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Out-of-Distribution Multi-set Generation with Context Extrapolation for Amortized Simulation and Inverse Problems

Friday 2 February 2024 09:20 (20 minutes)

Addressing the challenge of Out-of-Distribution (OOD) multi-set generation, we introduce YonedaVAE, a novel equivariant deep generative model inspired by Category Theory, motivating the Yoneda-Pooling mechanism. This approach presents a learnable Yoneda Embedding to encode the relationships between objects in a category, providing a dynamic and generalizable representation of complex relational data sets. YonedaVAE introduces a self-distilled set generator, capable of zero-shot creating sets with variable inter-category and intra-category cardinality, facilitated by the new Adaptive Top-p Sampling. We demonstrate that YonedaVAE can produce new point clouds with cardinalities well beyond the training data and achieve context extrapolation. Trained on low luminosity ultra-high-granularity data of PXD at Belle II, YonedaVAE can generate high luminosity valid signatures with the correct intra-event correlation without exposure to similar data during training. Being able to generalize to out-of-distribution samples, YonedaVAE stands as a valuable method for extrapolative multi-set generation tasks in scientific discovery, including de novo protein design, Drug Discovery, and simulating geometry-independent detector responses beyond experimental limits.

Would you like to be considered for an oral presentation?

Yes

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Track Classification: 3 ML for simulation and surrogate model : Application of Machine Learning to simulation or other cases where it is deemed to replace an existing complex model