

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

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**Noam Razin**

Joint work with Tom Verbin & Nadav Cohen

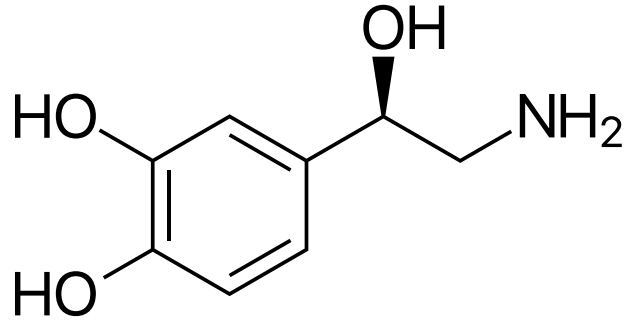
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Tel Aviv University



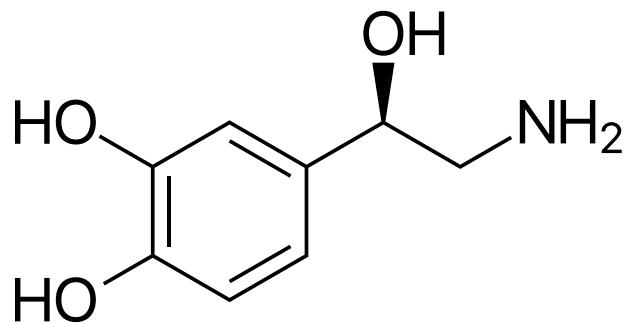
# Graph Neural Networks (GNNs)

Neural networks purposed for **modeling interactions over graph data**

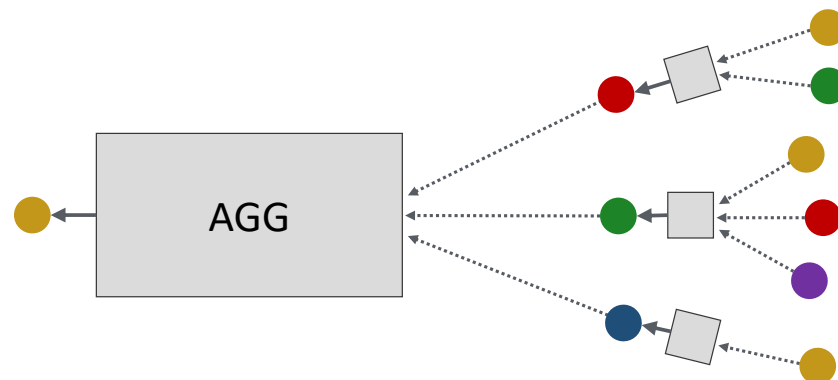


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Vast majority of GNNs follow the **message-passing paradigm**



# Expressivity of GNNs

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Fundamental Question: *Expressivity* – which functions can GNNs realize?

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Q: How do graph structure and GNN architecture affect modeled interactions?

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Widely used measure for the **interaction modeled across a partition of input variables**

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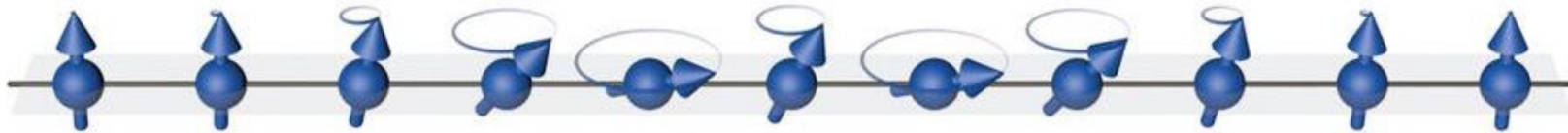
vertices of an input graph

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- Measure of **entanglement** in quantum mechanics

