SpeqNets:

Sparsity-aware Permutation-equivariant Graph Networks

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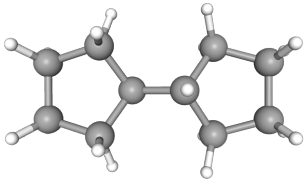
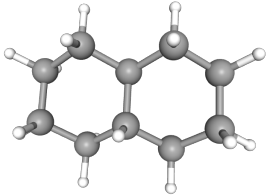
Expressivity of Graph Neural Networks



(a) Bicyclopentyl



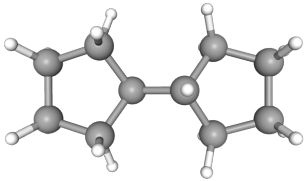
(b) Decalin

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

A hierarchy of more powerful models



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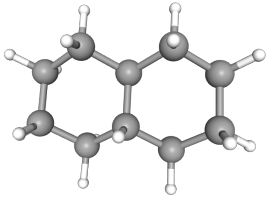
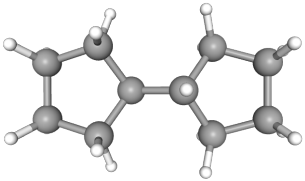


(b) Decalin

A hierarchy of more powerful models



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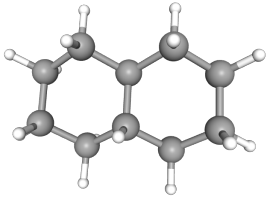
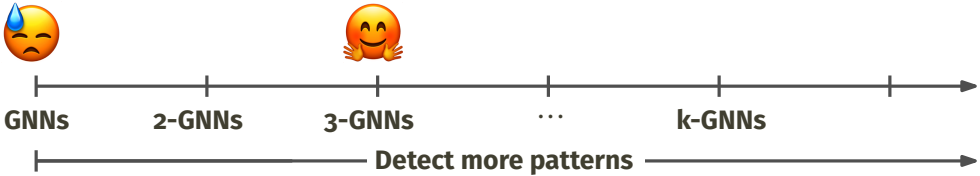
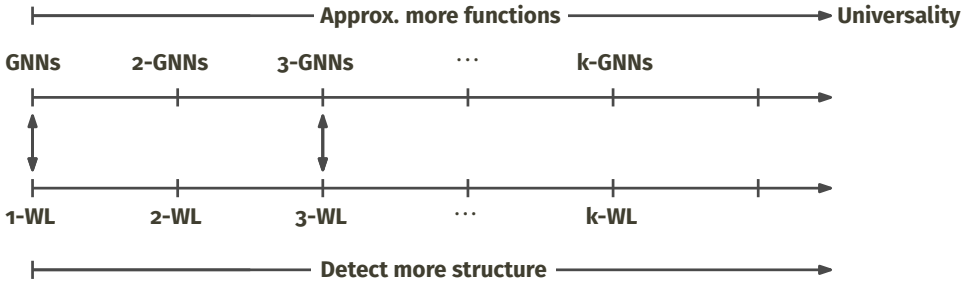


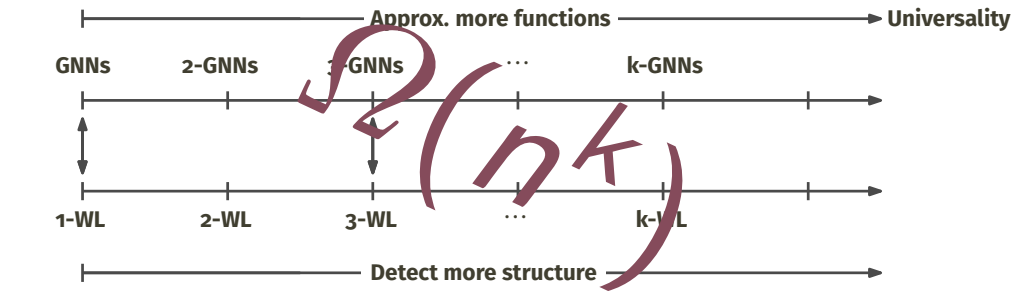
(b) Decalin



A hierarchy of more powerful algorithms



A hierarchy of more powerful algorithms

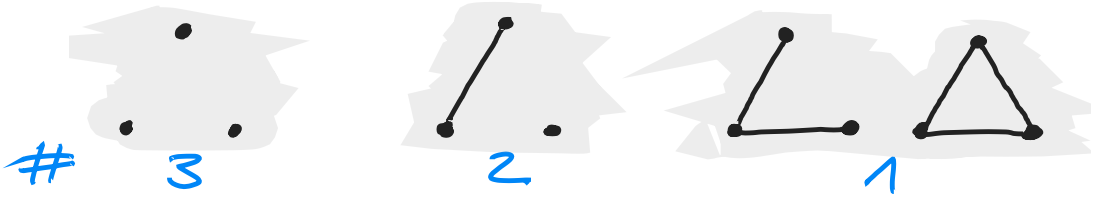


Problem

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*. 2021

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



(k, s)-LWL

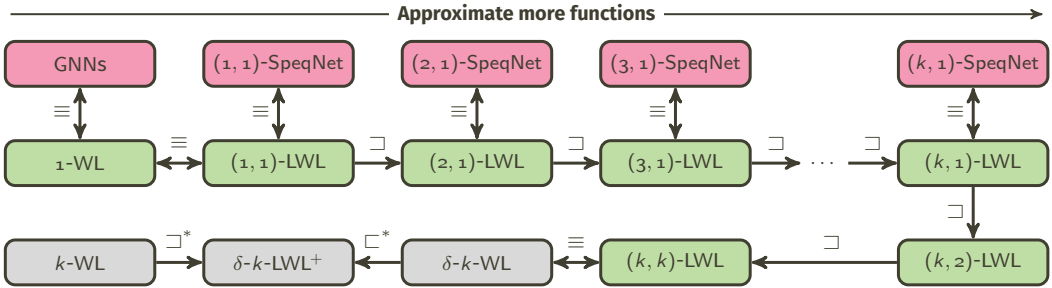
- Considers only k-tuples inducing **subgraphs** with at most s **connected components**

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

- 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 :)