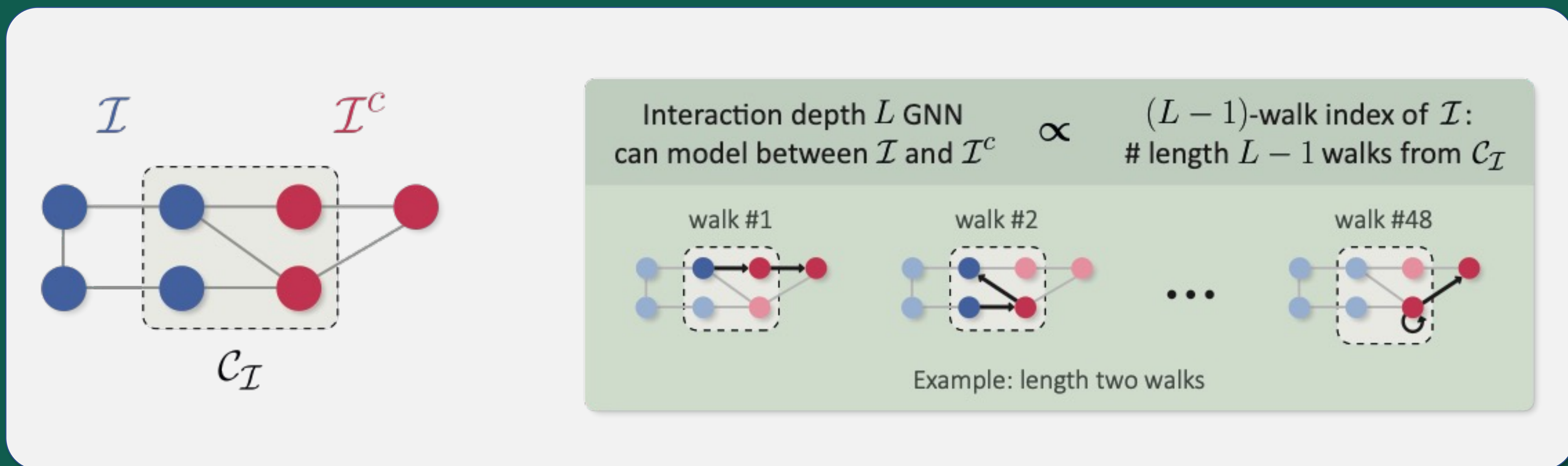
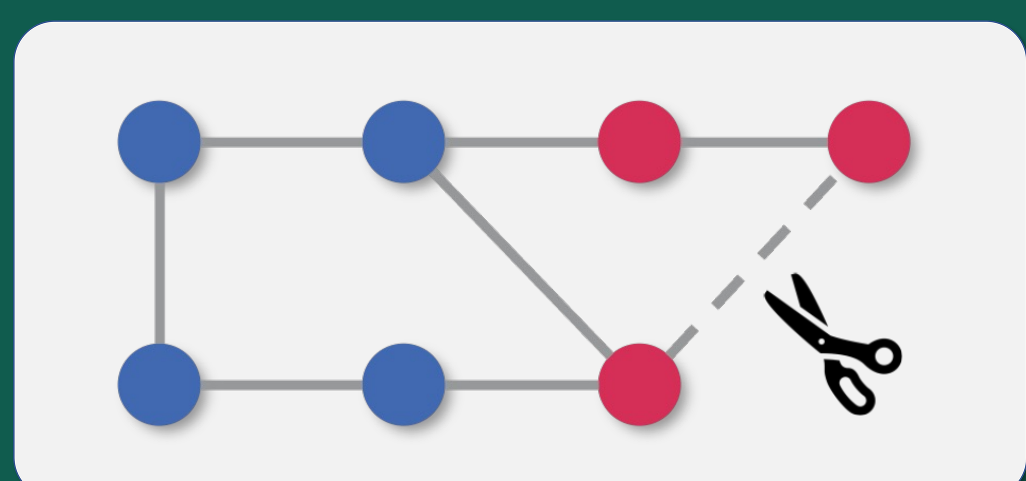
We **quantify the ability** of **Graph Neural Networks** to **model interactions** between vertices



Our theory leads to a **simple & efficient edge sparsification** algorithm that **outperforms** alternative methods



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

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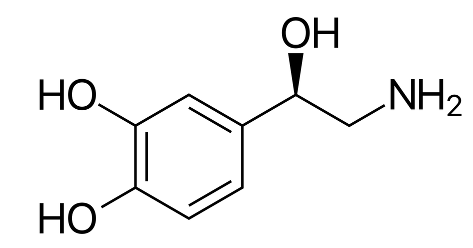
link to paper

1) Expressivity in Graph Neural Networks (GNNs)

GNNs are purposed for **modeling interactions between vertices**

Molecular Data – Graph Prediction



Social Networks – Vertex Prediction

Fundamental Question: ***expressivity*** — which functions can GNNs realize?