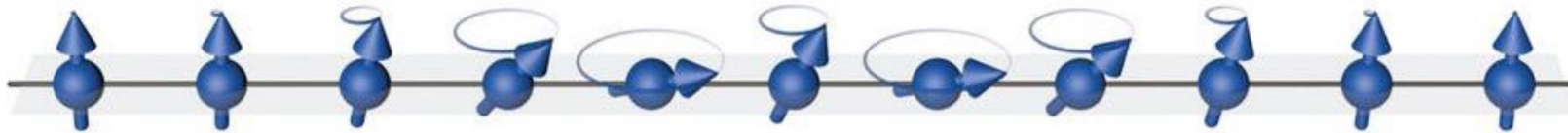


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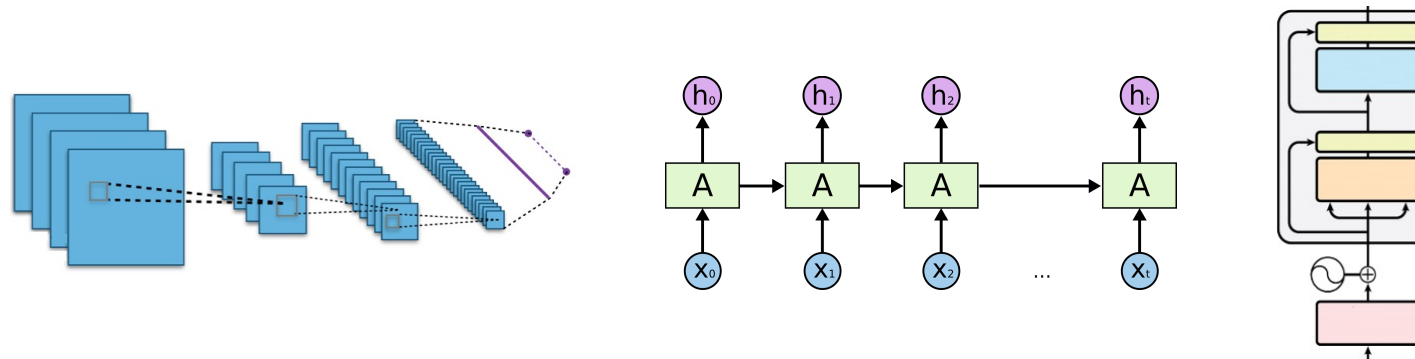
  
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- Analyses of convolutional, recurrent, and self-attention NNs

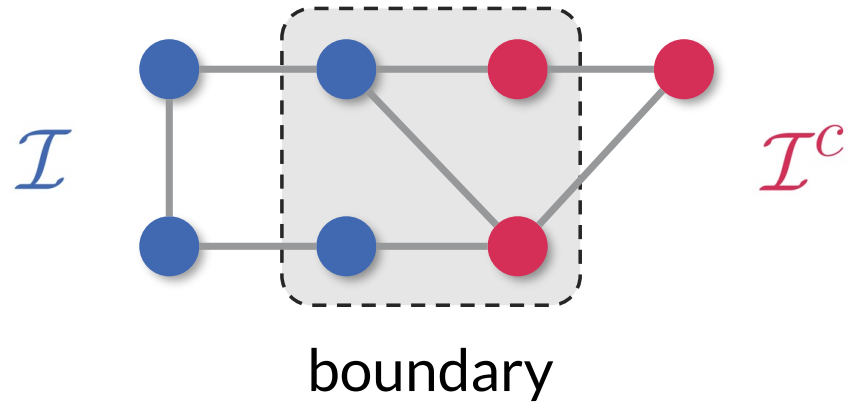
(e.g. Cohen & Shashua 2017, Levine et al. 2018;2020, R et al. 2022)



