On the Ability of Graph Neural Networks to Model Interactions Between Vertices

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Joint work with Tom Verbin & Nadav Cohen

Tel Aviv University

Learning on Graphs and Geometry Reading Group

16 January 2023

Outline

Graph Neural Networks (GNNs)

Neural networks purposed for modeling interactions over graph data

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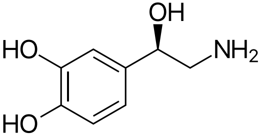
- Molecular data — graph prediction



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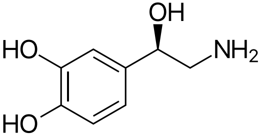

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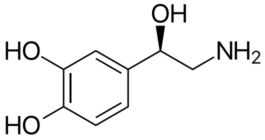

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- Many more applications: recommender systems, ETA prediction,...

Mathematical Theory of GNNs

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Challenge

Develop mathematical theory for GNNs

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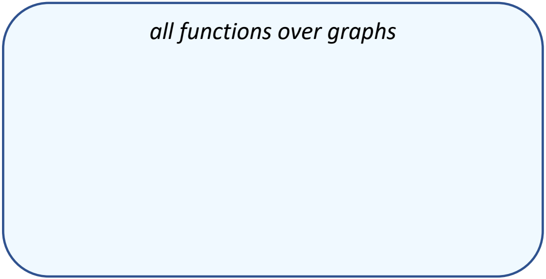

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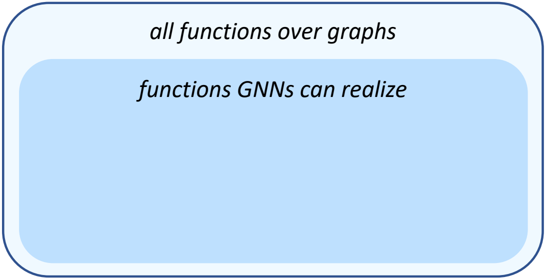

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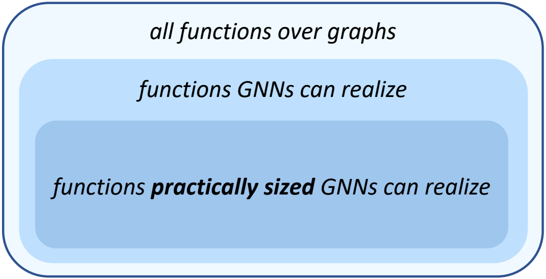

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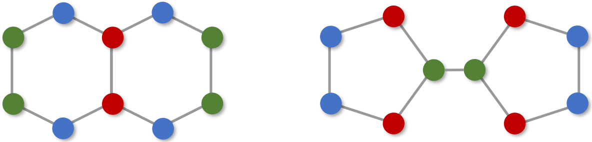
(*e.g.* Xu et al. 2019, Morris et al. 2019, Maron et al. 2019b, Geerts & Reutter 2022)



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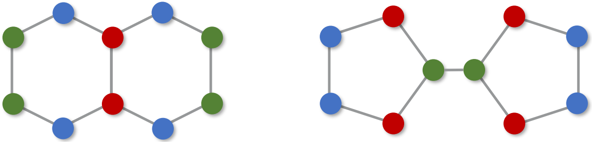

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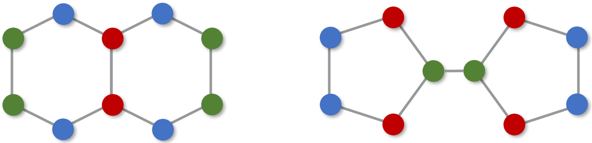

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(3) Computability of graph properties: shortest paths, diameter,...

(e.g. Dehmamy et al. 2019, Garg et al. 2020, Loukas 2020, Chen et al. 2020)

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Question

How do graph structure and GNN architecture affect interactions?

