Universität Basel

SADA signals and data group

Joint Graph Rewiring and Feature Denoising via Spectral Resonance

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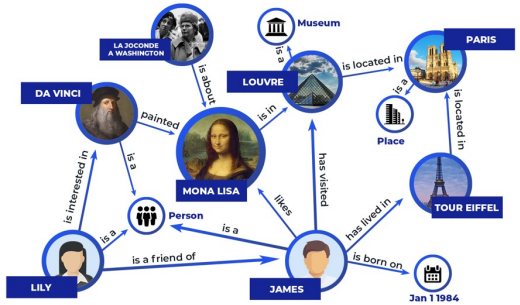
ICLR 2025

Oral Session E 4:30pm
Poster Session 4 3:00 – 5:30pm

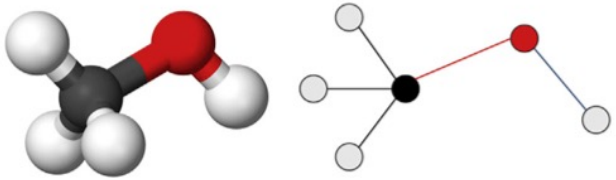
Thu April 24, 2025
Fri April 25, 2025

Singapore EXPO

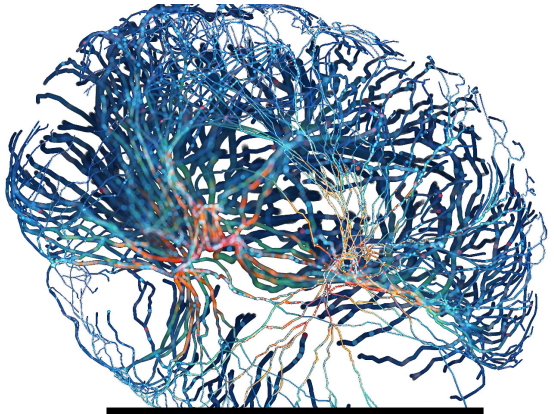
Graphs



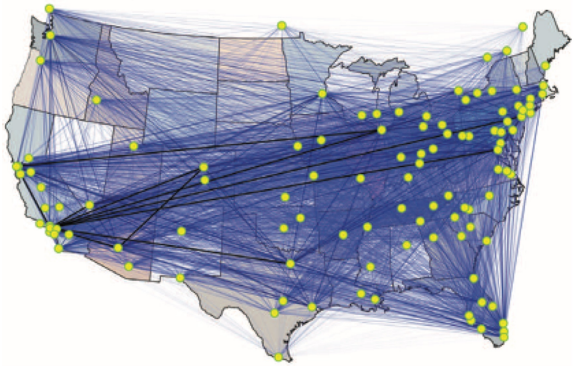
Knowledge



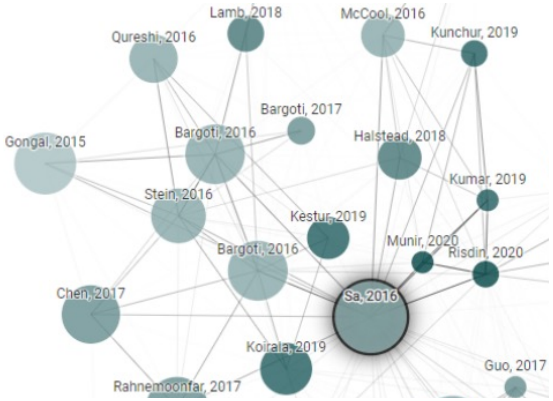
Molecules



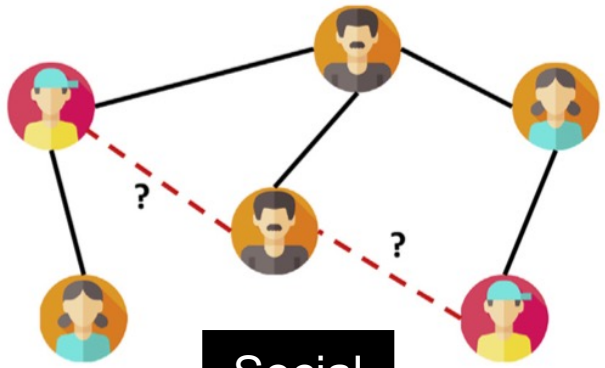
Brain/Neurons



Transport



Citations



Social

