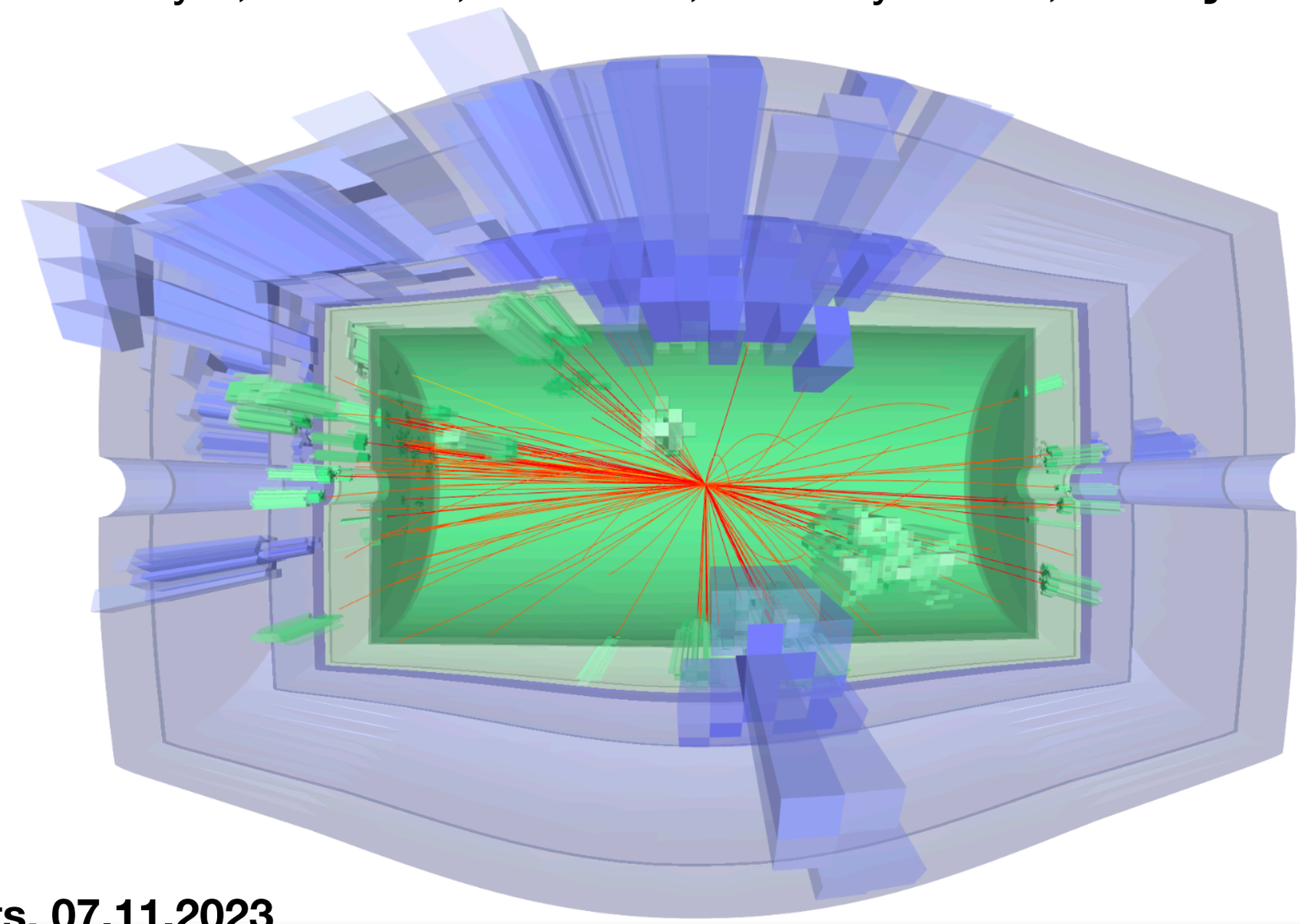
Fast Simulation using Graph Diffusion and Graph-to-Graph Translation

E. Dreyer, E. Gross, N. Kakati, D. Kobylianskii, **N. Soybelman**



ML4Jets, 07.11.2023

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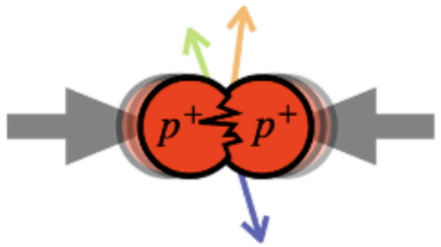
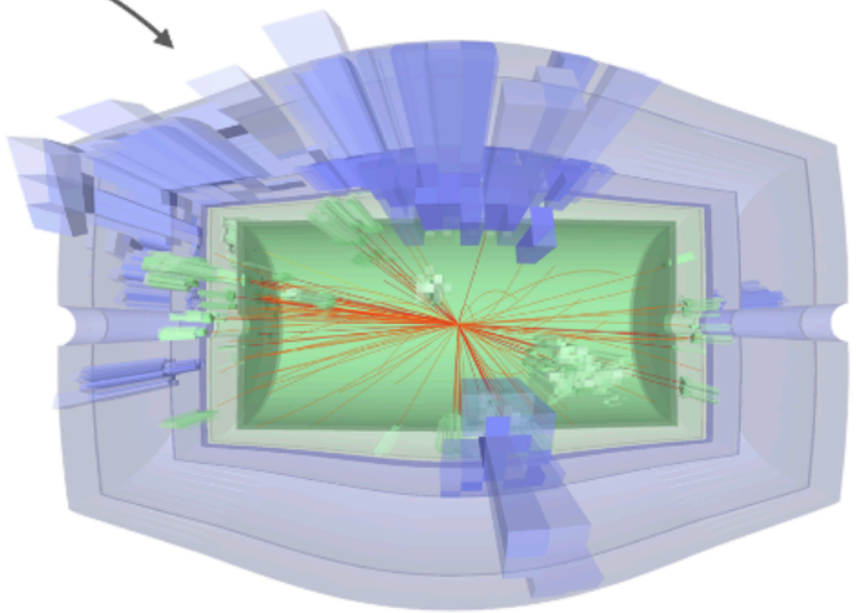
Motivation