Promo: Our Contributions

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Theory

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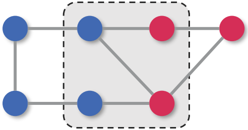
Characterize ability of certain GNNs to model interactions between vertices



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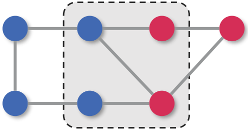
formalized via *separation rank*



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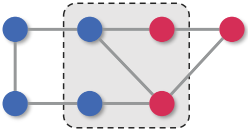

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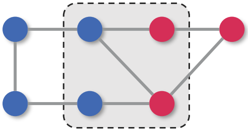

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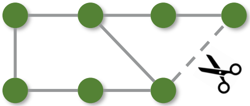
Use theory to derive an *edge sparsification* method preserving interactions



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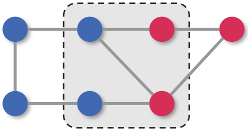

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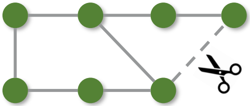

It is simple, efficient, and outperforms alternative methods

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Known measure for interaction modeled across partition of input variables

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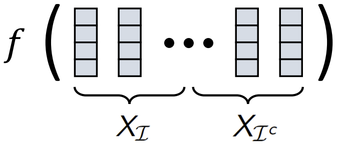
Let $f : (\mathbb{R}^D)^N \to \mathbb{R}$ and subset of variables $\mathcal{I} \subseteq [N]$



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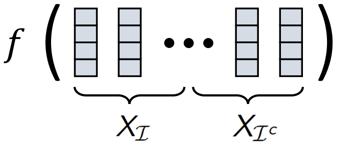

$$\mathrm{sep}(f; \mathcal{I}) := \min R \text{ s.t. } f(X) = \sum_{r=1}^{R} g_r(X_{\mathcal{I}}) \cdot \bar{g}_r(X_{\mathcal{I}^c})$$

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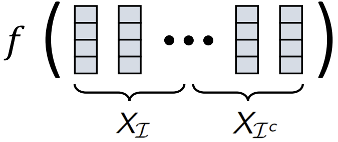

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Higher $\mathrm{sep}(f;\mathcal{I}) \implies$ stronger interaction between $X_{\mathcal{I}}$ and $X_{\mathcal{I}^c}$

Usages of Separation Rank

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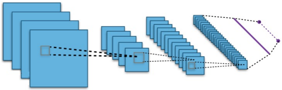
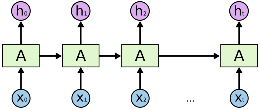
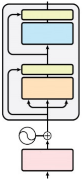
- Analyses of convolutional, recurrent, and self-attention NNs
  (*e.g.* Cohen & Shashua 2017, Levine et al. 2018;2020, **R** et al. 2022)







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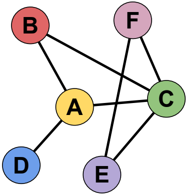

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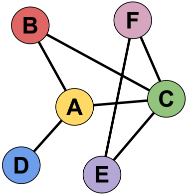

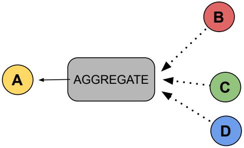

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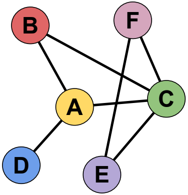

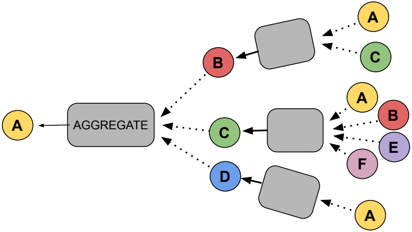

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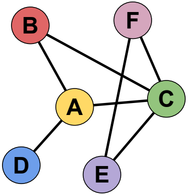

