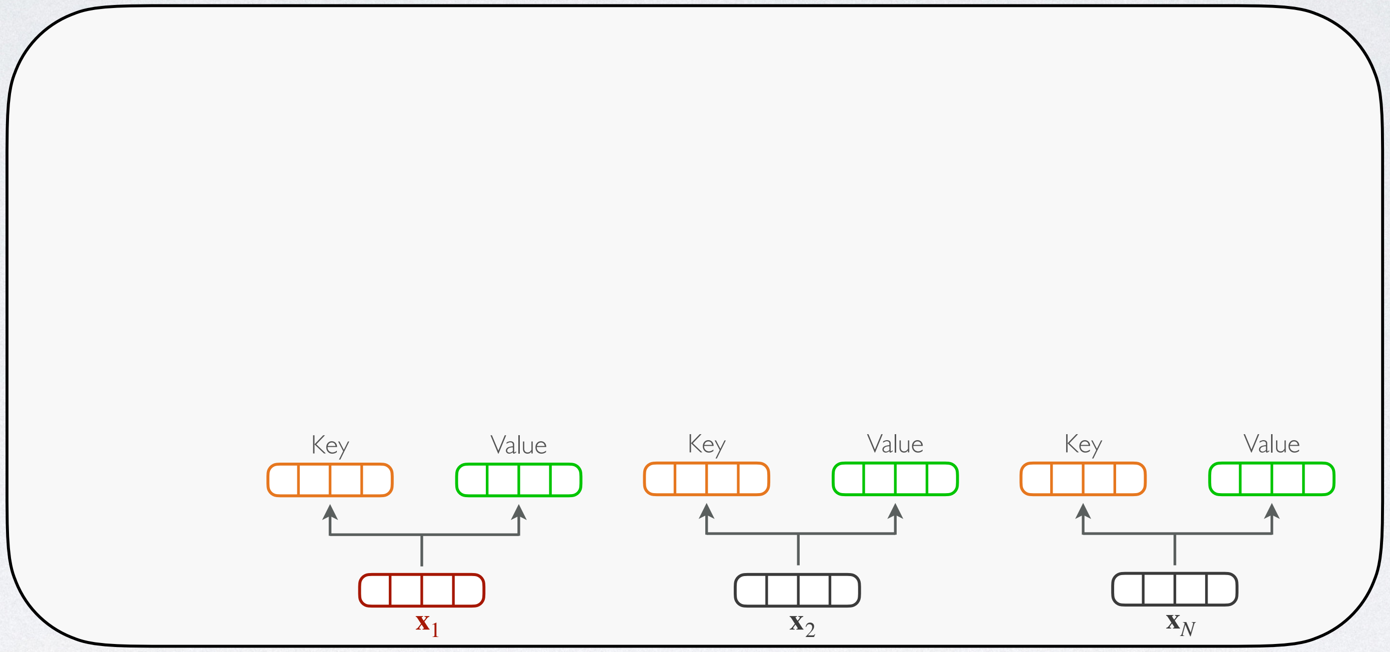

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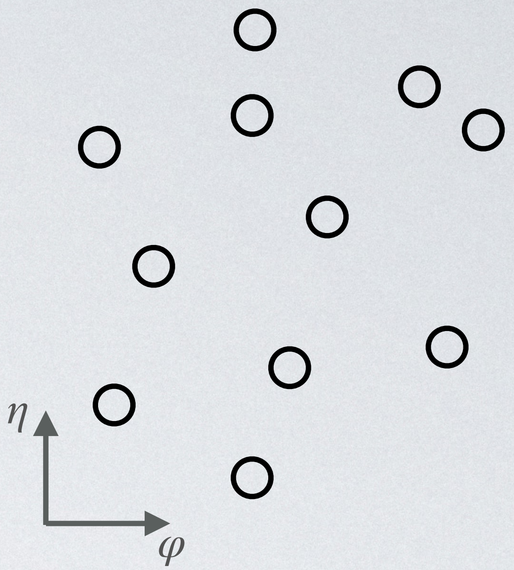

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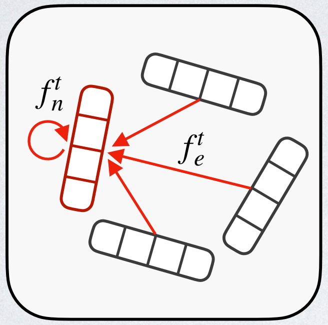

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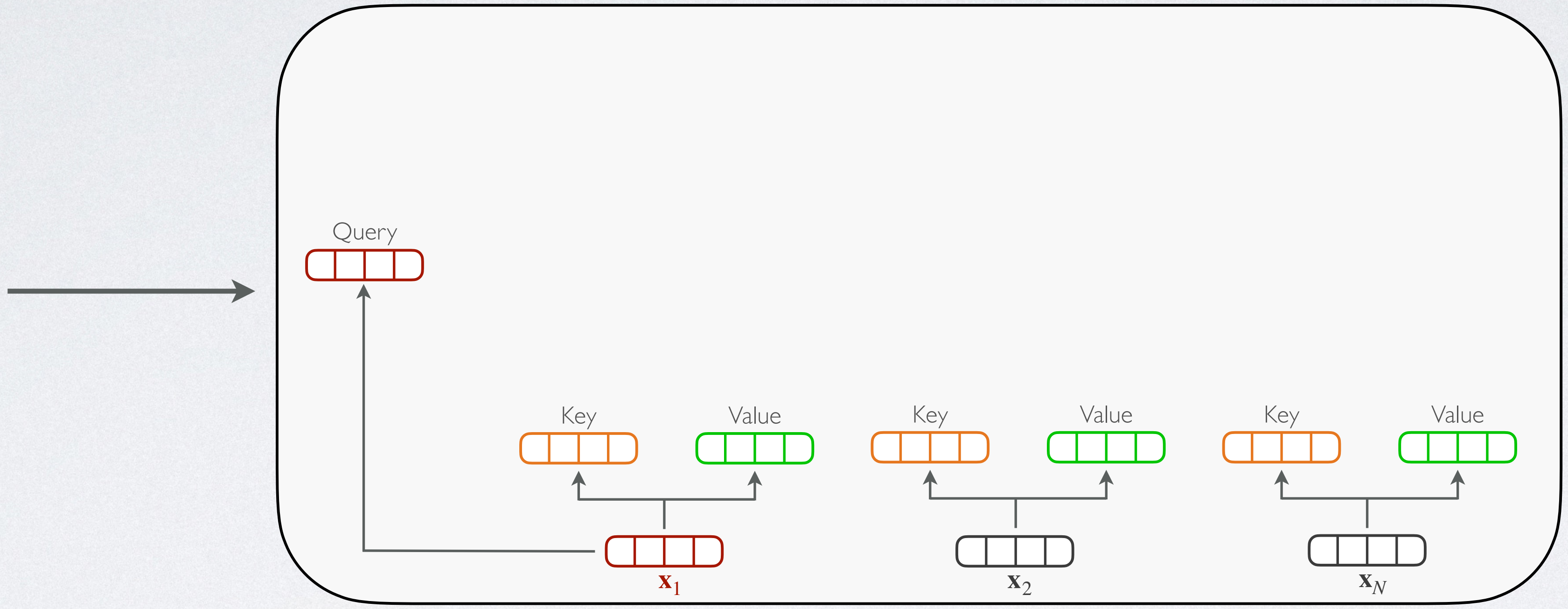

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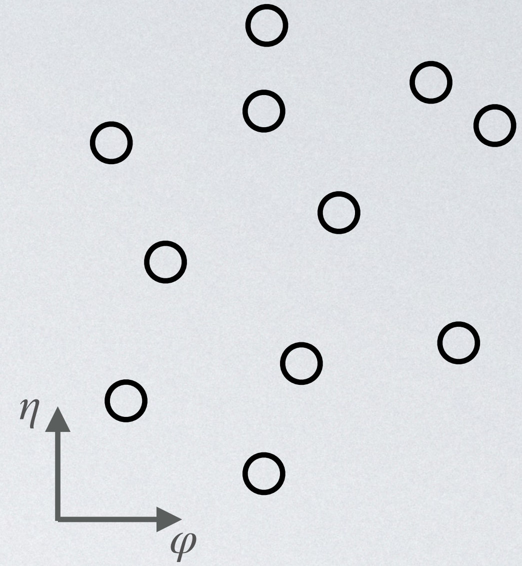

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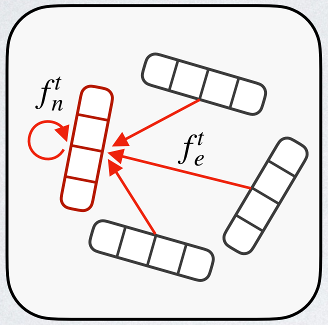

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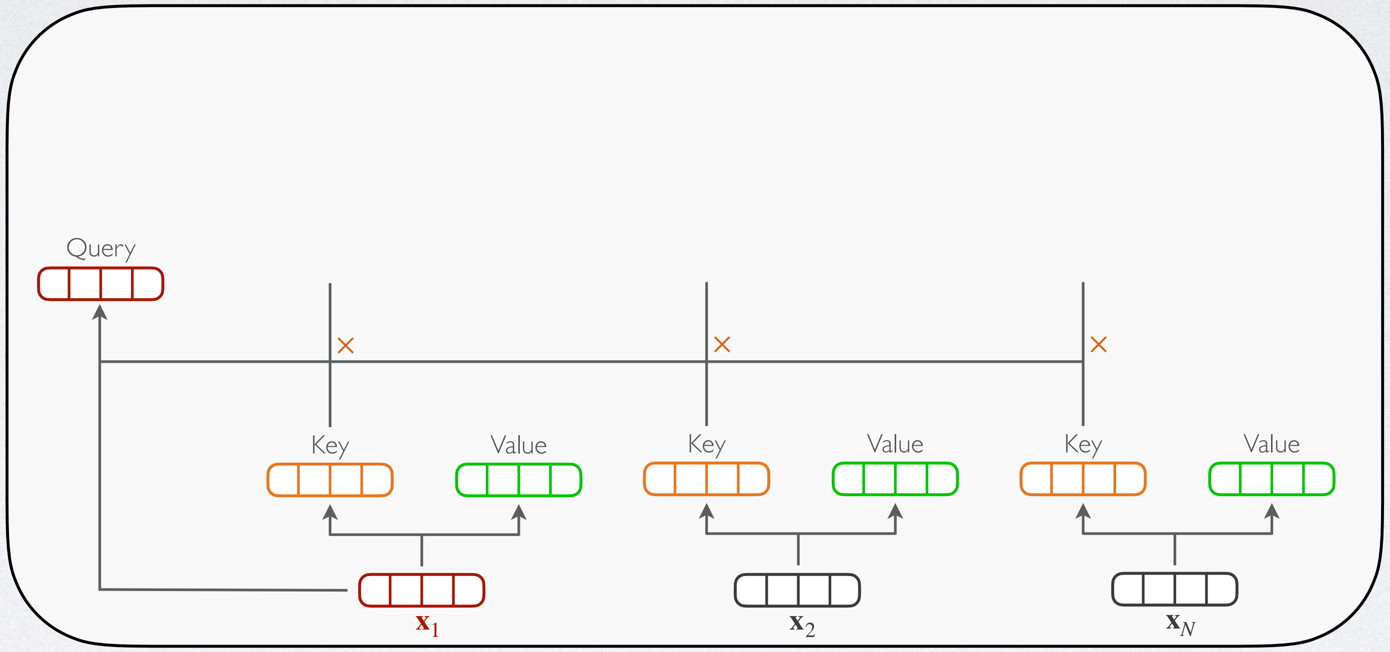

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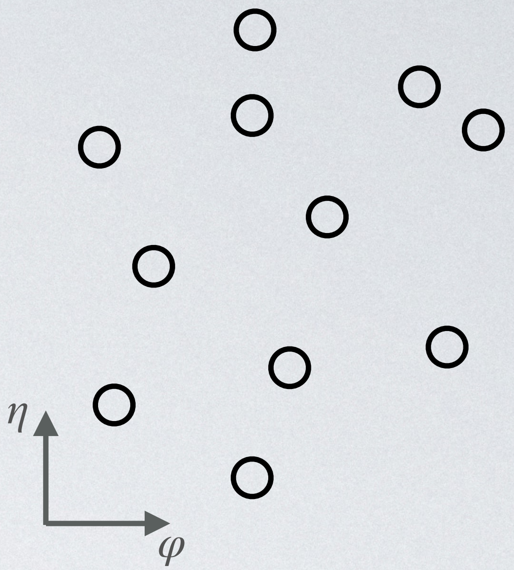

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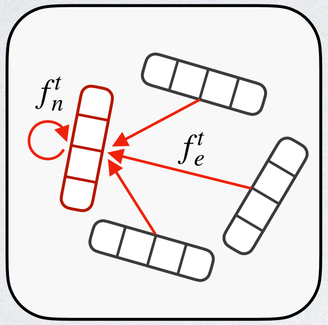

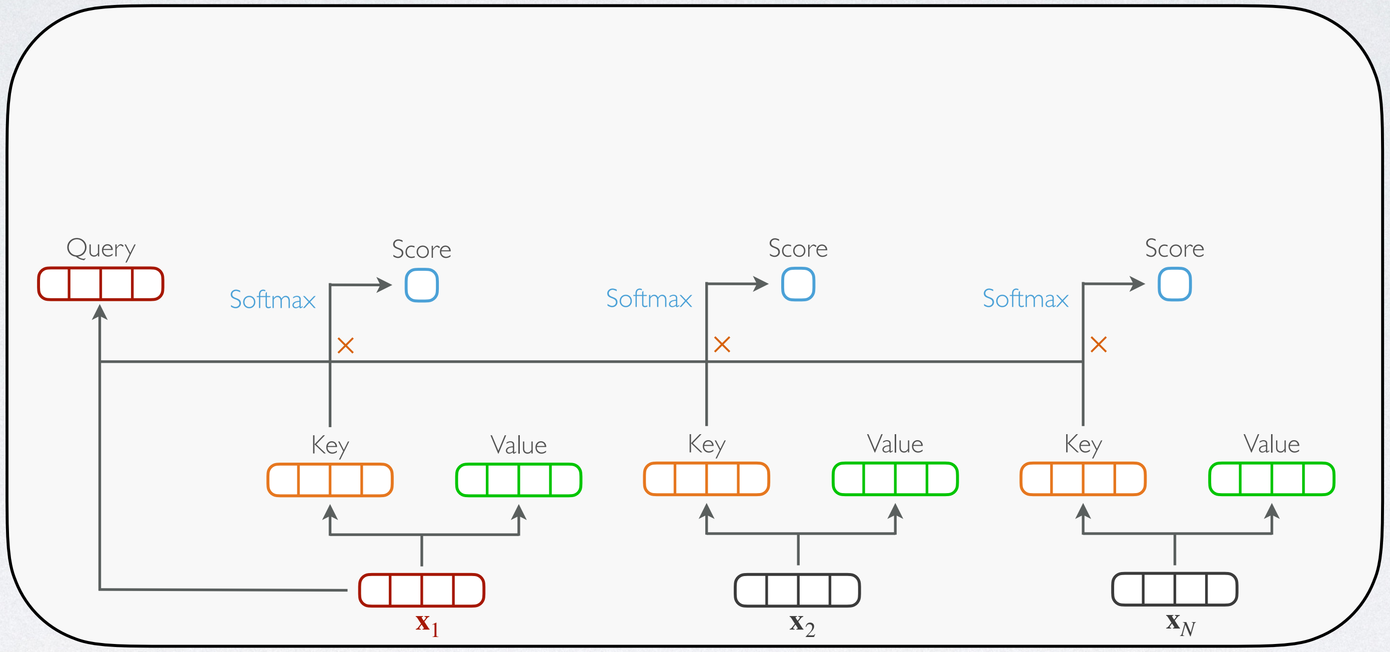

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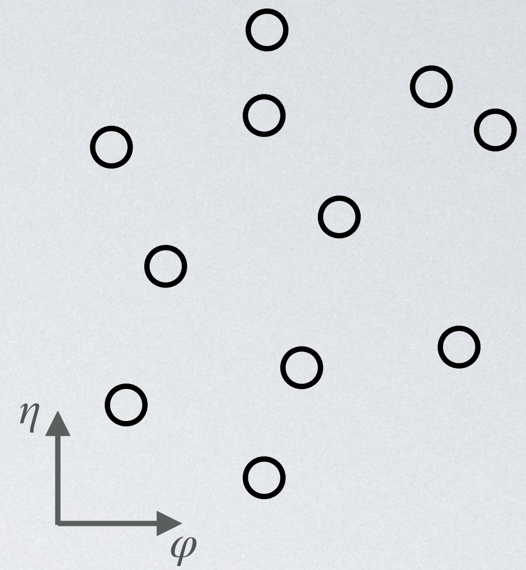

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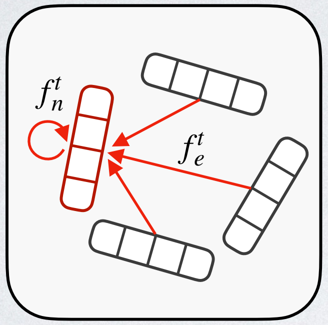

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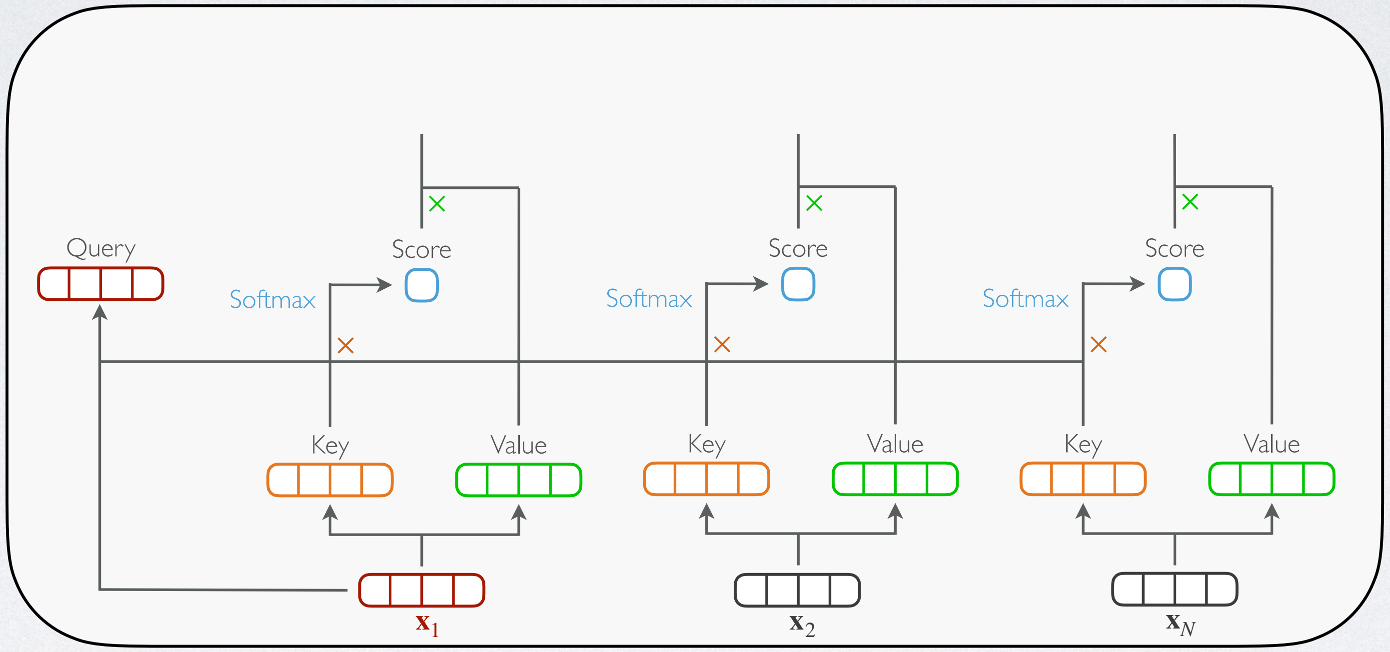

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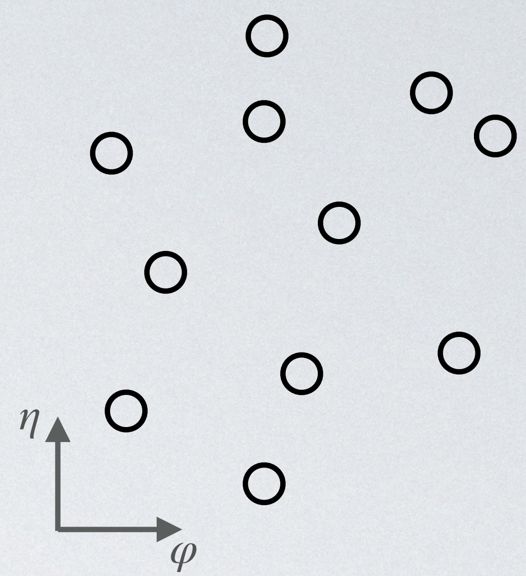

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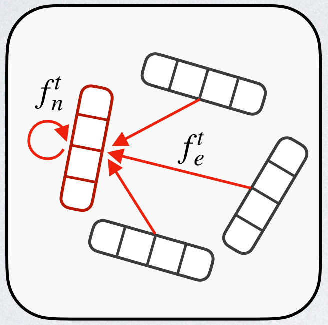

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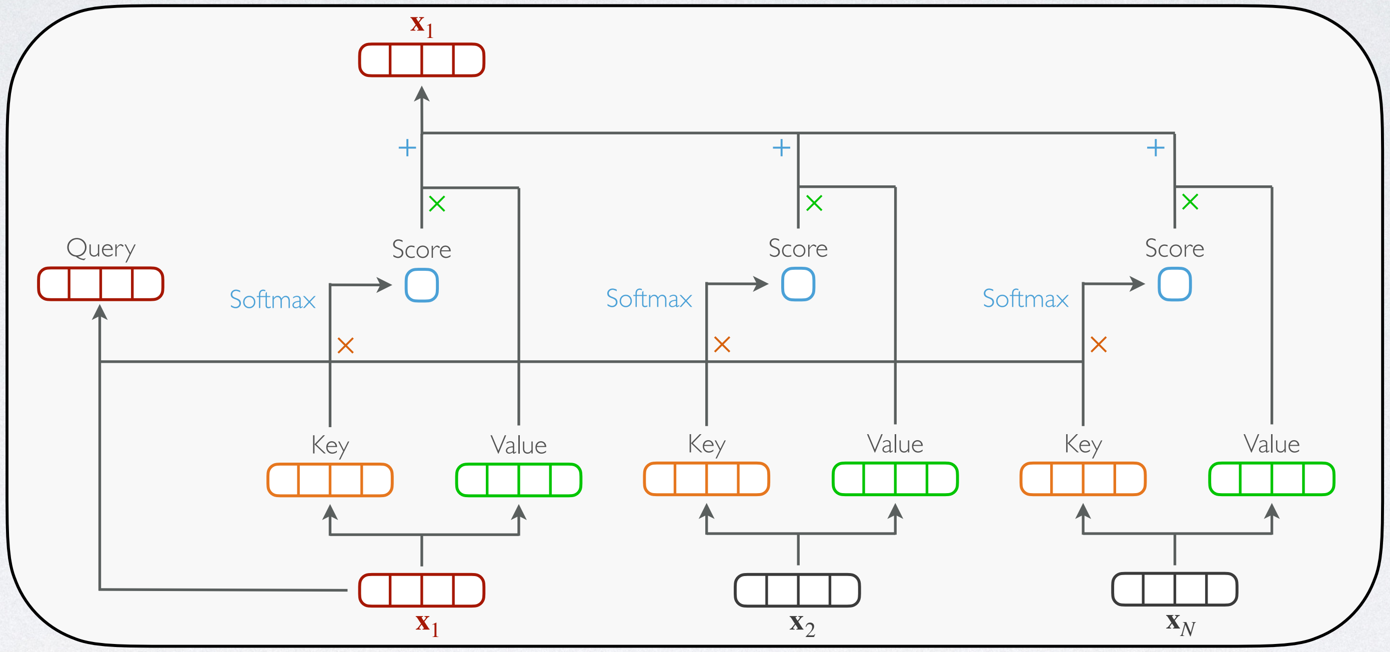

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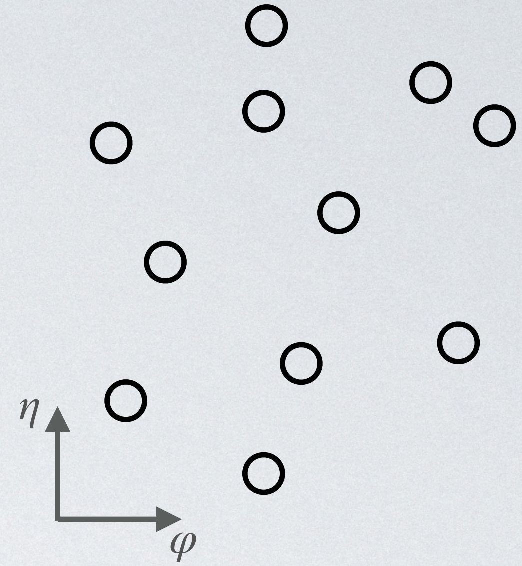

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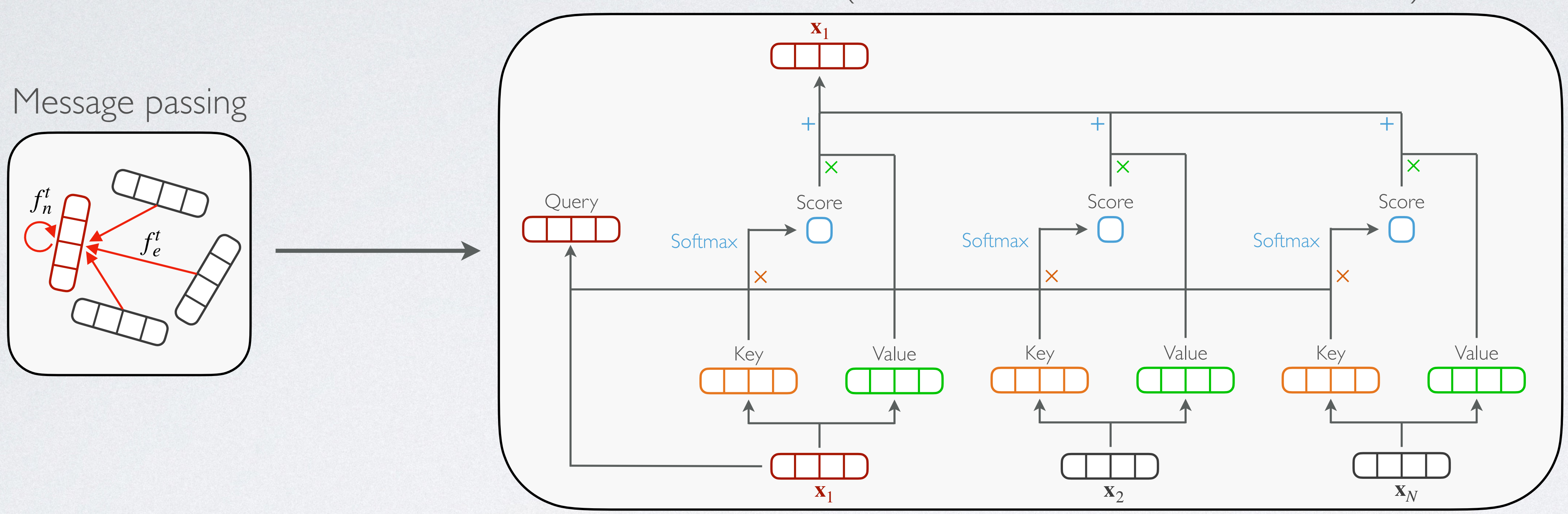

