Learning the Geometry of Collider Events with Metric Aware Deep Sets

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Motivation

- Collider events are represented as an **energy flow**

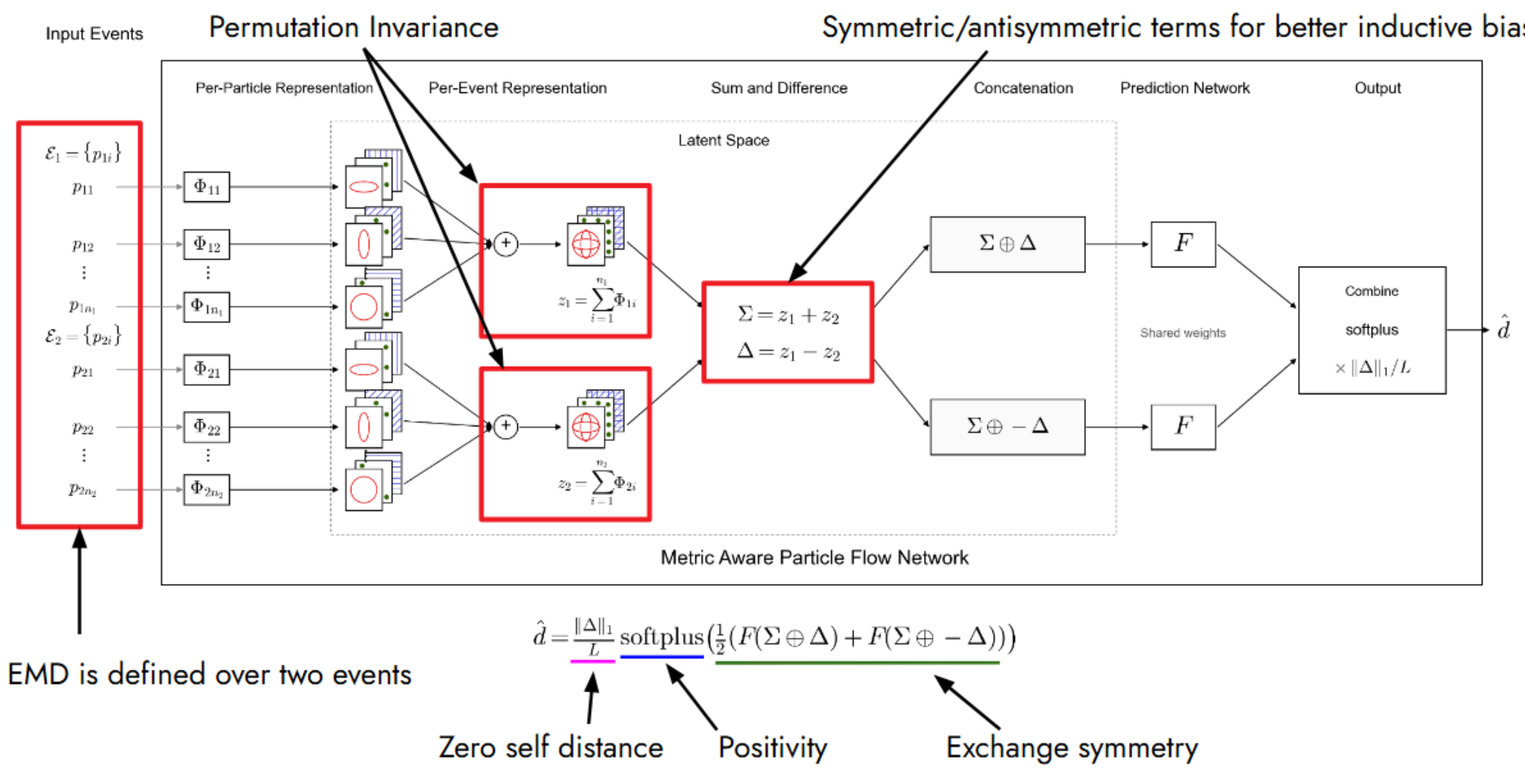
$$\mathcal{E} = \sum_{i=1}^{M} E_i \delta(x - \vec{x}) \tag{1}$$

- Optimal transport between energy flows is the **Energy Movers Distance** (EMD) [1]
  - Infrared and collinear (IRC) safe
  - but $\mathcal{O}(M^3 \log M)$ scaling with particle multiplicity

$$\mathrm{EMD}(\mathcal{E}, \mathcal{E}') = \min \sum_{i=1}^{M} \sum_{j=1}^{M'} f_{ij} \left(\frac{\theta_{ij}}{R}\right)^{\beta} + |\Delta E_{\mathrm{total}}| \tag{2}$$

- EMD calculations are computationally intractable for large datasets with complicated final states!
  - Solution: replace numerical solver with ML surrogate!