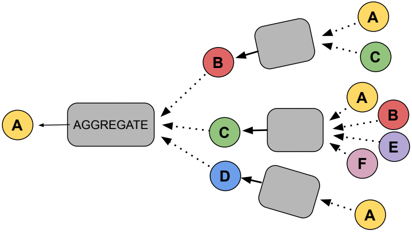

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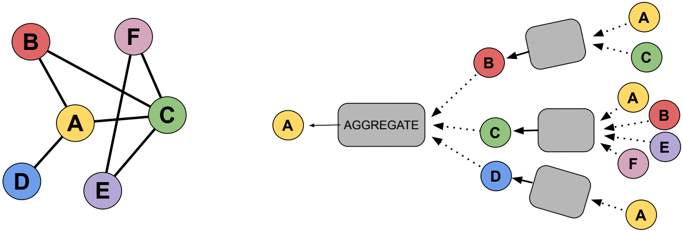

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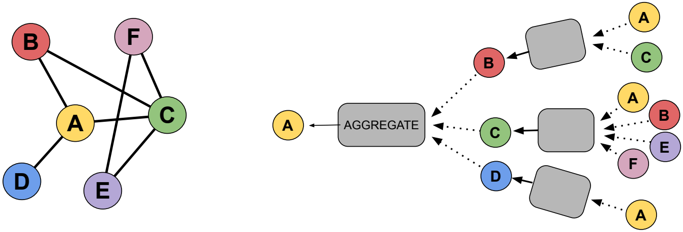

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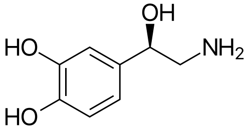

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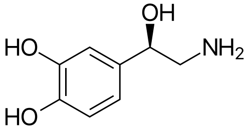

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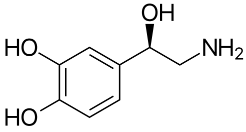

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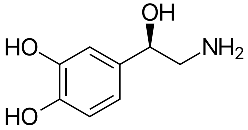

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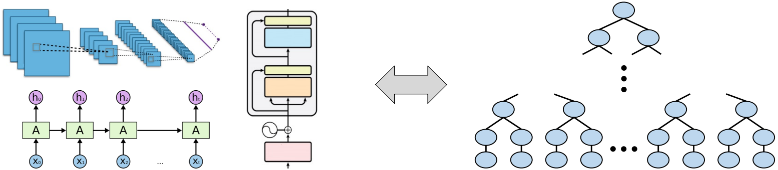

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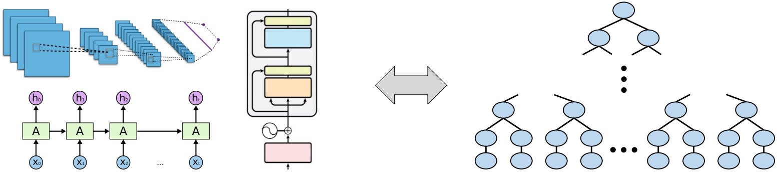

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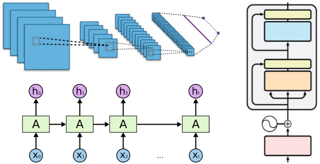

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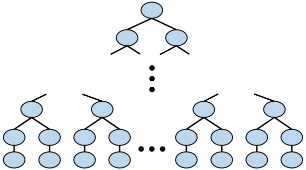

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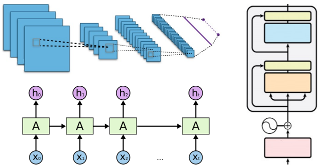

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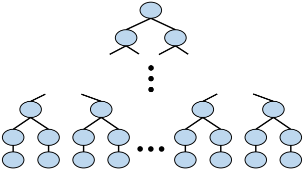

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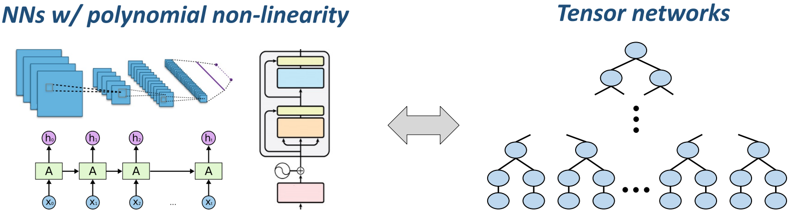