Zhou et al. Graph neural networks: A review of methods and applications, 2018
Benson et al. Higher-order organization of complex networks, 2016
Brain: Andriy Onufriyenko / Getty Images / Moment

https://yashuseth.wordpress.com/2019/10/08/introduction-question-answering-knowledge-graphs-kgqa/
https://www.connectedpapers.com
https://link.springer.com/article/10.1007/s10910-023-01511-6/figures/3

Graphs

Graph: $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ with $|\mathcal{V}| = N$

Adjacency matrix:

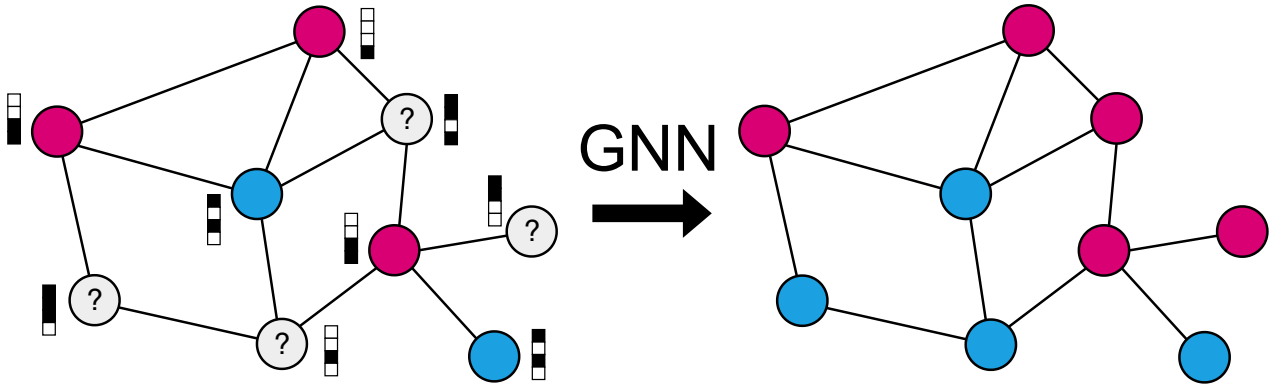
$$\boldsymbol{A} = \begin{cases} 1 & \text{if } e_{ij} \in \mathcal{E} \\ 0 & \text{otherwise} \end{cases} \in \mathbb{R}^{N \times N}$$