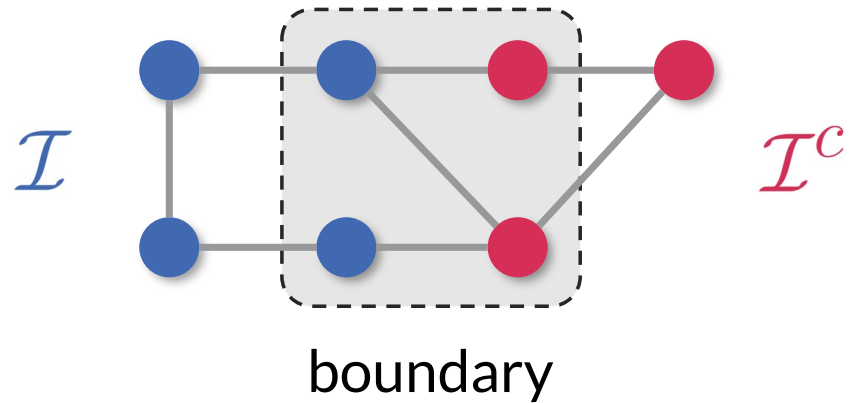
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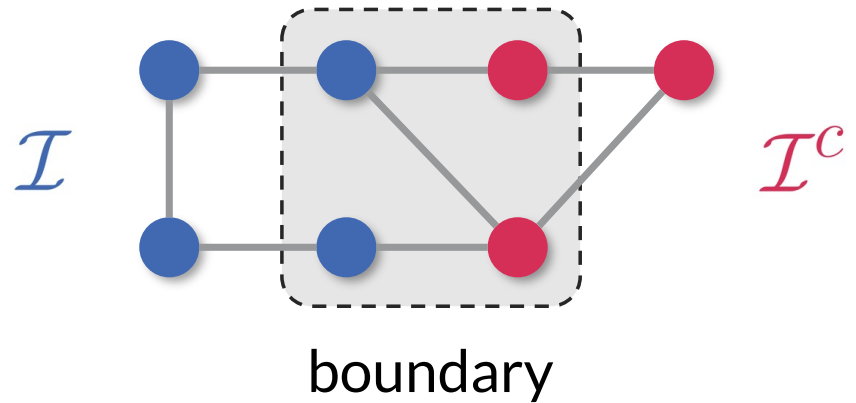


