Ordered Subgraph Aggregation Networks

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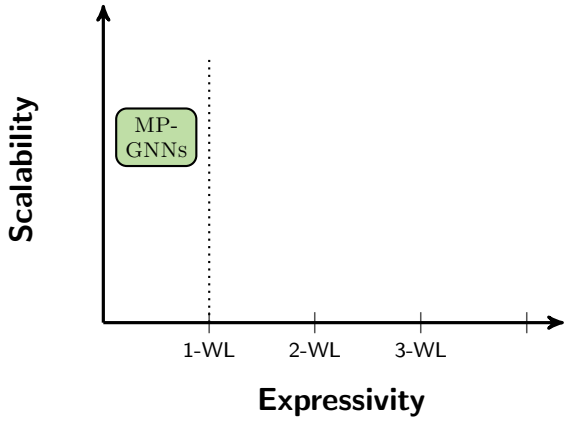
GNNs: Expressivity vs Scalability



[1] 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.* AAAI 2019.

[2] K. Xu et. al. *How Powerful are Graph Neural Networks?* ICLR 2019

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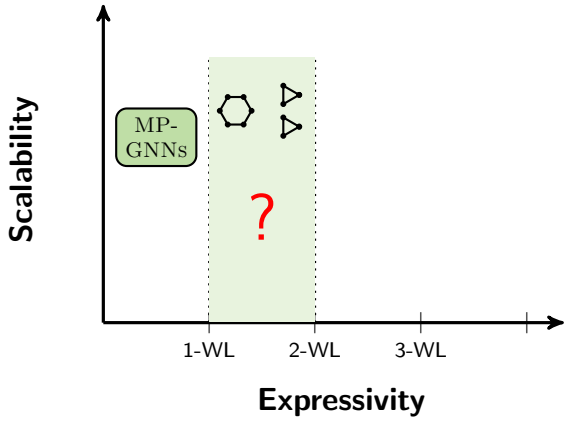

GNN Models

- Sparsity Awareness
- Substructure Counting
- Positional Encoding
- Random Initialization
- ...
- **Subgraph Enhancement**

[1] 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.* AAAI 2019.

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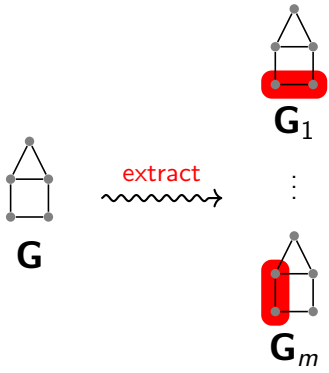
Subgraph-Enhanced GNNs



Methodology

Enrich the graph representation using representations of such derived graphs ...

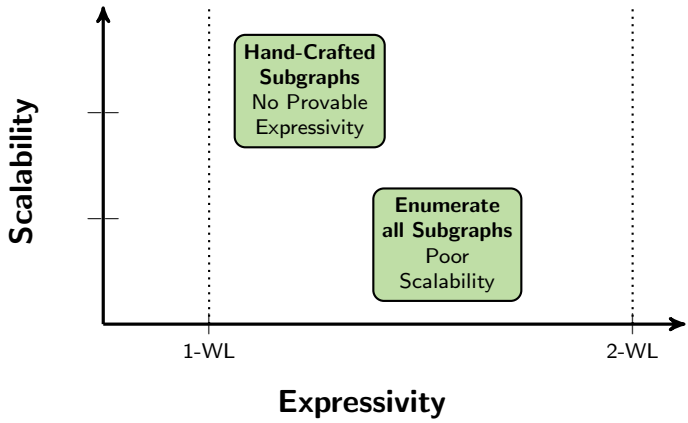
Multiple Avatars

- Reconstruction GNNs [1]
- ESAN [2]
- ID-Aware GNNs
- Nested GNNs
- ...

[1] L. Cotta and C. Morris and B. Ribeiro. *Reconstruction for Powerful Graph Representations*. NeurIPS 2021