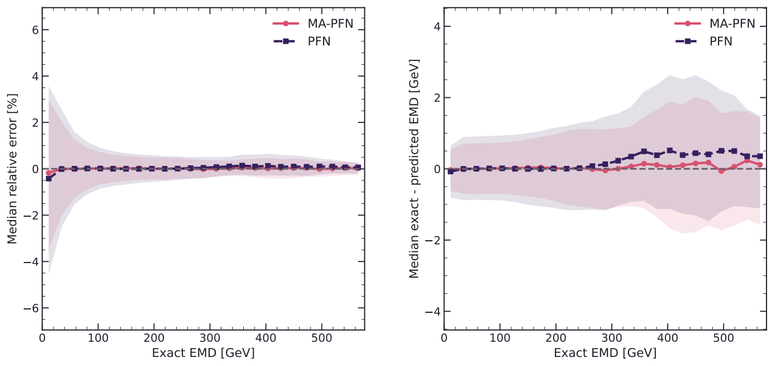
Metric Aware Particle Flow Network (MA-PFN)



MA-PFN is a multisets neural network [2] with zero self distance, positivity, and exchange symmetry enforced.

We compare MA-PFN performance to baseline PFN [3] and other EMD computation methods.

Accuracy

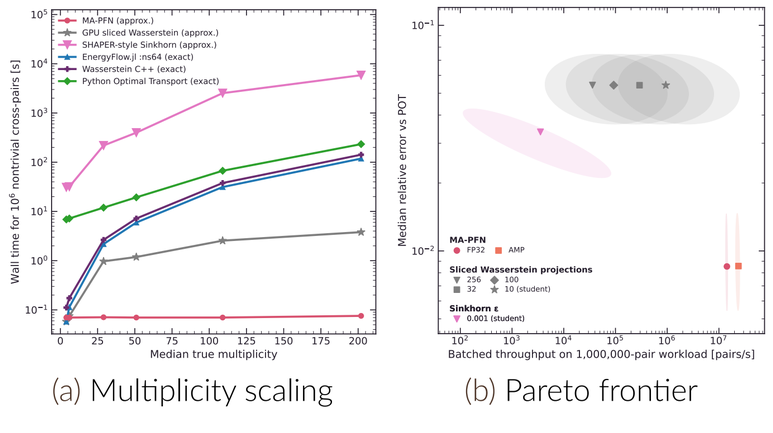


(a) Relative residual (b) Residual

Figure 1. Predictive residuals vs exact EMD. Curves show binned median and central 68%.

- MA-PFN is **more accurate** for large EMDs
- MA-PFN is more accurate and has **smaller error** for small EMDs

Timing Study



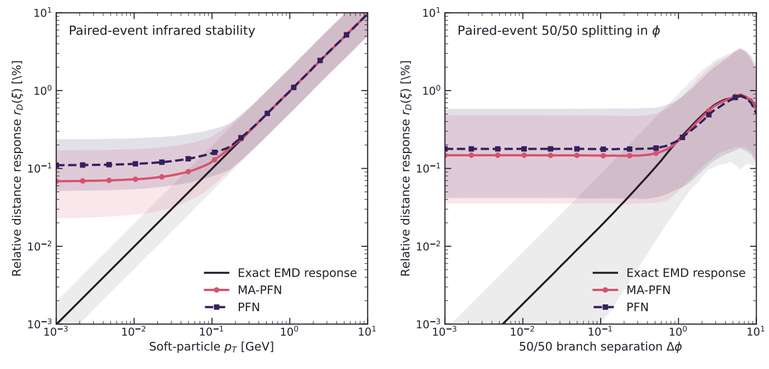
(a) Multiplicity scaling (b) Pareto frontier

Figure 2. Left: Timing study over varied multiplicities with 10^6 event pairs for several computation methods. Right: Accuracy-throughput Pareto frontier with median and dispersion over 10 trials.