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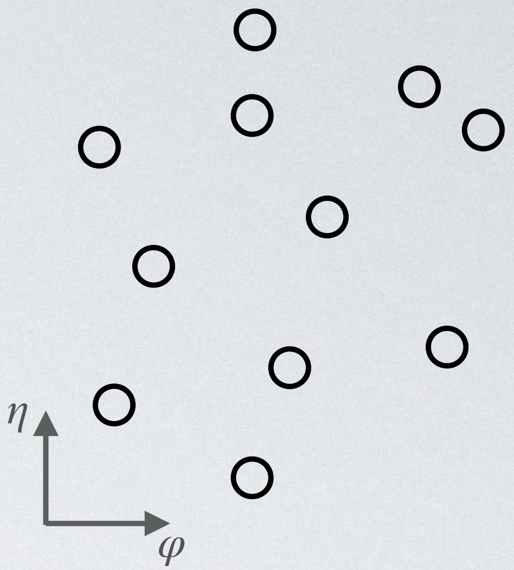
RK et al., 2022

APPROACH 2: GAPT



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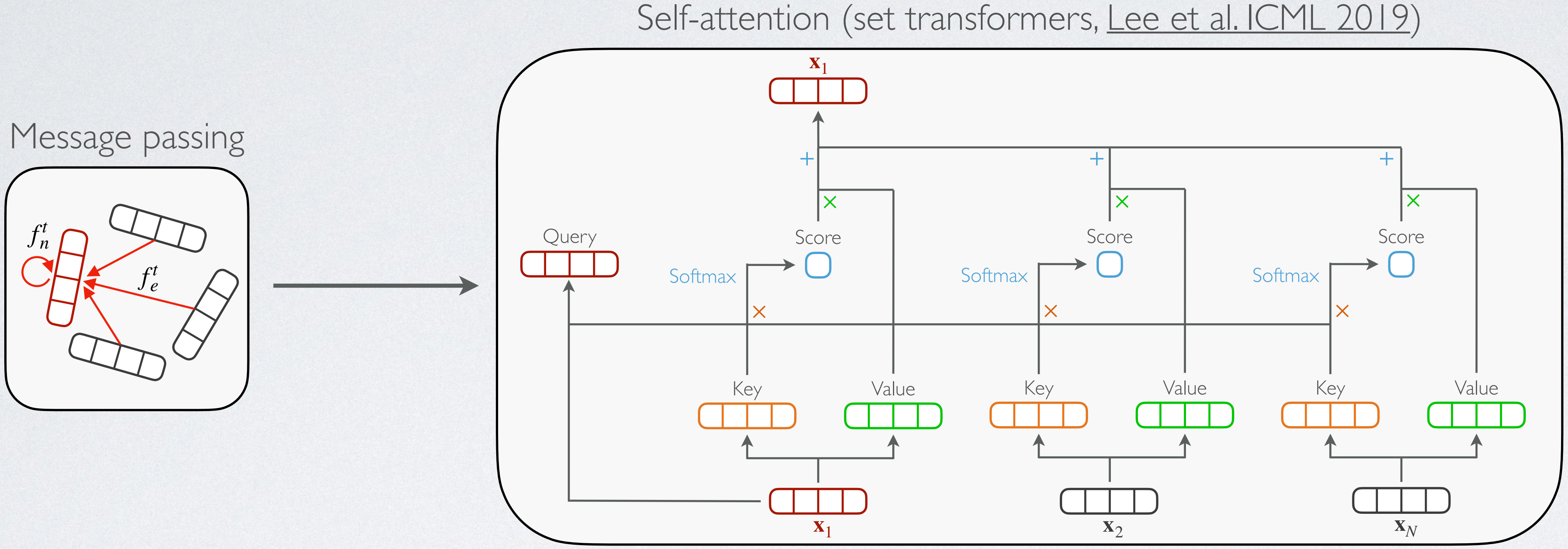

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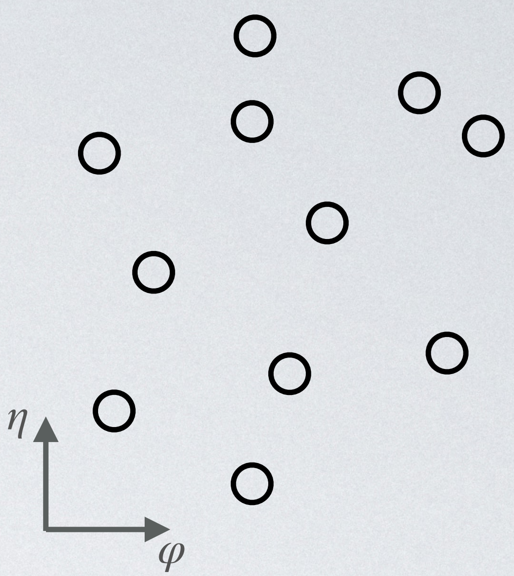
APPROACH 2: GAPT

[RK et al., 2022](#)



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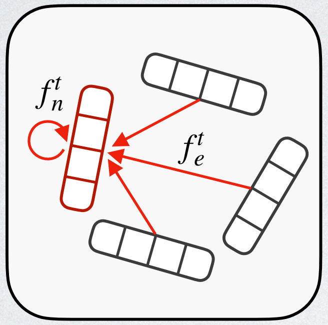

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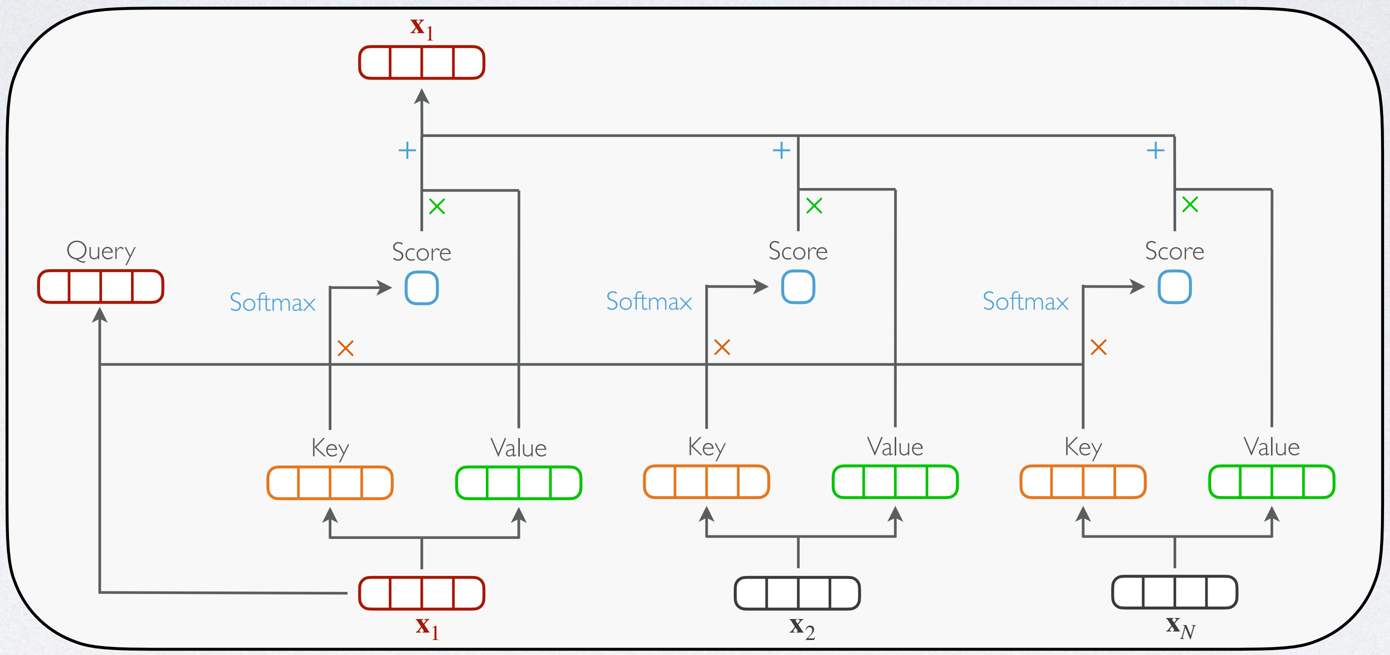

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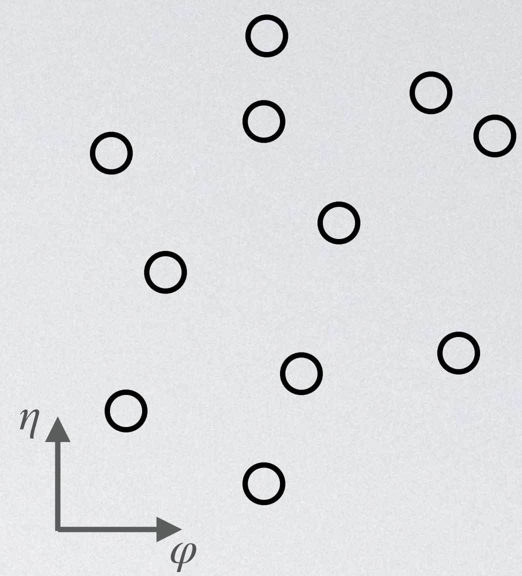
- 5-15x faster than MPGAN
- MPGAN and naive GAPT scale as $O(N^2)$ with # of nodes

APPROACH 2: GAPT

RK et al., 2022



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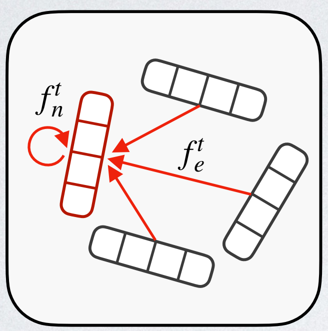
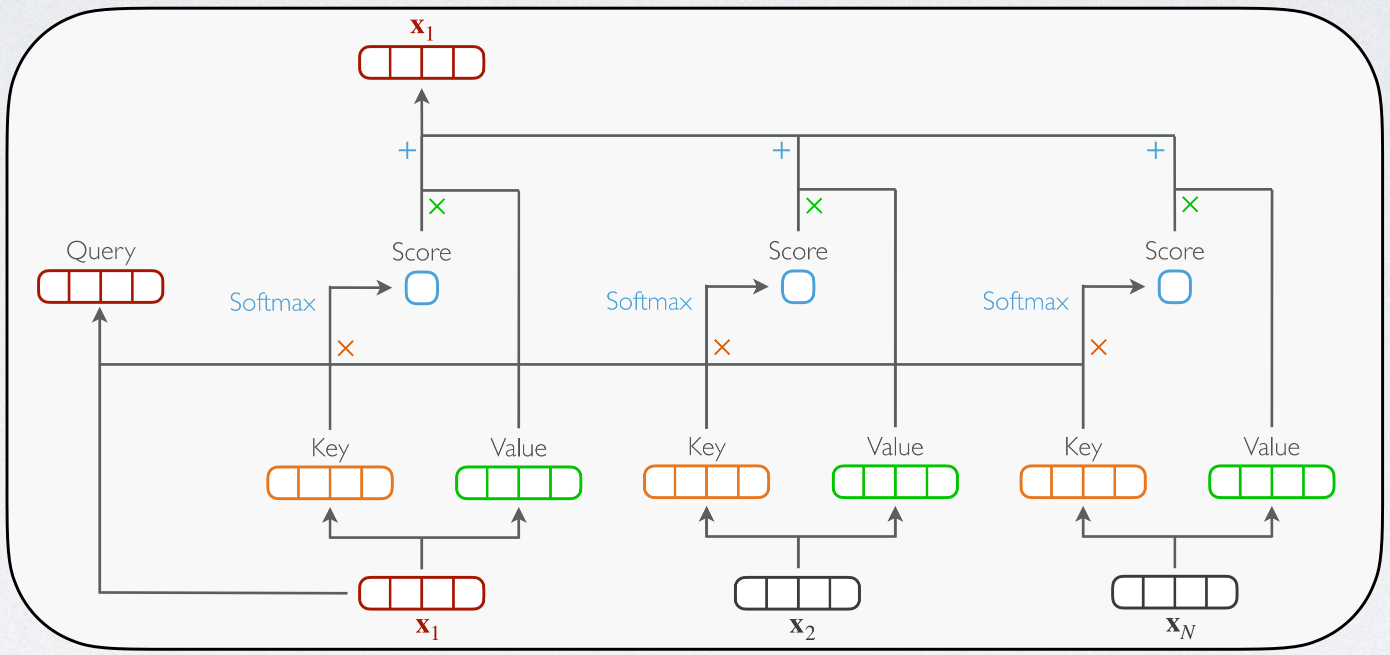
Message passing

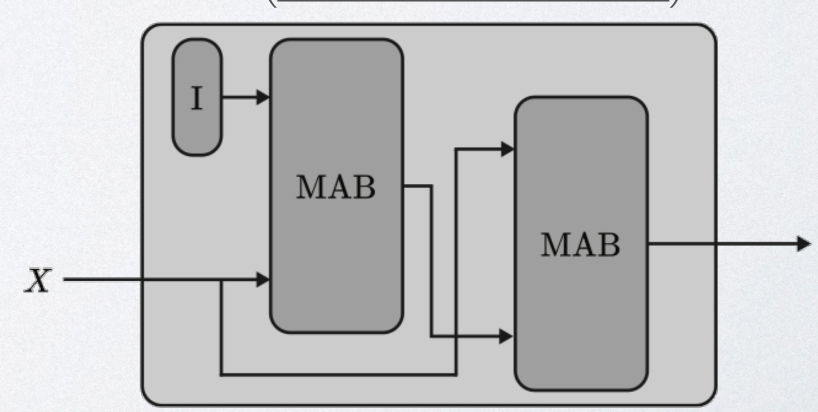


Self-attention (set transformers, Lee et al. ICML 2019)



- Based on GAST (Stelzner et al. 2020), "Generative adversarial particle transformer" (GAPT)
- 5-15x faster than MPGAN
- MPGAN and naive GAPT scale as $O(N^2)$ with # of nodes
- But linear scaling with induced self-attention blocks (ISAB)

ISAB (Lee et al. ICML 2019)



MPGAN VS GAPT

RK et al., 2022

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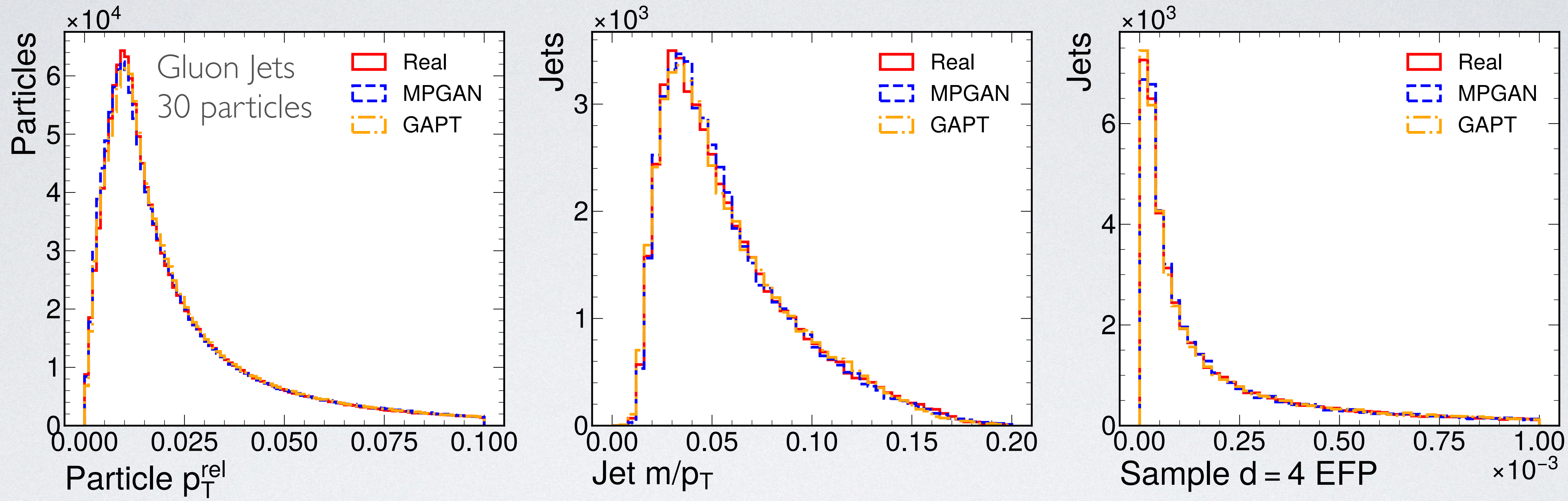

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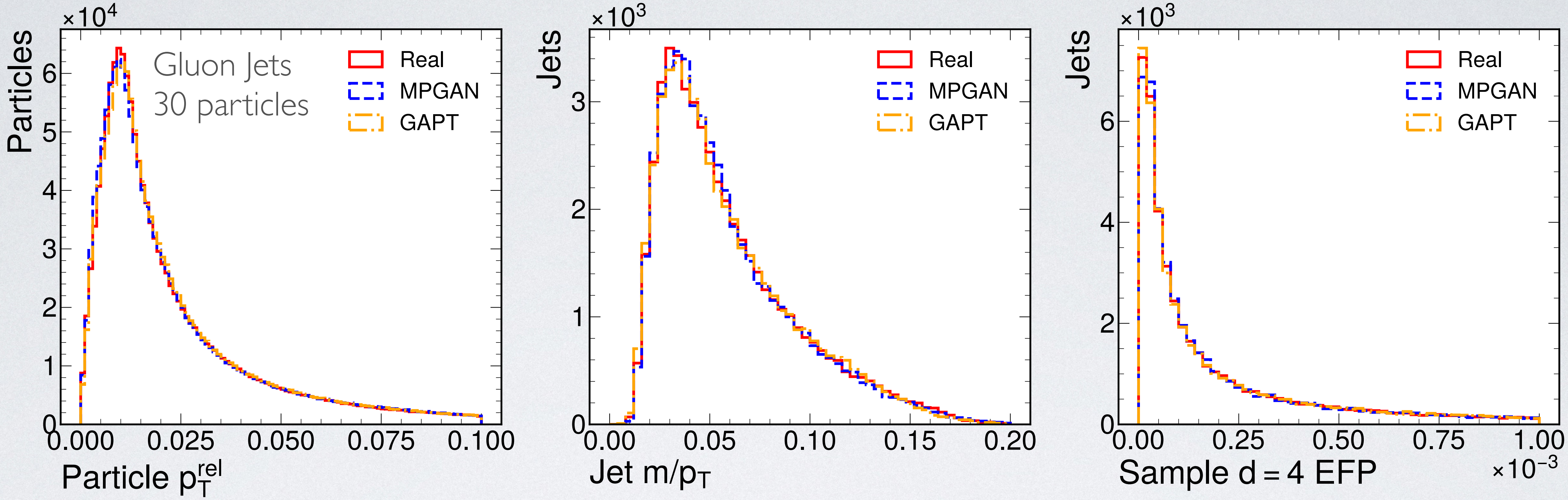

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RK et al., 2022

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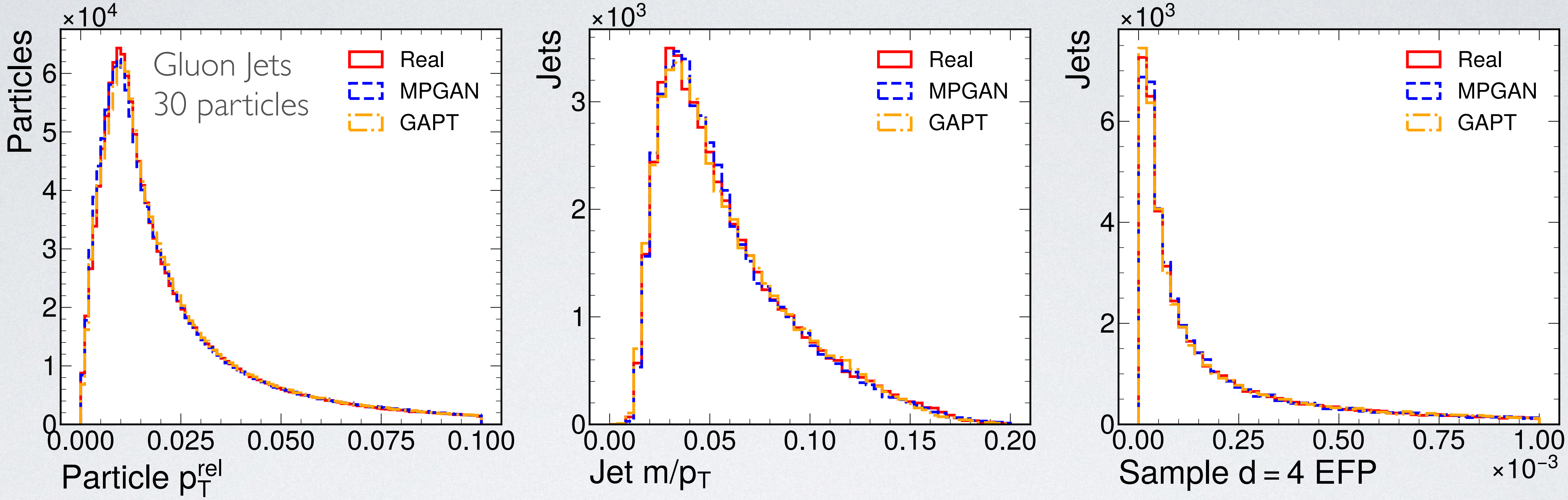

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Truth	0.08 ± 0.03	−0.006 ± 0.005	0.28 ± 0.05	-
MPGAN	0.30 ± 0.06	−0.001 ± 0.004	0.54 ± 0.06	41
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*On an A6000

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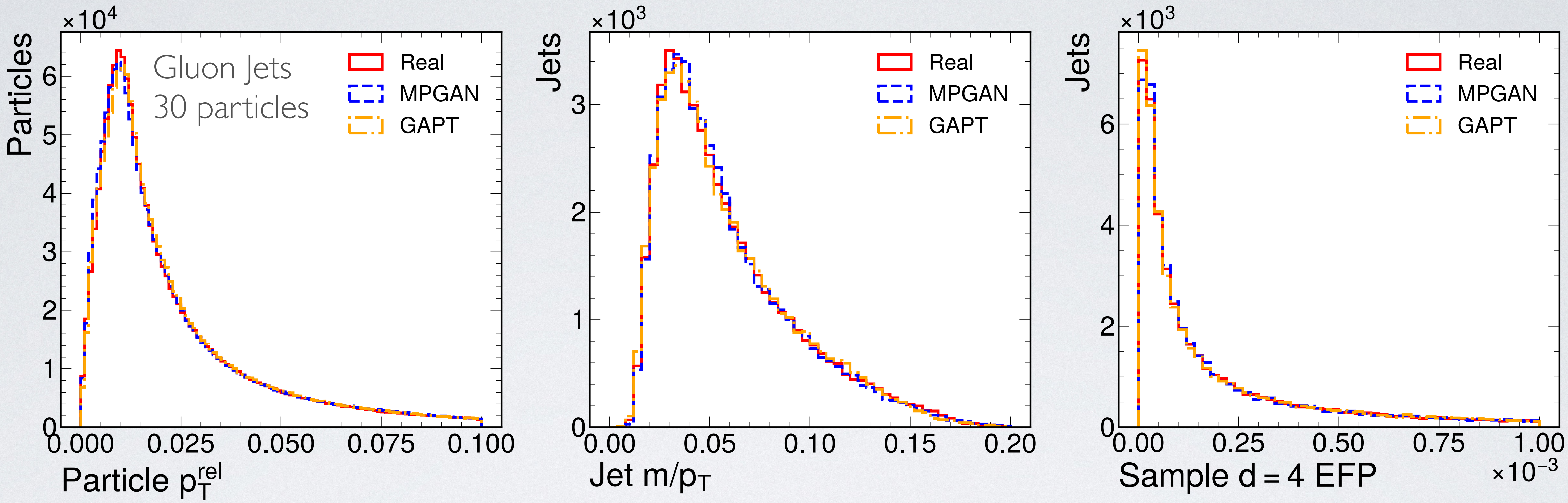

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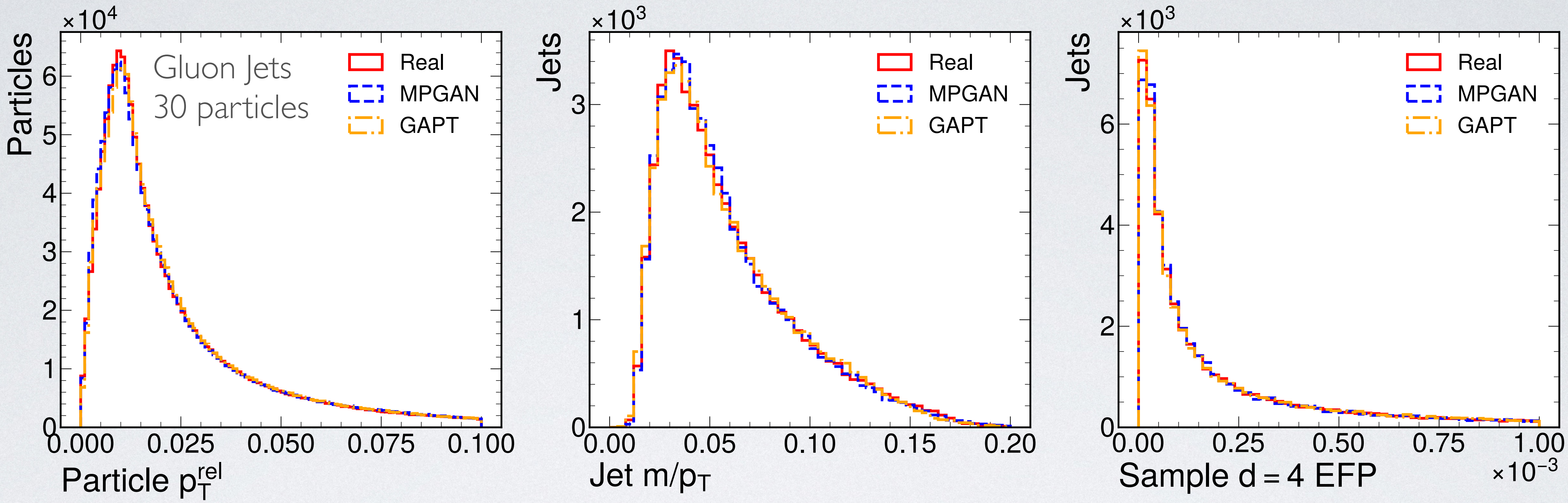

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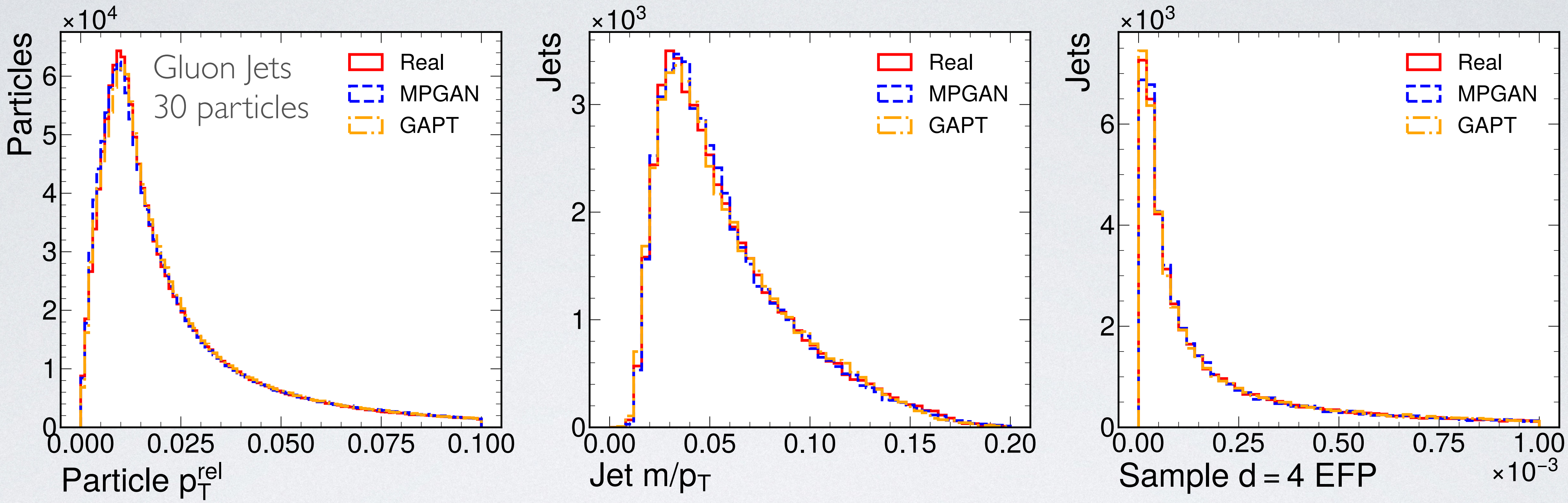