Features: $\boldsymbol{X} : \mathcal{V} \to \mathbb{R}^{N \times F}$

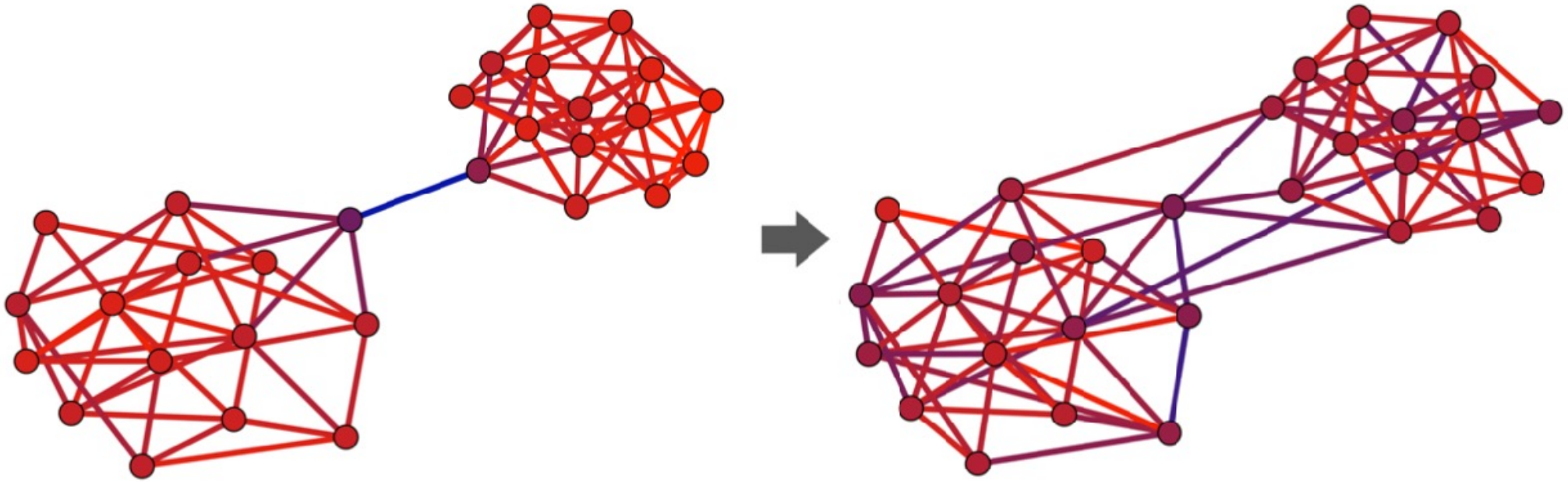
Labels: $\boldsymbol{y} : \mathcal{V} \to C$

Node Classification

- Given: $\mathcal{G}, \boldsymbol{X}, \boldsymbol{y}_{\text{train}}$
- Estimate labels in $\mathcal{V} \backslash \mathcal{V}_{\text{train}}$