- Multiplicity-dependent encoding is only done **once per event**. Then all distance computations are multiplicity-independent
- The MA-PFN scales best with multiplicity
- MA-PFN sits on the accuracy-throughput Pareto frontier

Infrared and Collinear (IRC) Safety

- IRC safety ensures that an observable is perturbatively calculable [4, 5]
- IRC safety ↔ **EMD is continuous on event space** [1]
- We introduce soft/collinear distortion and measure response as function of distortion
  - Soft distortion: Introduce new particle with transverse momentum (p_T)
  - Collinear distortion: Evenly split highest p_T particle into two daughters with angular separation $\Delta\phi$

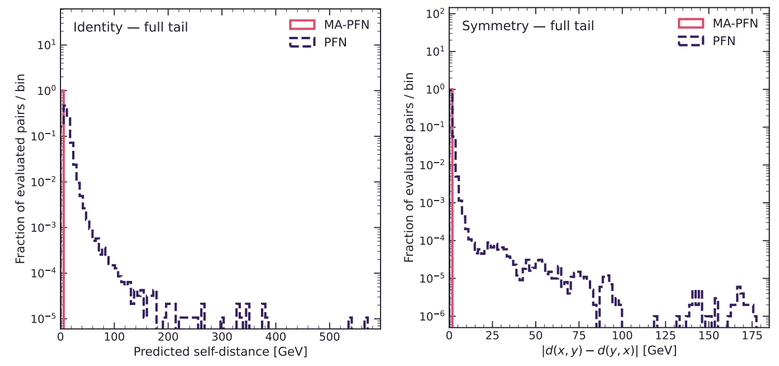


(a) Soft response (b) Collinear response

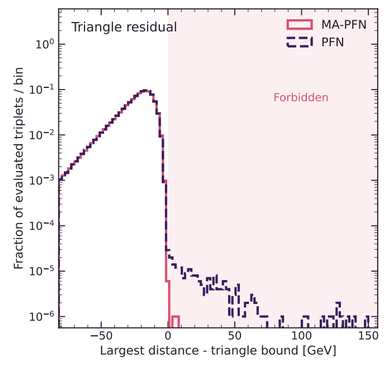
Figure 3. Relative response for 10^4 event pairs with soft/collinear distortion. Median and central 68% shown.

- In the exact soft/collinear limit both models plateau away from exact response
- Models are learning **'discrete' approximation** of event phase space
- But MA-PFN plateaus lower than PFN → **'higher resolution' approximation**

Metric Properties



(a) Identity (b) Exchange symmetry



(c) Triangle inequality

Figure 4. Metric-property benchmarks for the MA-PFN and matched baseline PFN.

- Identity and exchange symmetry are badly broken by PFN
- Triangle inequality is not enforced in either model but is **better constrained** by MA-PFN

Conclusion and Future Work

- MA-PFN is a multisets network with **enforced metric properties** to predict EMDs
- MA-PFN has **best multiplicity-scaling** and sits on accuracy-throughput Pareto frontier
- MA-PFN is **approximately IRC safe** and constrains triangle inequality better than PFN
- **Next**: extend MA-PFN to be exactly IRC safe
- **Next**: apply MA-PFN to realistic physics task

References

[1] Patrick T. Komiske, Eric M. Metodiev, and Jesse Thaler. Metric Space of Collider Events. *Phys. Rev. Lett.*, 123(4):041801, 2019.

[2] Puoya Tabaghi and Yusu Wang. Universal representation of permutation-invariant functions on vectors and tensors. In Claire Vernade and Daniel Hsu, editors, *Proceedings of The 35th International Conference on Algorithmic Learning Theory*, volume 237 of *Proceedings of Machine Learning Research*, pages 1134–1187. PMLR, 25–28 Feb 2024.

[3] Patrick T. Komiske, Eric M. Metodiev, and Jesse Thaler. Energy Flow Networks: Deep Sets for Particle Jets. *JHEP*, 01:121, 2019.

[4] Toichiro Kinoshita. Mass Singularities of Feynman Amplitudes. *Journal of Mathematical Physics*, 3(4):650–677, July 1962.

[5] T. D. Lee and M. Nauenberg. Degenerate Systems and Mass Singularities. *Physical Review*, 133(6B):B1549–B1562, March 1964.

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