$L$  – GNN depth

$WI(\mathcal{I}) := \# \text{ length } L - 1 \text{ walks from boundary}$

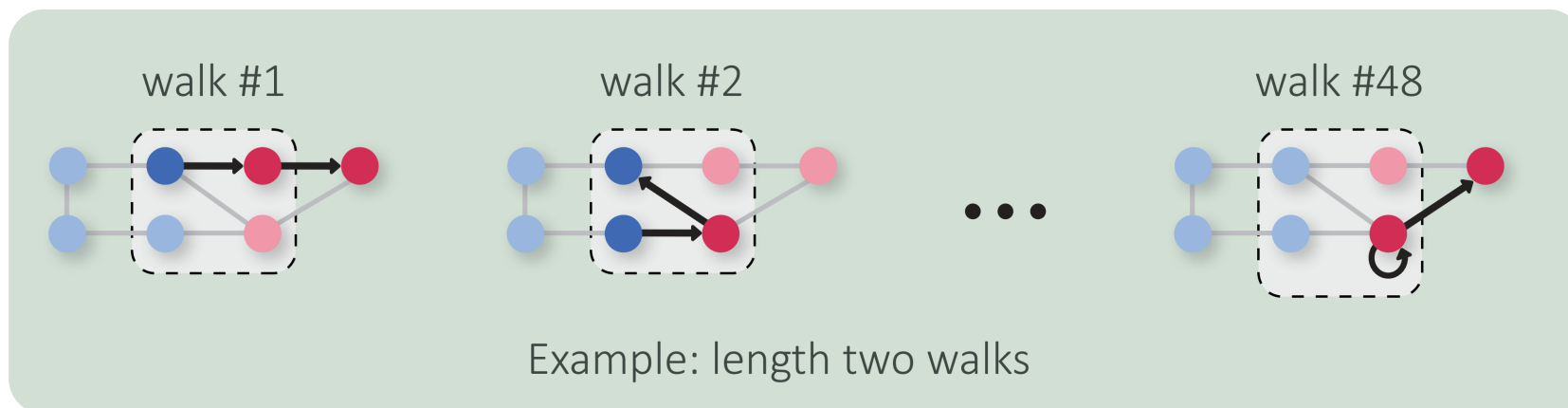


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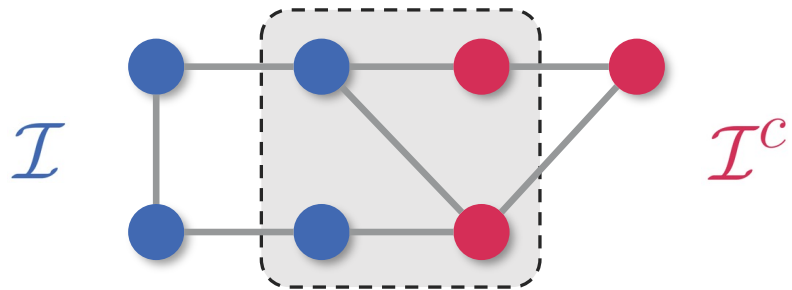
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# Main Result: Strength of Interaction $\propto$ Walk Index

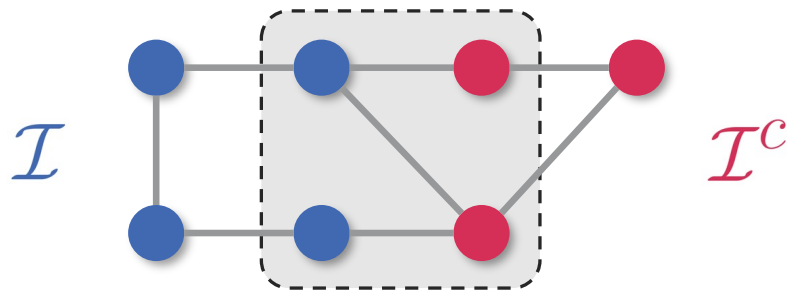
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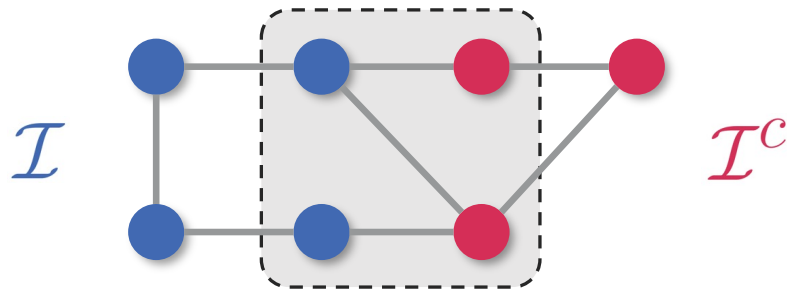