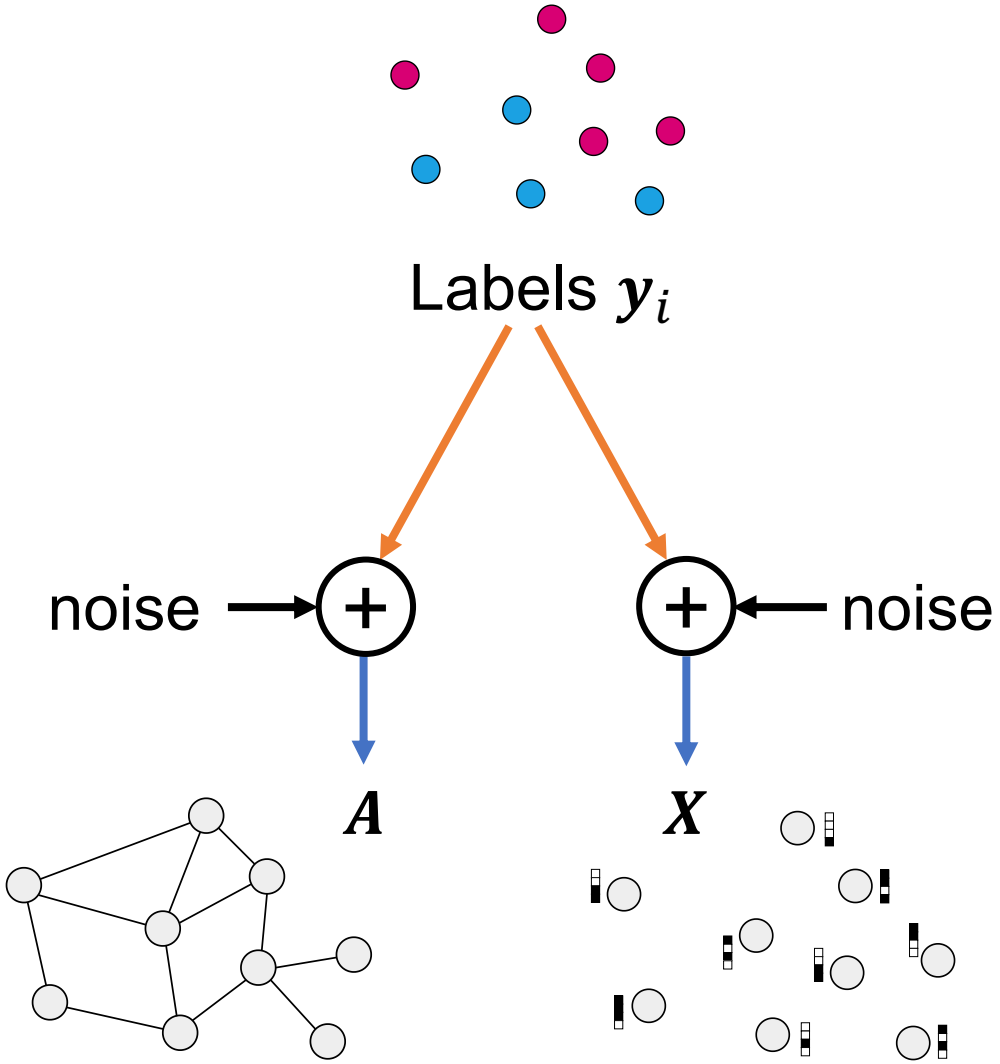


The rewiring idea

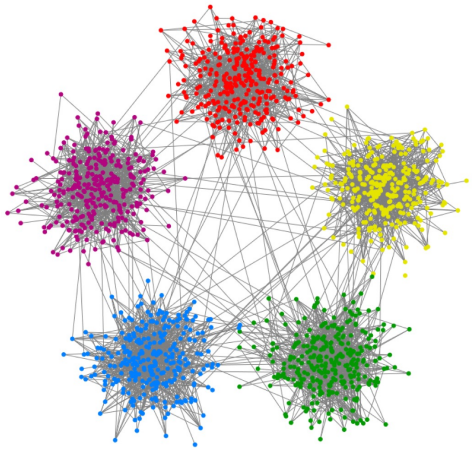


[1] Topping et al. Understanding over-squashing and bottlenecks on graphs via curvature, ICLR 2022
[2] Nguyen et al. Revisiting Over-smoothing and Over-squashing Using Ollivier-Ricci Curvature, ICML 2023
[3] Karhadkar et al. FoSR: First-order spectral rewiring for addressing oversquashing in GNNs, ICLR 2023

Denoising problem: Intuition



(contextual) stochastic block model



$$\mathbb{P}(A_{ij}=1)=\begin{cases}\frac{c_{\text{in}}}{N} & y_i=y_j\\ \frac{c_{\text{out}}}{N} & y_i\neq y_j\end{cases}$$

$$X_i=\sqrt{\frac{\mu}{N}}\,y_i\xi+\frac{z_i}{\sqrt{F}}$$

$$\text{Alignment}_L(A,X)=\left\|V_A^L\left(V_X^L\right)^T\right\|_{\text{sp}}$$

Joint **d**enoising and **r**ewiring (**JDR**) algorithm

Analysis

$$\boldsymbol{A} = \mathbf{V}\boldsymbol{\Lambda}\boldsymbol{V}^{\boldsymbol{T}} \text{ and } \boldsymbol{X} = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{W}^{\boldsymbol{T}}$$

Interpolation

$$\forall i \in [L] \quad \begin{aligned} \widetilde{\boldsymbol{v}}_i &= (1-\eta_A)\boldsymbol{v}_i + \eta_A \mathrm{sign}\big(\langle \boldsymbol{v}_i, \boldsymbol{u}_j \rangle\big)\boldsymbol{u}_j \quad j = \mathrm{argmax}_{\mathrm{j}\in[\mathrm{L}]} \big|\langle \boldsymbol{v}_i, \boldsymbol{u}_j \rangle\big| \\ \widetilde{\boldsymbol{u}}_i &= (1-\eta_X)\boldsymbol{u}_i + \eta_X \mathrm{sign}\big(\langle \boldsymbol{u}_i, \boldsymbol{v}_j \rangle\big)\boldsymbol{v}_j \quad j = \mathrm{argmax}_{\mathrm{j}\in[\mathrm{L}]} \big|\langle \boldsymbol{u}_i, \boldsymbol{v}_j \rangle\big| \end{aligned}$$

