

Equivariant Subgraph Aggregation Networks

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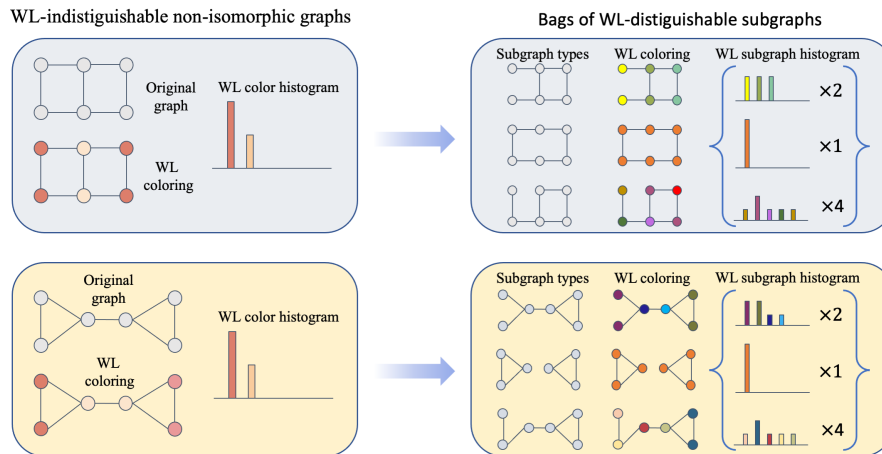


Figure 1: We present a provably expressive graph learning framework based on representing graphs as bags of subgraphs and processing them with an equivariant architecture, composed of GNNs and set networks. **Left panel:** A pair of graphs not distinguishable by the WL test. **Right panel:** The corresponding bags (multisets) of all edge-deleted subgraphs, which can be distinguished by our framework.

Message-passing neural networks (MPNNs) are the leading architecture for deep learning on graph-structured data, in large part due to their simplicity and scalability. Unfortunately, it was shown that these architectures are limited in their expressive power [2].

This work proposes a novel framework called Equivariant Subgraph Aggregation Networks (ESAN) to address this issue. Our main observation is that while two graphs may not be distinguishable by an MPNN, they often contain distinguishable subgraphs. Thus, we propose to represent each graph as a bag (multiset) of subgraphs derived by some predefined policy, and to process it using a suitable equivariant architecture. To deal with the increased computational cost, we propose a subgraph sampling scheme, which can be viewed as a stochastic version of our framework.

We develop novel variants of the 1-dimensional Weisfeiler-Leman (1-WL) [1] test for graph isomorphism, and prove lower bounds on the expressiveness of ESAN in terms of these new WL variants. We further prove that our approach increases the expressive power of both MPNNs and more expressive architectures. Moreover, we provide theoretical results that describe how design choices such as the subgraph selection policy and equivariant neural architecture affect our architecture’s expressive power.

A comprehensive set of experiments on real and synthetic datasets demonstrates that our framework improves the expressive power and overall performance of popular GNN architectures.

Joint work with: Beatrice Bevilacqua, Fabrizio Frasca, Derek Lim, Balasubramaniam Srinivasan, Chen Cai, Gopinath Balamurugan, Michael M. Bronstein.

References

- [1] B. Weisfeiler and A. Leman. The reduction of a graph to canonical form and the algebra which appears therein. *NTI, Series*, 2(9):12–16, 1968.
- [2] K. Xu, W. Hu, J. Leskovec, and S. Jegelka. How powerful are graph neural networks? In *International Conference on Learning Representations*, 2019.