Existing Analyses of Expressivity: mostly focus on

Distinguishing non-isomorphic graphs *(e.g. Xu et al. 2019, Morris et al. 2019)*

Computability of graph properties *(e.g. Chen et al. 2020, Garg et al. 2020)*

Limitations of Existing Analyses

(1) Often treat asymptotic regimes of unbounded width or depth

(2) No formalization for ability of GNNs to model interactions

Q: how do graph structure and GNN size affect modeled interactions?

2) Formalizing Strength of Interaction via Separation Rank

Separation Rank: measure of interaction modeled between input variables

For $f : (\mathbb{R}^D)^N \to \mathbb{R}$ and $\mathcal{I} \subseteq \{1, \ldots, N\}$:

$$\mathrm{sep}(f; \mathcal{I}) := \min R \text{ s.t. } f(x_1, \ldots, x_N) = \sum_{r=1}^{R} g_r(\{x_u\}_{u \in \mathcal{I}}) \cdot \bar{g}_r(\{x_v\}_{v \in \mathcal{I}^c})$$

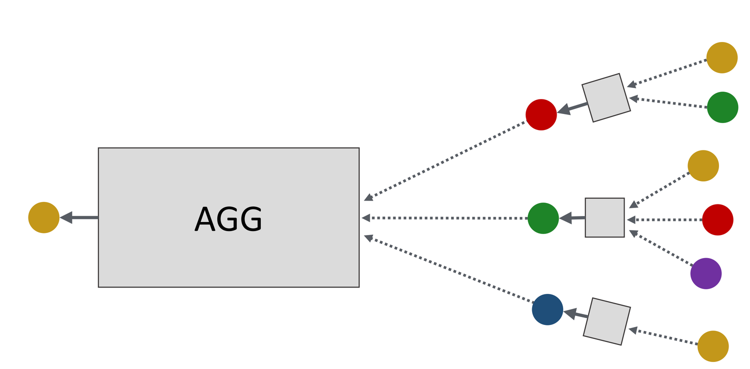
Usages:

(1) Entanglement in physics (2) Analyses of various NN architectures

(e.g. Cohen & Shashua 2017, Levine et al. 2018;2020, R et al. 2022)

3) Analyzed GNN Architecture

Vast majority of GNNs follow message-passing paradigm



$\mathcal{V} := \{1, \ldots, |\mathcal{V}|\}$ — vertices of input graph

$x_1, \ldots, x_{|\mathcal{V}|}$ — input vertex features

$h^{(l,u)}$ — hidden embedding of $u \in \mathcal{V}$ at layer l

$h^{(l,u)} = \mathrm{AGG}(\{ W^{(l)} h^{(l-1,v)} : v \in \mathrm{neigh}(u) \})$

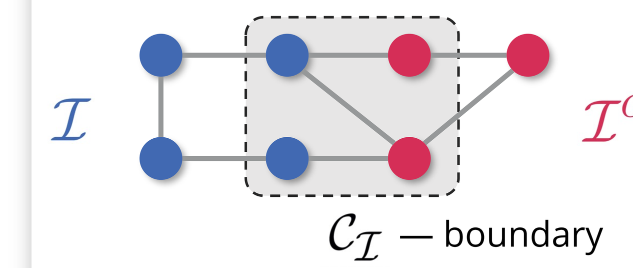
Prior work: studied interactions modeled by other NNs w/ poly non-linearity

(e.g. Cohen & Shashua 2017, Levine et al. 2018;2020, R et al. 2022)

Our theory: message-passing GNNs w/ product aggregation

4) Theory: Quantifying Ability of GNNs to Model Interactions

Walk Index (WI)



$\mathrm{WI}_{L-1}(\mathcal{I}) :=$ # length $L-1$ walks from $\mathcal{C}_\mathcal{I}$

$\mathrm{WI}_{L-1,t}(\mathcal{I}) :=$ # length $L-1$ walks from $\mathcal{C}_\mathcal{I}$ to $t \in \mathcal{V}$

Theorem

For depth L GNN of width D_h, subset of vertices $\mathcal{I} \subseteq \mathcal{V}$, and target $t \in \mathcal{V}$