Proton collisions



Truth particles, T

Detector simulation
$p(H \mid T)$

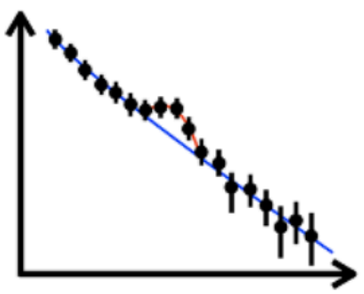


Computationally expensive

Reconstruction
$p(R \mid H)$

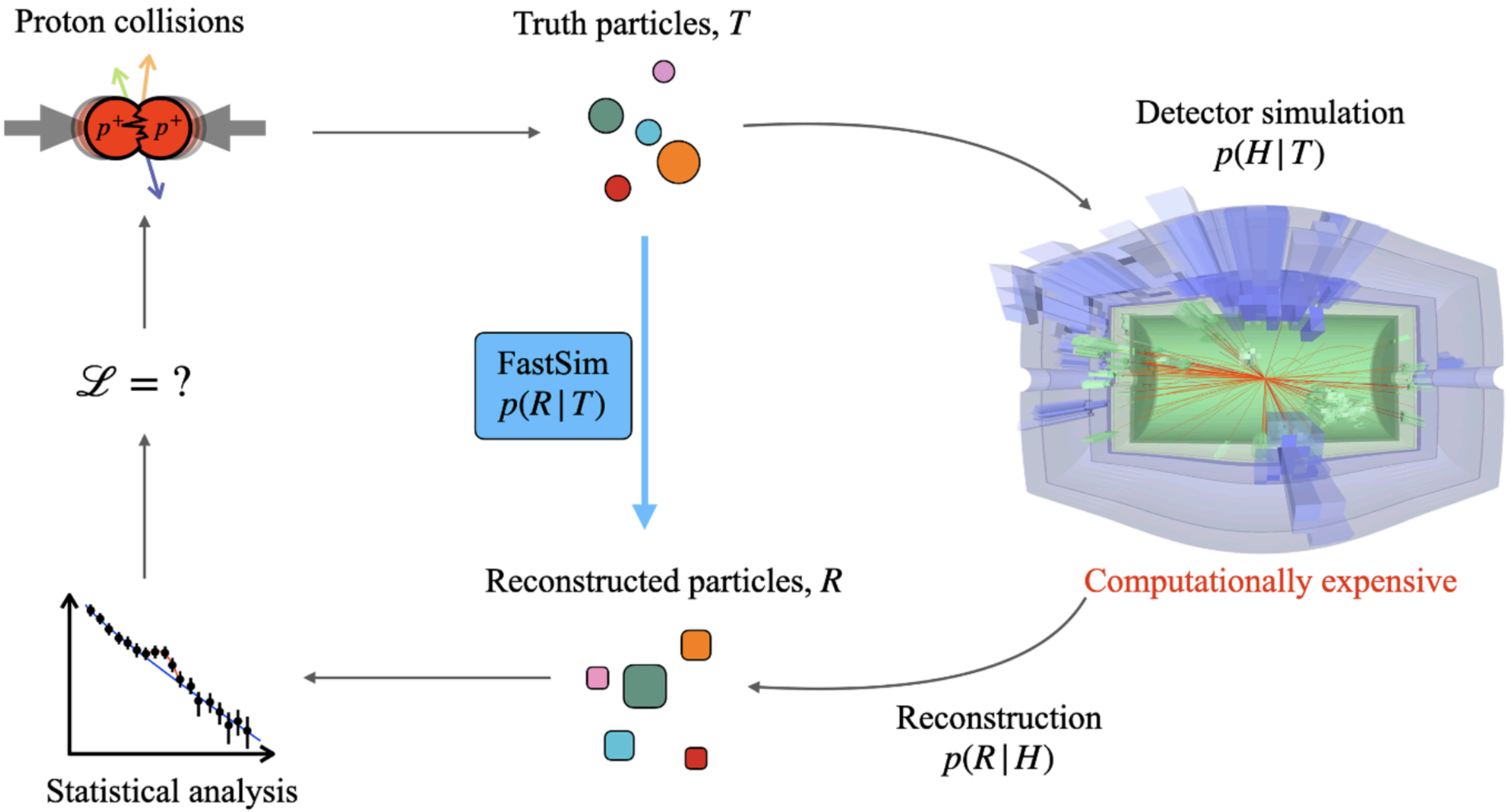
Reconstructed particles, R

Statistical analysis



$\mathscr{L} = ?$

Motivation


Proton collisions
p^+ p^+
Truth particles, T
Detector simulation
$p(H \mid T)$
$\mathscr{L} = ?$
FastSim
$p(R \mid T)$
Reconstructed particles, R
Computationally expensive
Statistical analysis
Reconstruction
$p(R \mid H)$

Previous work

arXiv: 2211.06406

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Set-Conditional Set Generation for Particle Physics

Nathalie Soybelman[1], Nilotpal Kakati[1], Lukas Heinrich[2], Francesco Armando Di Bello[3], Etienne Dreyer[1], Sanmay Ganguly[4], Eilam Gross[1], Marumi Kado[5] and Jonathan Shlomi[6]

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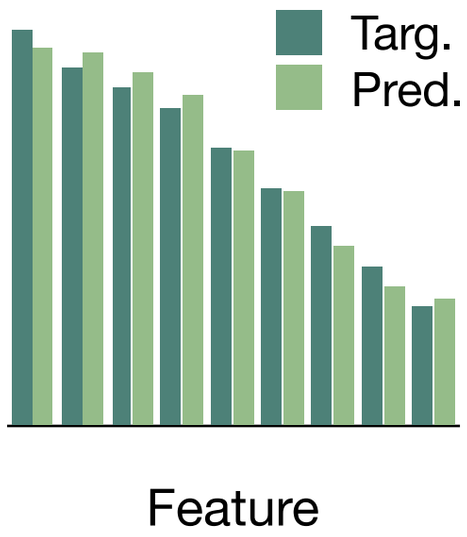
	Previously	Now
Dataset	Toy model — emulated tracks	Full simulation & reconstruction
Particles	charged only	charged + neutral
Architecture	GNN with Slot-Attention	Graph Diffusion Graph-to-Graph Translation