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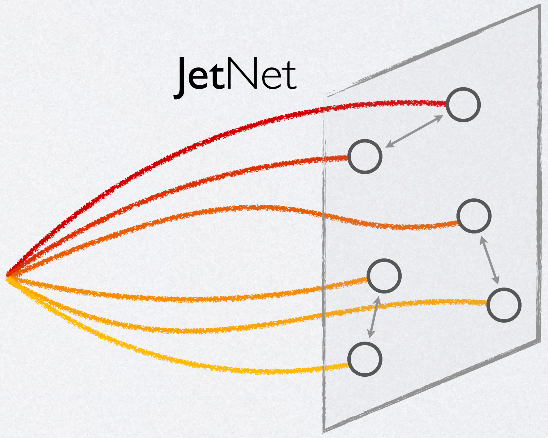

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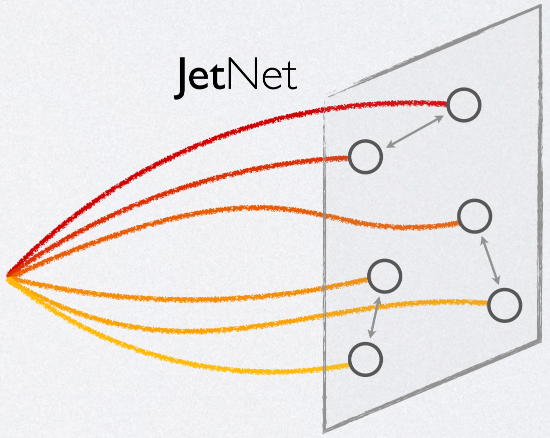
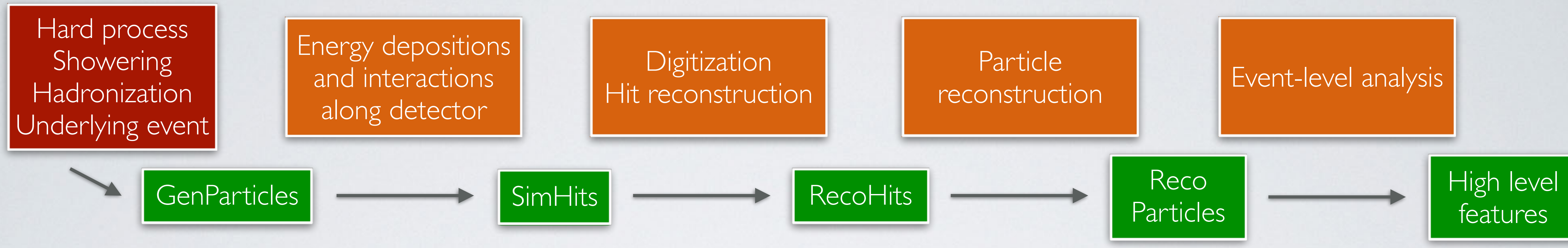


BACKUP

LHC SIMULATIONS



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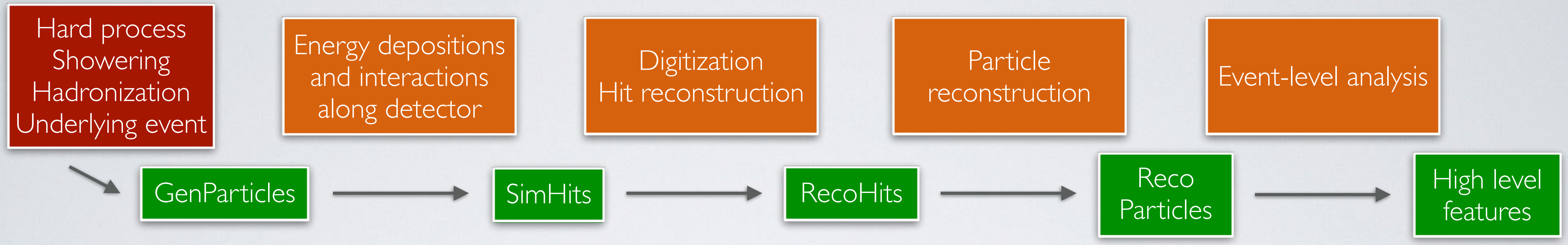

- Want model $p_\theta(\mathbf{x})$ for underlying data distribution $p(\mathbf{x})$

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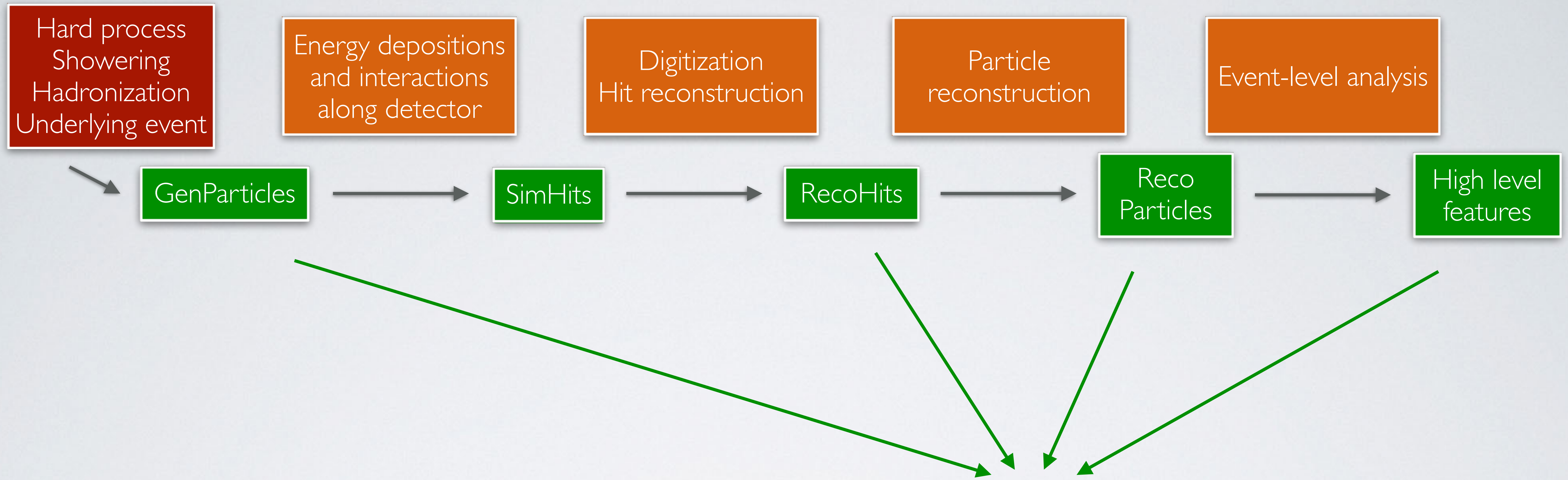

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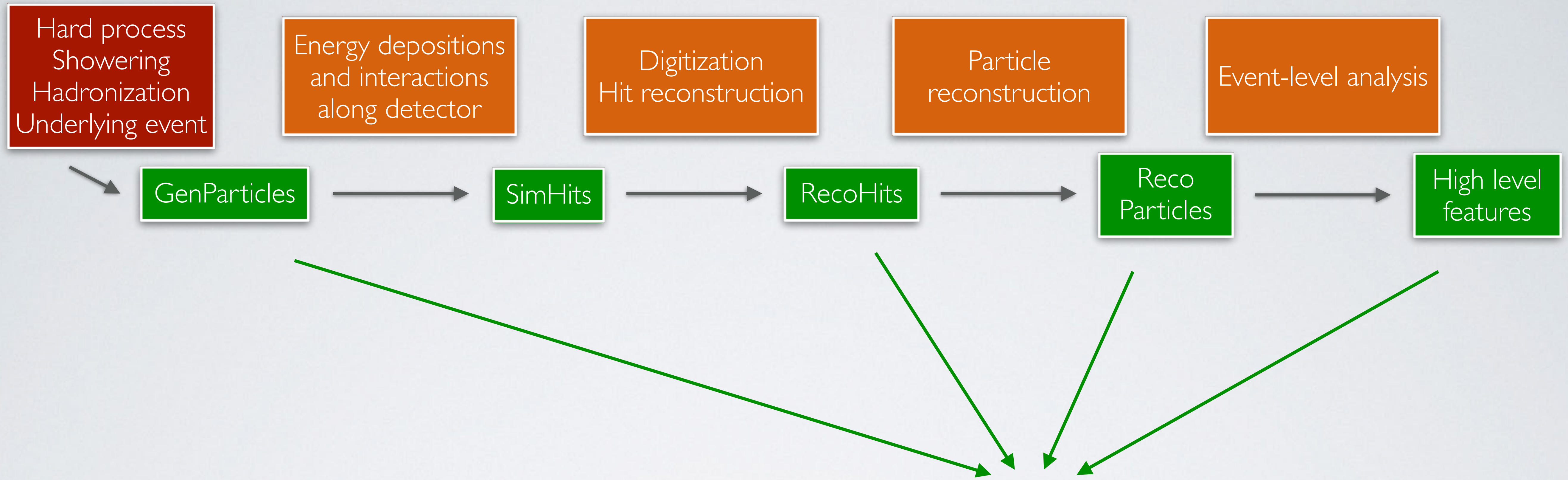

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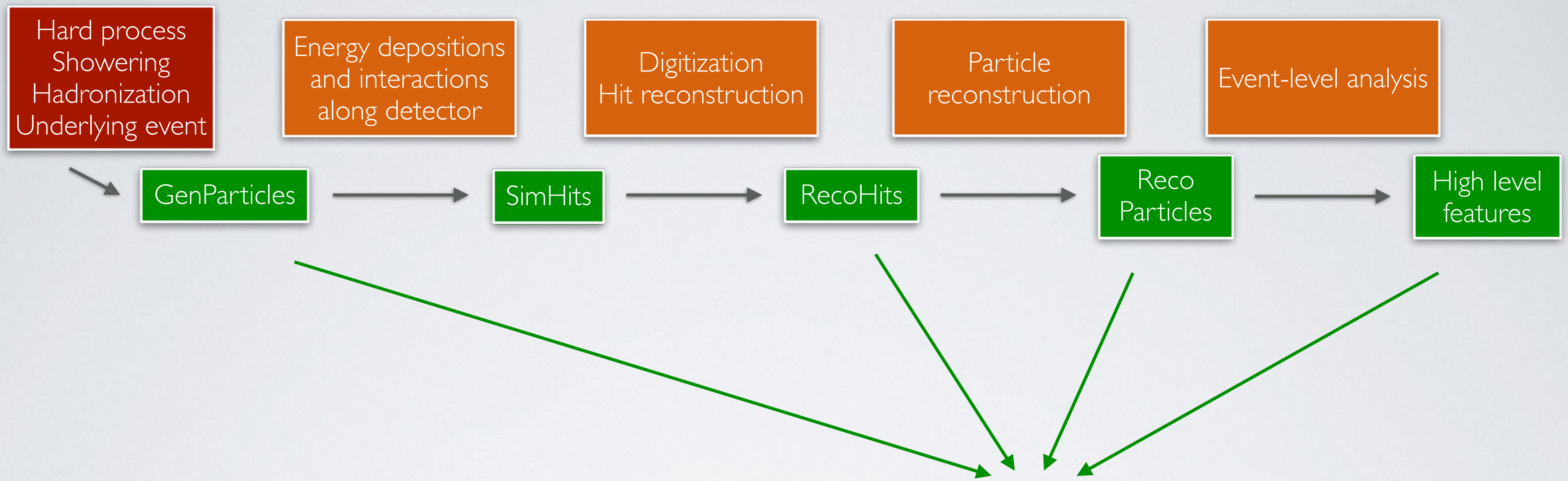

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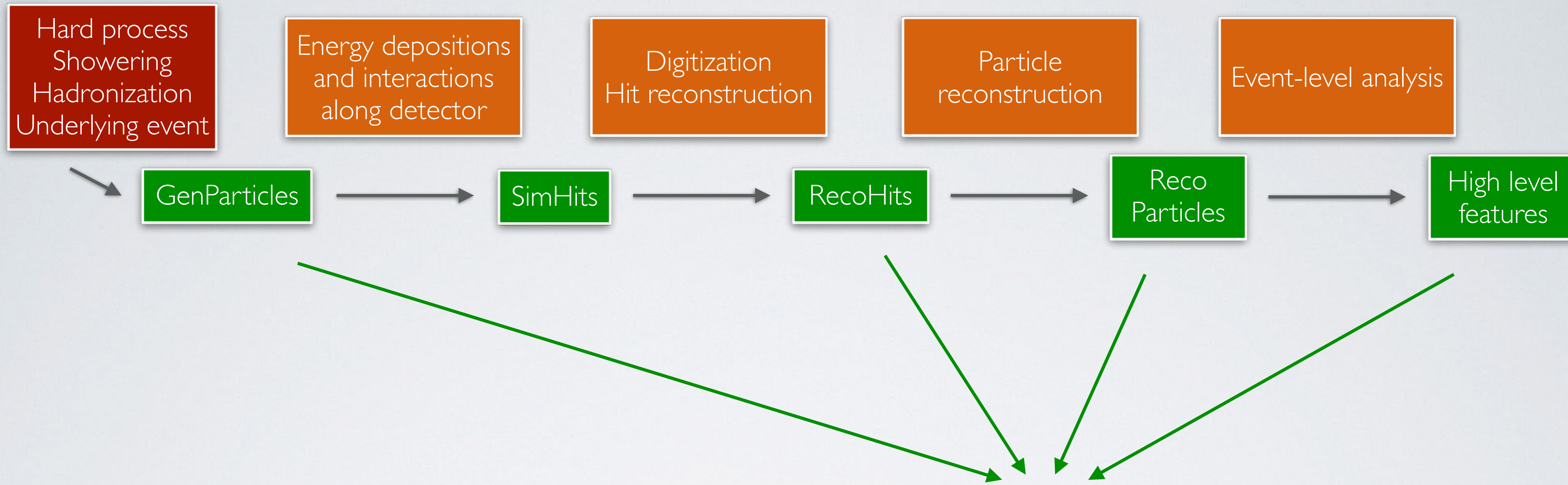

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  - $p_\theta(\mathbf{x})$ typically modelled with high-capacity DNNs

MORE ON IPMS

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$\{\mathbf{x}_{\text{real}}\}$ $\{\mathbf{x}_{\text{gen}}\}$

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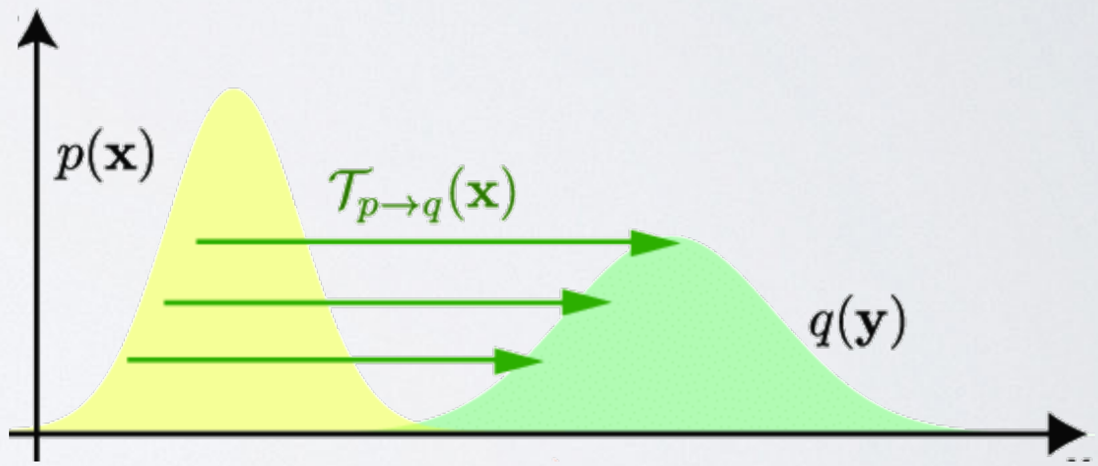

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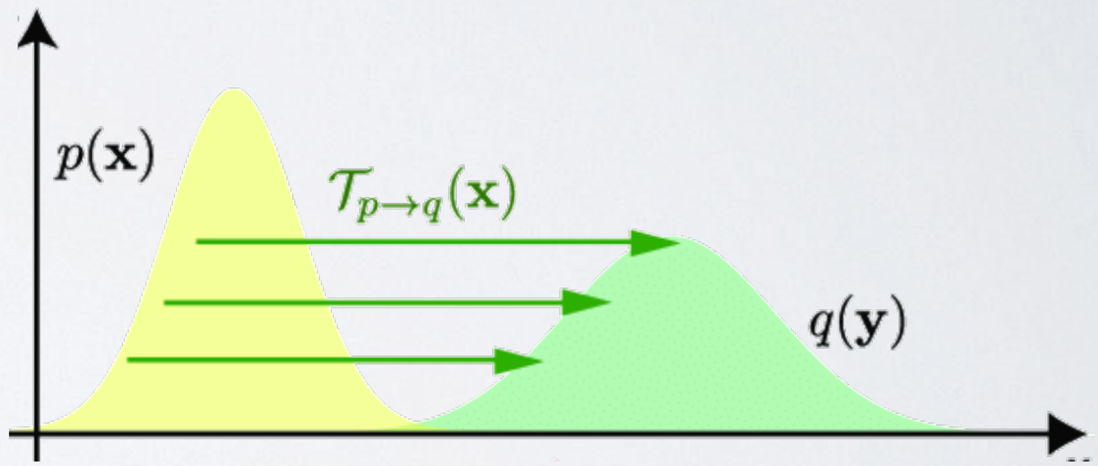

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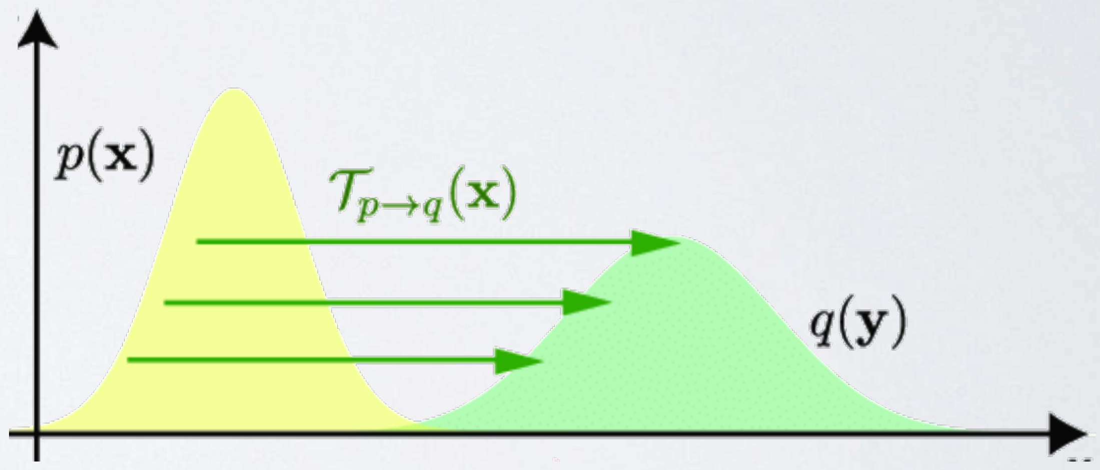

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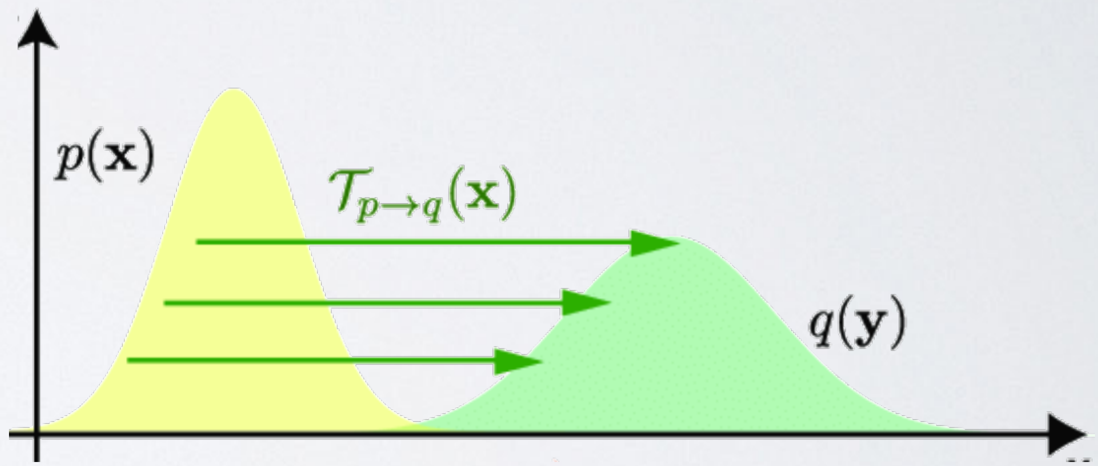

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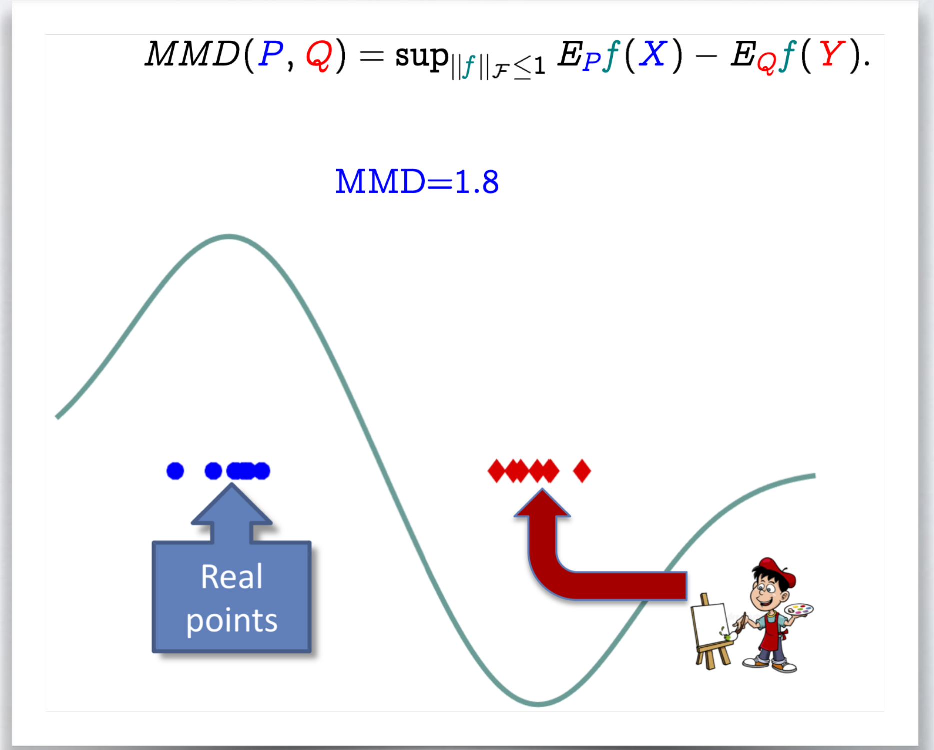
Gretton 2020



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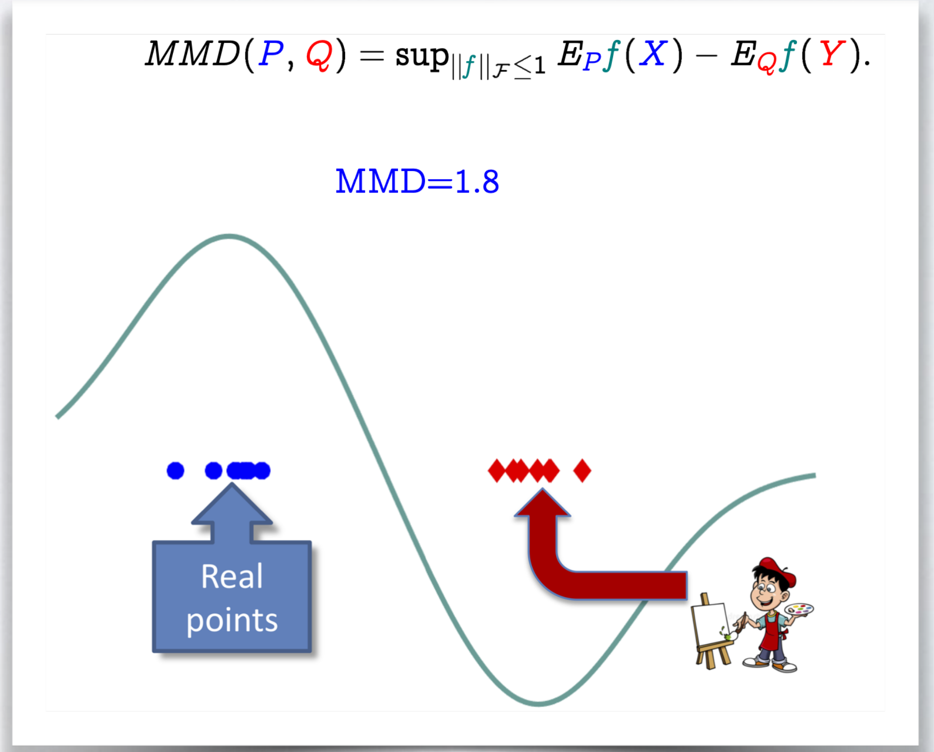

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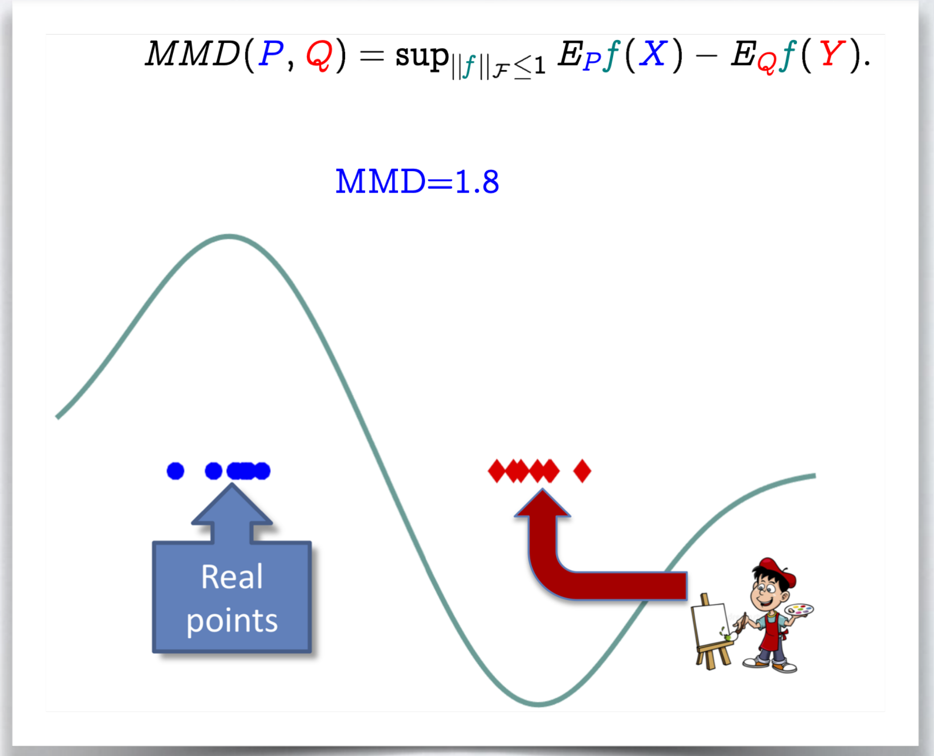