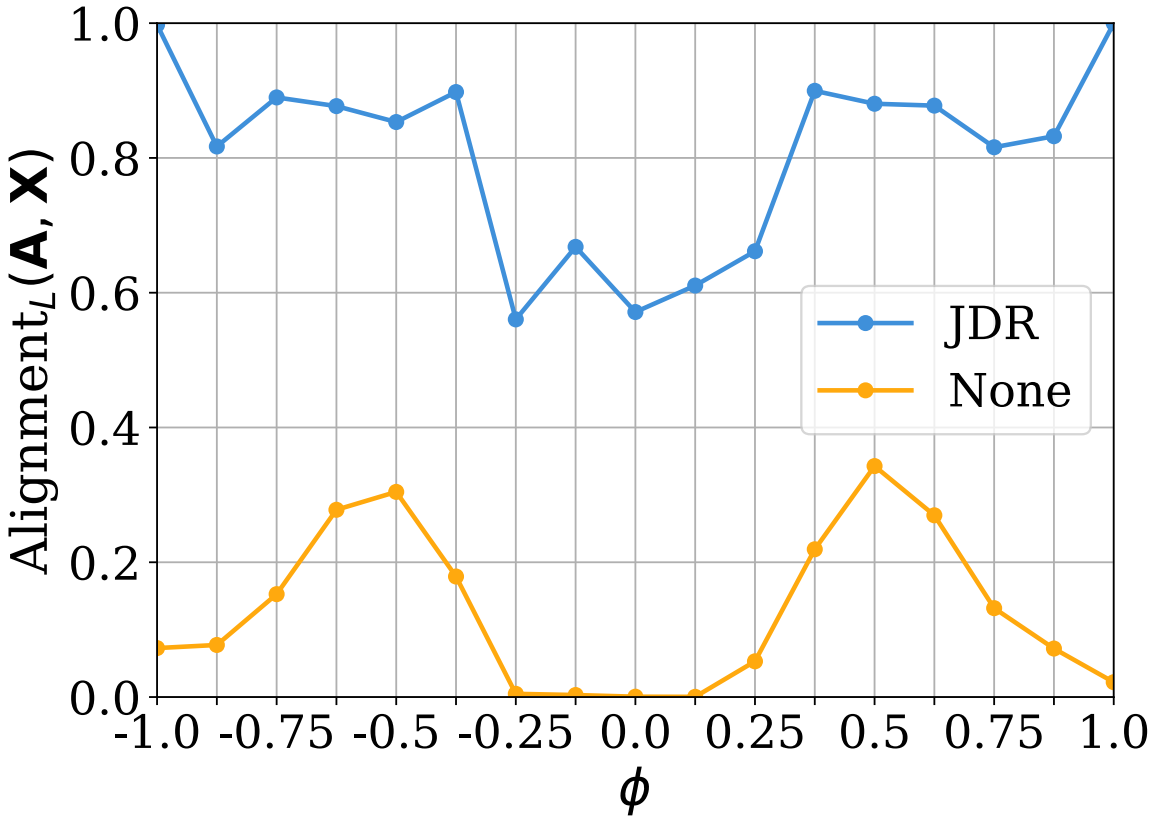
Synthesis

$$\widetilde{\boldsymbol{A}} = \widetilde{\mathbf{V}}\boldsymbol{\Lambda}\widetilde{\boldsymbol{V}}^{\boldsymbol{T}} \text{and } \widetilde{\boldsymbol{X}} = \widetilde{\boldsymbol{U}}\boldsymbol{\Sigma}\boldsymbol{W}^{\boldsymbol{T}}$$