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- Insights and practical tools for more common models

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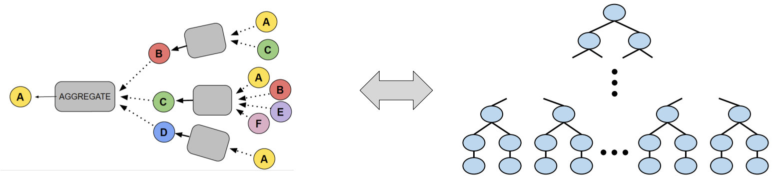

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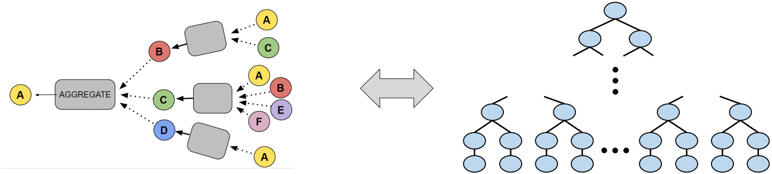

- Variant of the competitive Tensorized GNN (Hua et al. 2022)

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We theoretically study GNNs with product aggregation (polynomial in X)

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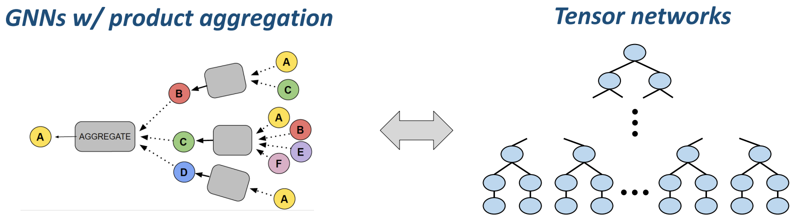

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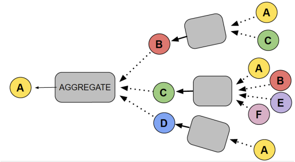

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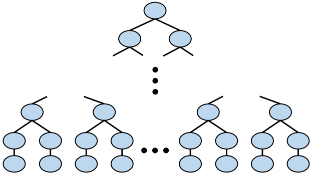

- Variant of the competitive Tensorized GNN (Hua et al. 2022)
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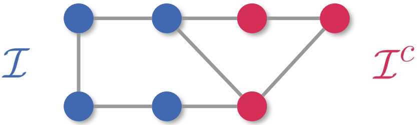
- Based on theory: derive an edge sparsification algorithm

Outline

Walk Index (WI) of a Partition of Vertices



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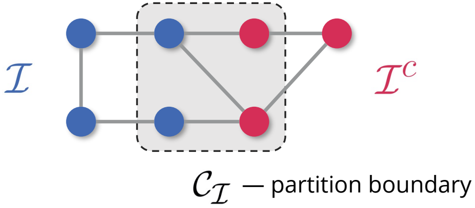

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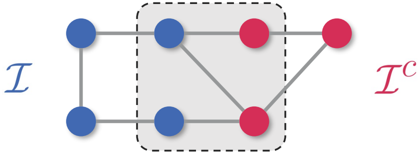

L — GNN depth

$\mathcal{C}_{\mathcal{I}}$ — partition boundary

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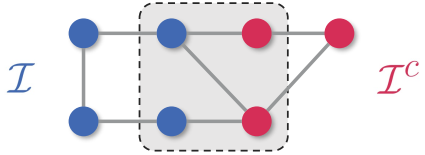

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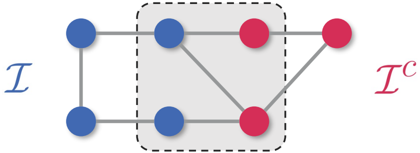