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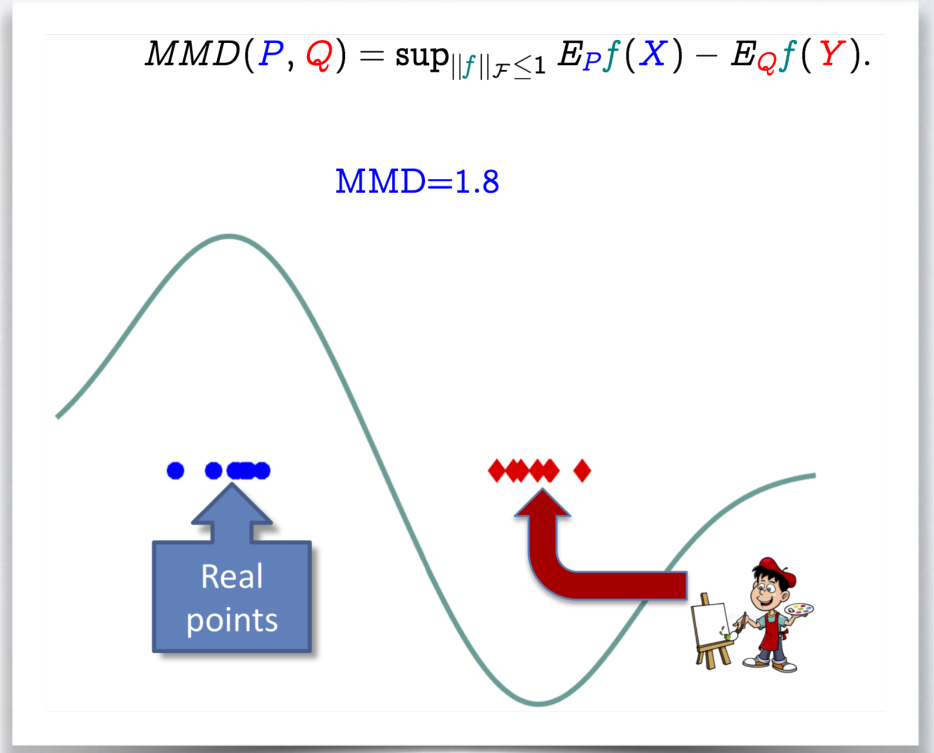

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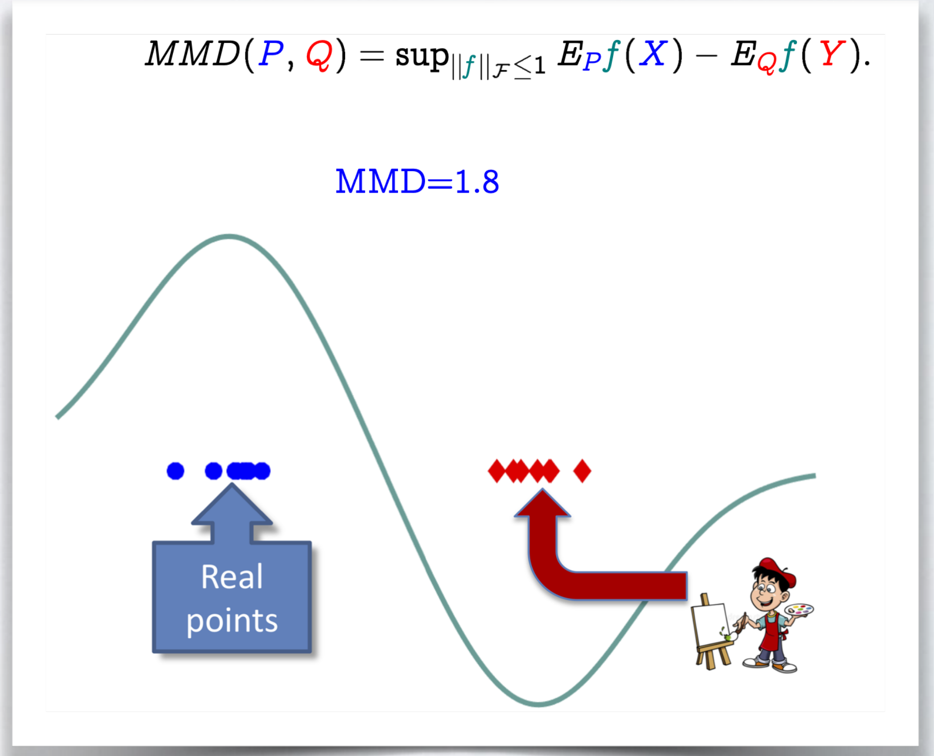

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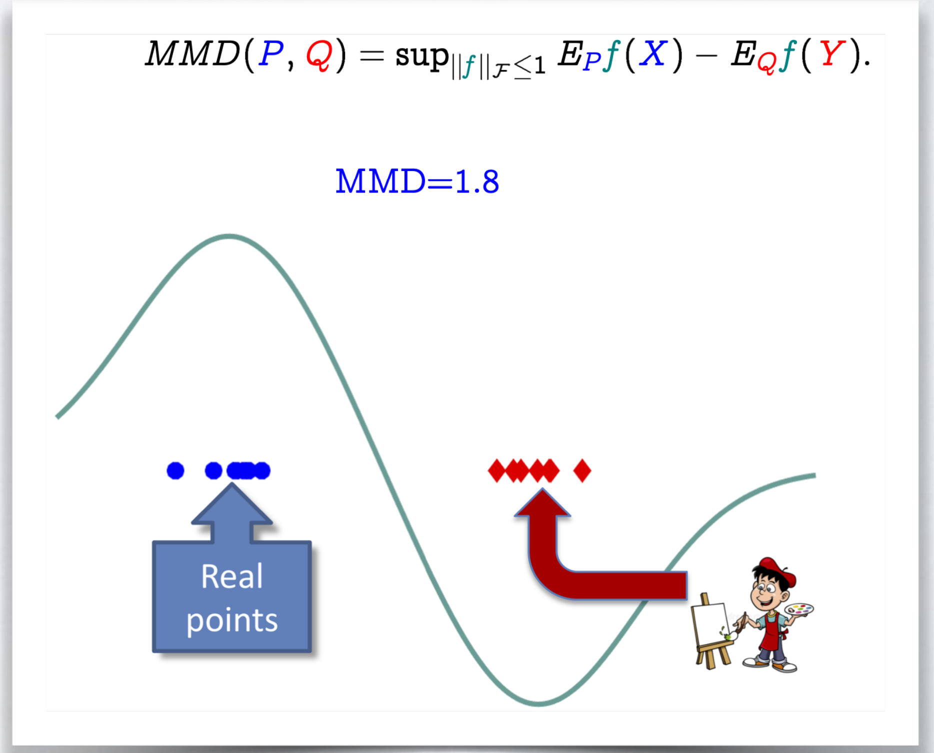

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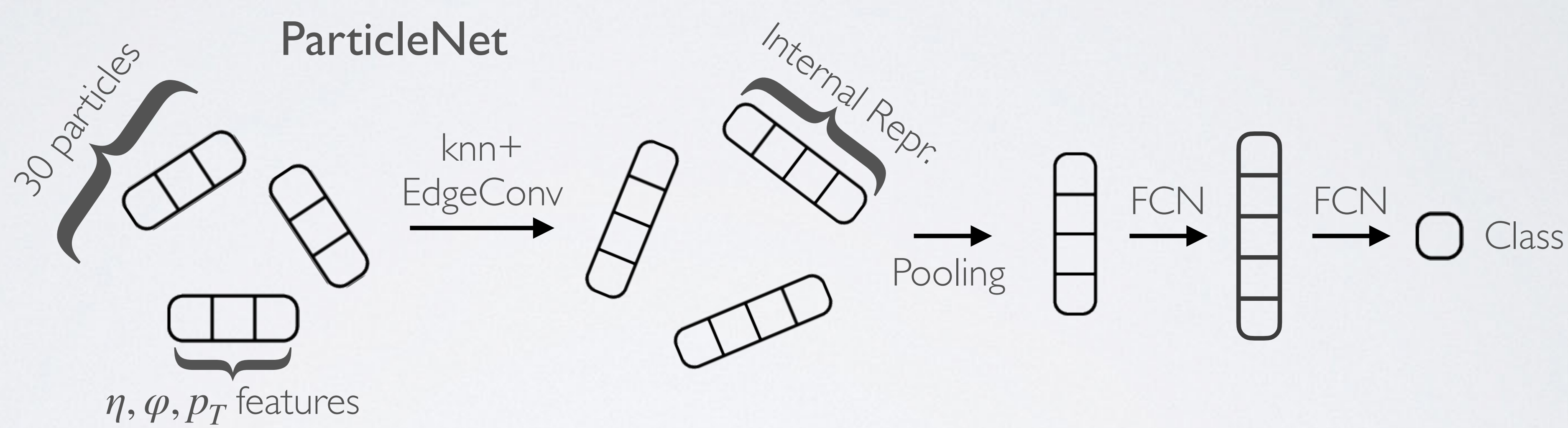

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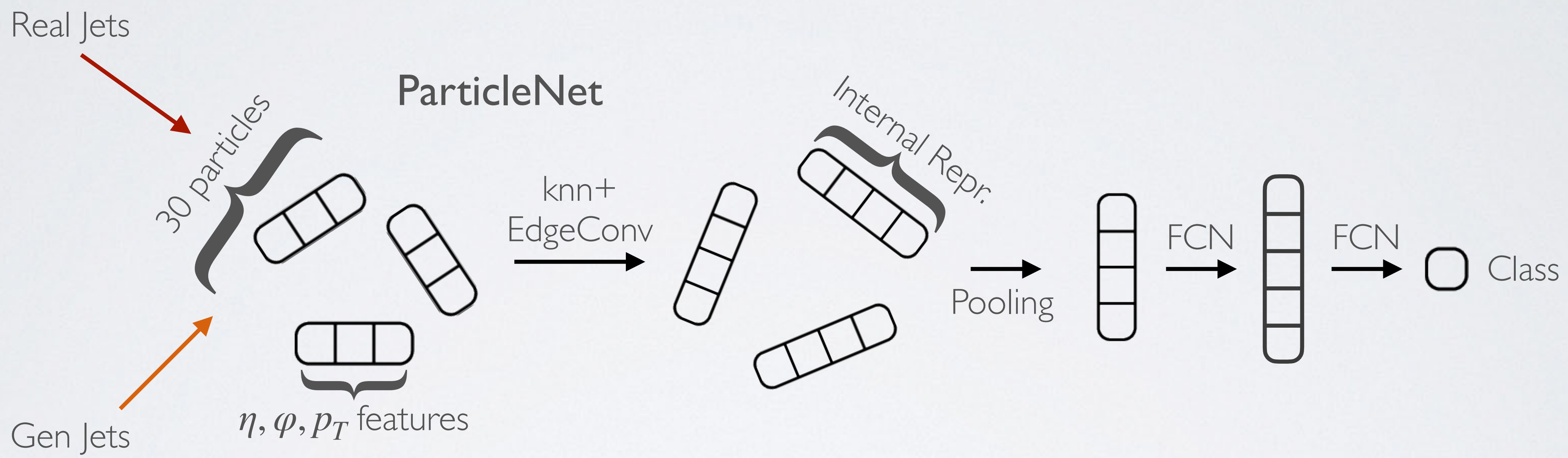

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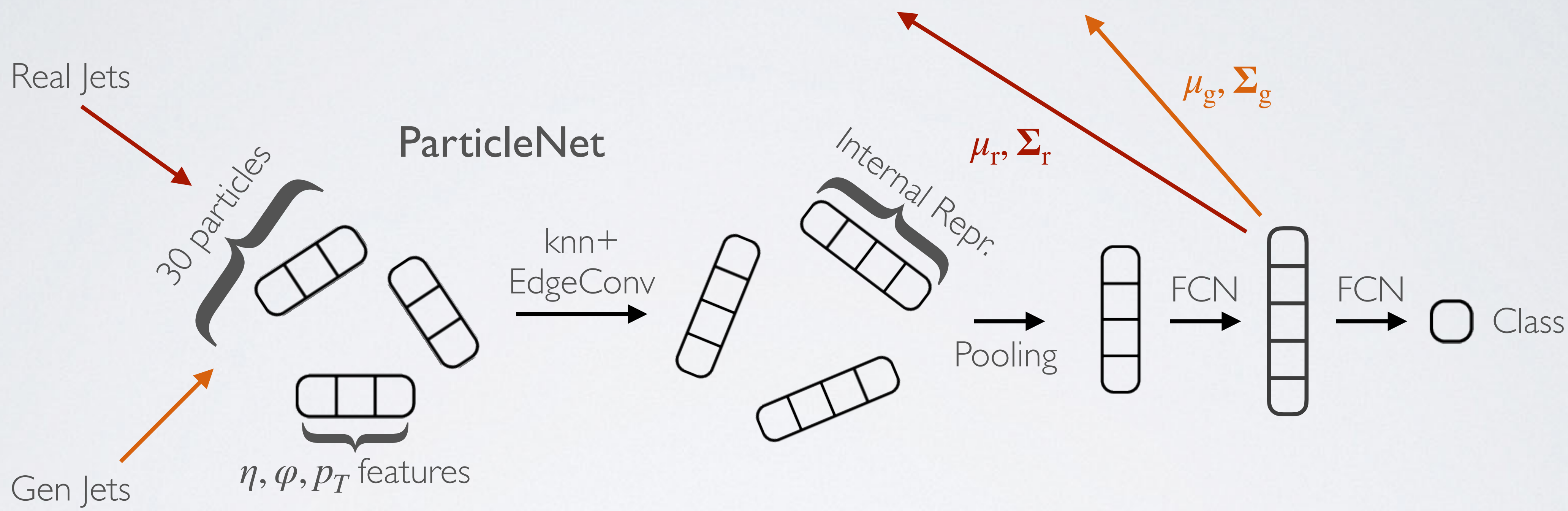

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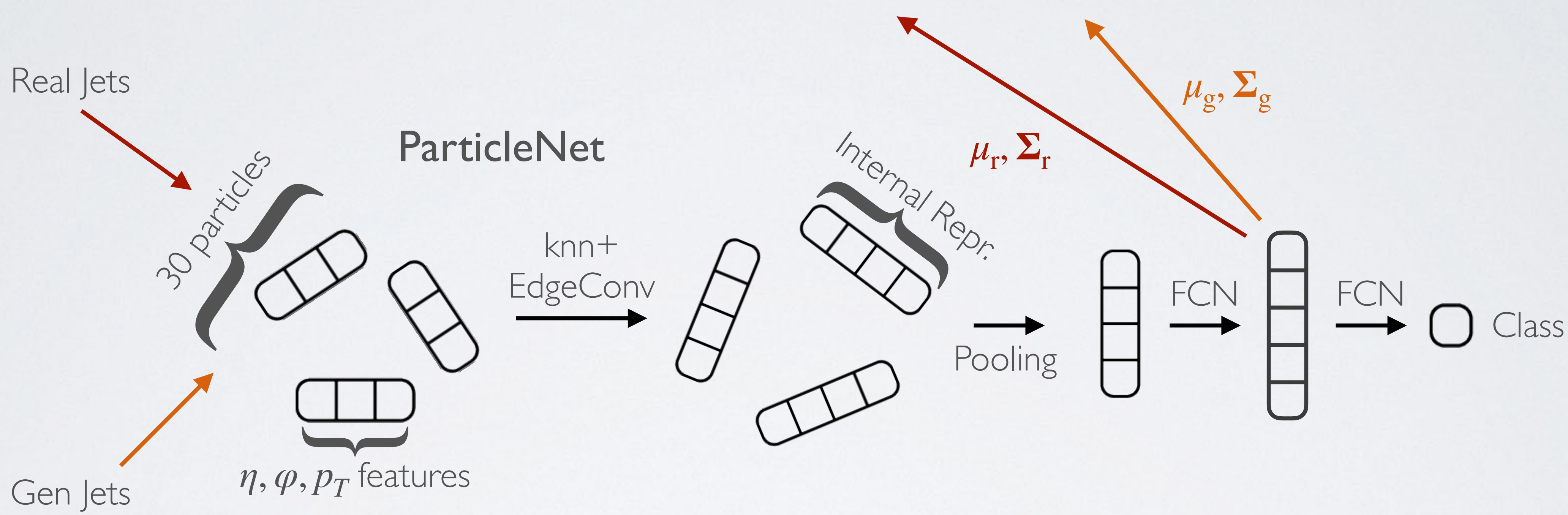

- High-performing classifier learns salient hidden features from data

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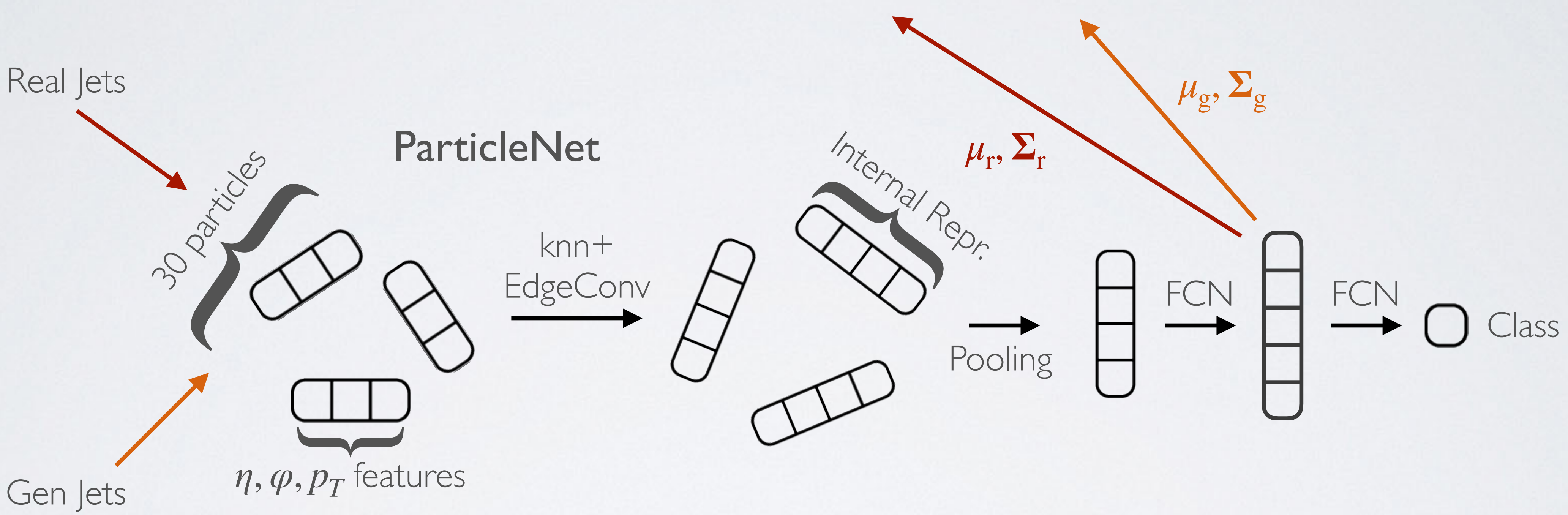

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- Retain sensitivity to **quality, diversity** from W_1, **reproducible** and **efficient** plus:

FRÉCHET <CLASSIFIER> DISTANCES

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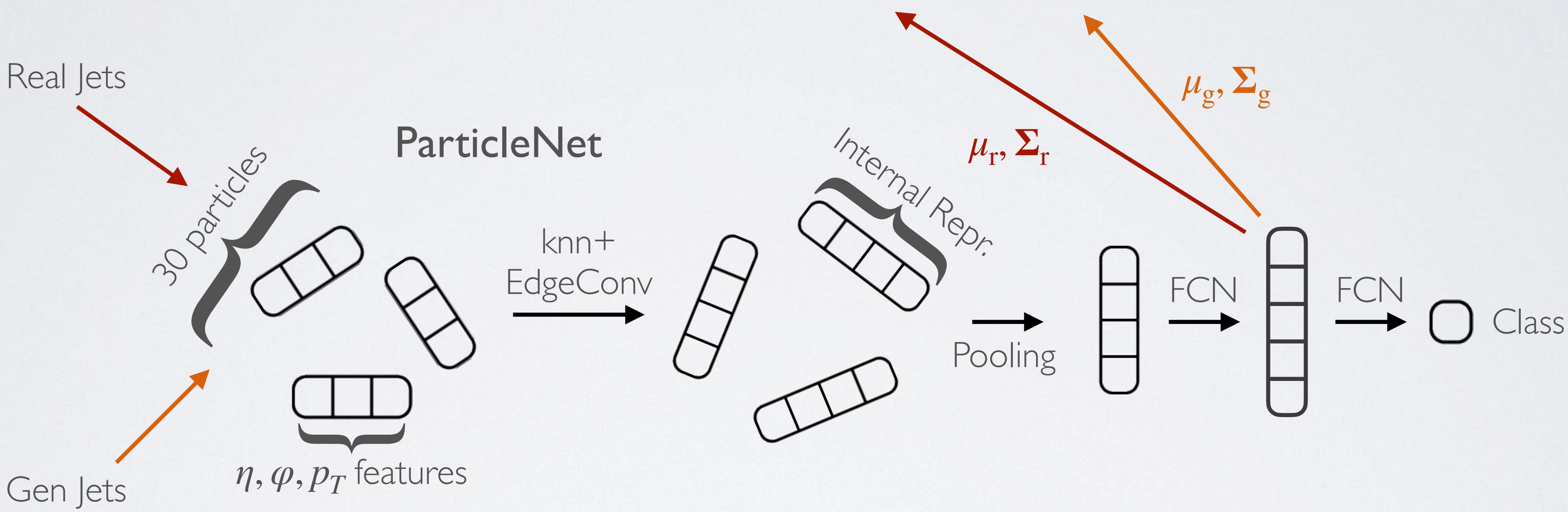
$$\mathrm{FGD} = \mathrm{Frechet}(\mathcal{N}(\mu_r, \Sigma_r), \mathcal{N}(\mu_g, \Sigma_g)) = ||\mu_r - \mu_g||^2 + \mathrm{Tr}\left[\Sigma_r + \Sigma_g - 2(\Sigma_r\Sigma_g)^{1/2}\right]$$



- High-performing classifier learns salient hidden features from data
- Retain sensitivity to **quality, diversity** from W_1, **reproducible** and **efficient** plus:
  - Single aggregate score, correlations (Σ) between features, easy to scale

MAXIMUM MEAN DISCREPANCY

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- MMD: distance between means in embedding space
- Very powerful method for calculating distance between distributions

TESTS FOR QUALITY / DIVERSITY

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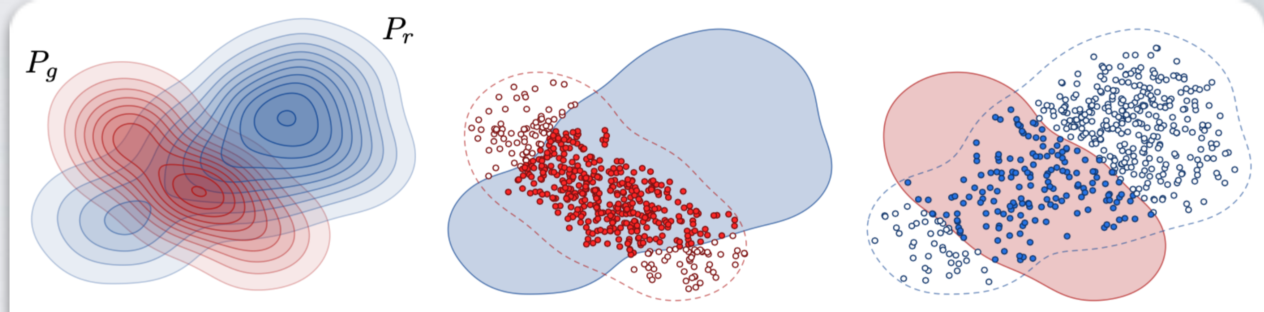

(a) Example distributions (b) Precision (c) Recall

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    - Estimate real and generated manifold using k-nearest-neighbours
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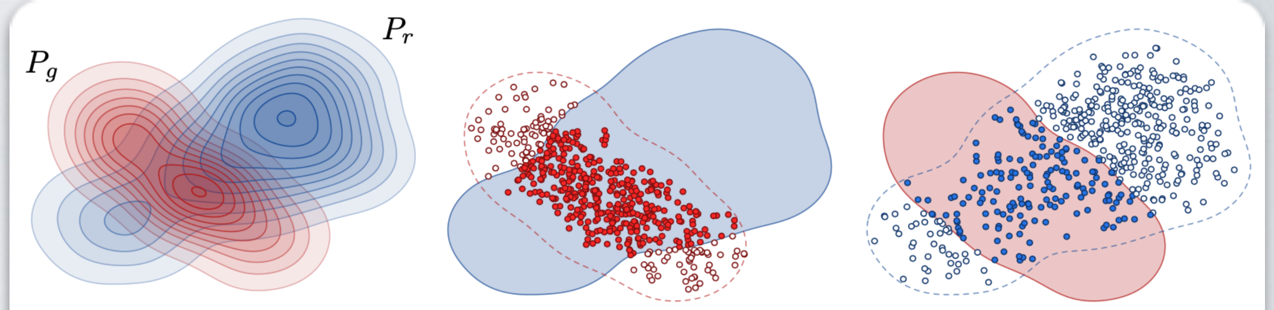

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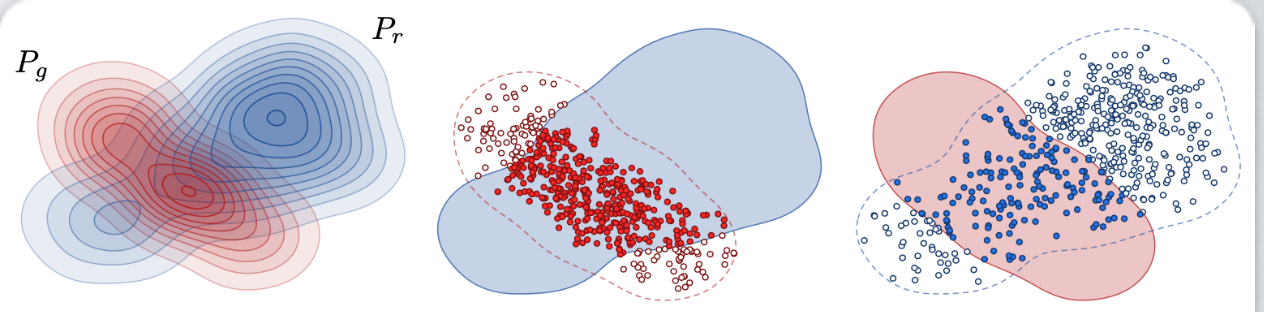

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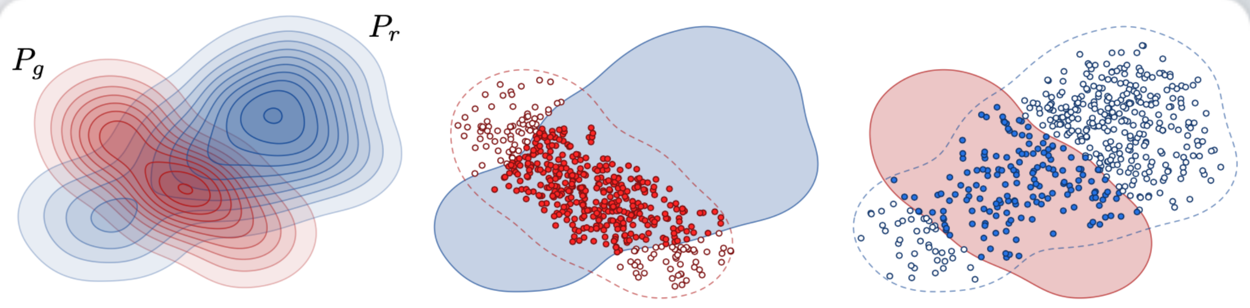

