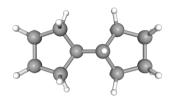
SpeqNets:

Sparsity-aware Permutation-equivariant Graph Networks

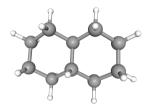
Christopher Morris, Gaurav Rattan, Sandra Kiefer, Siamak Ravanbakhsh

RWTH Aachen University, RWTH Aachen University, MPI SWS, McGill University and Quebec AI Institute (Mila)

Expressivity of Graph Neural Networks



(a) Bicyclopentyl



(b) Decalin

Insight

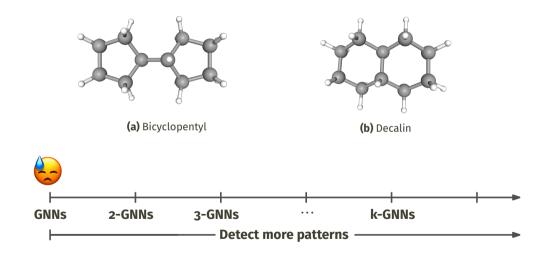
Any possible **GNN** architecture **misses crucial patterns** in the data!

C. Morris, M. Ritzert, M. Fey, W. L. Hamilton, J. Eric Lenssen, G. Rattan, and M. Grohe. "Weisfeiler and Leman Go Neural: Higher-order Graph Neural Networks". In: AAAI. 2019

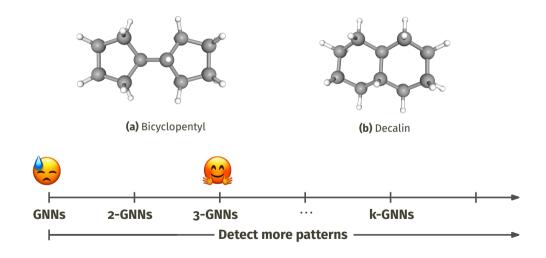
K. Xu, W. Hu, J. Leskovec, and S. Jegelka. "How Powerful are Graph Neural Networks?" In: ICLR. 2019

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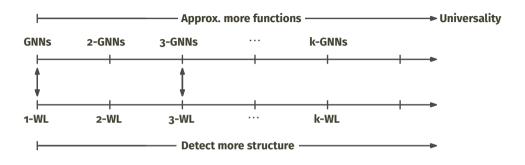
A hierarchy of more powerful models



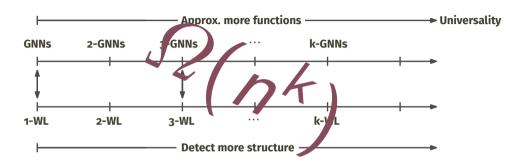
A hierarchy of more powerful models



A hierarchy of more powerful algorithms



A hierarchy of more powerful algorithms



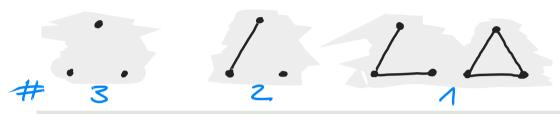
Problem

Exponential dependence on k, *i.e.*, space complexity $\Omega(n^k)$.

C. Morris, G. Rattan, and P. Mutzel. "Weisfeiler and Leman Go Sparse: Higher-order Graph Embeddings". In: *NeurIPS*. 2020
C. Morris, M. Ritzert, M. Fey, W. L. Hamilton, J. Eric Lenssen, G. Rattan, and M. Grohe. "Weisfeiler and Leman Go Neural: Higher-order Graph Neural Networks". In: *AAAI*. 2019
W. Azizian and M. Lelarge. "Characterizing the Expressive Power of Invariant and Equivariant Graph Neural Networks". In: *ICLR*.

w. Azizian and M. Letarge. Characterizing the expressive Power of Invariant and Equivariant Graph Neural Networks . III. ICER 2021

Let's go more sparse: Trading off expressivity and scalability



(k,s)-LWL

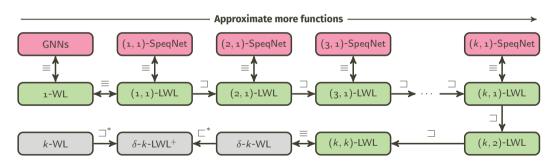
• Considers only k-tuples inducing **subgraphs** with at most s **connected components**

$$V(G)_s^k = \{ \mathbf{v} \in V(G)^k \mid \#\mathsf{com}(G[\mathbf{v}]) \le s \}$$

- Uses neighborhood of local k-WL [MRM20]
- Running time in $\tilde{\mathcal{O}}(n^s)$ instead of $\Omega(n^k)$

Our contribution: (k, s)-LWL and (k, s)-SpeqNet

A better tradeoff between expressivity and scalability for permutation-equivariant function approximation



I am also looking for PhD students! Come talk to me:)