Graph Prediction	Vertex Prediction
$\mathrm{sep}(GNN; \mathcal{I}) = D_h^{\mathcal{O}(\mathrm{WI}_{L-1}(\mathcal{I}))}$	$\mathrm{sep}(GNN^{(t)}; \mathcal{I}) = D_h^{\mathcal{O}(\mathrm{WI}_{L-1,t}(\mathcal{I}))}$

* Nearly matching lower bounds

Interaction GNNs model across partition is determined by walk index

Experiment: implications of theory apply to various GNNs (e.g. GCN & GIN)

5) Application: Expressivity Preserving Edge Sparsification

Edge Sparsification: remove edges to reduce compute/memory costs

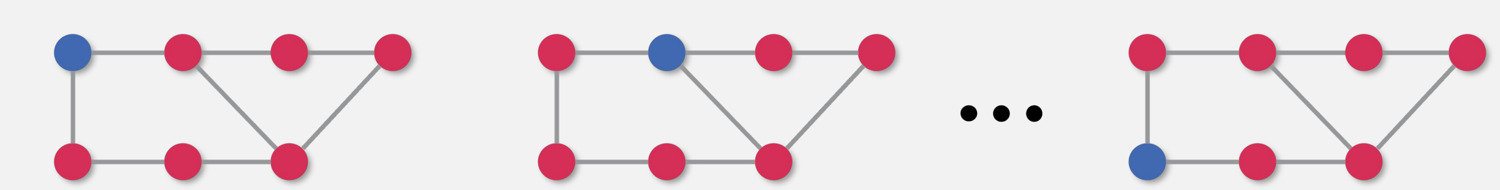
Theory: walk index of $\mathcal{I} \subseteq \mathcal{V}$ key for modeling interaction between $\mathcal{I}$ & $\mathcal{I}^c$

(L – 1)-Walk Index Sparsification (WIS)

Idea: greedily prune edge whose removal harms interactions the least

Algorithm: until desired # edges are removed:

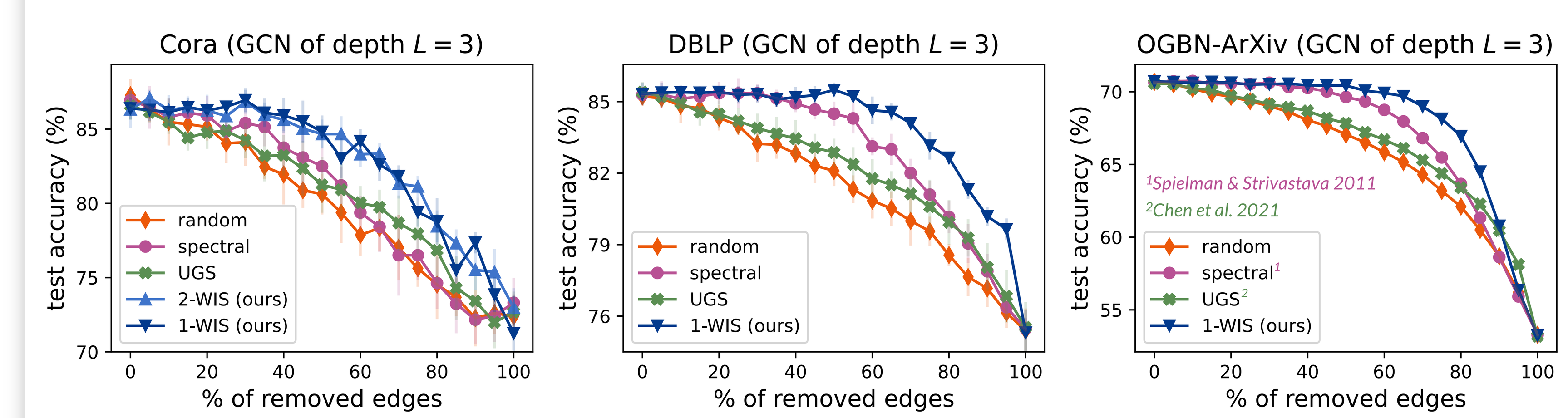
- Per edge, compute tuple holding what the *(L – 1)*-walk indices of $\{1\}, \ldots, \{|\mathcal{V}|\}$ will be if the edge is removed



- Remove edge w/ maximal walk index tuple (by some order over tuples)

1-WIS: particularly simple & efficient implementation

Experiment: comparison of edge sparsification algorithms



WIS outperforms existing methods while being simple & efficient