Learned Aggregations Functions for Graph Neural Networks

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Background

Many problems can be modeled using graphs. There, we have nodes representing entities and edges between nodes representing relationships between nodes. Graph neural networks (GNNs) offer a neat way to do machine learning on graph data structures. Since there is no order in a graph, a central concept is *permutation invariance*, meaning it should not matter in which order we process the nodes. This invariance plays a role within the aggregation function within the message passing in GNNs. The aggregation function is thus a mean, max, or sum (Bishop and Bishop, 2023). In this project, we want to explore learned aggregation functions. Specifically, we are interested in using a generalized f-mean, where we use an invertible neural network (see, *e.g.*, Papamakarios et al. (2021)) for f of which we learn the parameters.

Research questions

- Is the generalized f-mean beneficial as a learned aggregation function in graph neural networks?
- What type of invertible neural network is suited best to model f?

Eligibility requirements

- Sound knowledge of machine learning (very good grades in relevant courses)
- Very good programming skills in Python
- Knowledge of Graph Neural Networks is extremely beneficial
- Knowledge of frameworks such as PyTorch/JAX is beneficial

Please attach your CV and transcripts when applying.

References

Bishop, C. M. and Bishop, H. (2023). *Deep learning: Foundations and concepts*. Springer Nature.

Papamakarios, G., Nalisnick, E., Rezende, D. J., Mohamed, S., and Lakshminarayanan, B. (2021). Normalizing flows for probabilistic modeling and inference. *Journal of Machine Learning Research*, 22(57):1–64.