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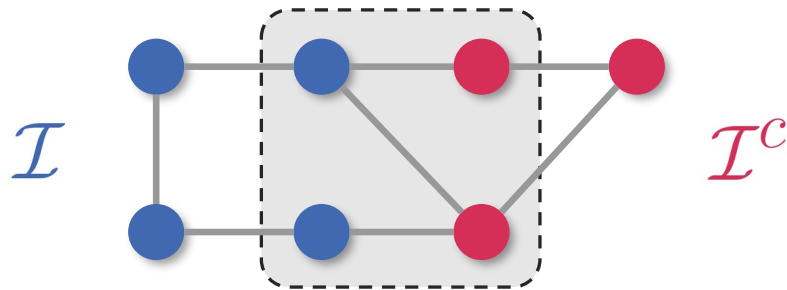
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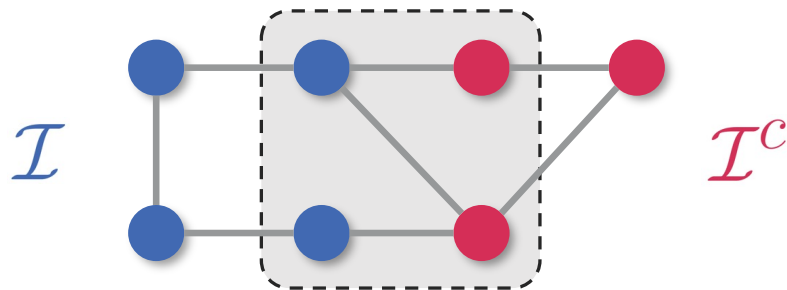
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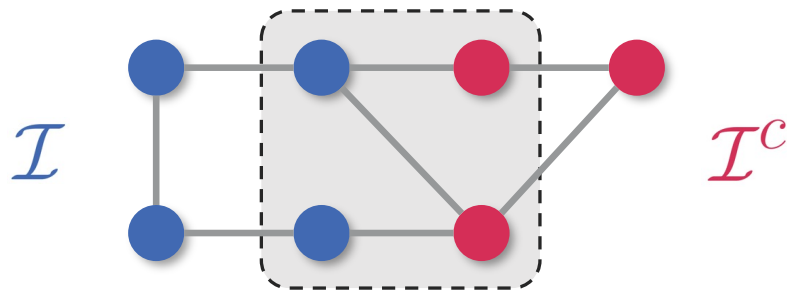
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Theory applies to GNNs with product aggregation

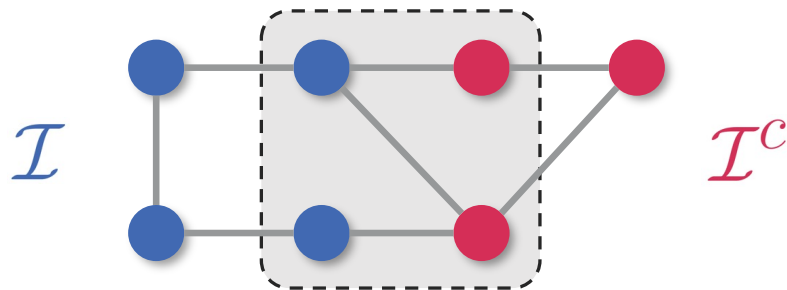
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**Experiment:** Implications of theory apply to GNNs with ReLU non-linearity (GCN, GAT, GIN)



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**Edge Sparsification:** Remove edges to reduce compute/memory costs

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**Algorithm:** Walk Index Sparsification (WIS)