[2] B. Bevilacqua et. al. *Equivariant Subgraph Aggregation Networks*. ICLR 2022

Limitations of Subgraph Enhancement



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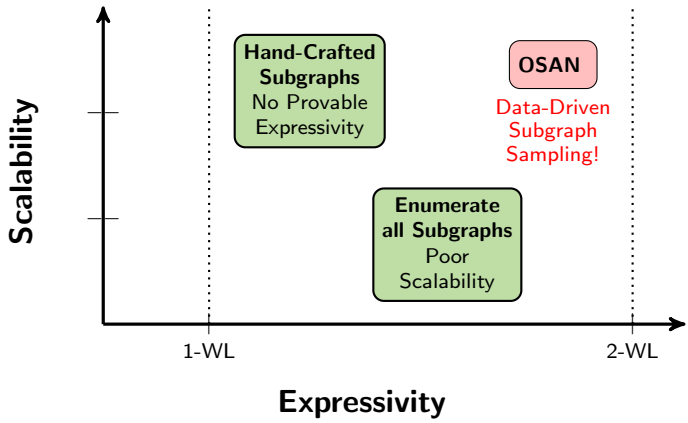
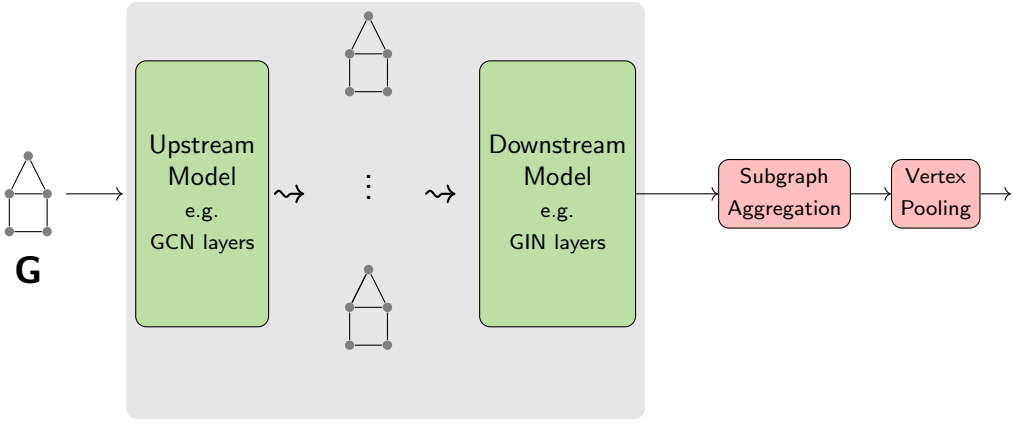


k-OSAN: The Architecture



[1] Niepert et. al. *Implicit MLE: Backpropagating Through Discrete Exponential Family Distributions*. NeurIPS 2021

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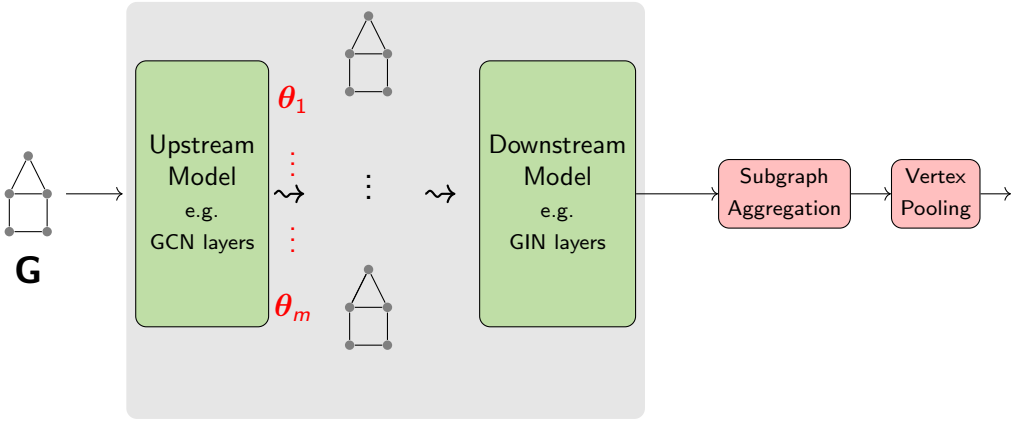

I-MLE[1]

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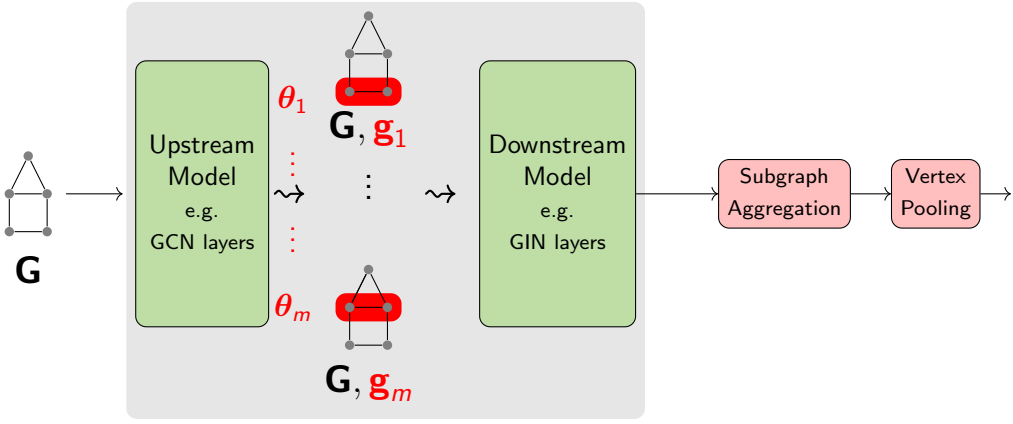