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Main Result: Strength of Interaction $\propto$ Walk Index

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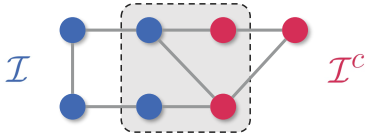
For a depth L GNN with width D_h and $\mathcal{I} \subseteq \mathcal{V}$:



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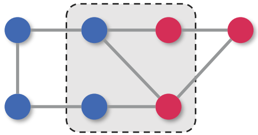
$\mathcal{I}$  $\mathcal{I}^c$

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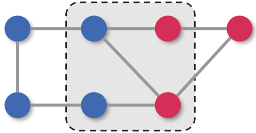
$\mathcal{I}$  $\mathcal{I}^c$

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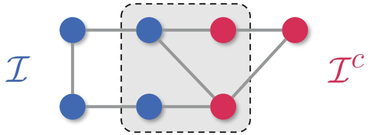
* *Nearly matching lower bounds*



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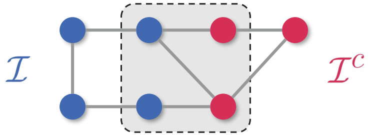

Strength of interaction modeled across partition of vertices is determined by its walk index

Main Result — Proof Sketch

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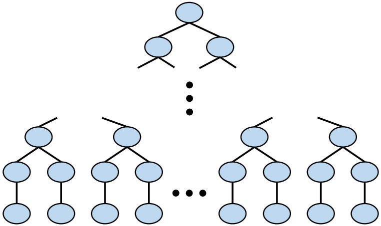

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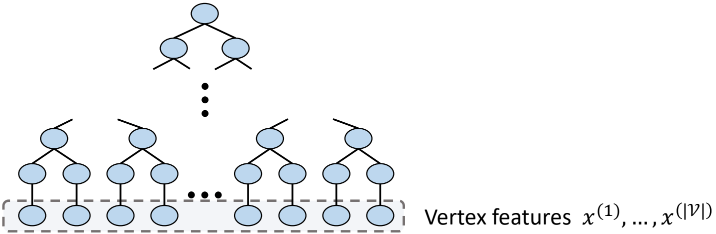

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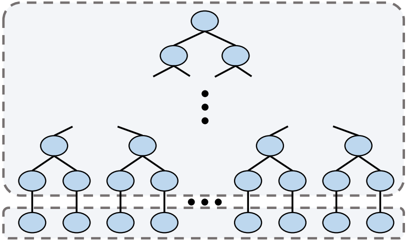

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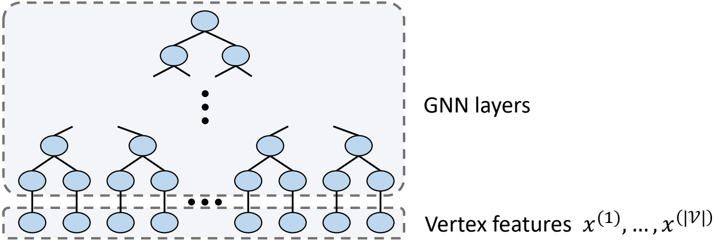

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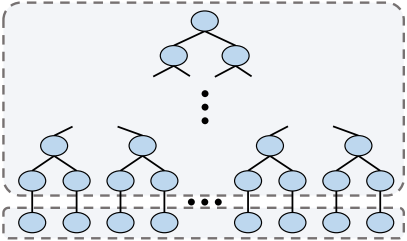

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$\uparrow$

separating leaves in $\mathcal{I}$ from leaves in $\mathcal{I}^c$

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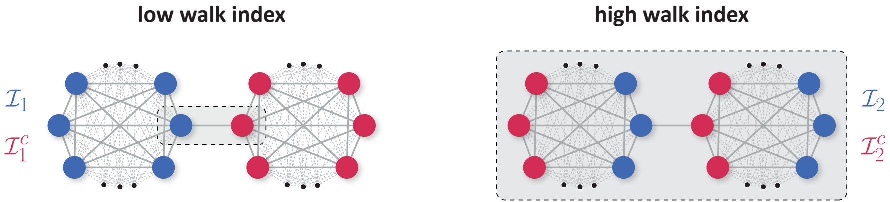