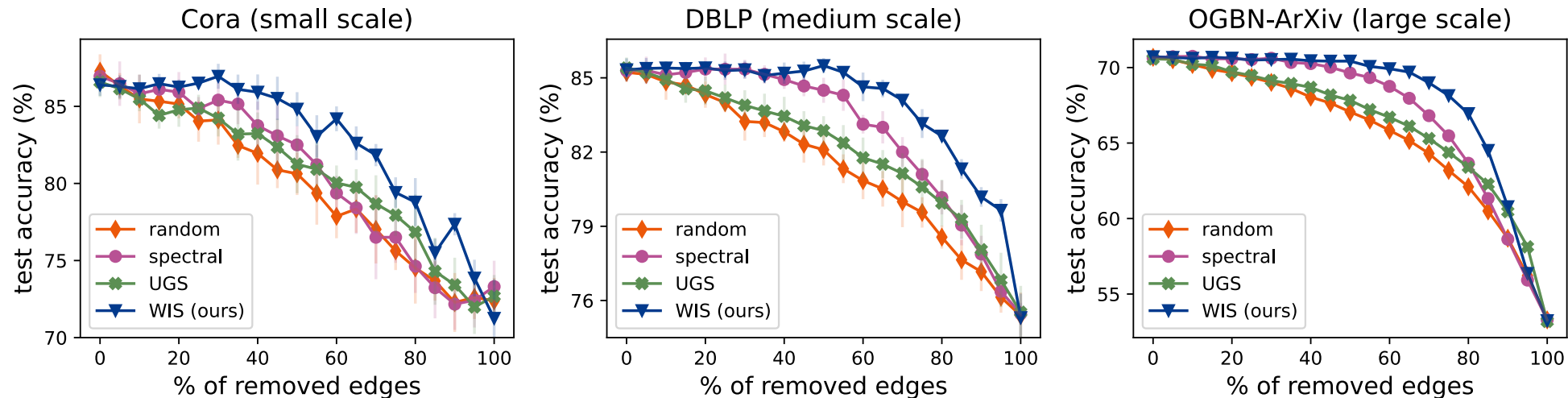
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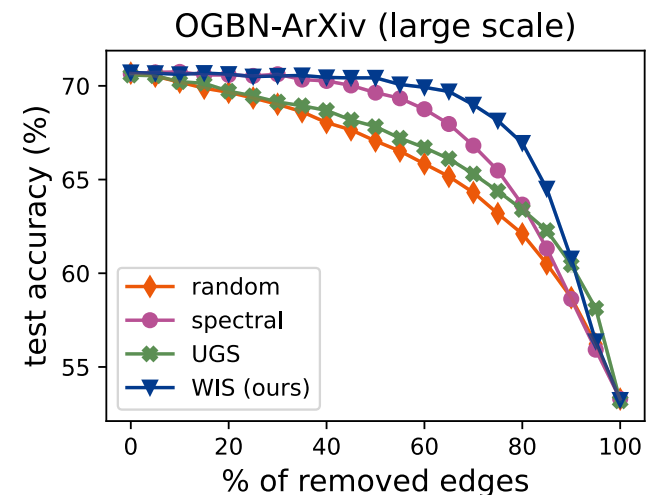
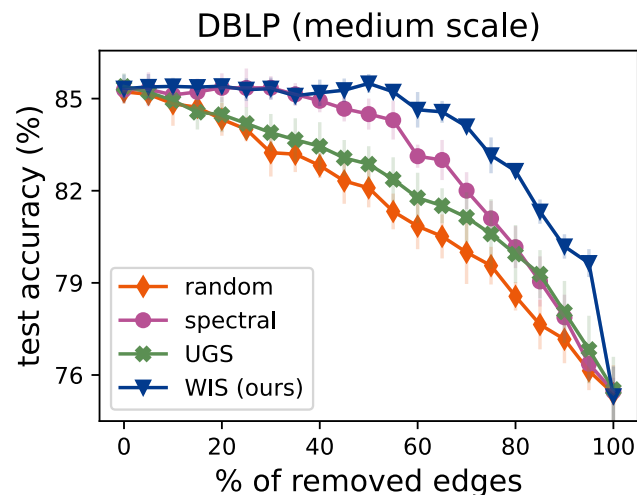
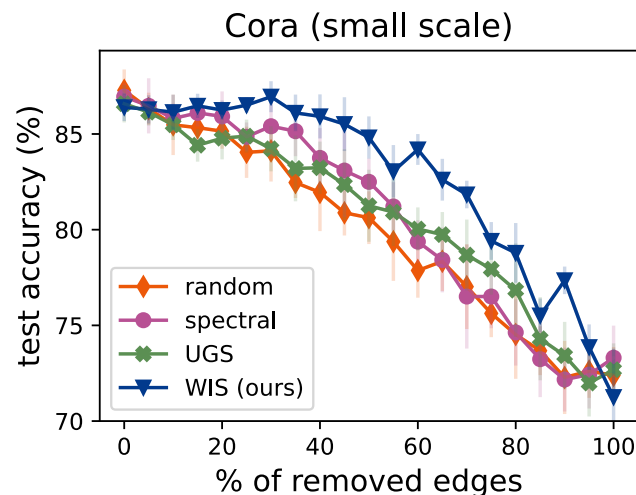
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Code