Goals

Goals

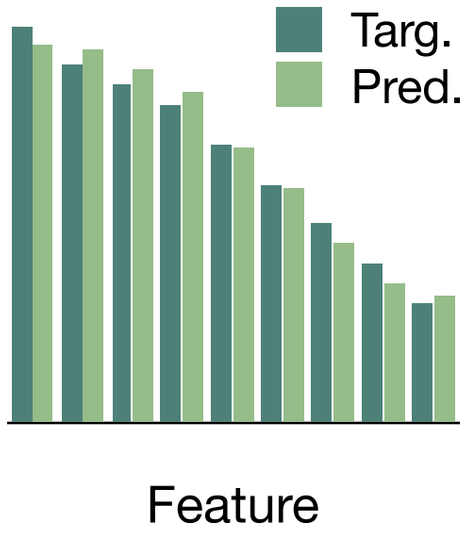
Marginal distributions

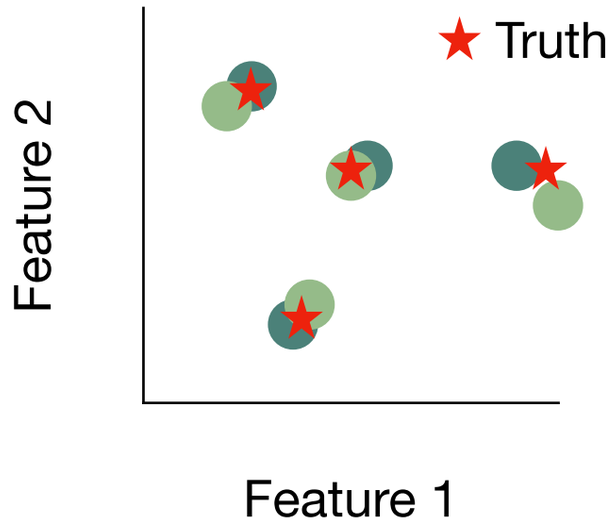


Goals

Marginal distributions

Reconstruct constituents



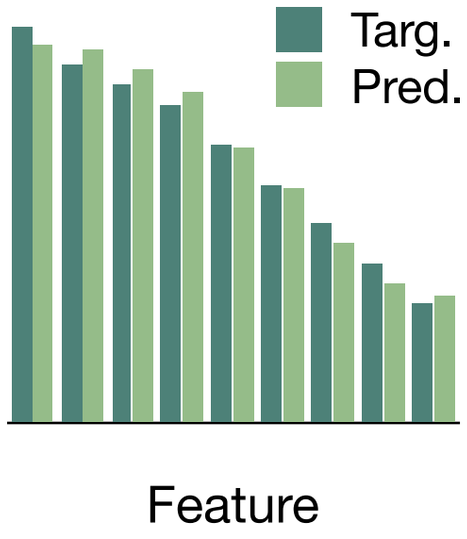


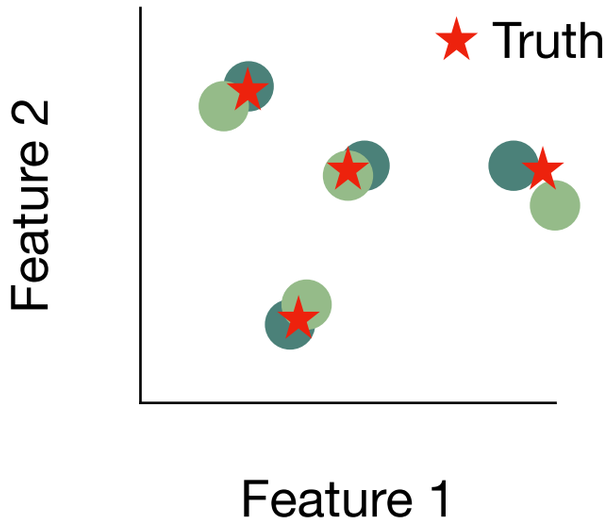
Goals

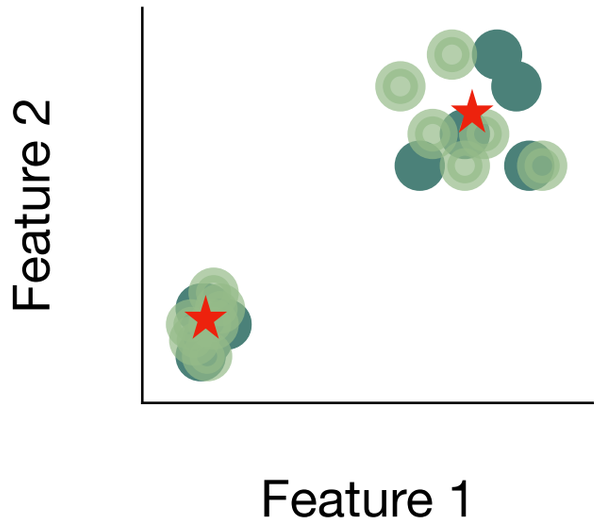
Marginal distributions

Reconstruct constituents

Resolution







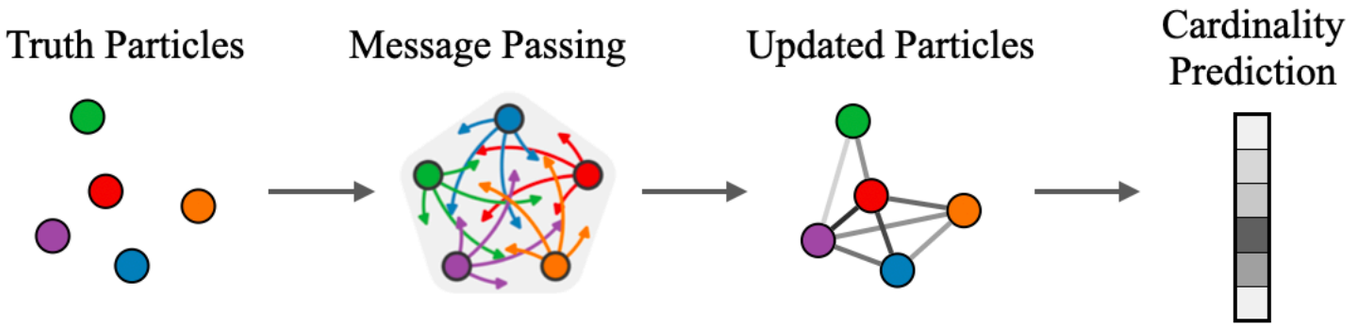
Dataset

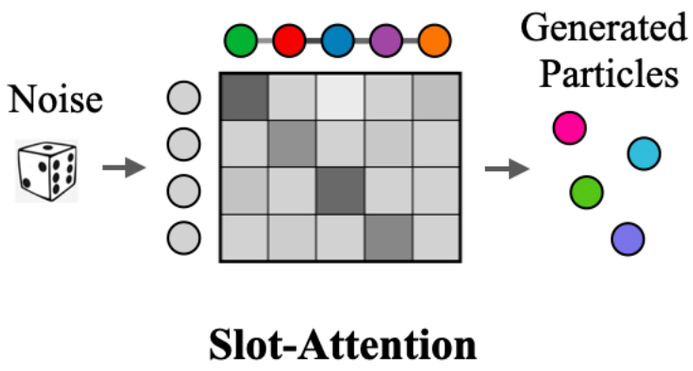
- Single jet events
- COCOA detector simulation — 2303.02101
- HGPflow reconstruction — 2212.01328, Nilotpal's talk