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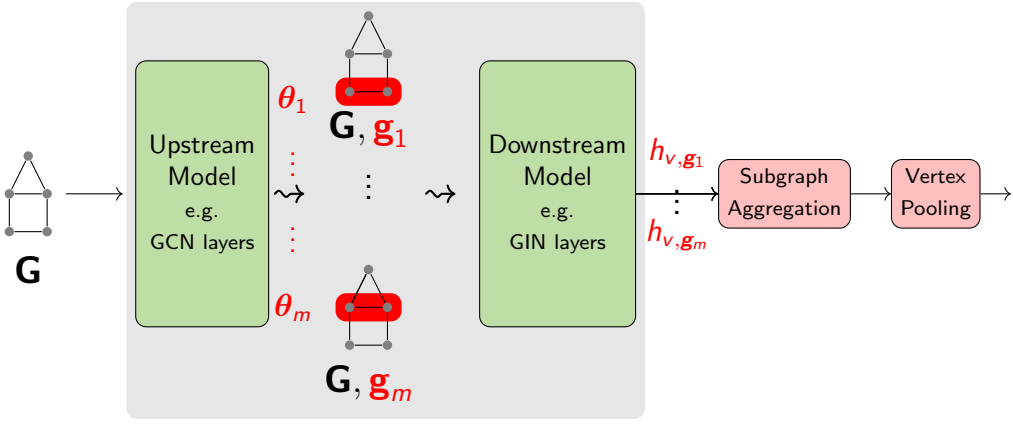

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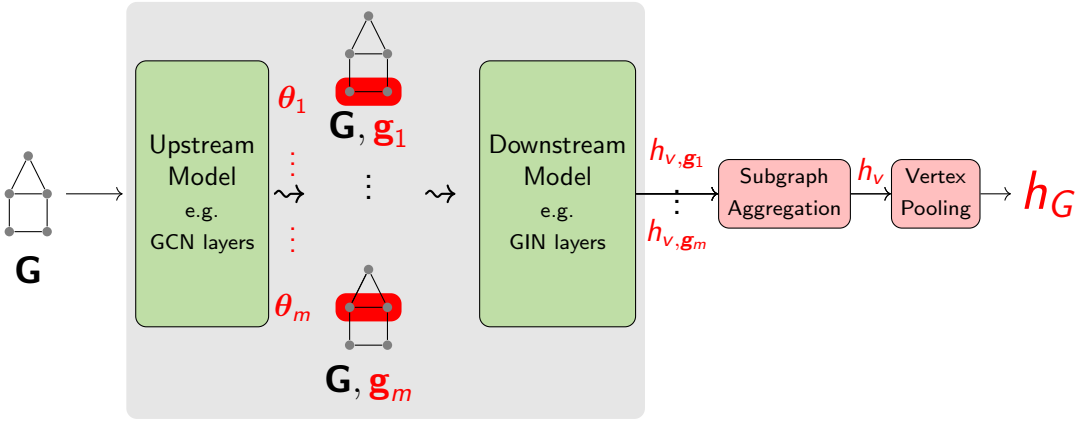

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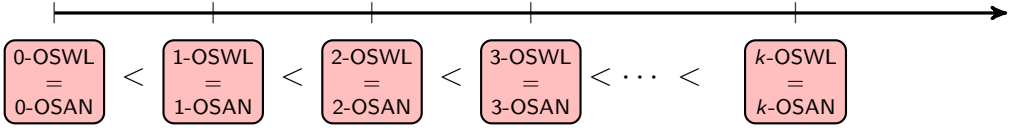
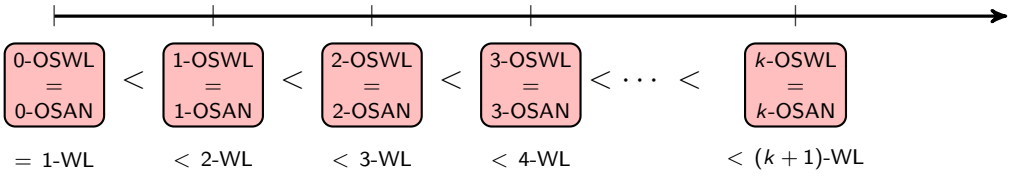
Our Results: The Expressivity Landscape



For $k \geq 1$, k-OSAN form a hierarchy of GNNs with strictly increasing expressive power.