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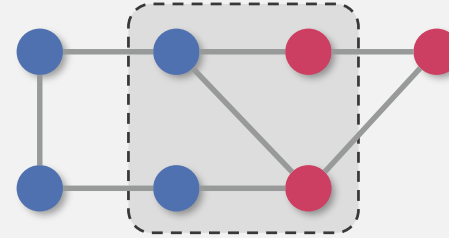
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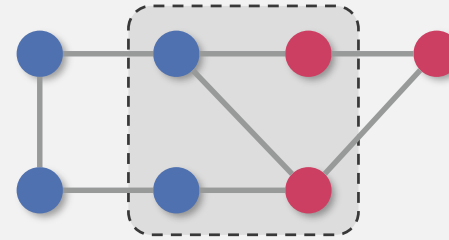
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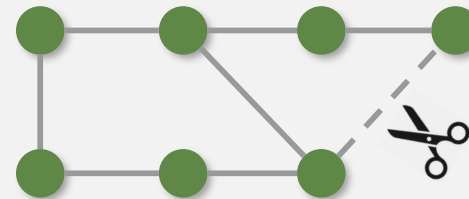
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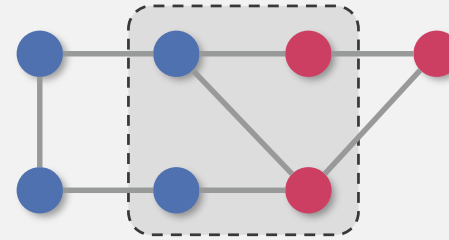




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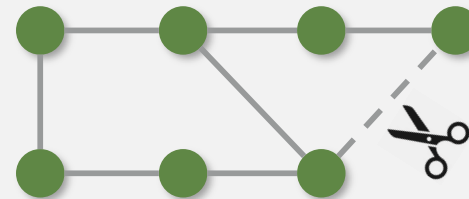
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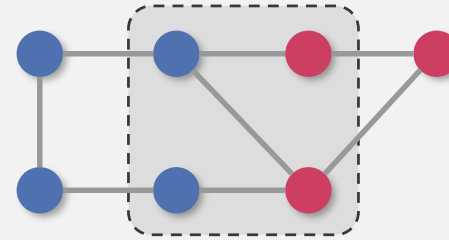


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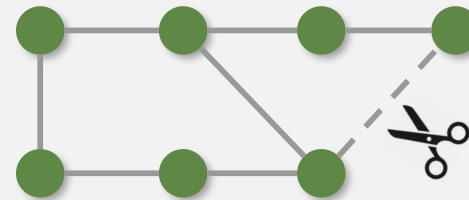
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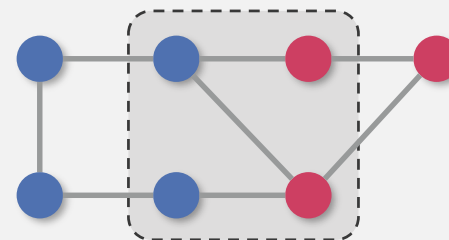
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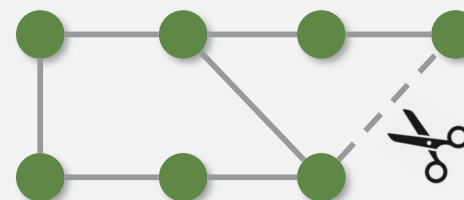
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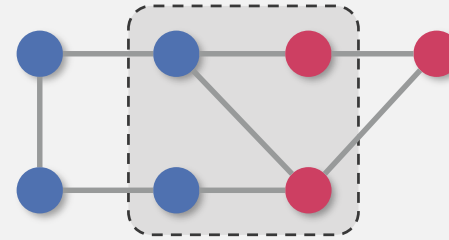
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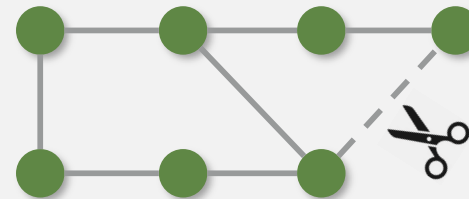
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Thank You!