- **100 *replicas*** per event

  repeat detector simulation for the same truth event

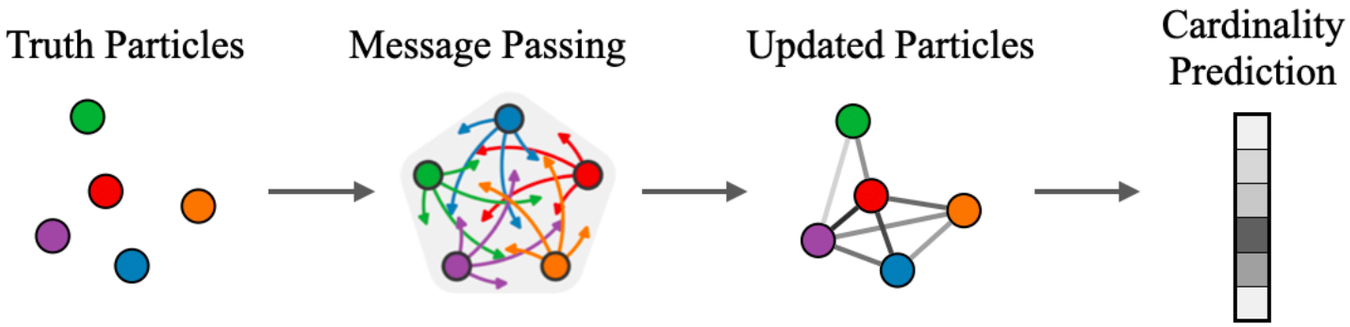
Architectures

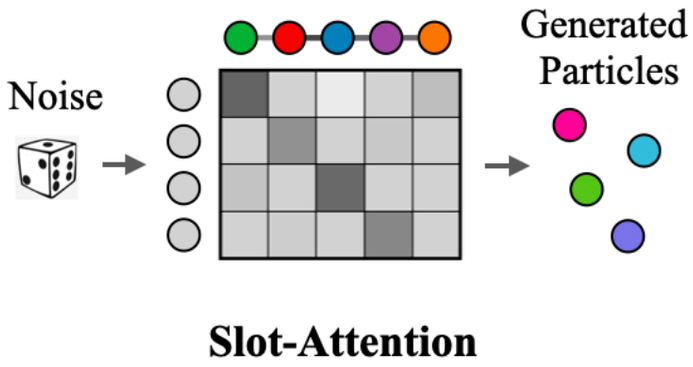


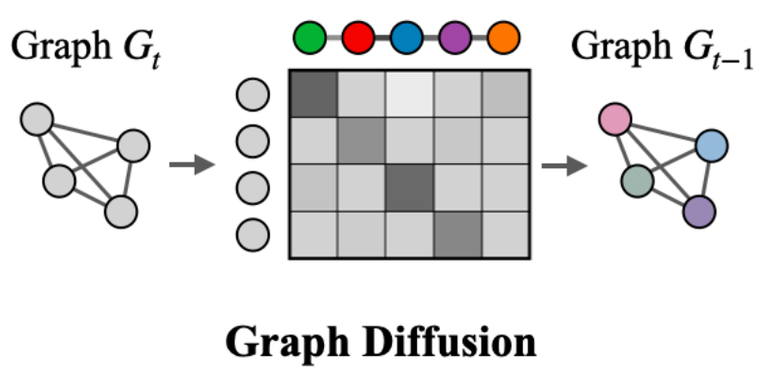


Set-based loss through Hungarian matching (LSA) using particle features

Architectures

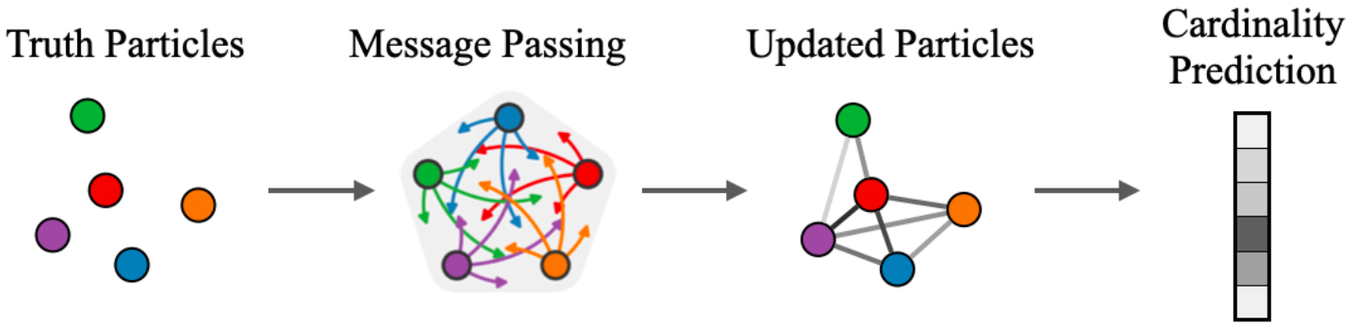


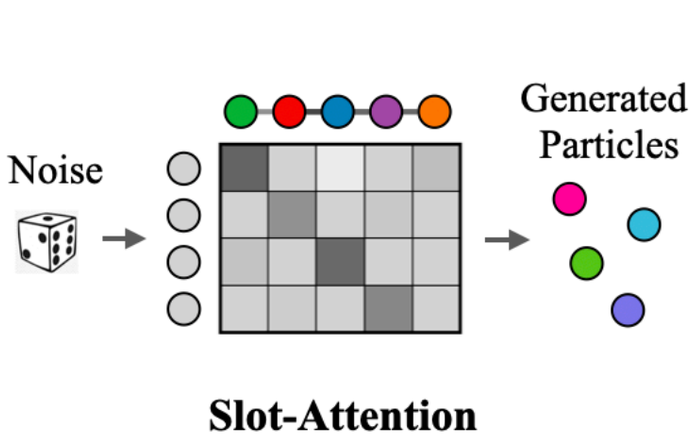


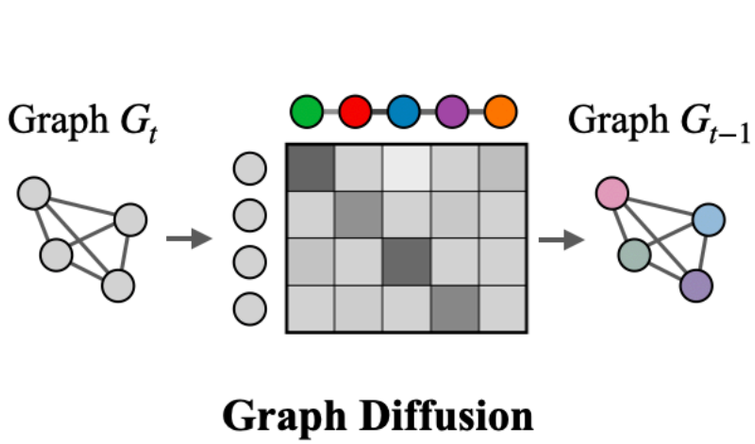


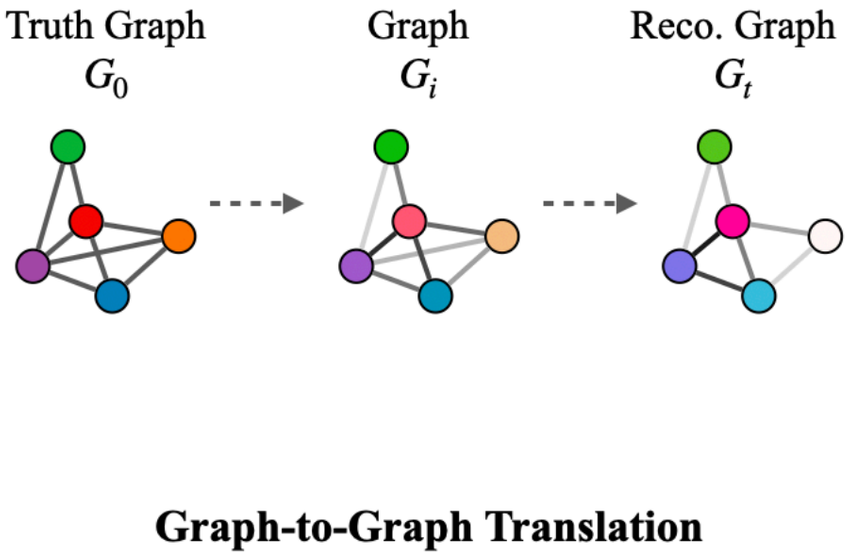
Set-based loss through Hungarian matching (LSA) using particle features