Our Results: The Expressivity Landscape



For every $k \geq 1$, k-OSAN is strictly less powerful than $(k+1)$-WL.

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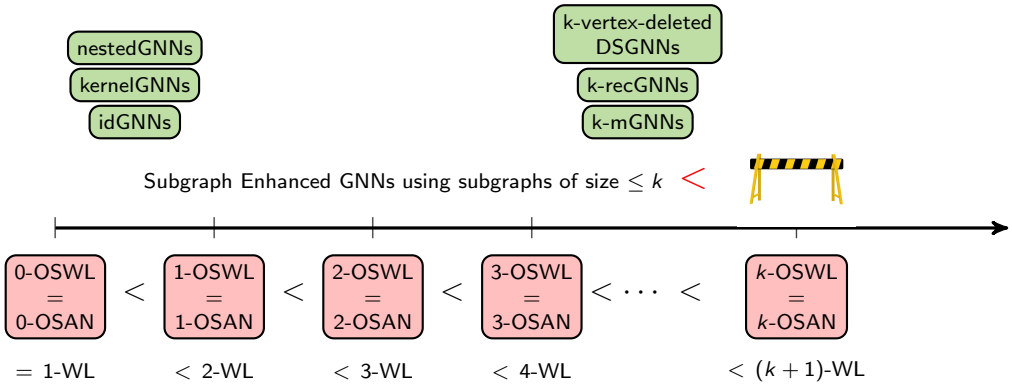
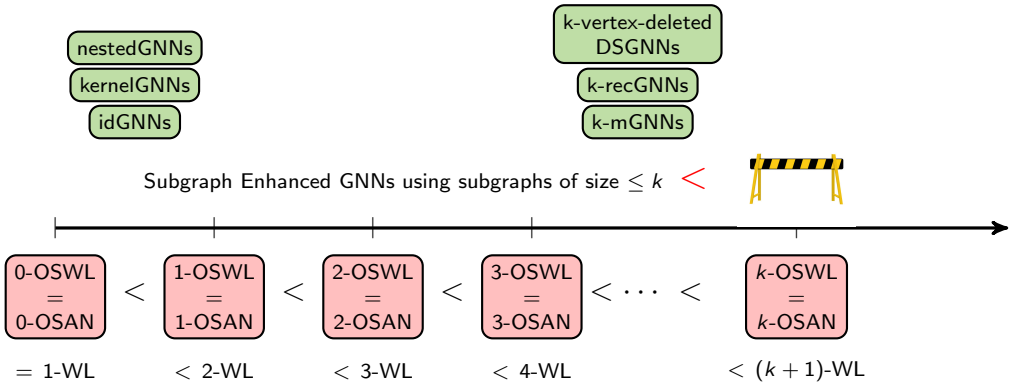


The k-OSAN forms a unified framework for capturing known subgraph-enhanced GNNs.

Our Results: The Expressivity Landscape



Data-driven sampling of subgraphs leads to better generalization than random sampling.

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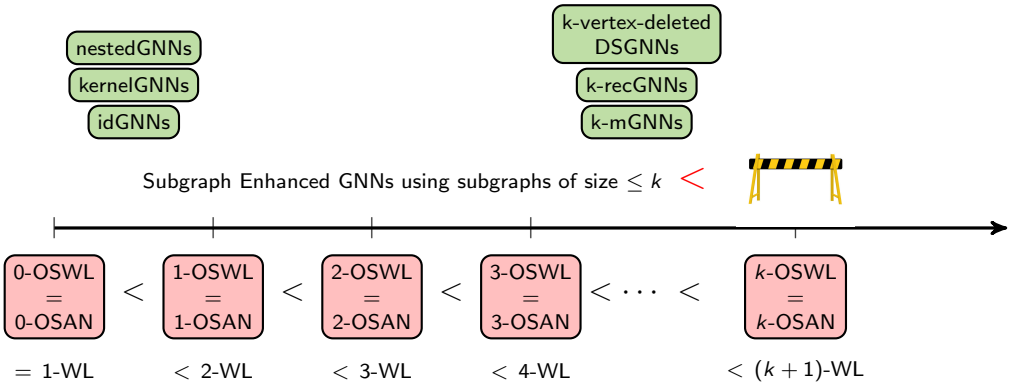

The I-MLE framework can improve the scalability of subgraph-enhanced GNNs.