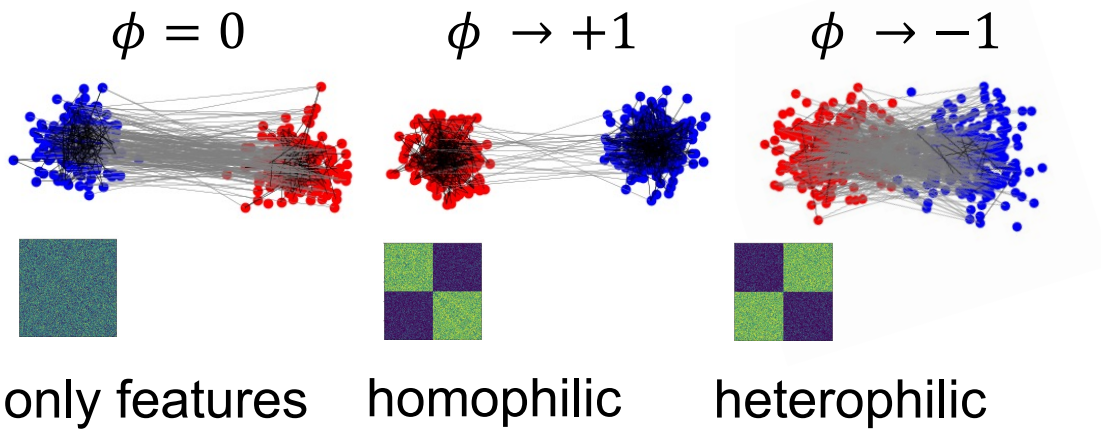
Iterate

Does JDR increase alignment?