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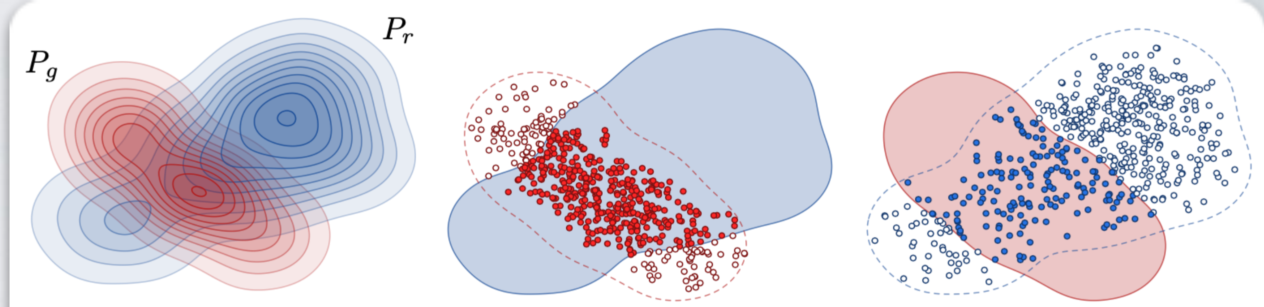

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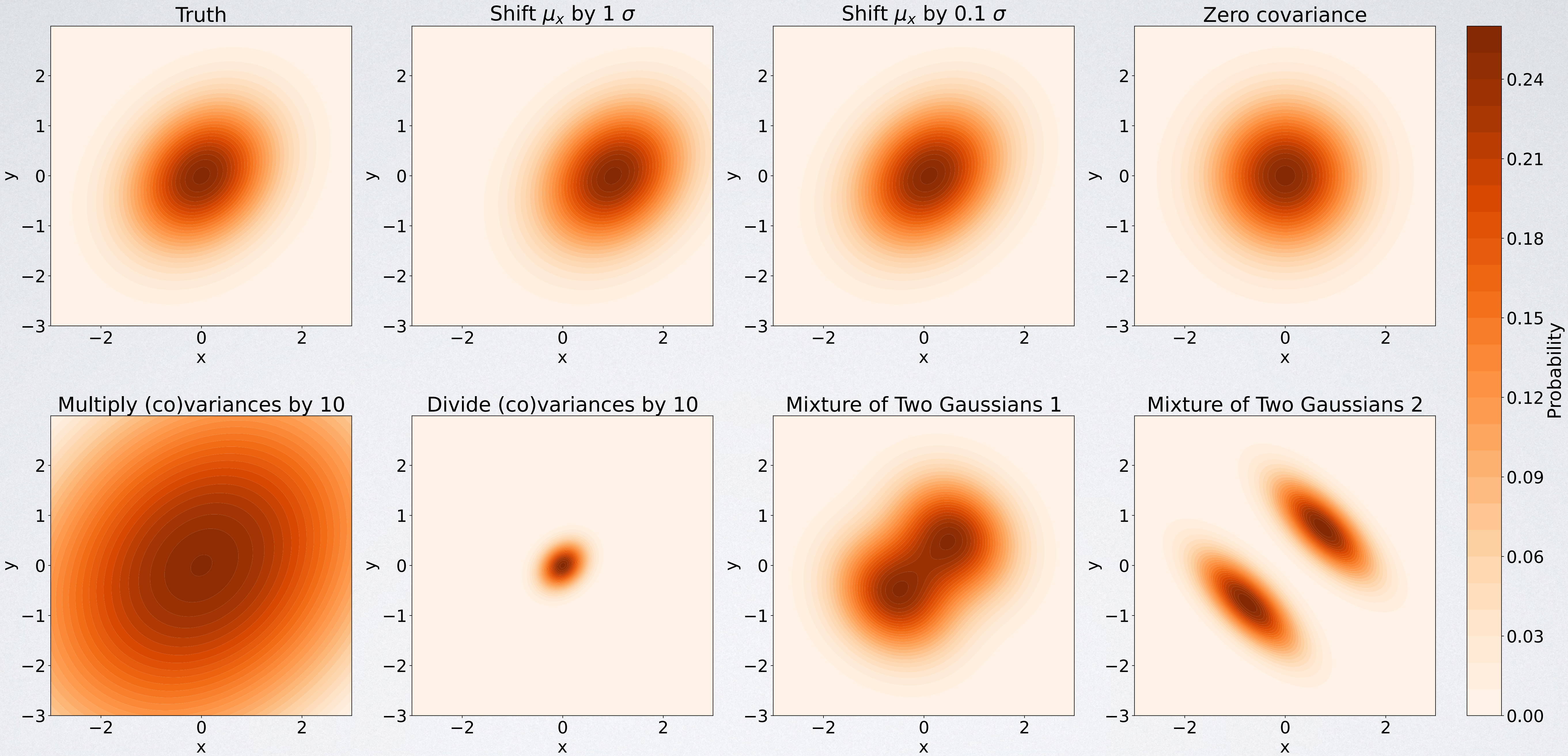
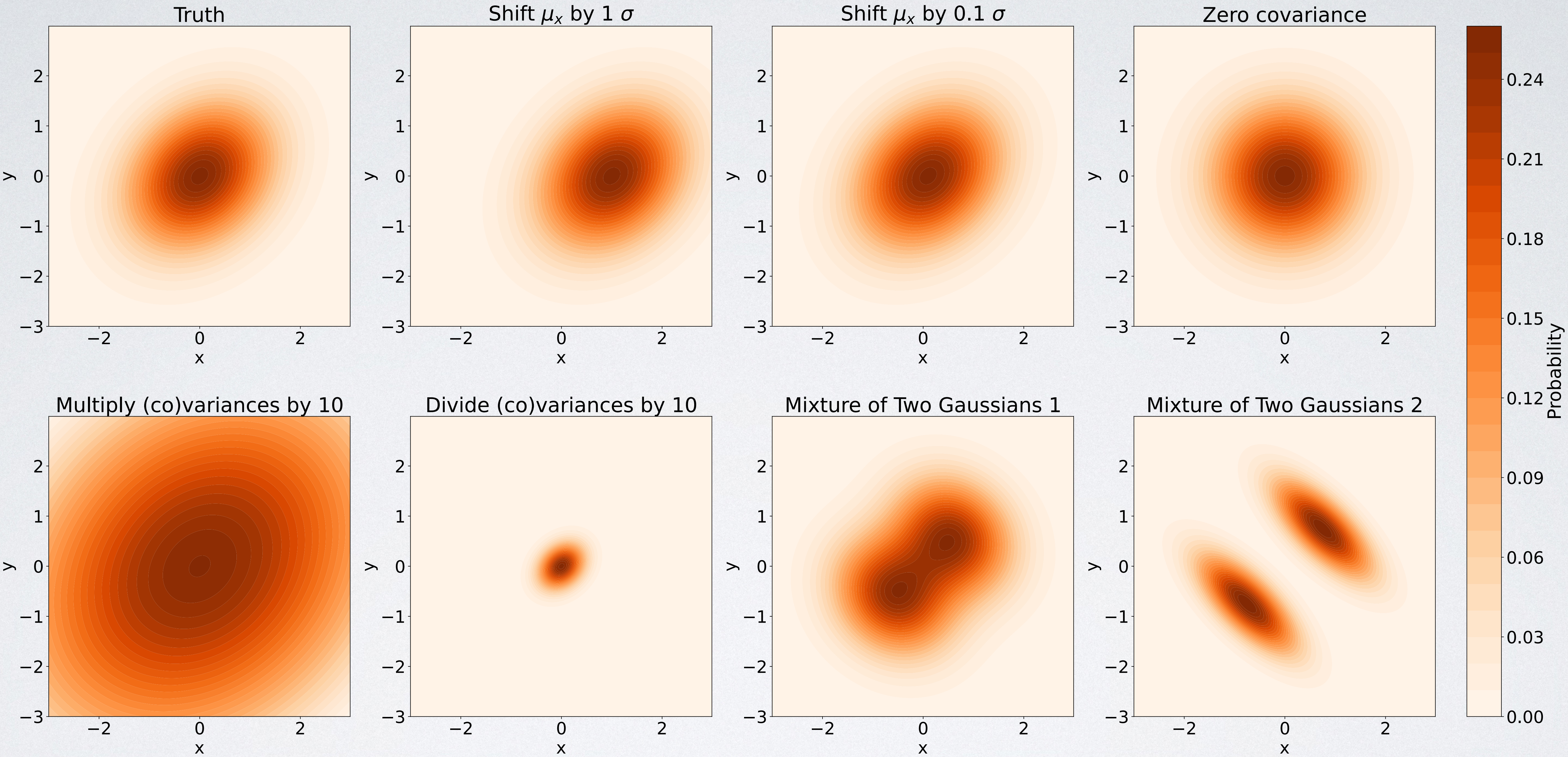
  - Like P&R, but takes into account density of real manifold

TOY DISTRIBUTIONS



TOY DISTRIBUTIONS

- We first test on toy Gaussian distributions



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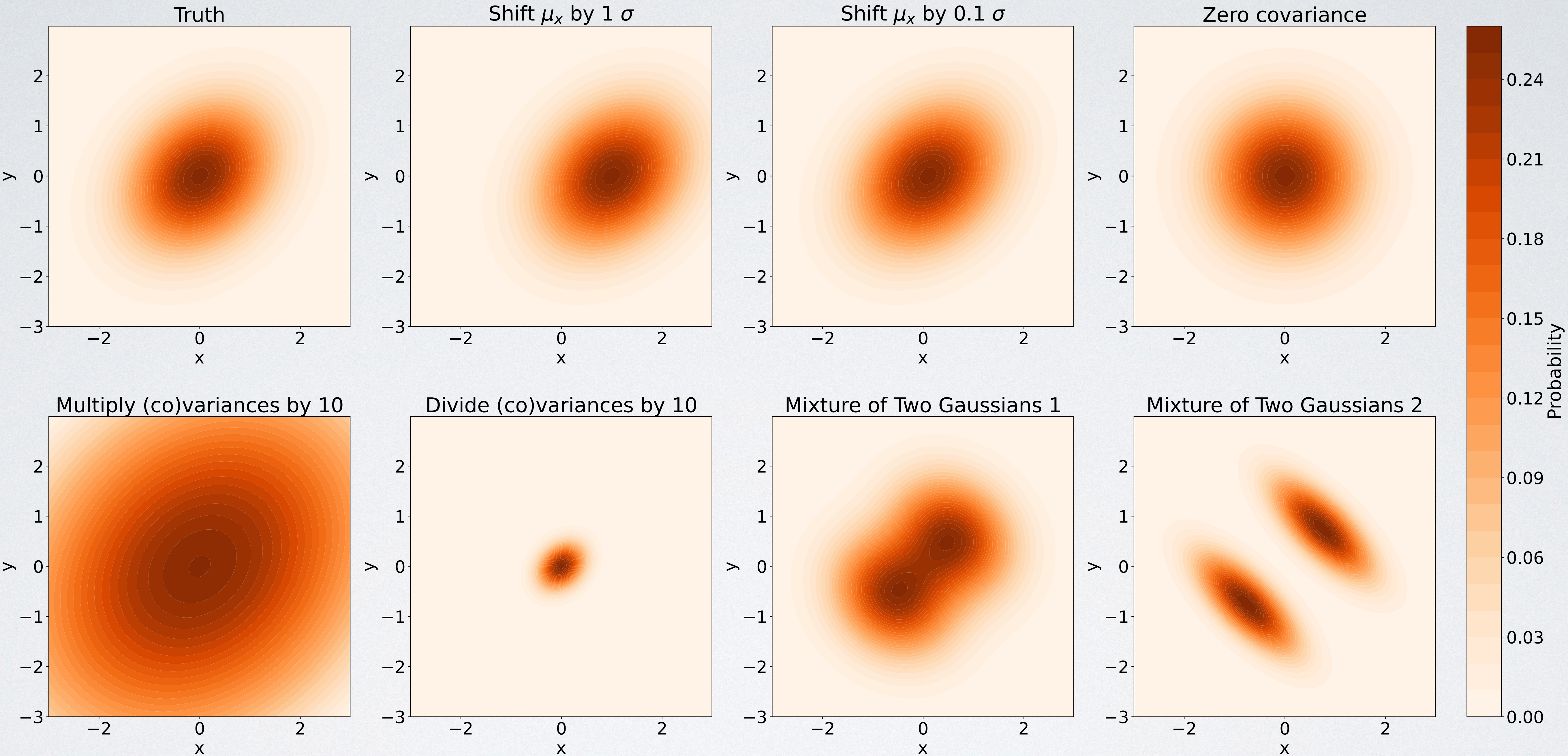

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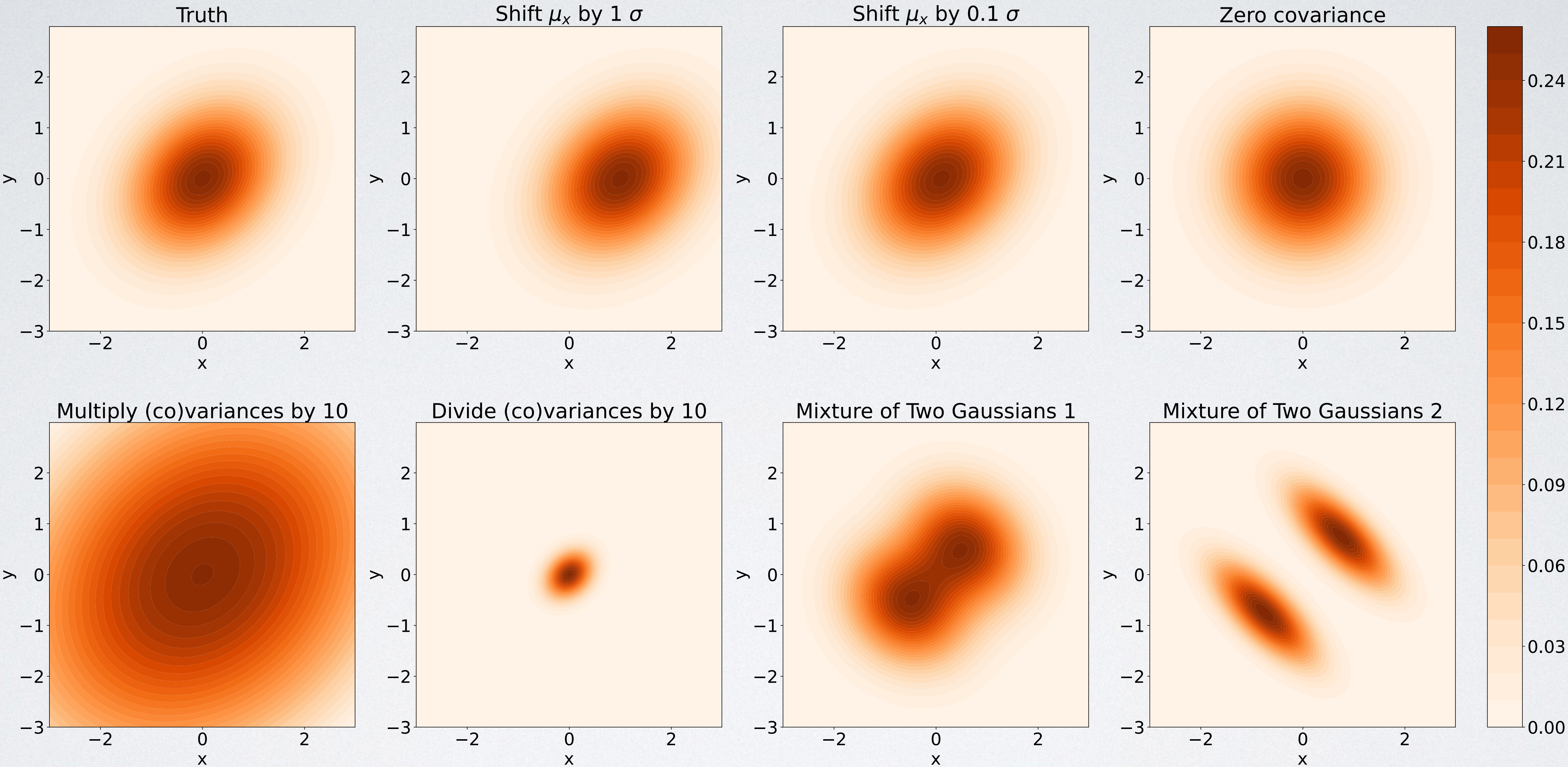

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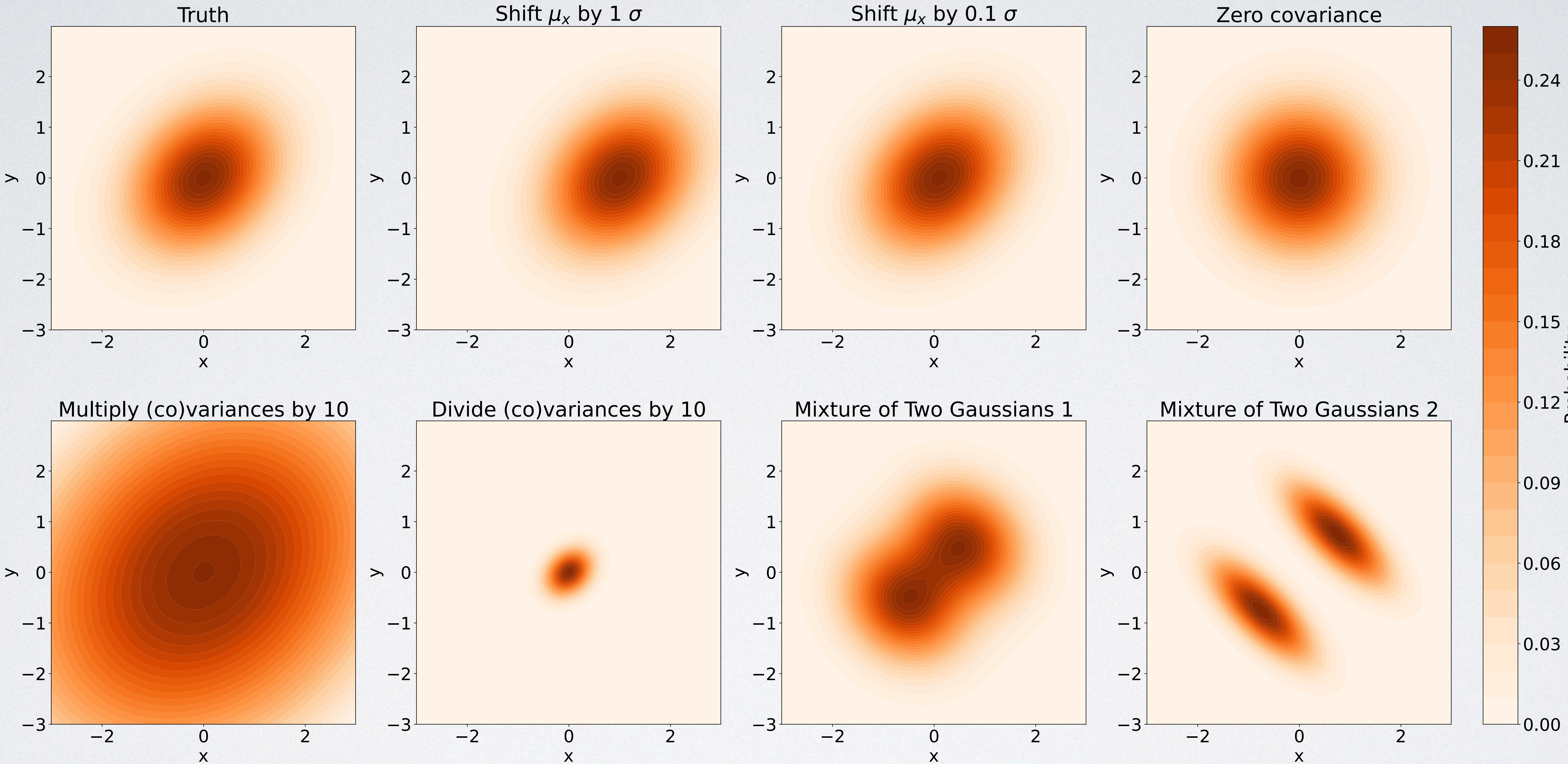

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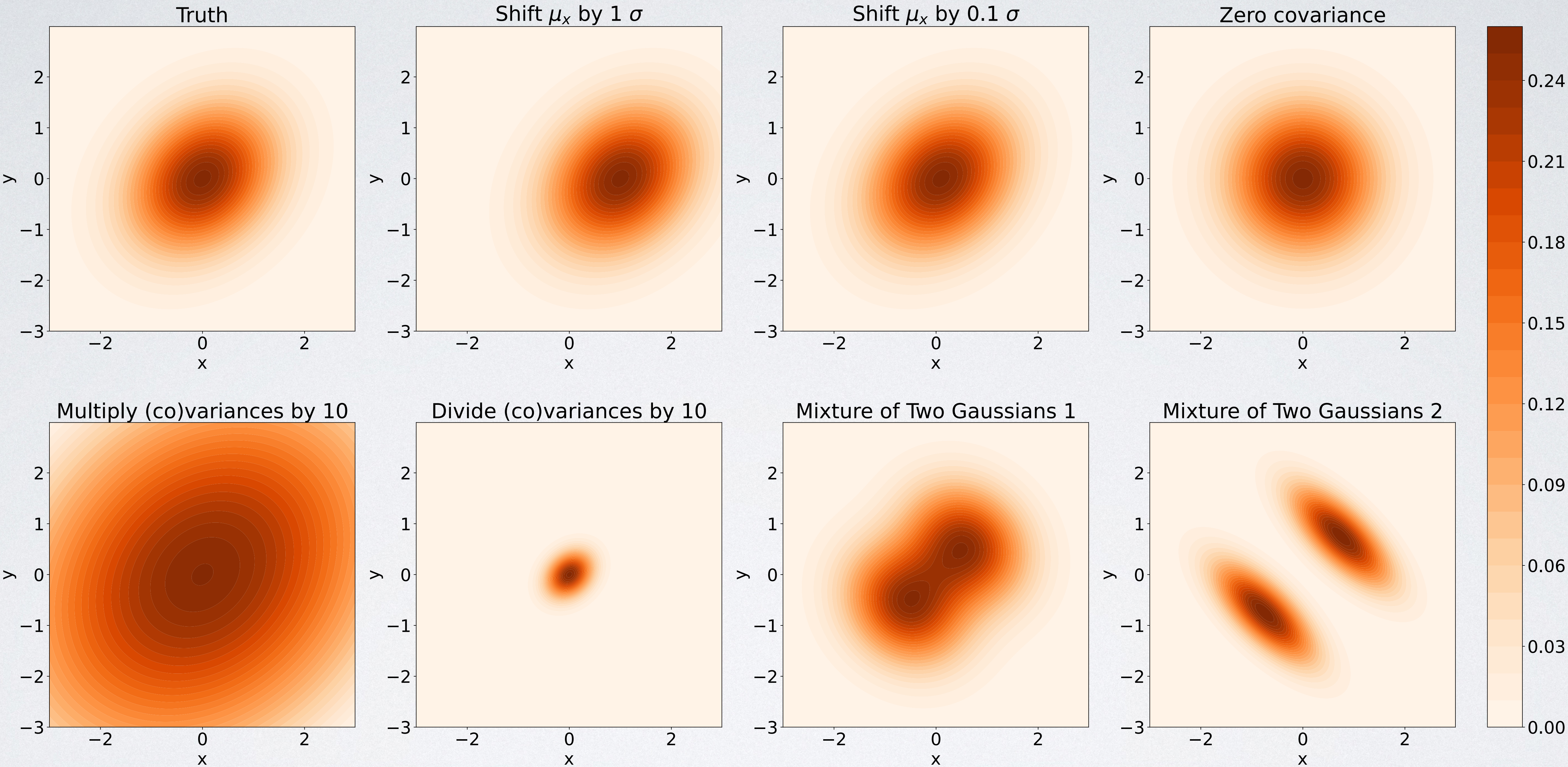

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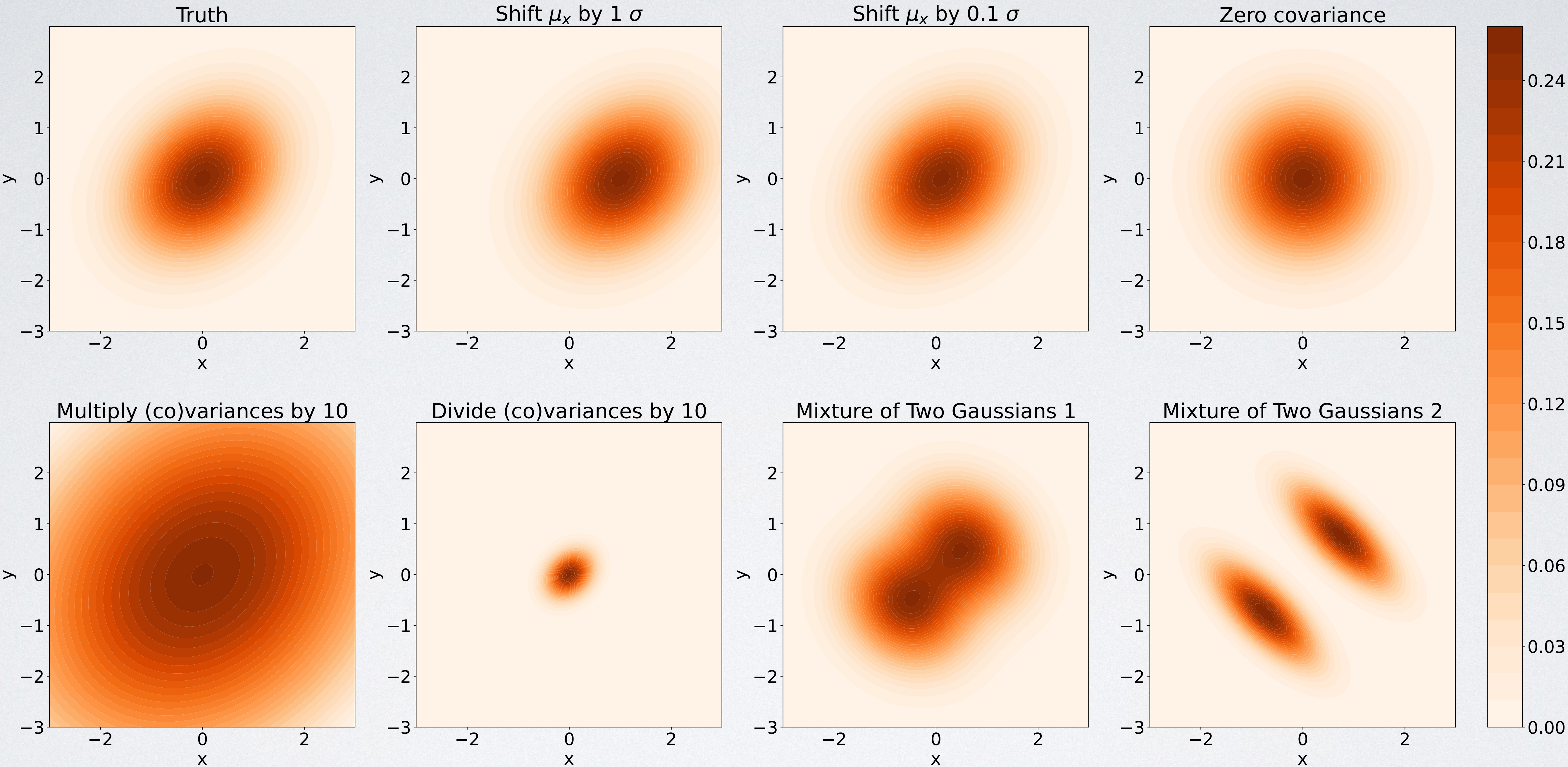