Architectures



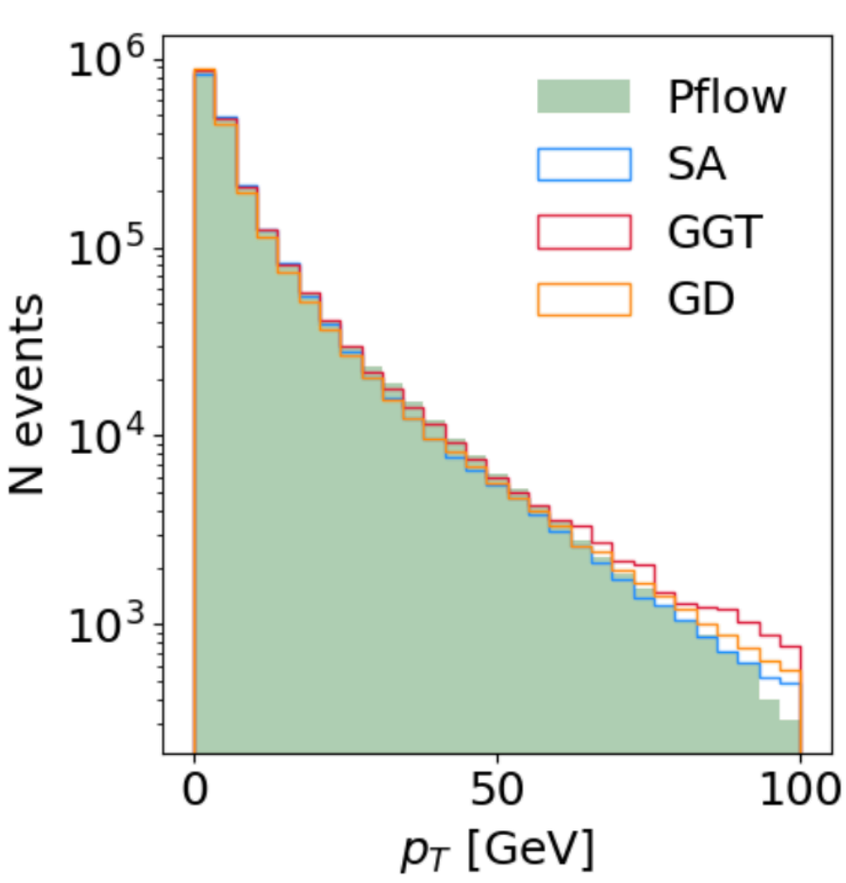


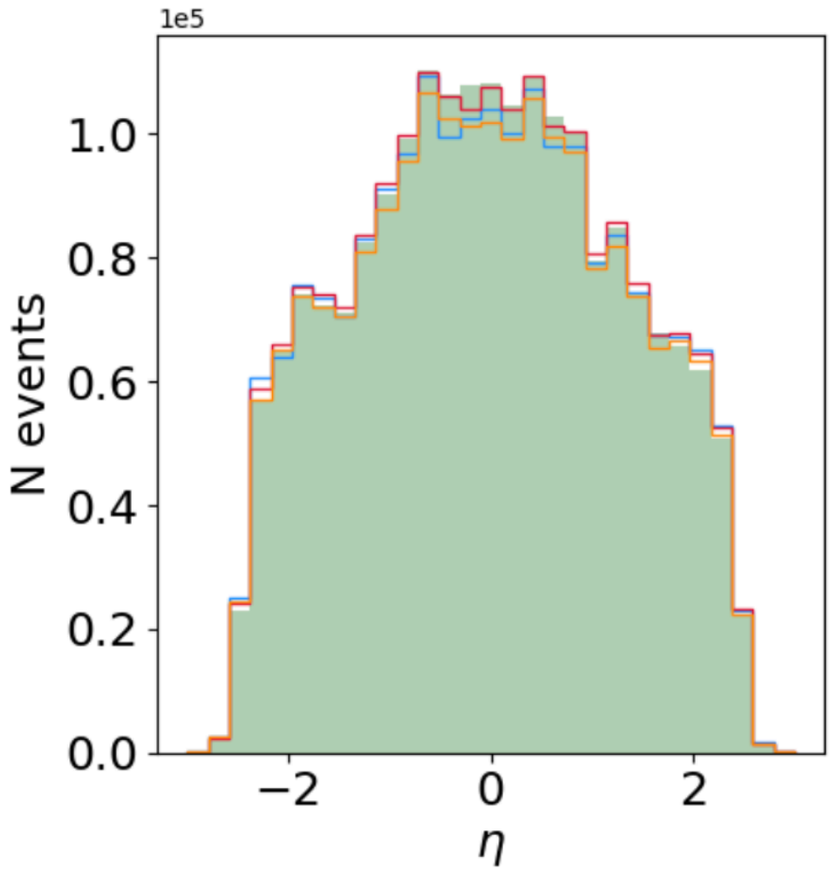


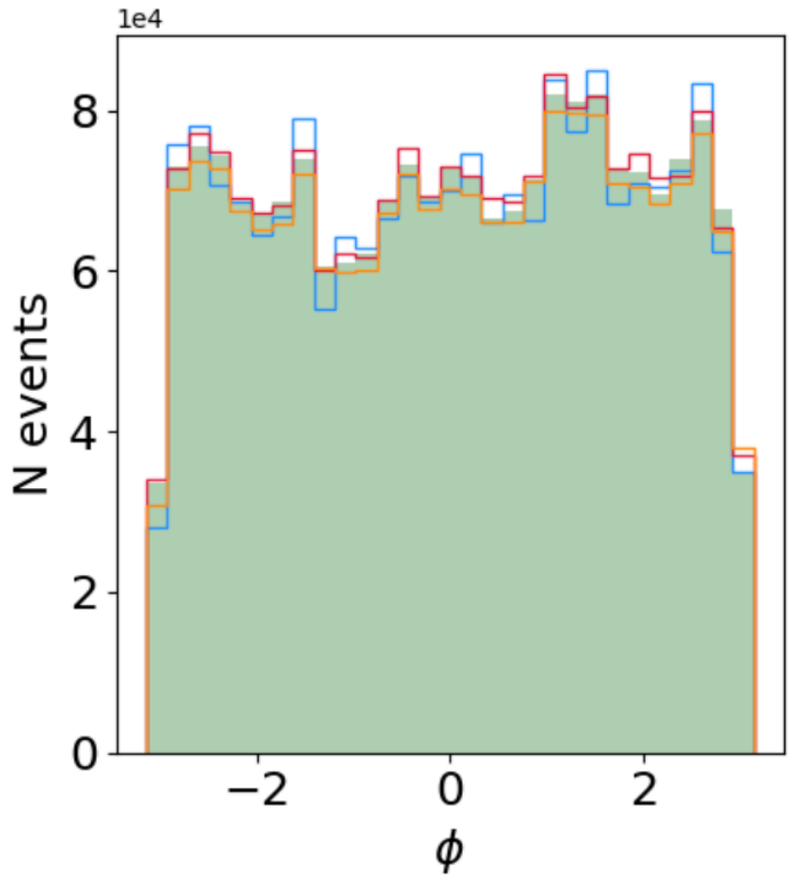


Set-based loss through Hungarian matching (LSA) using particle features

Marginal distributions

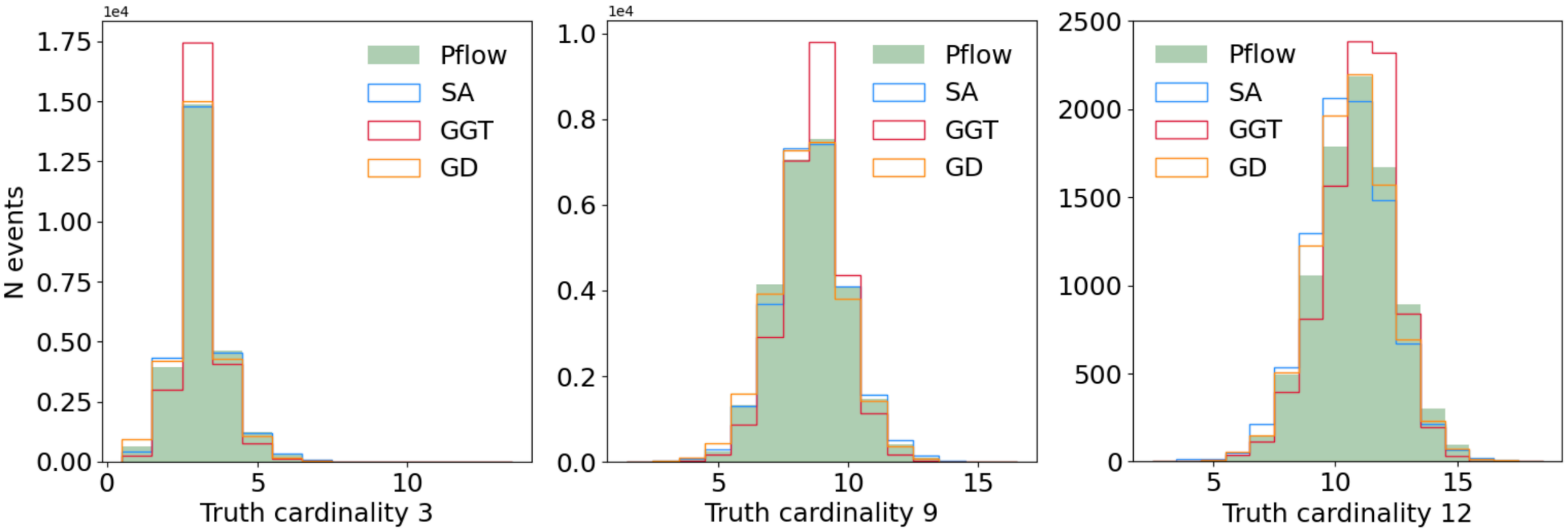