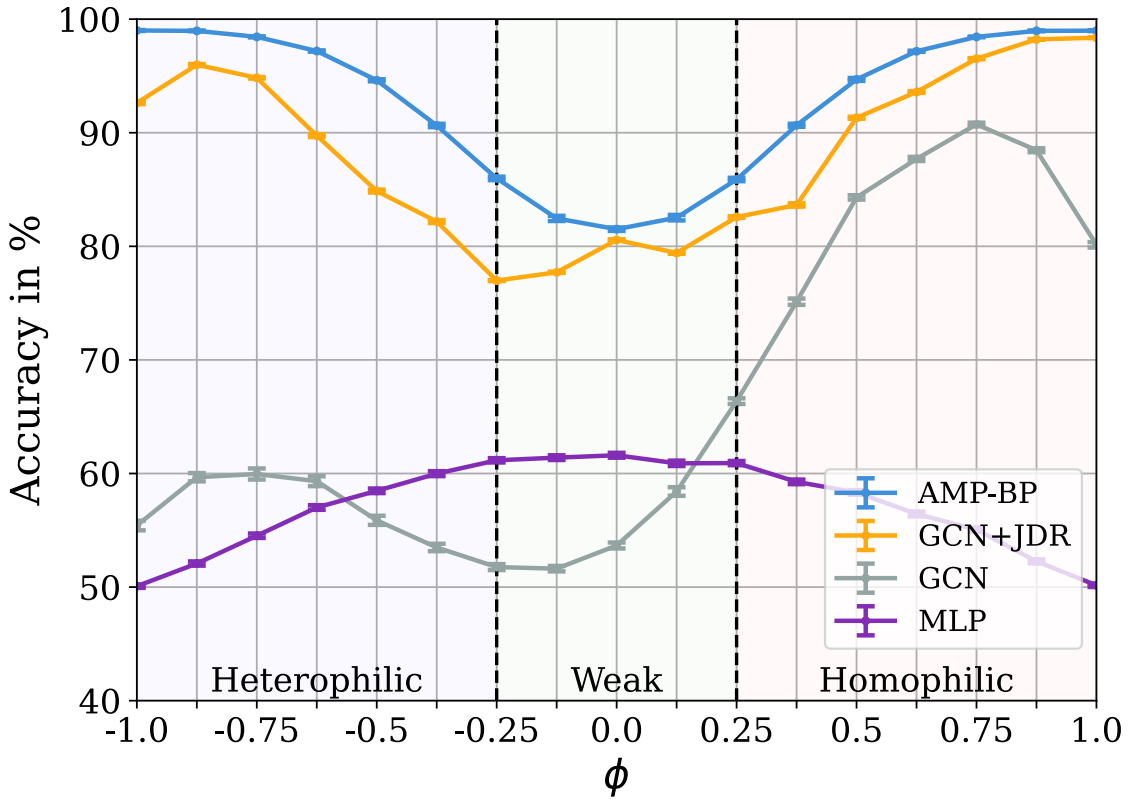
Theory ✓



Graphs from cSBM with ϕ



Experiments



Method	Cora	CiteSeer	PubMed	Computers	Photo
GCN	77.26±0.35	67.16±0.37	84.22±0.09	84.42±0.31	91.33±0.29
GCN+DIGL	79.27±0.26	68.03±0.33	84.60±0.09	**86.00±0.24**	92.00±0.23
GCN+FoSR	77.23±0.34	67.03±0.34	84.21±0.09	84.34±0.27	91.36±0.28
GCN+BORF	77.23±0.35	66.96±0.38	84.22±0.09	84.46±0.30	91.26±0.30
GCN+JDR	**79.96±0.26**	**69.35±0.28**	**84.79±0.08**	85.66±0.36	**92.52±0.23**
GPRGNN	79.65±0.33	67.50±0.35	84.33±0.10	84.06±0.48	92.01±0.41
GPRGNN+DIGL	79.77±0.30	67.50±0.35	84.72±0.10	**86.25±0.28**	92.31±0.25
GPRGNN+FoSR	79.22±0.31	67.30±0.38	84.32±0.09	84.21±0.46	92.07±0.37
GPRGNN+BORF	79.43±0.30	67.48±0.36	84.36±0.10	84.08±0.43	92.11±0.38
GPRGNN+JDR	**80.77±0.29**	**69.17±0.30**	**85.05±0.08**	84.77±0.35	**92.68±0.25**

Method	Chameleon	Squirrel	Actor	Texas	Cornell
GCN	67.65±0.42	57.94±0.31	34.00±0.31	75.62±1.12	64.68±1.25
GCN+DIGL	58.04±0.48	39.64±0.34	39.57±0.29	**91.05±0.73**	**88.49±0.74**
GCN+FoSR	67.67±0.39	58.12±0.35	33.98±0.30	78.31±1.07	65.64±1.06
GCN+BORF	67.78±0.43	OOM	33.95±0.31	76.66±1.10	68.72±1.11
GCN+JDR	**69.76±0.50**	**61.76±0.39**	**40.47±0.31**	85.12±0.74	84.51±1.06
GPRGNN	69.15±0.51	53.44±0.37	39.52±0.22	92.82±0.67	87.79±0.89
GPRGNN+DIGL	66.57±0.46	42.98±0.37	39.61±0.21	91.11±0.72	88.06±0.81
GPRGNN+FoSR	68.96±0.45	52.34±0.37	39.47±0.21	93.16±0.66	87.51±1.04
GPRGNN+BORF	69.44±0.56	OOM	39.55±0.20	93.53±0.68	88.83±1.06
GPRGNN+JDR	**71.00±0.50**	**60.62±0.38**	**41.89±0.24**	**93.85±0.54**	**89.45±0.84**

…and many more

AMP-BP: O. Duranthon and L. Zdeborová. Optimal inference in contextual stochastic block models, 2023
GCN: Kipf and Welling. Semi-supervised classification with graph convolutional networks, ICLR 2017
GPRGNN: Chien et al. Adaptive universal generalized pagerank graph neural network, ICLR 2021

Thank you for watching!

paper

code

lab

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