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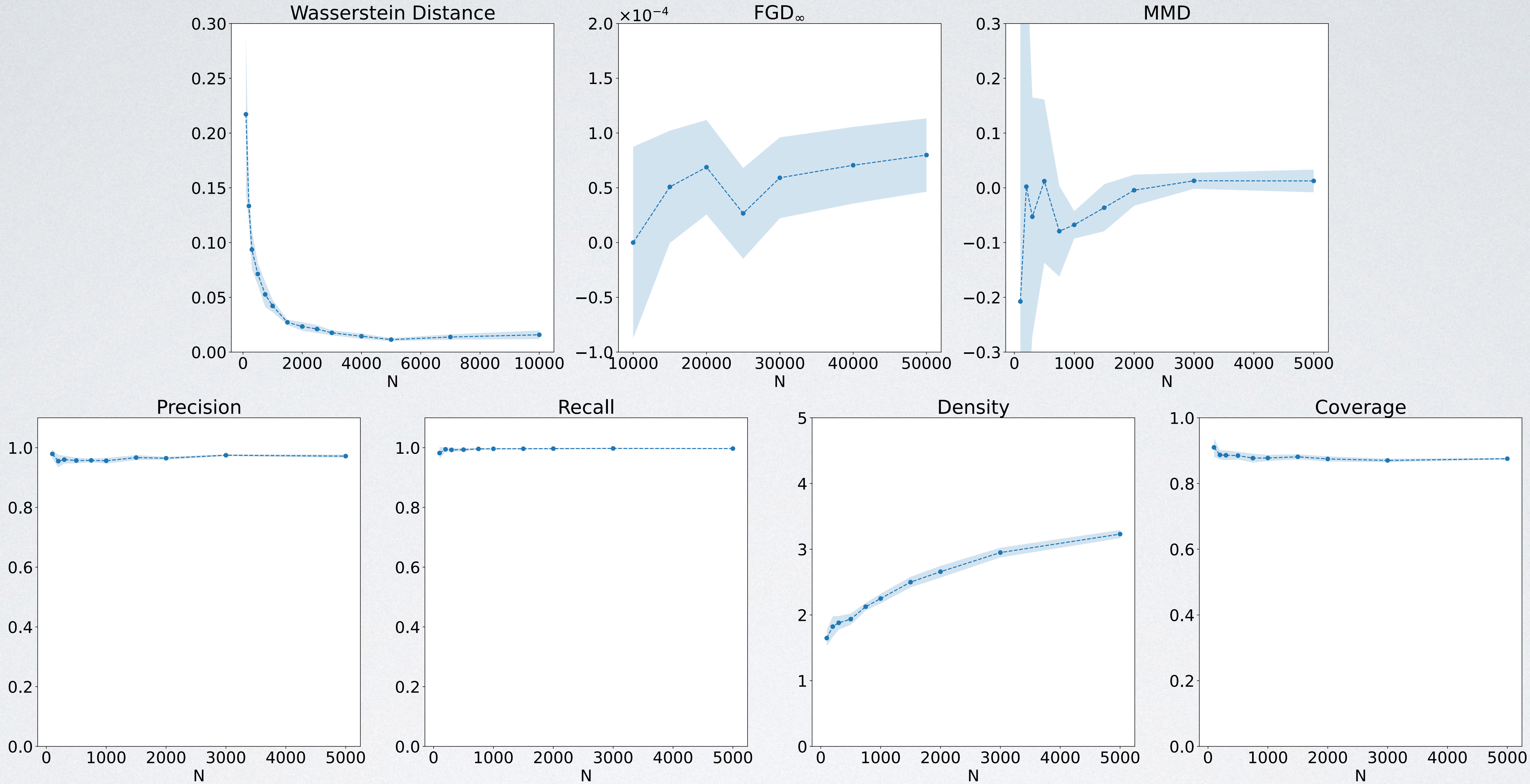
Same statistics, but easier to distinguish (by eye)

TRUTH SCORES

Scores vs sample size comparing samples of the true distribution



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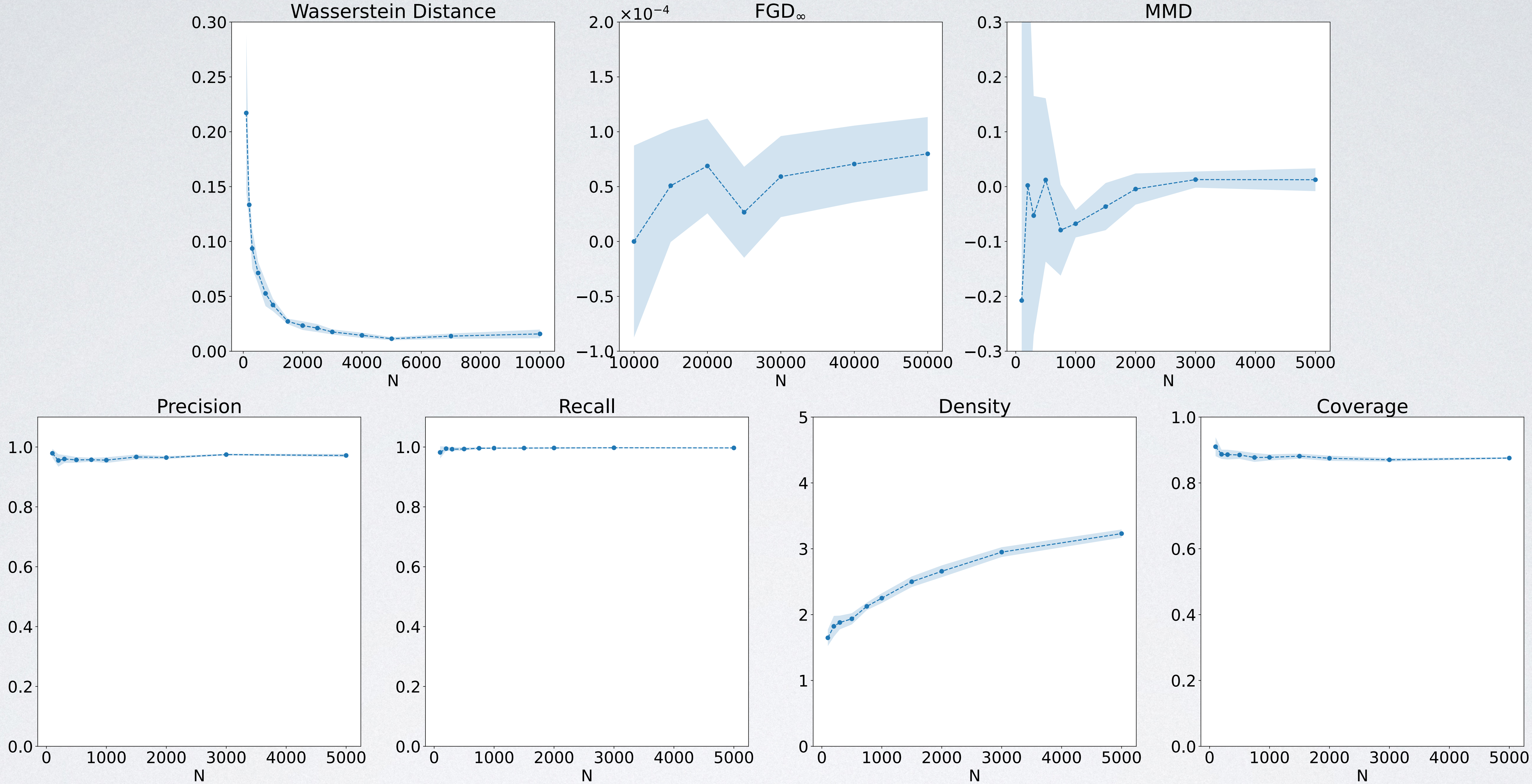

- FGD_∞ and MMD are effectively unbiased
- Wasserstein, density, and coverage very slow to converge

TRUTH SCORES

Most sensitive metric per distribution in bold

Metric	Truth	Shift μ_x by 1σ	Shift μ_x by 0.1σ	Zero covariance	Multiply (co)variances by 10	Divide (co)variances by 10	Mixture of Two Gaussians 1	Mixture of Two Gaussians 2
Wasserstein	0.016 ± 0.004	1.14 ± 0.02	0.043 ± 0.008	0.077 ± 0.006	9.8 ± 0.1	0.97 ± 0.01	$\mathbf{0.036 \pm 0.003}$	$\mathbf{0.191 \pm 0.005}$
FGD_∞ $\times 10^3$	0.08 ± 0.03	$\mathbf{1011 \pm 1}$	$\mathbf{11.0 \pm 0.1}$	$\mathbf{32.3 \pm 0.2}$	9400 ± 8	$\mathbf{935.1 \pm 0.7}$	0.07 ± 0.03	0.03 ± 0.03
MMD	0.01 ± 0.02	16.4 ± 0.9	0.07 ± 0.04	0.40 ± 0.08	$\mathbf{19k \pm 1k}$	4.3 ± 0.1	0.06 ± 0.02	0.35 ± 0.03
Precision	0.972 ± 0.005	0.91 ± 0.01	0.976 ± 0.004	0.969 ± 0.006	0.34 ± 0.01	1.0 ± 0.0	0.975 ± 0.003	0.9976 ± 0.0007
Recall	0.997 ± 0.001	0.992 ± 0.003	0.997 ± 0.001	0.9976 ± 0.0006	0.998 ± 0.001	0.58 ± 0.02	0.996 ± 0.001	0.9970 ± 0.0009
Density	3.23 ± 0.06	2.48 ± 0.08	3.19 ± 0.07	3.1 ± 0.1	0.60 ± 0.02	5.7 ± 0.3	2.99 ± 0.09	0.989 ± 0.009
Coverage	0.876 ± 0.002	0.780 ± 0.006	0.872 ± 0.005	0.872 ± 0.004	0.60 ± 0.01	0.406 ± 0.008	0.871 ± 0.002	0.956 ± 0.006

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- Wasserstein, $\mathbf{FGD}_\infty$, MMD find all alternatives discrepant, except $\mathbf{FGD}_\infty$ on mixtures
- $\mathbf{FGD}_\infty$ generally the most sensitive otherwise, but misses shape distortions
- Precision and recall do their job, density and coverage give unintuitive results

EFP SCORES VS SAMPLE SIZE

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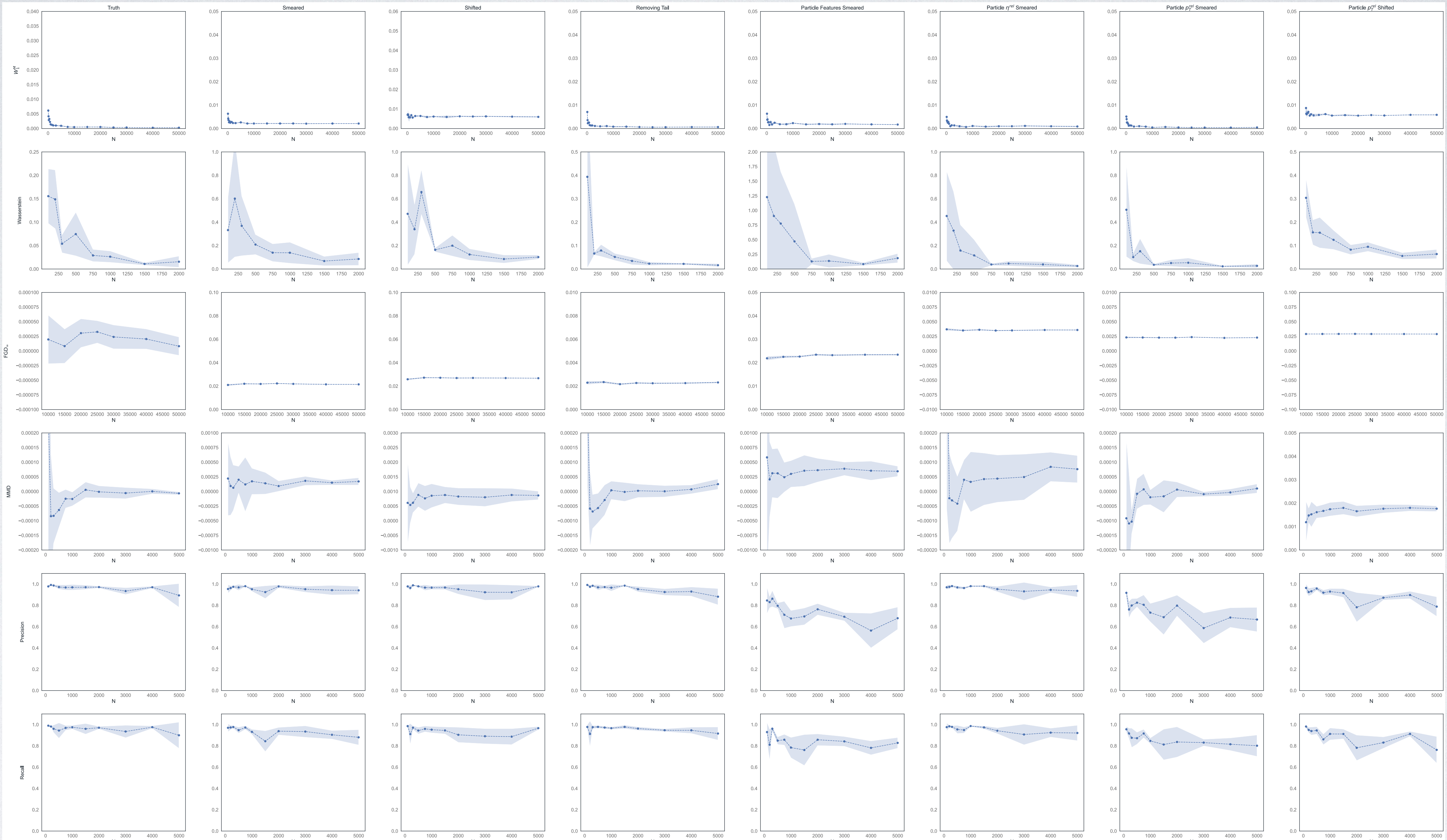

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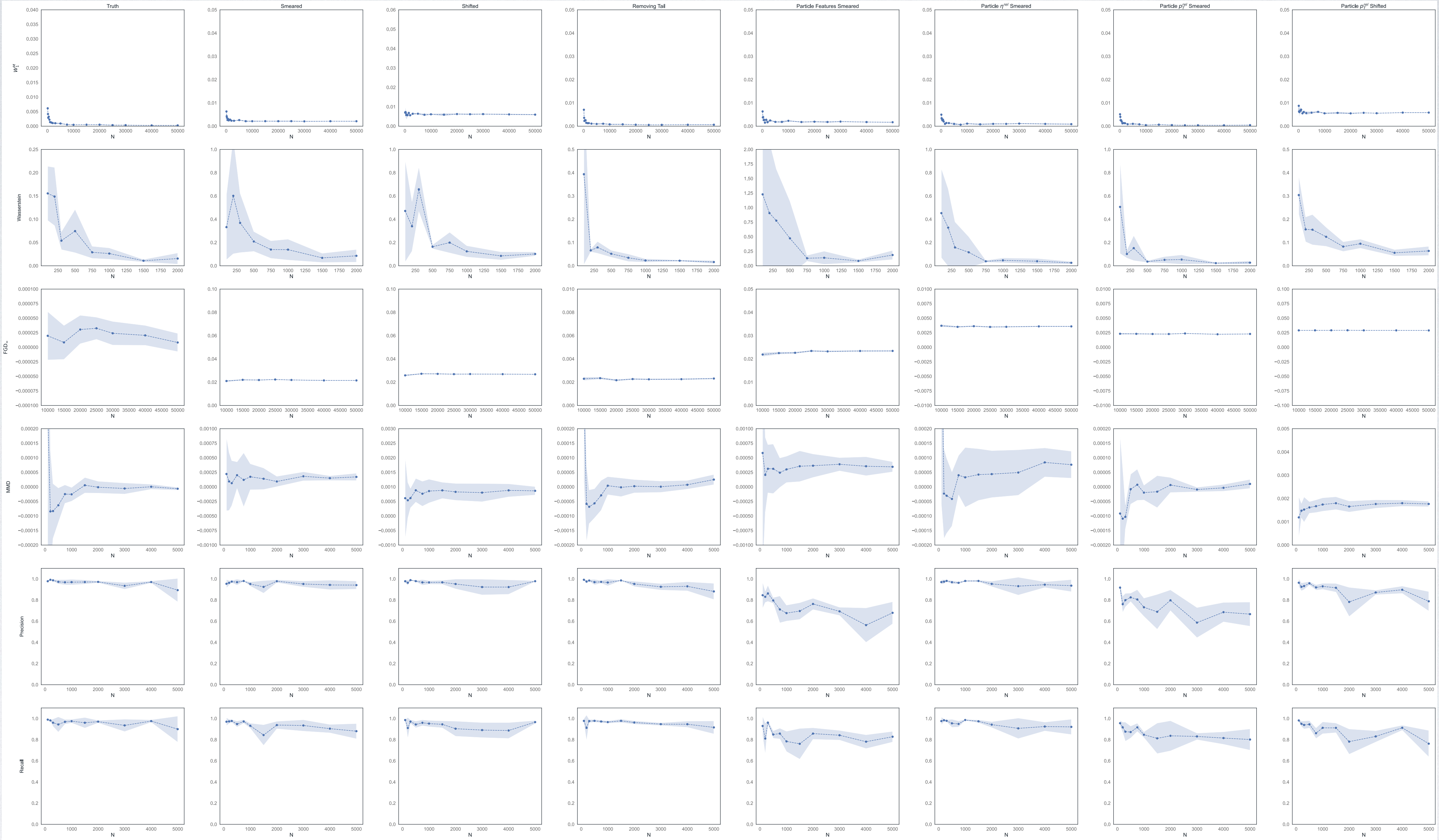

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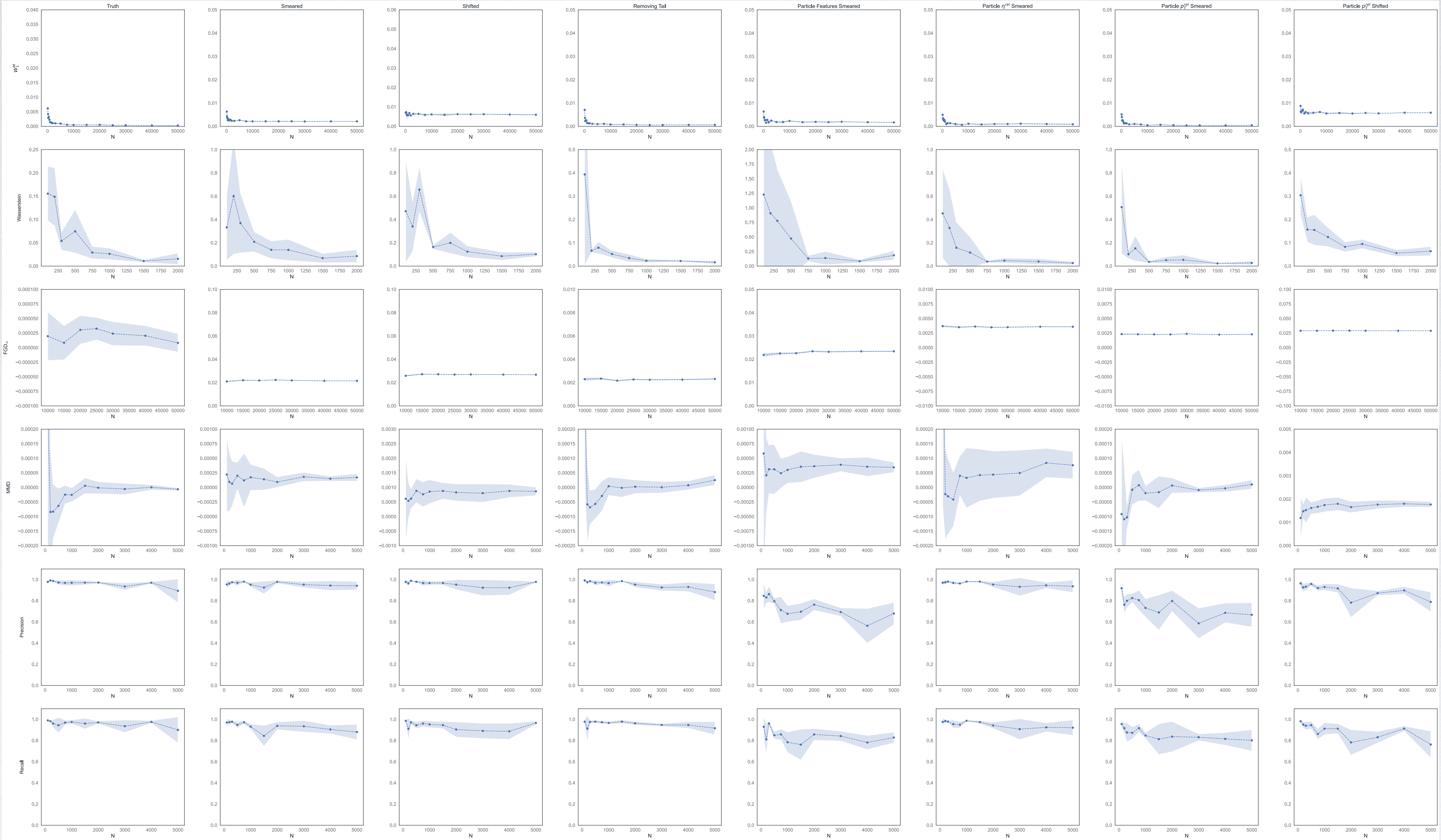

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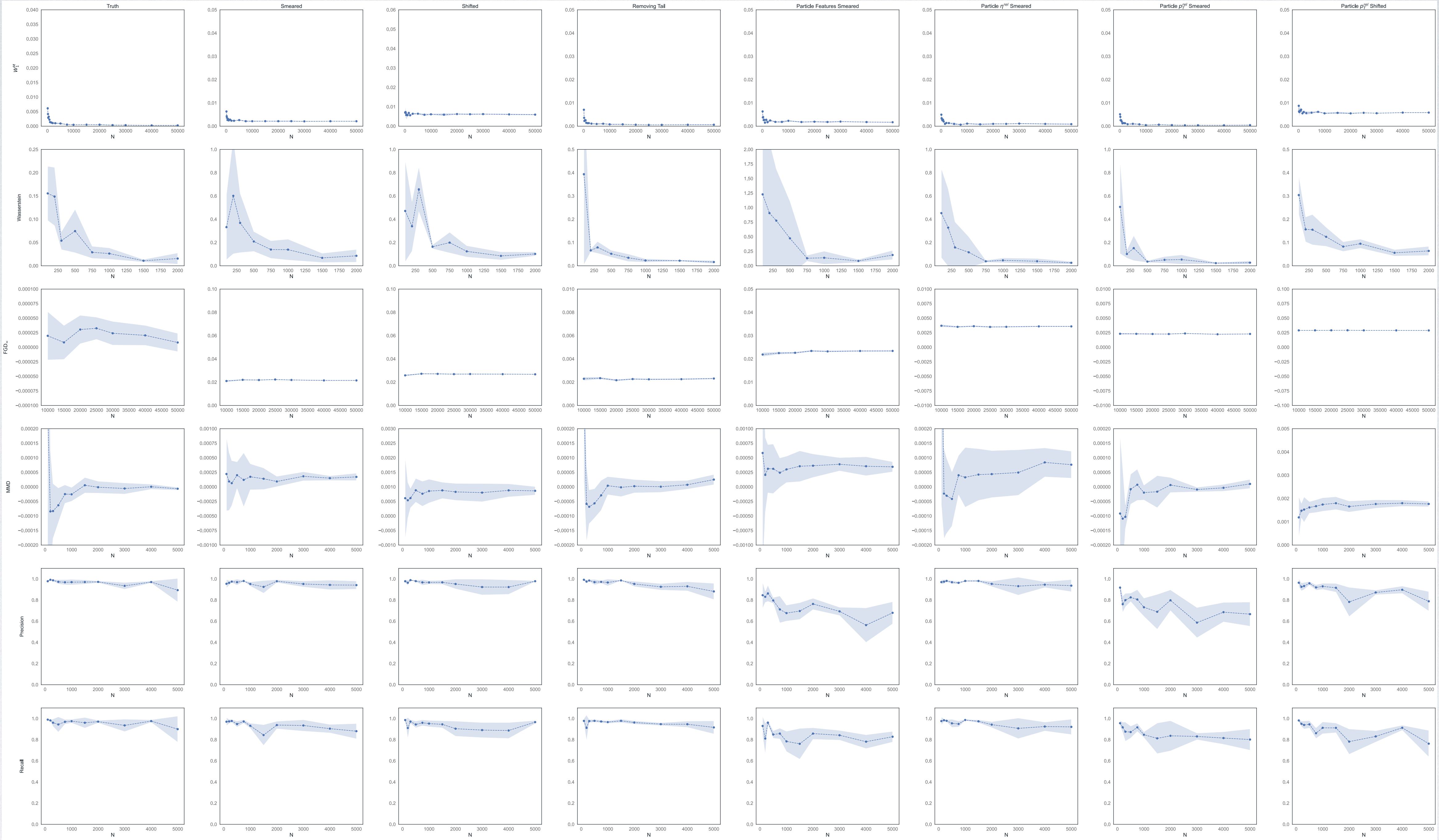

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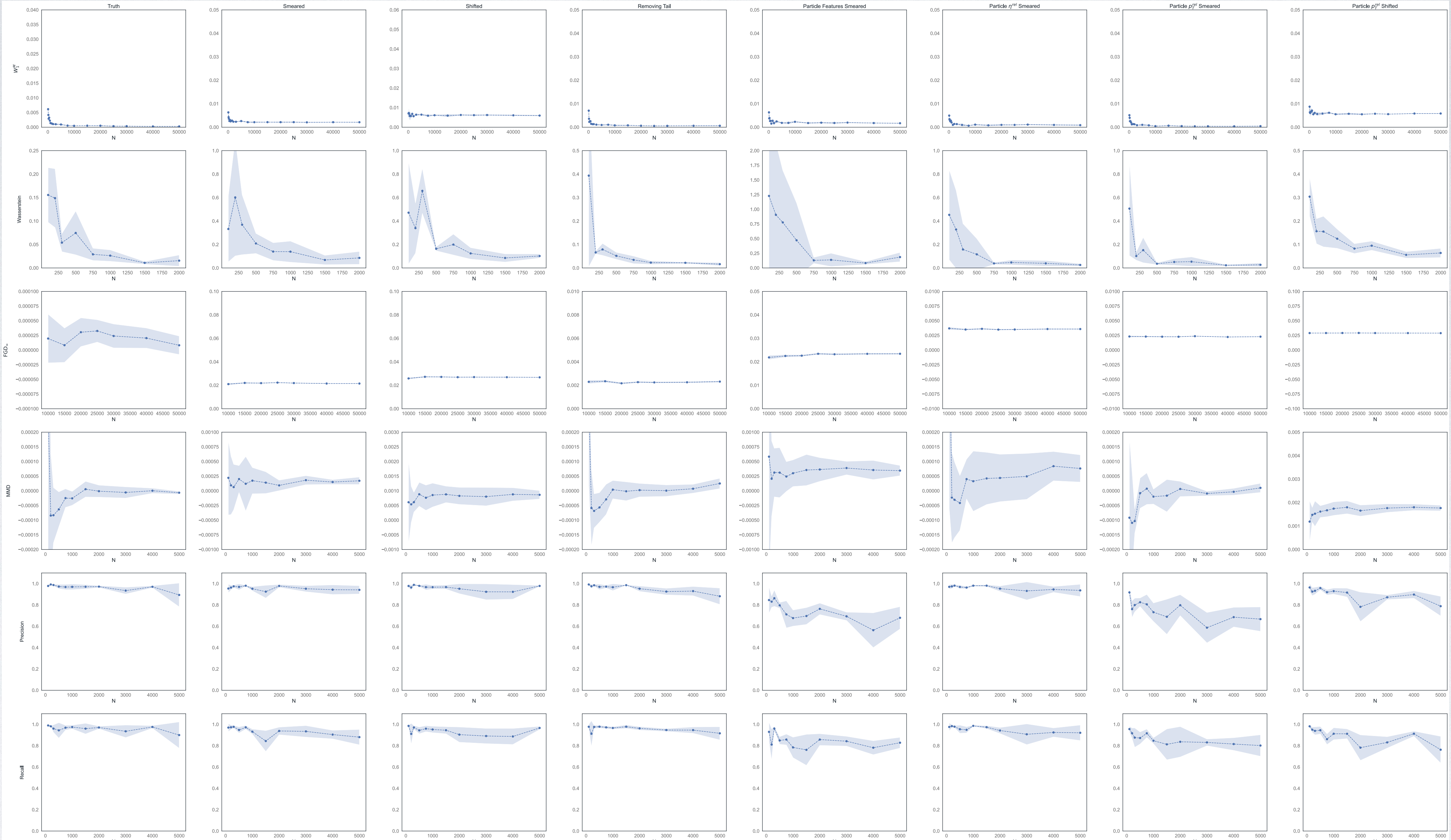