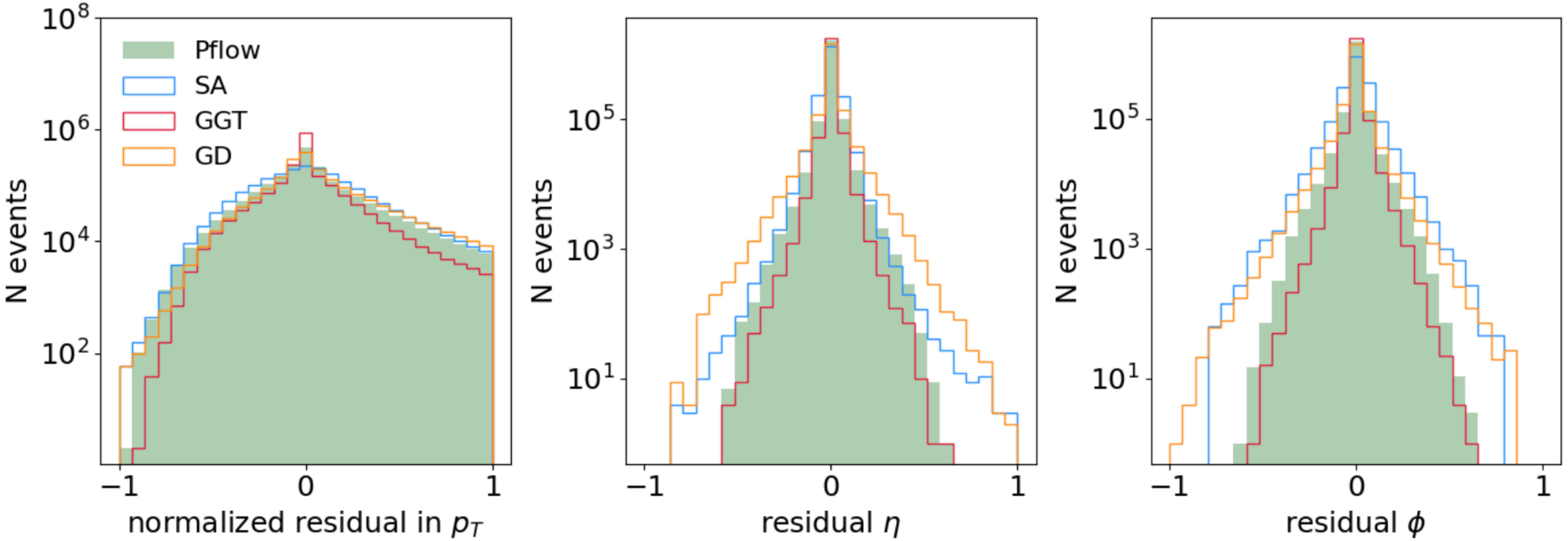
- Overall good agreement
- Some issues in p_T tail — under investigation

Cardinality

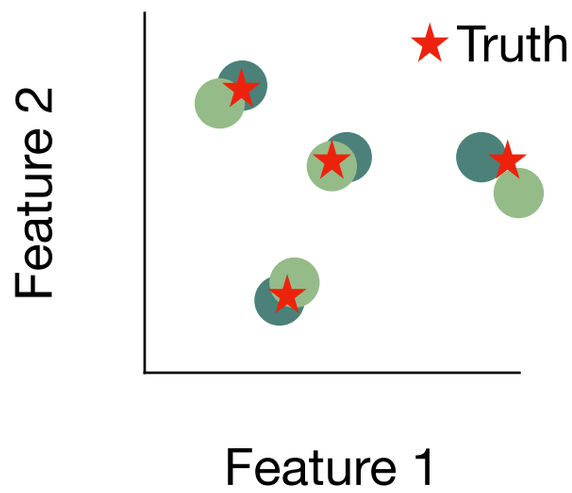


- SA & GD very similar — expected since its the same network
- GGT to close to the truth