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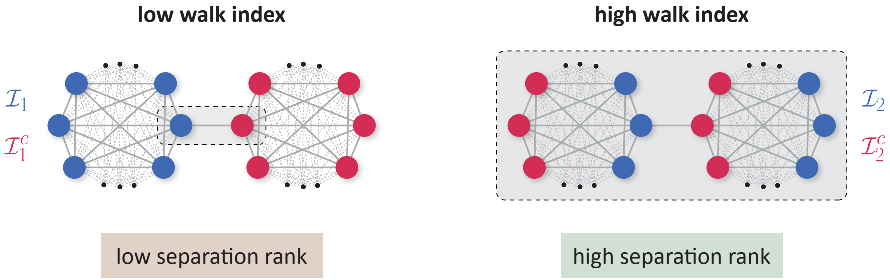

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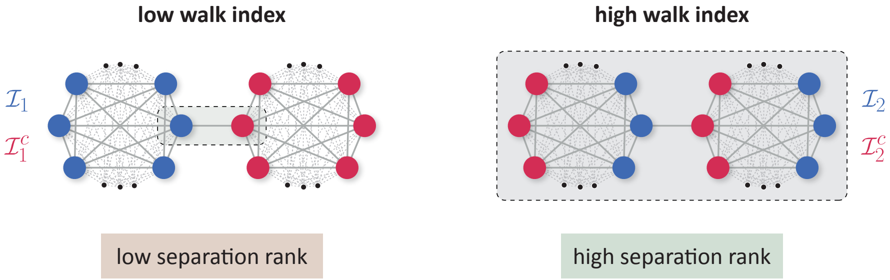

GNNs can model stronger interactions across partitions with higher walk index

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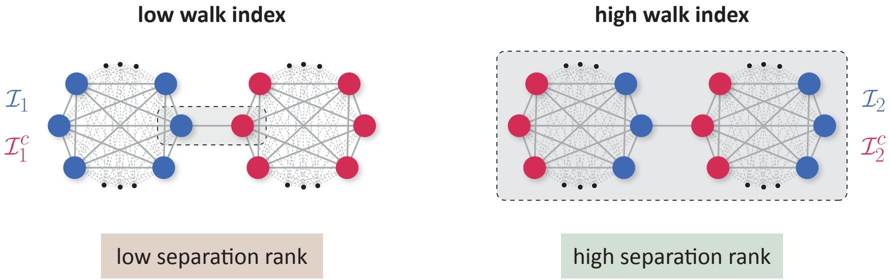

GNNs can model stronger interactions across partitions with higher walk index

Formalizes intuition: more interconnected $\Longrightarrow$ stronger interaction

Empirical Demonstration on GNNs with ReLU

Theory Suggests

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GNNs perform better on datasets requiring strong interactions across higher walk index partitions

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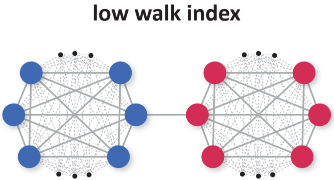

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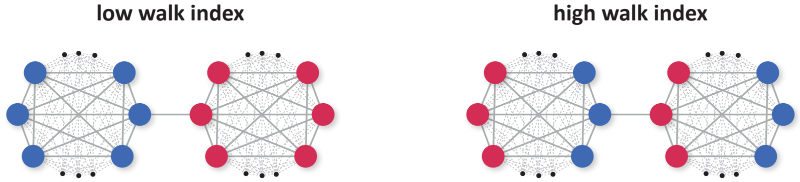

blue vertices: patches of 1st image | red vertices: patches of 2nd image

Empirical Demonstration on GNNs with ReLU

Experiment Results

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Experiment Results

		Partition Walk Index	
		Low	High
GCN	Train	70.4 ± 1.7	$\mathbf{81.4} \pm 2.0$
	Test	52.7 ± 1.9	$\mathbf{66.2} \pm 1.1$
GAT	Train	82.8 ± 2.6	$\mathbf{88.5} \pm 1.1$
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Empirical Demonstration on GNNs with ReLU