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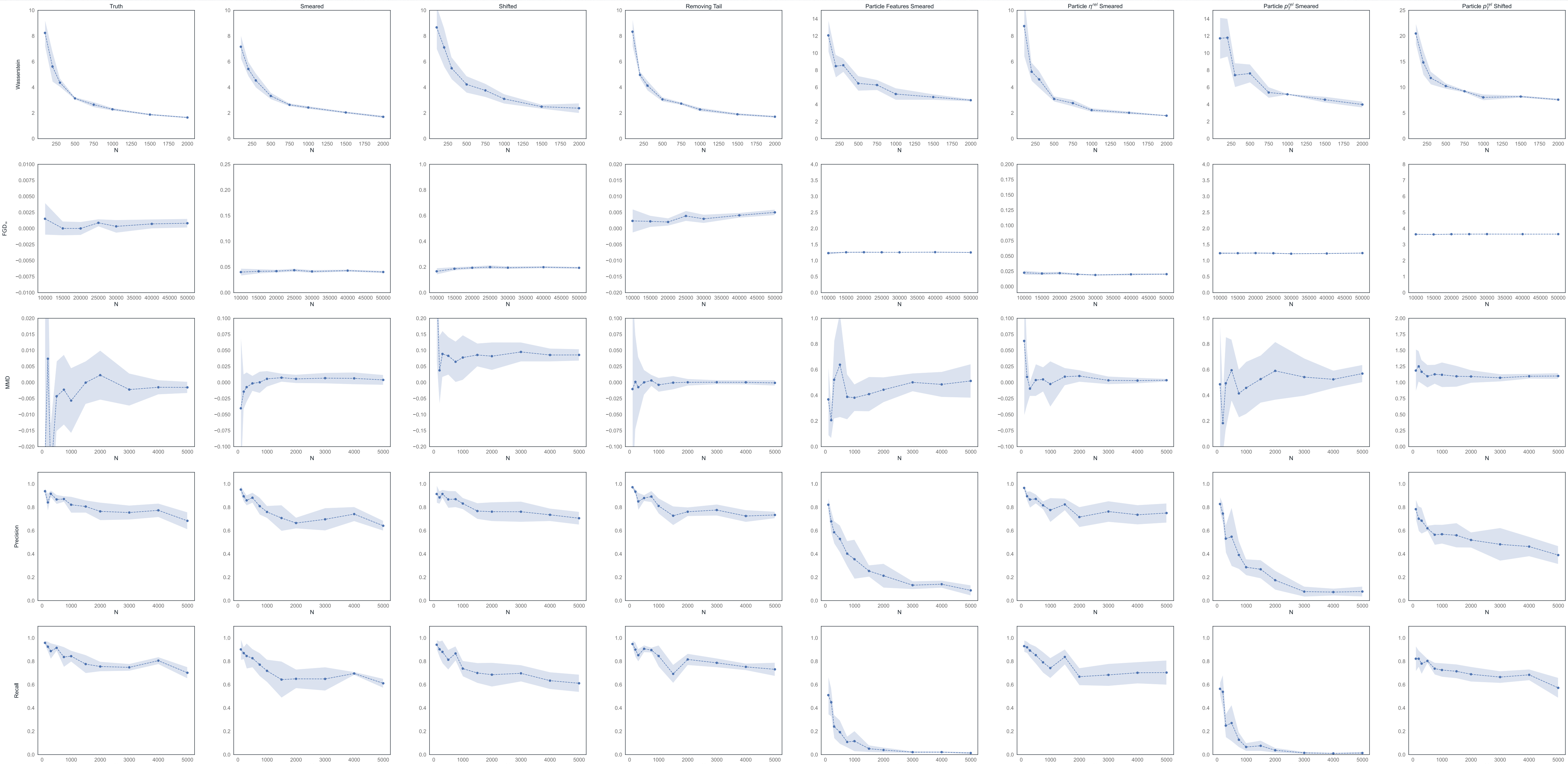
- FGD is the most sensitive
- MMD reasonable

PARTICLENET ACTIVATION SCORES



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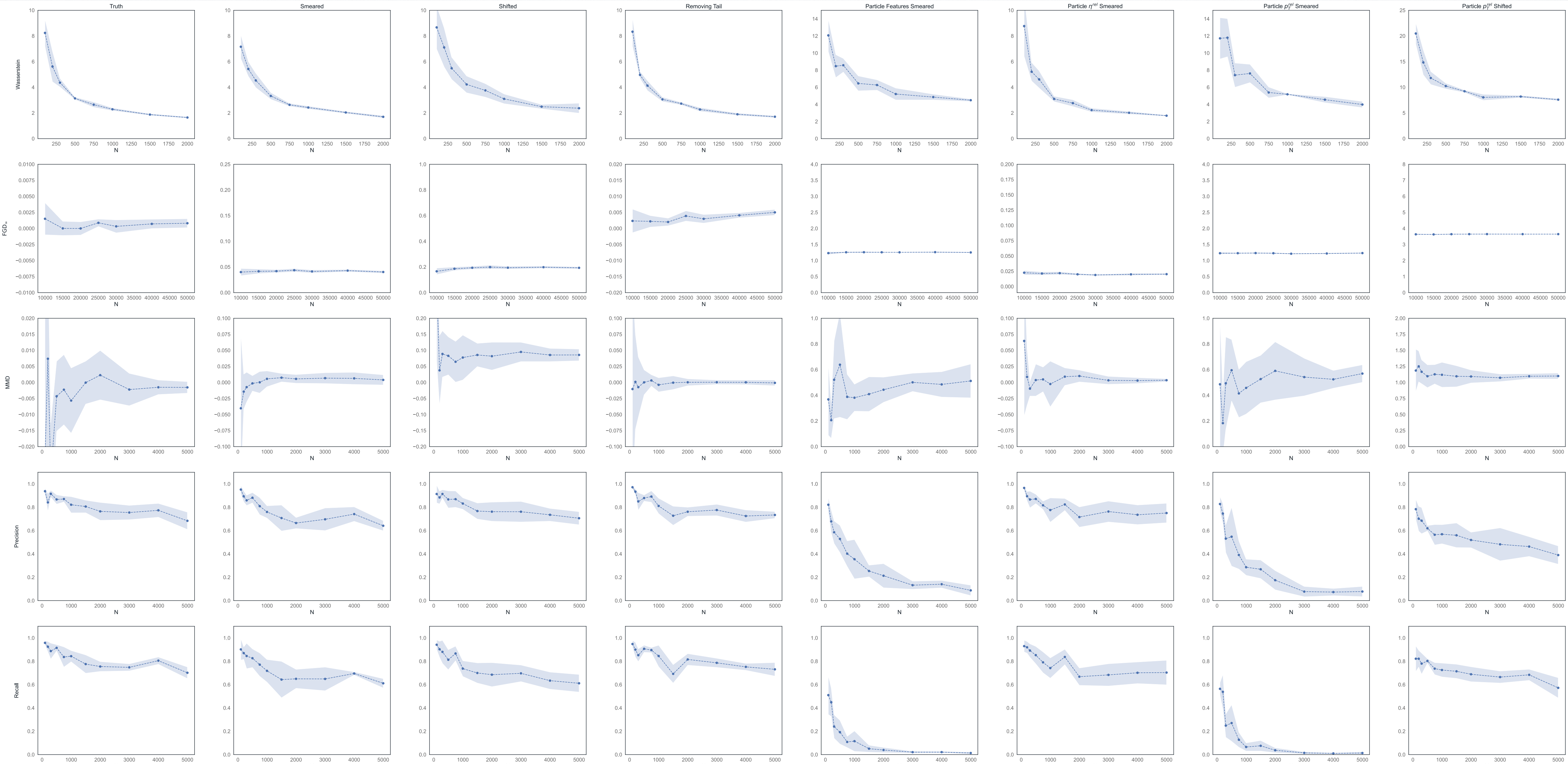

- Same conclusions overall as for EFPs
- FGD the best, MMD reasonable, P&R are OK for diagnosing failure modes

RESULTS: GLUON JETS

Kansal et al., ML4PS @ NeurIPS 2020
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Sample feature distributions, with MPGAN compared to baseline point cloud generators

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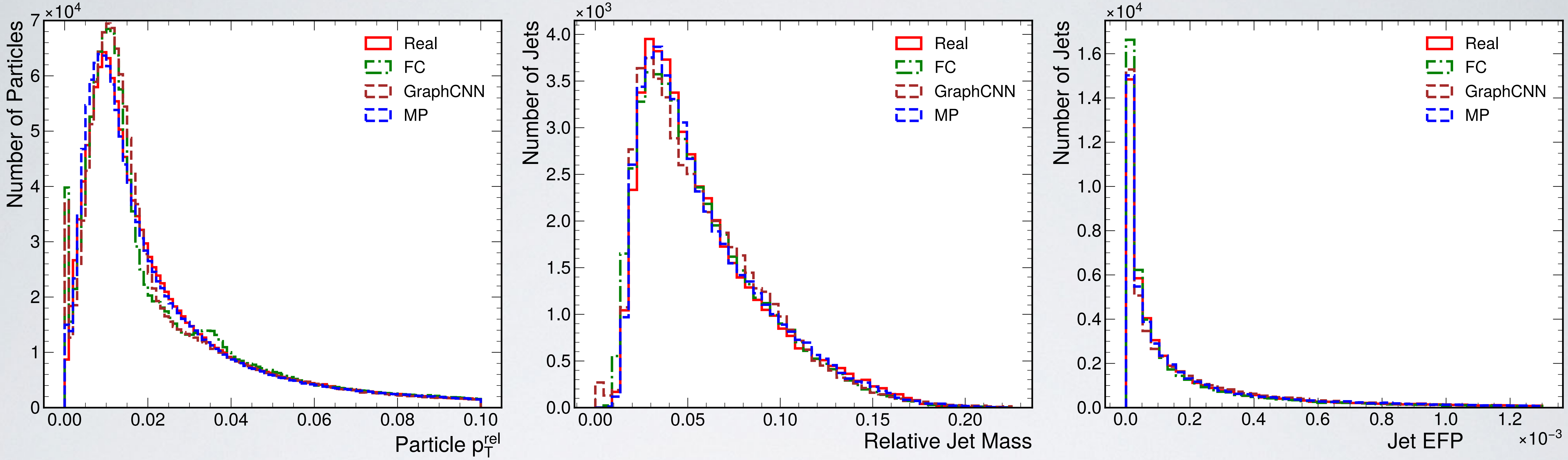

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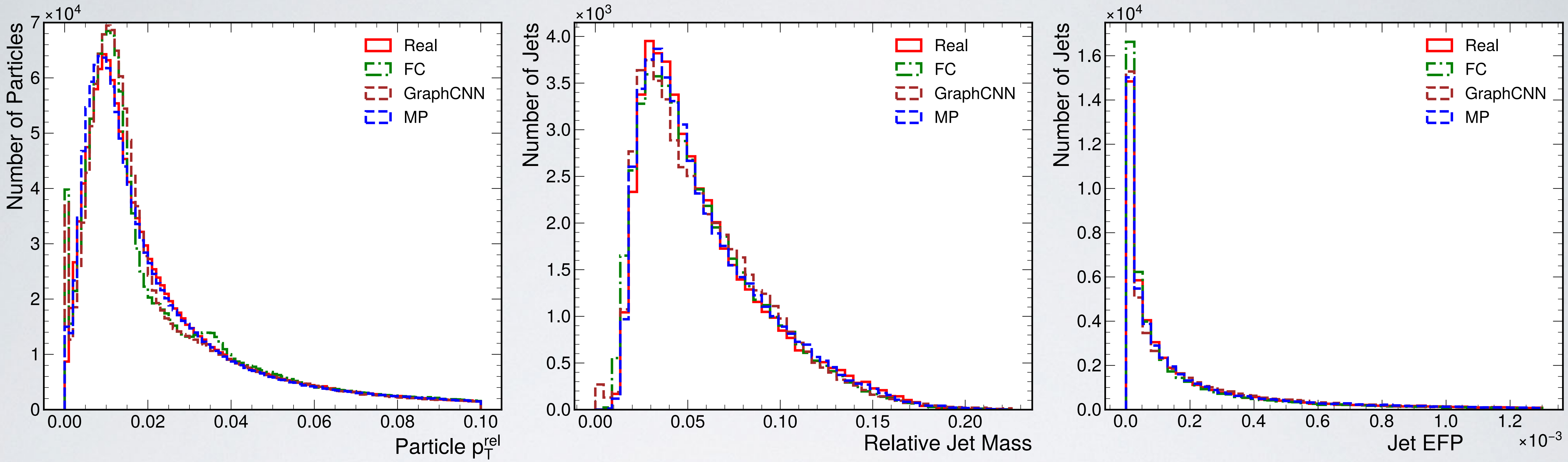

Generator	Discriminator	W1-P (10^{-3})	W1-M (10^{-3})	W1-EFP (10^{-5})	FPND
FC	PointNet	1.3 ± 0.2	1.3 ± 0.4	1.5 ± 0.9	5.0
GraphCNN	PointNet	16 ± 6	1.9 ± 0.2	200 ± 1000	7k
MP	MP	0.9 ± 0.3	0.7 ± 0.2	0.7 ± 0.2	0.12
MP	PointNet	1.2 ± 0.4	1.3 ± 0.4	4 ± 2	18

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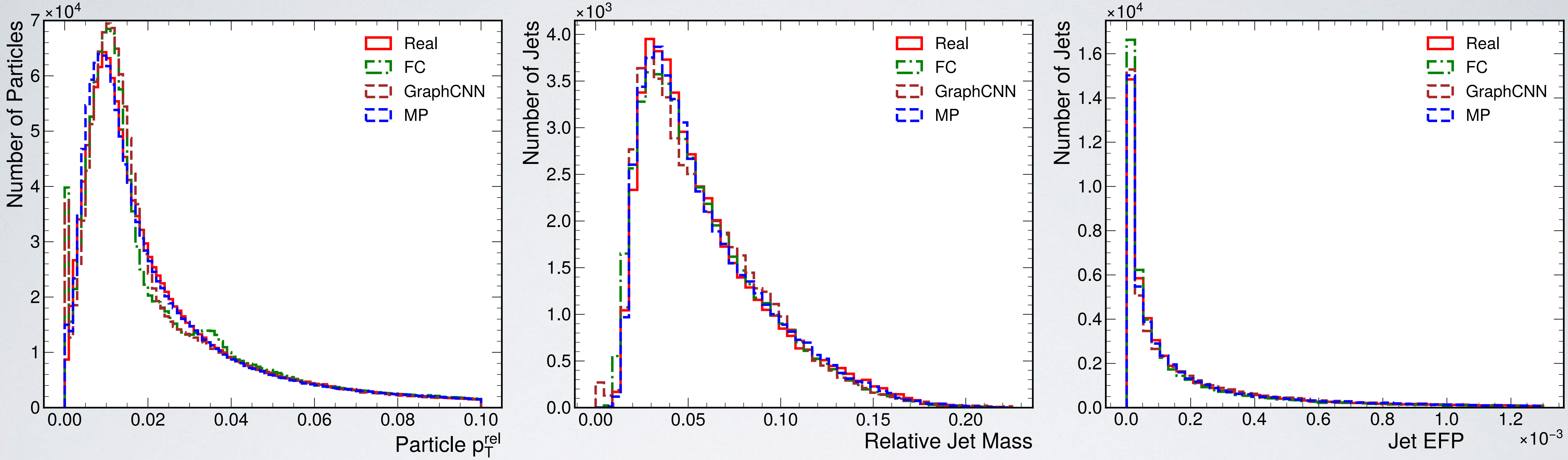

Generator	Discriminator	W1-P (10^{-3})	W1-M (10^{-3})	W1-EFP (10^{-5})	FPND
FC	PointNet	1.3 ± 0.2	1.3 ± 0.4	1.5 ± 0.9	5.0
GraphCNN	PointNet	16 ± 6	1.9 ± 0.2	200 ± 1000	7k
MP	MP	0.9 ± 0.3	0.7 ± 0.2	0.7 ± 0.2	0.12
MP	PointNet	1.2 ± 0.4	1.3 ± 0.4	4 ± 2	18

- MPGAN generator is the best performing on every metric

RESULTS: GLUON JETS

Kansal et al., ML4PS @ NeurIPS 2020
Kansal et al., NeurIPS 2021

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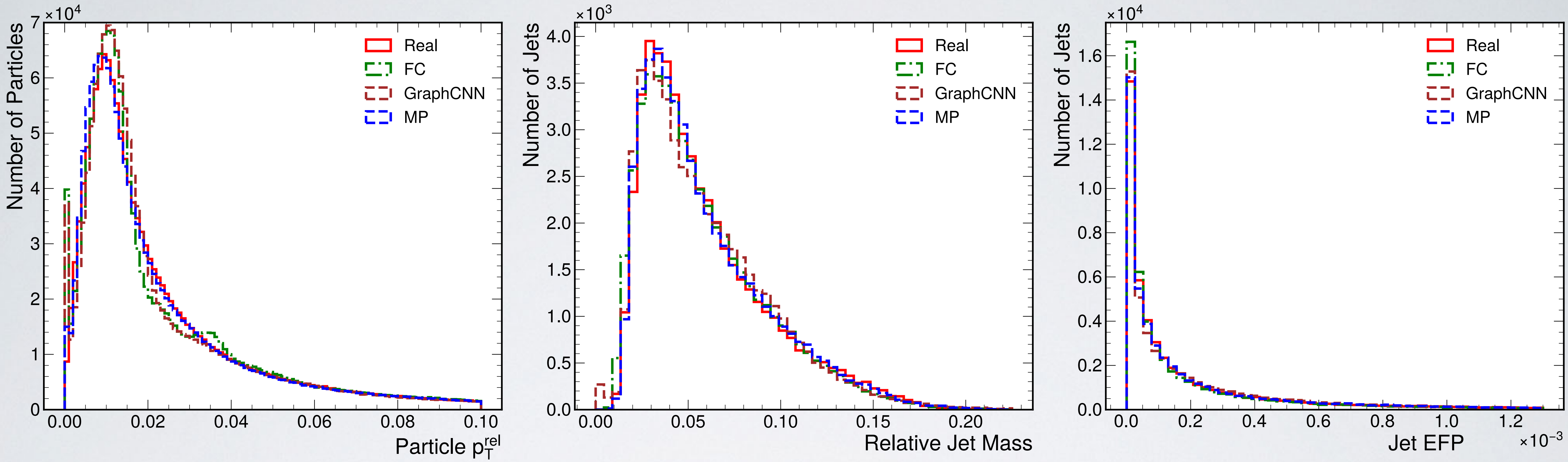

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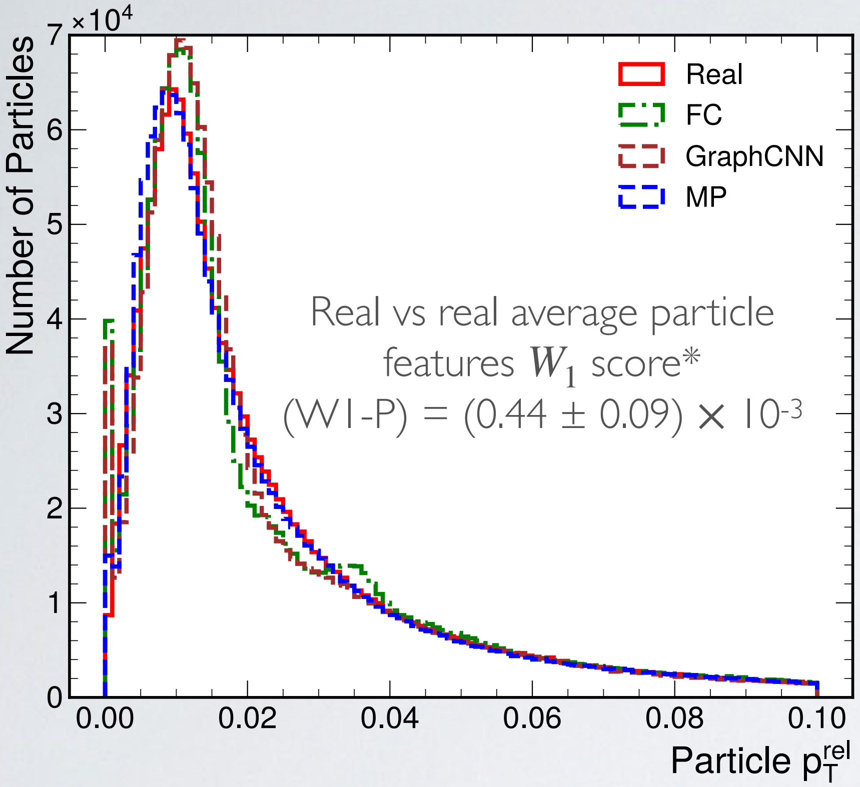
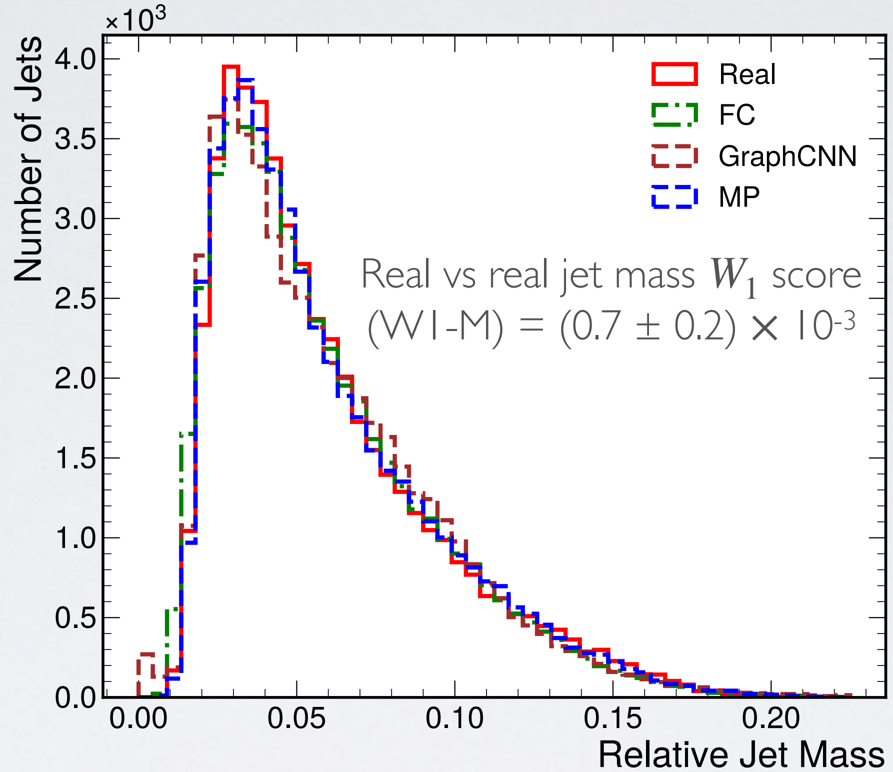
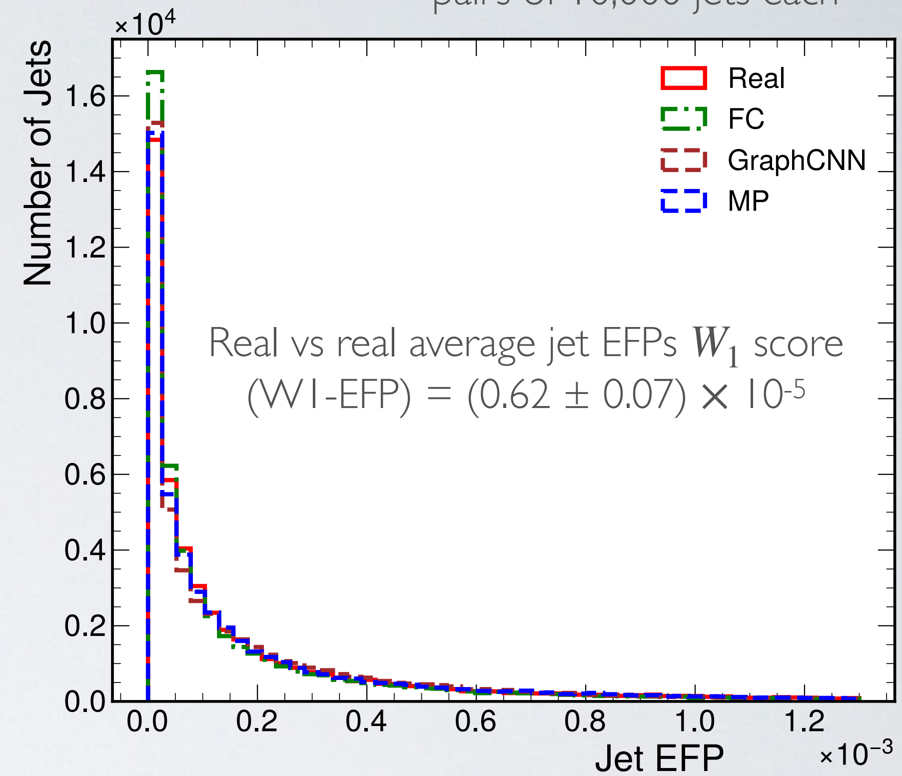
Sample feature distributions, with MPGAN compared to baseline point cloud generators

*Mean and error over 5 sets of pairs of 10,000 jets each







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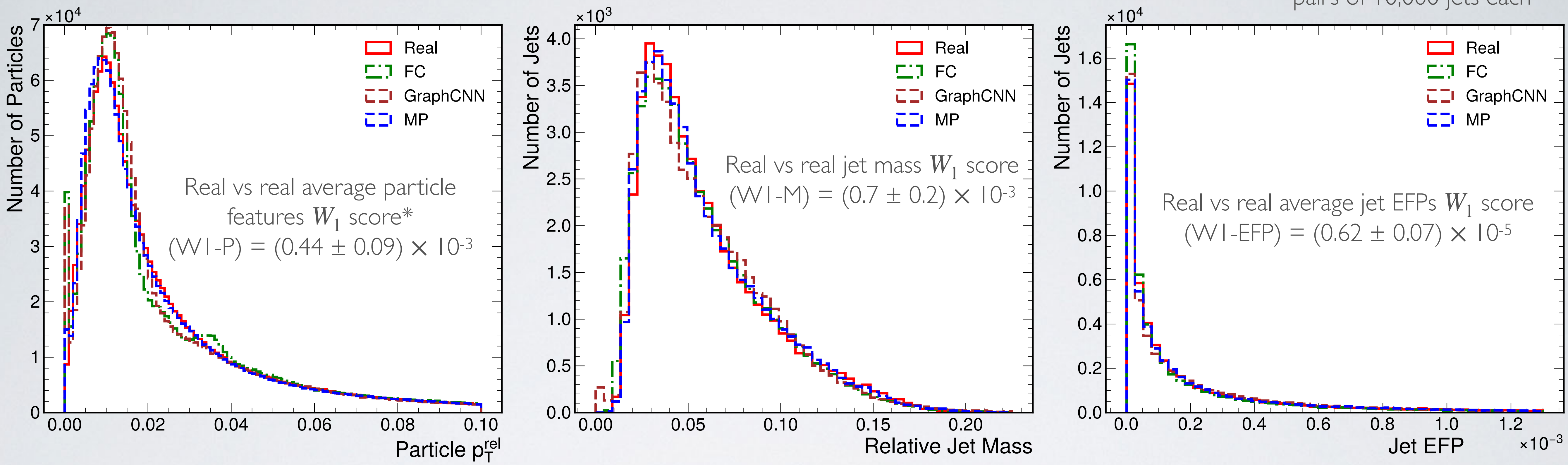