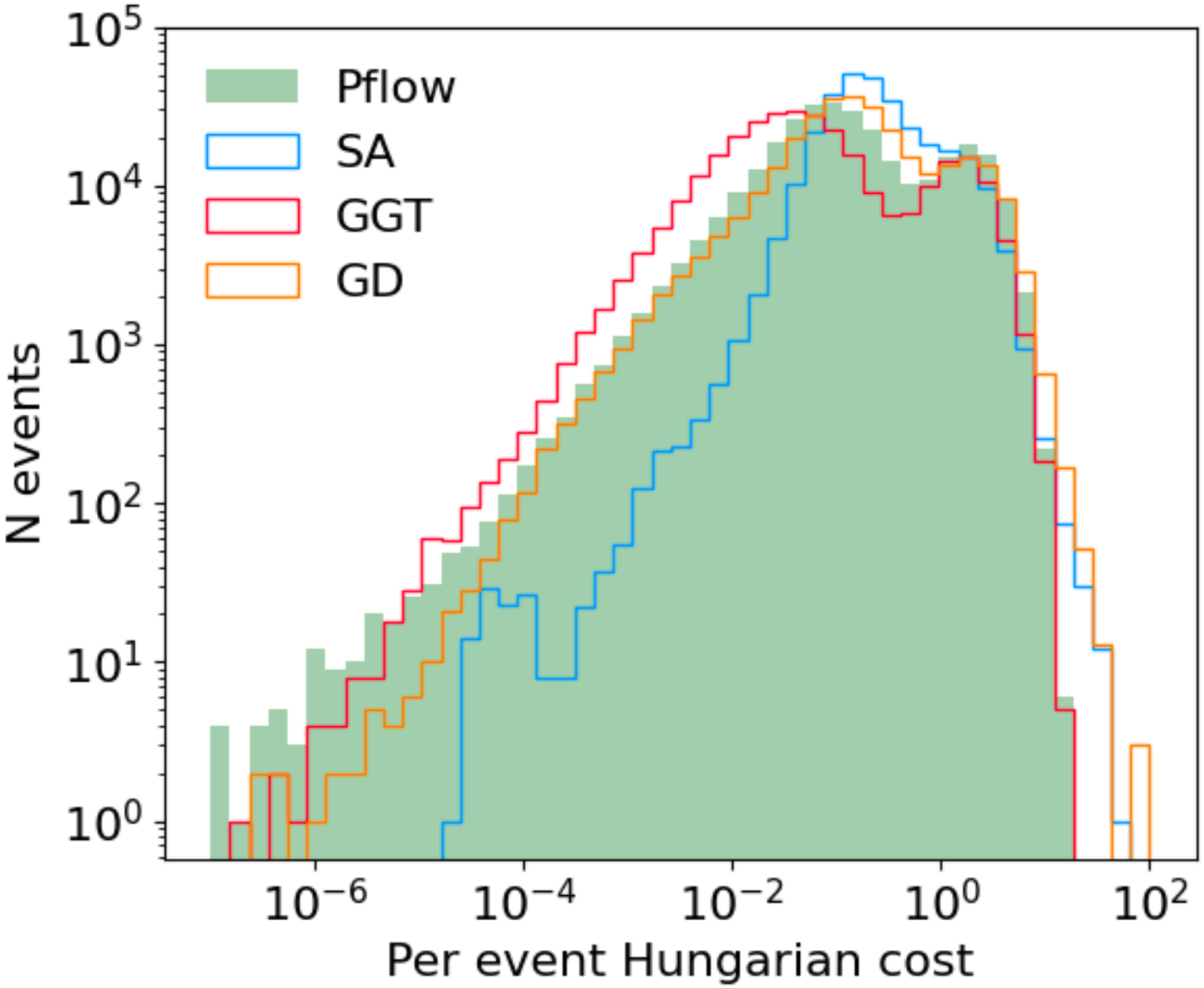
Residuals — ‘Distance to Truth’



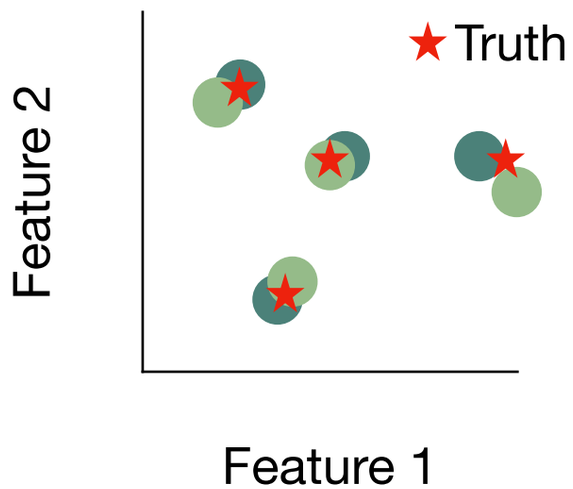
- Hungarian matching between truth and reconstruction
- GGT predictions are ‘to precise’
- SA & GD good agreement in p_T
- Need combined metric