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In accordance with our theory:

GNNs perform better on tasks entailing strong interactions across partitions with higher walk index

Outline

1. Expressivity in Graph Neural Networks (GNNs)
2. Theory: Quantifying Ability of GNNs to Model Interactions
   - Formalizing Interaction via Separation Rank
   - Analyzed GNN Architecture
   - Characterizing Strength of Modeled Interaction
3. Application: Expressivity Preserving Edge Sparsification
4. Conclusion

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Our theory $\implies$ simple & effective recipe for pruning edges

General Walk Index Sparsification Scheme

Theory: walk index of $\mathcal{I} \subseteq \mathcal{V}$ key for modeling interaction across $\mathcal{I}, \mathcal{I}^c$

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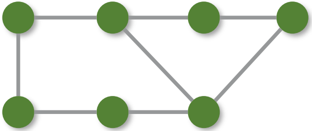

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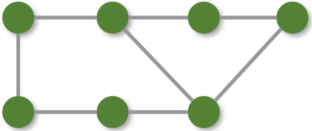

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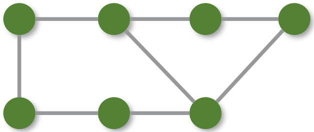

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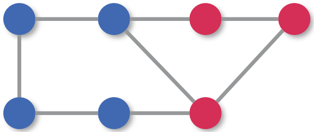

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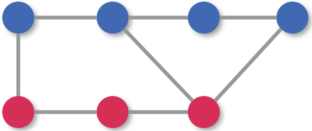

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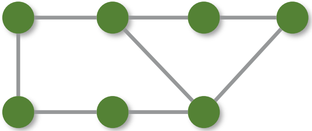

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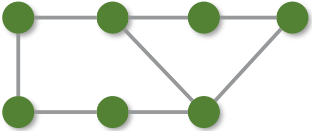

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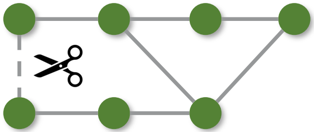

$s_1 =$

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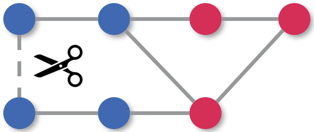

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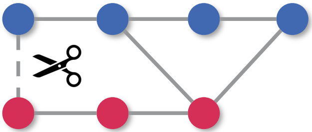

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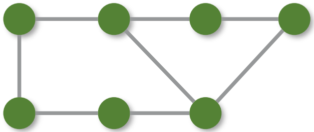

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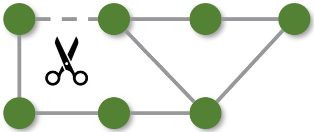

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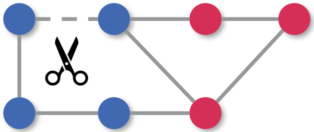

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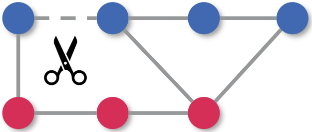

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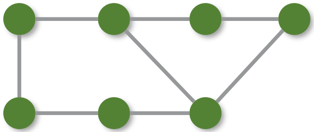

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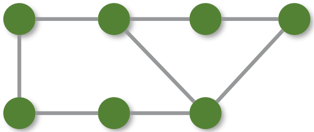

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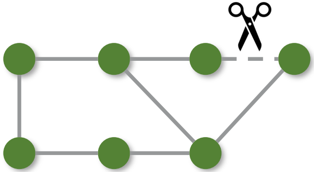