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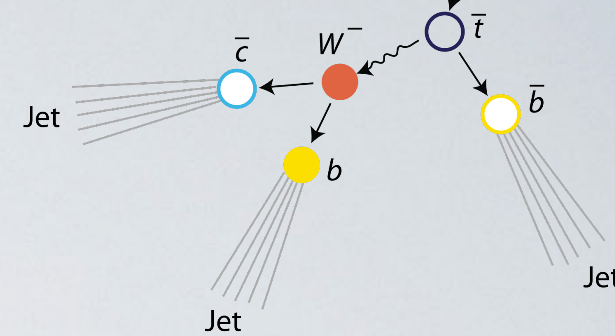
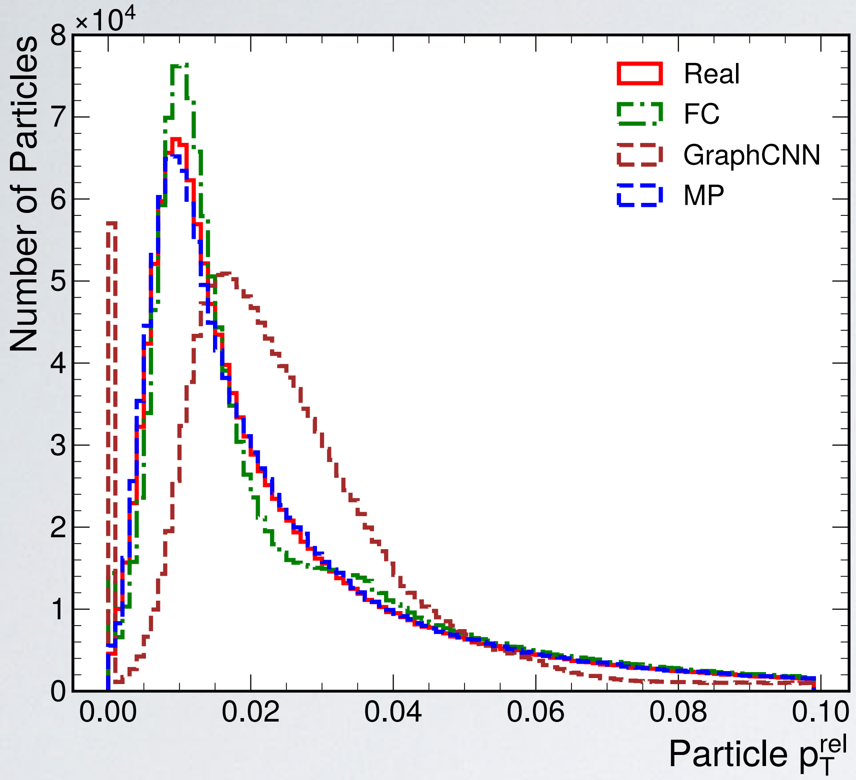
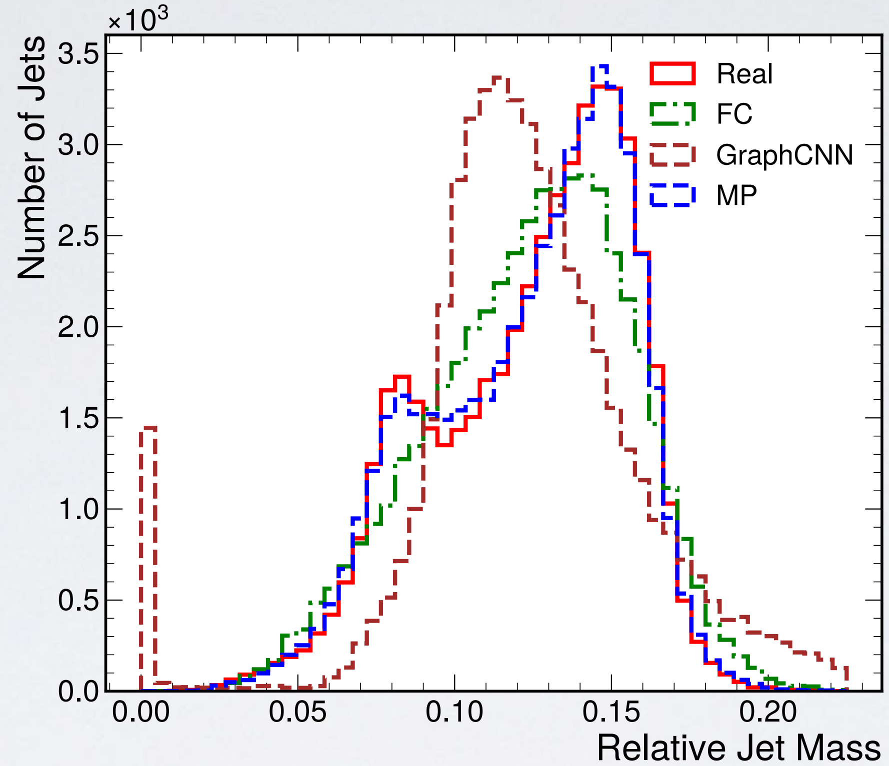
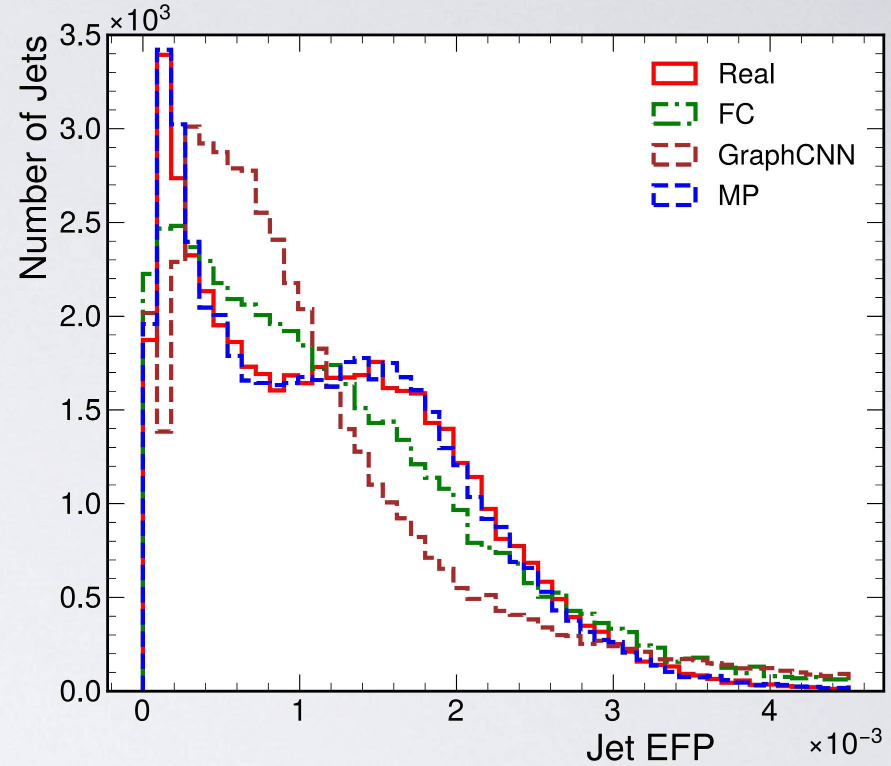
- MPGAN generator is the best performing on every metric
- Significantly outperforms alternatives on high level feature metrics (W1-M, W1-EFP, FPND)
- Mass and ave. EFP scores are within error of the real vs real baseline ⇒ learning jet substructure correctly

RESULTS: TOP QUARK JETS









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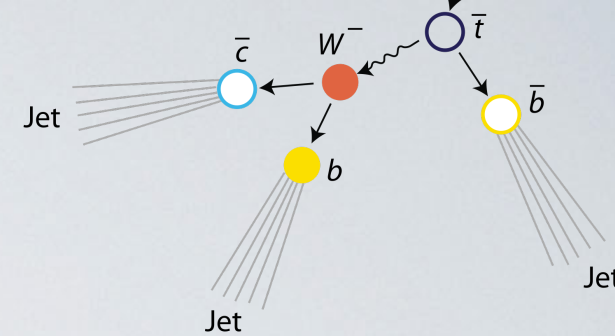
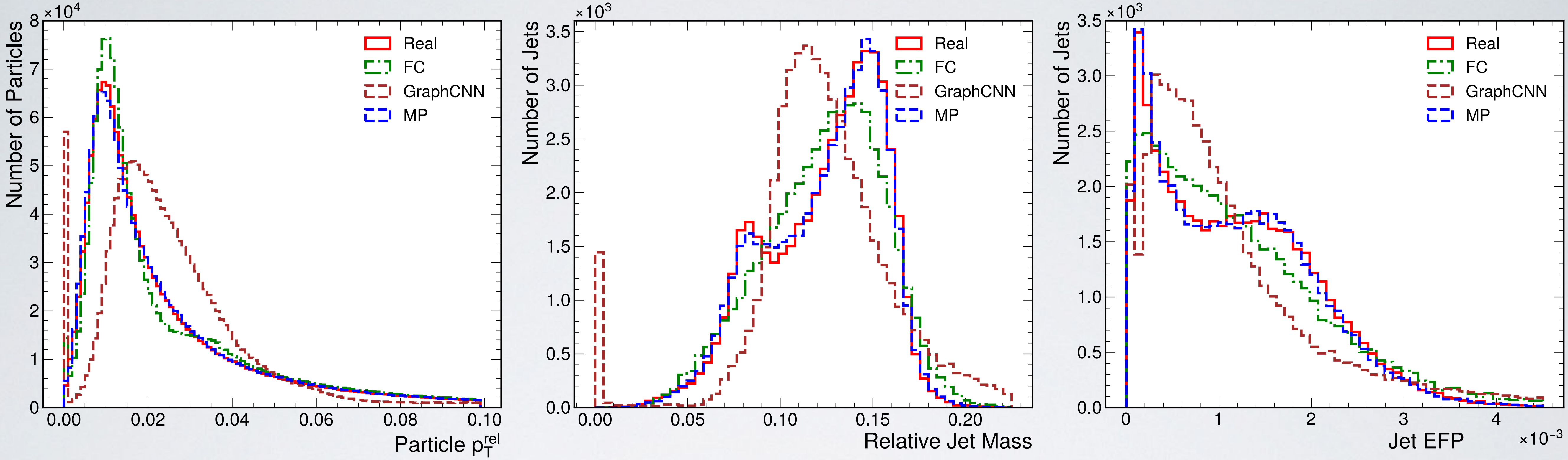
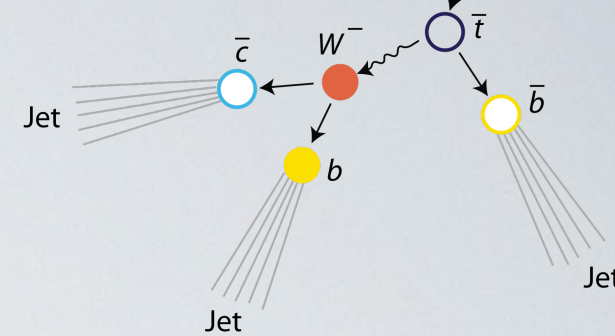
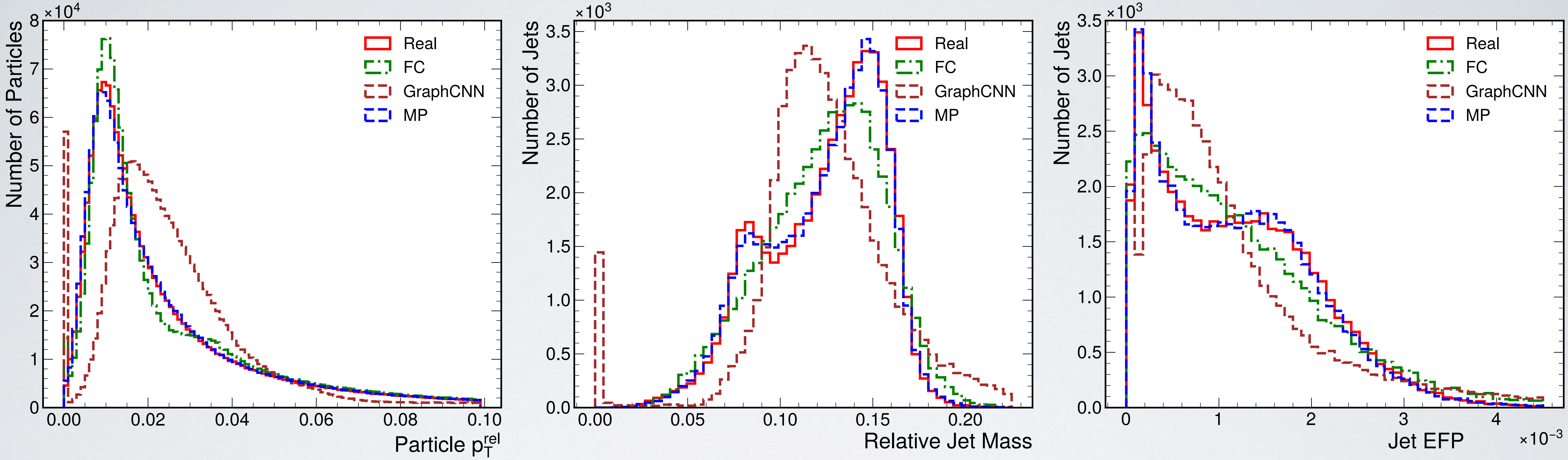




- MPGAN learns perfectly the complex bimodal jet feature distributions

RESULTS: TOP QUARK JETS





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GraphCNN	PointNet	30 ± 20	11.3 ± 0.9	37 ± 2	30k
MP	MP	2.3 ± 0.3	0.6 ± 0.2	2 ± 1	0.37
MP	PointNet	1.6 ± 0.4	0.76 ± 0.08	4 ± 1	3.7

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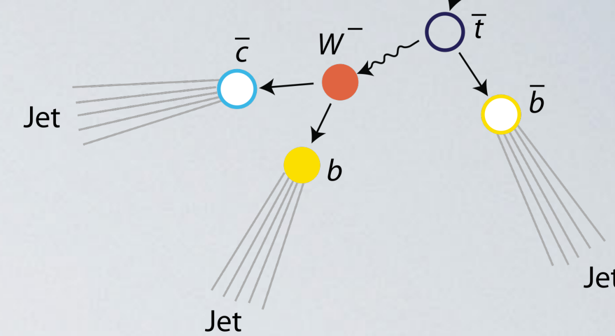
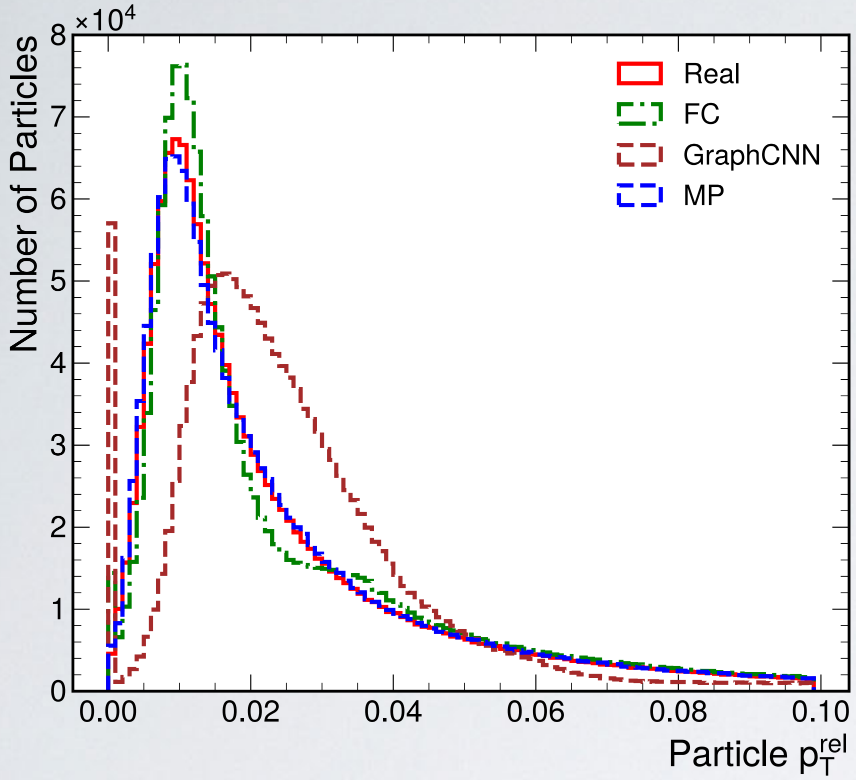
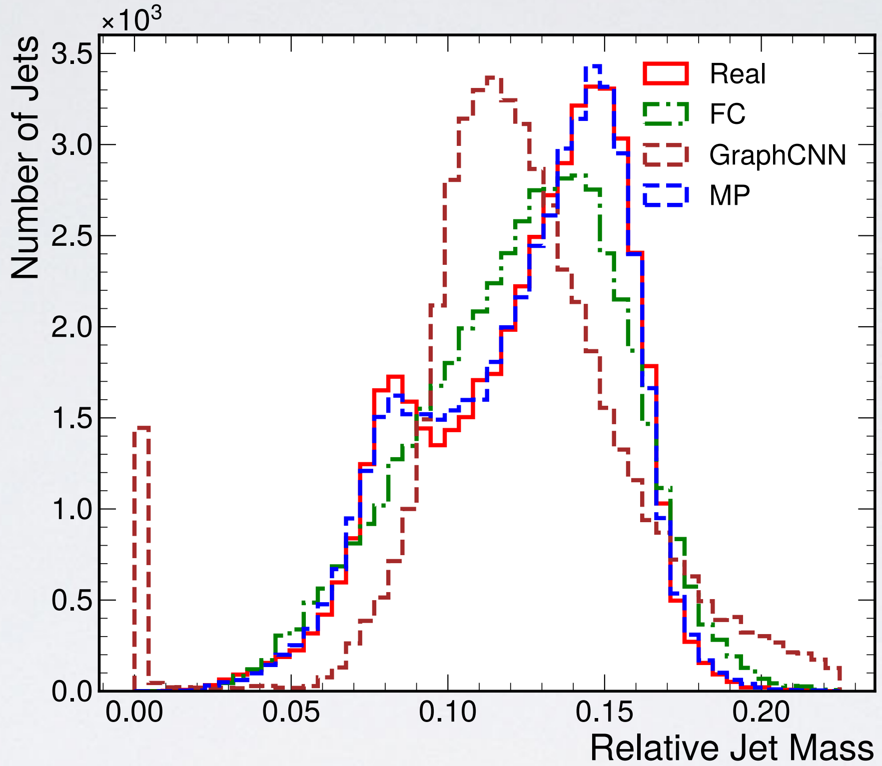




Real vs real
W1-P = (0.55 ± 0.07) × 10^{-3}



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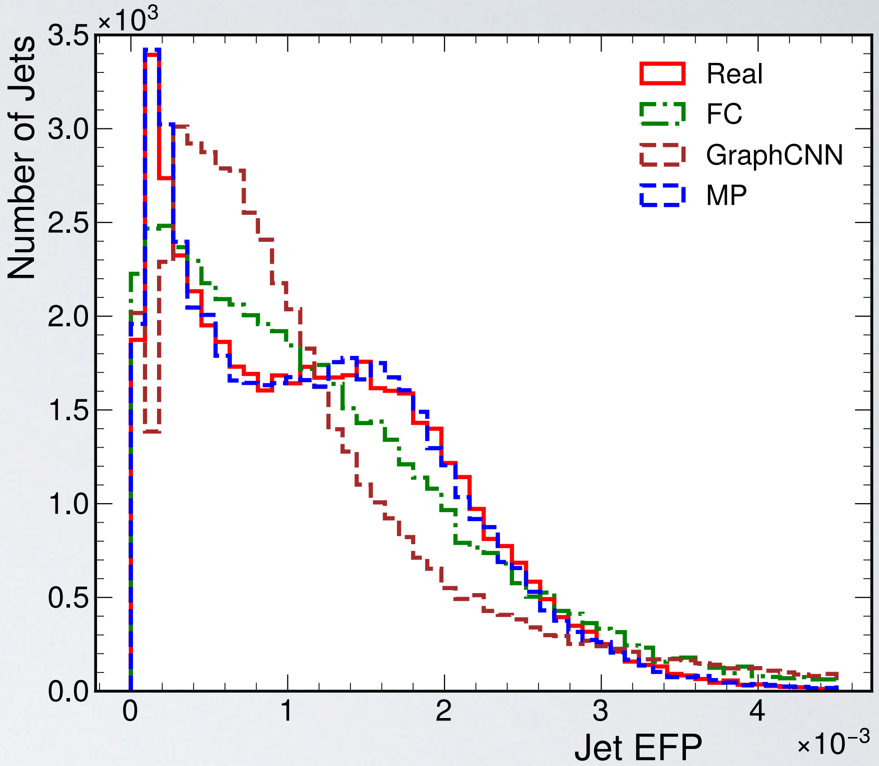

Real vs real
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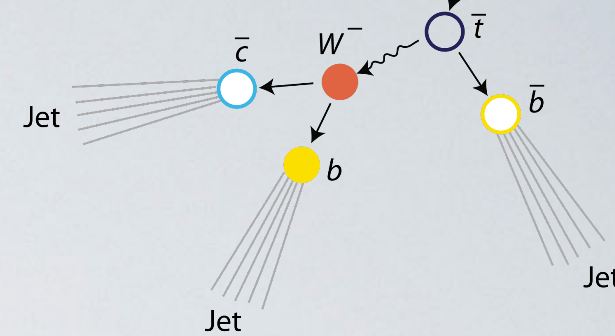

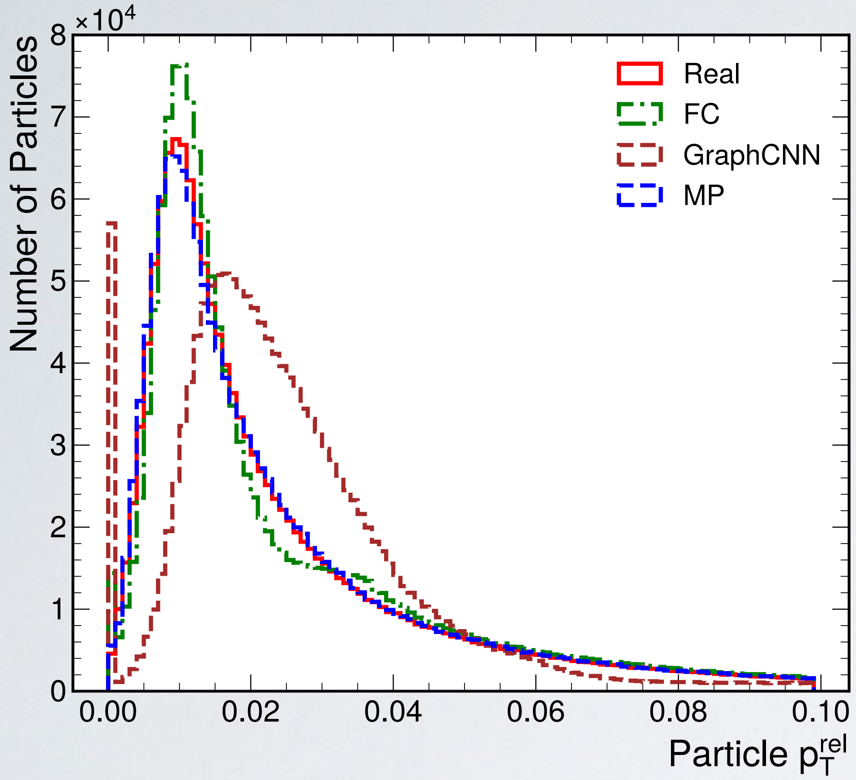

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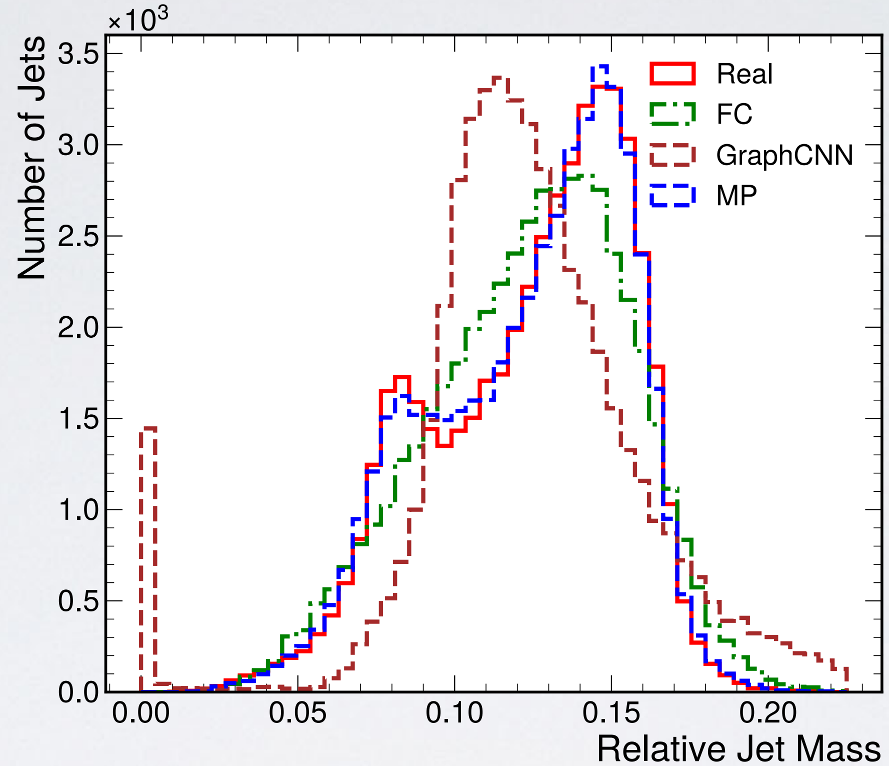

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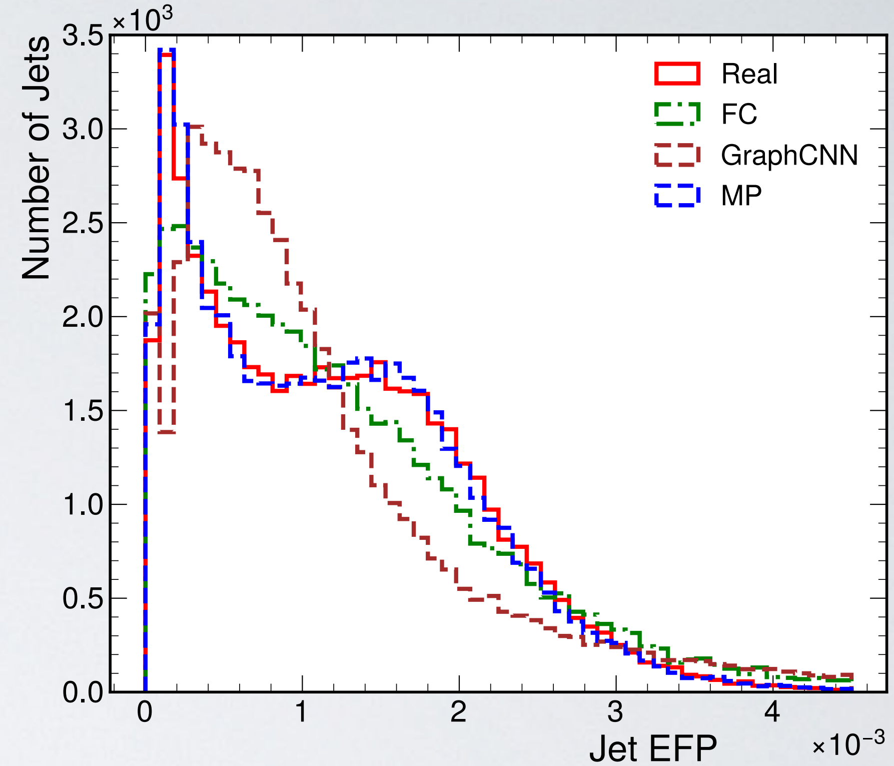

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