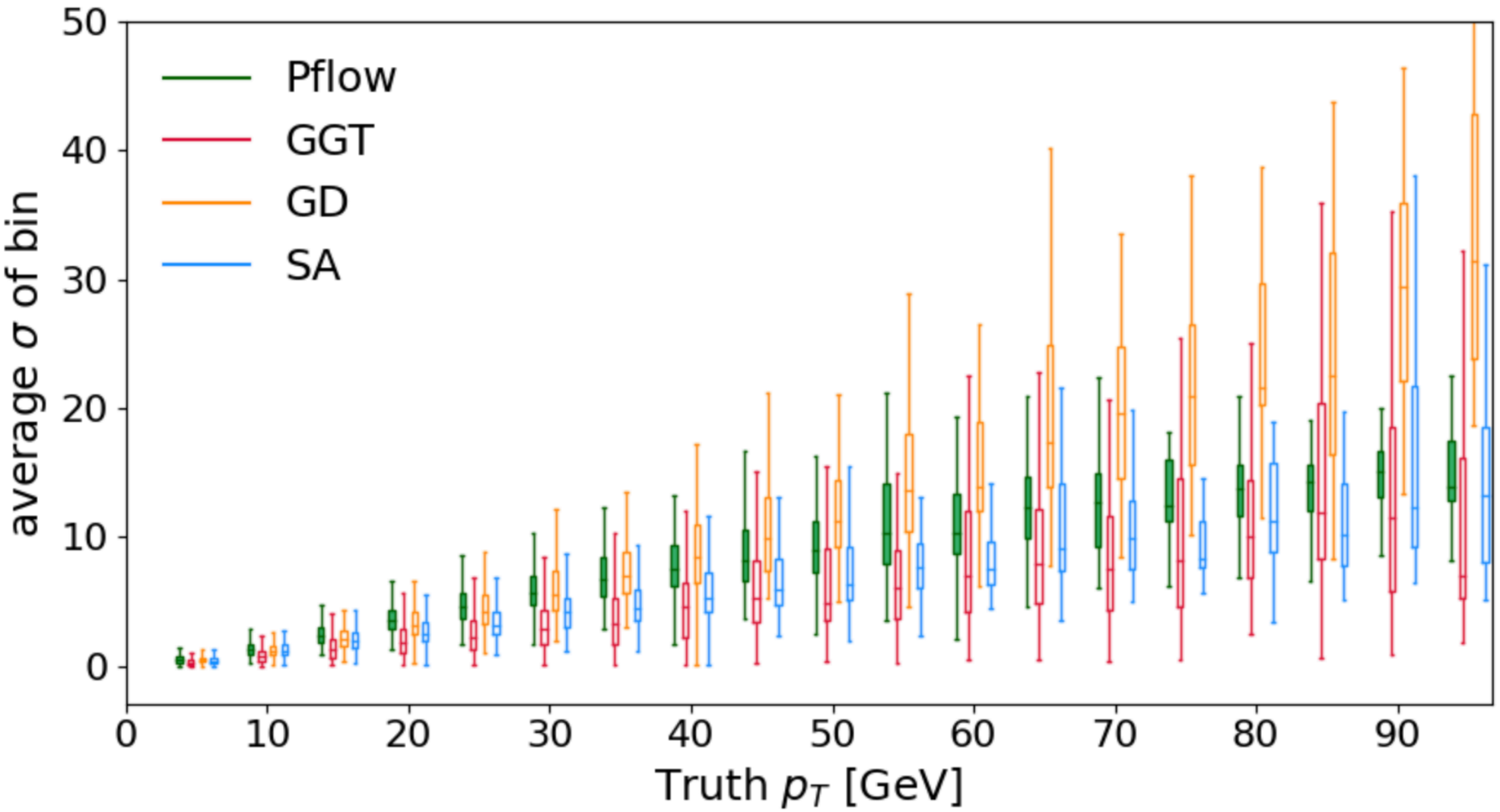
Matching with truth



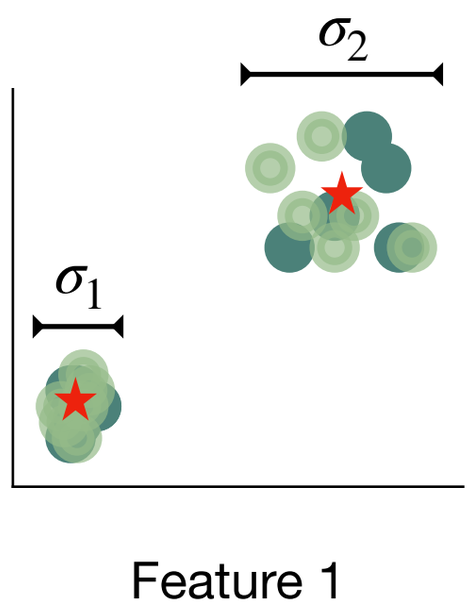
- Matching Cost — MSE of p_T, η, ϕ
- SA — to high cost
  GGT — to low cost
  GD — good agreement



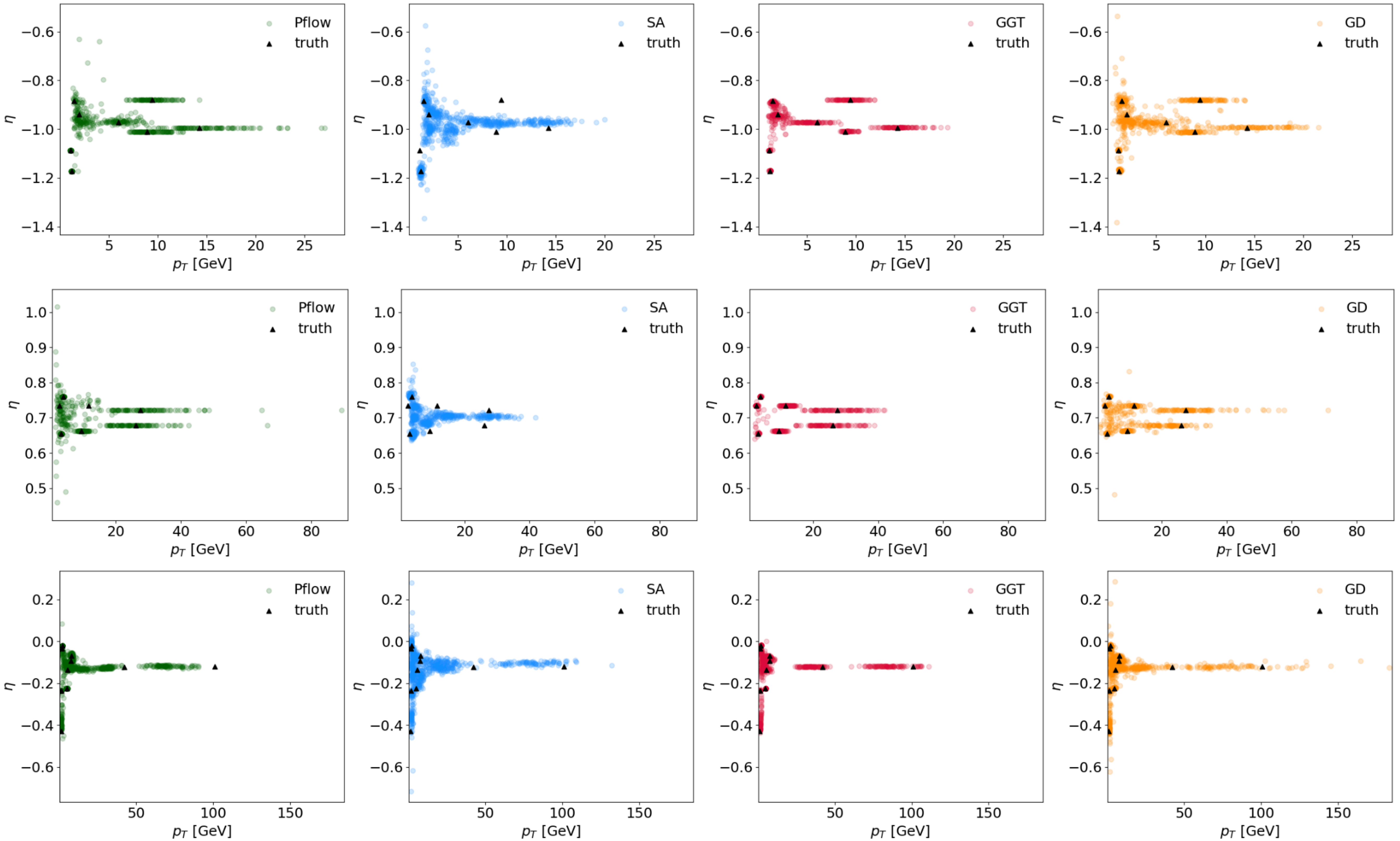
Resolution



- For each truth particle take σ of all associated replicas
- Difficulties at high p_T



Event displays



Summary

- 3 approaches for a conditional end-to-end generative model

  Slot-Attention, Graph Diffusion, Graph-to-Graph Translation

- Goal to reconstruct constituents and model detector resolution

- New models show significant improvement w.r.t. the original

- GGT work in progress — move it away from the truth