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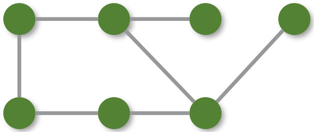

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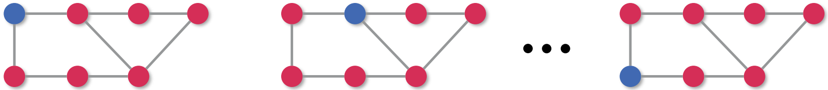

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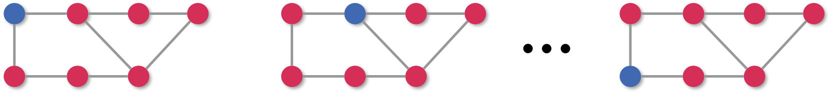

- Order tuples by minimal entry, breaking ties using second smallest,...

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(break ties via $\max\{\deg(i), \deg(j)\}$)

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Compare edge sparsification methods over standard benchmarks

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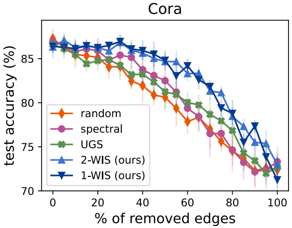

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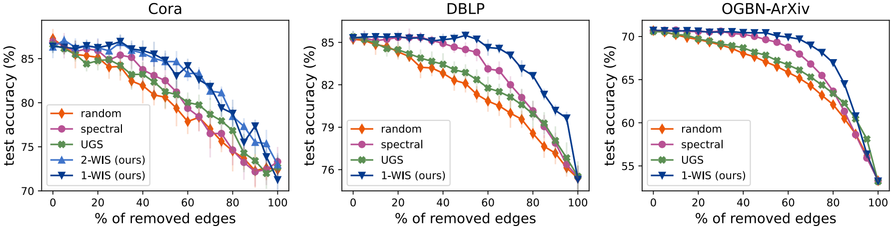

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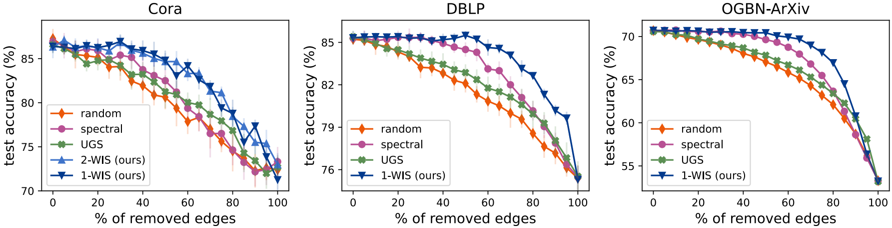

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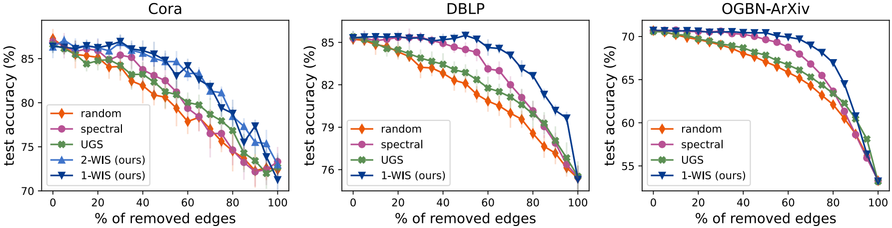

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Code: `https://github.com/noamrazin/gnn_interactions`

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Thank You!

Work supported by:
Apple Scholars in AI/ML PhD fellowship, Google Research Scholar Award, Google Research Gift, the Yandex Initiative in Machine Learning, the Israel Science Foundation (grant 1780/21), Len Blavatnik and the Blavatnik Family Foundation, Tel Aviv University Center for AI and Data Science, and Amnon and Anat Shashua.