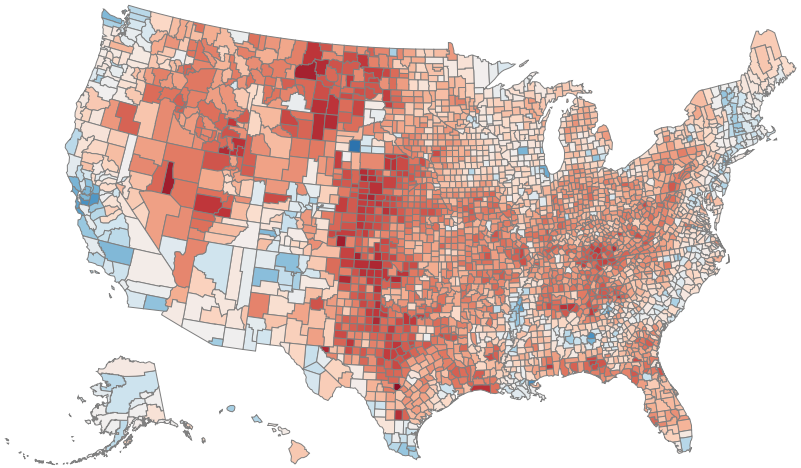
Modeling and Inferring Attributed Graphs

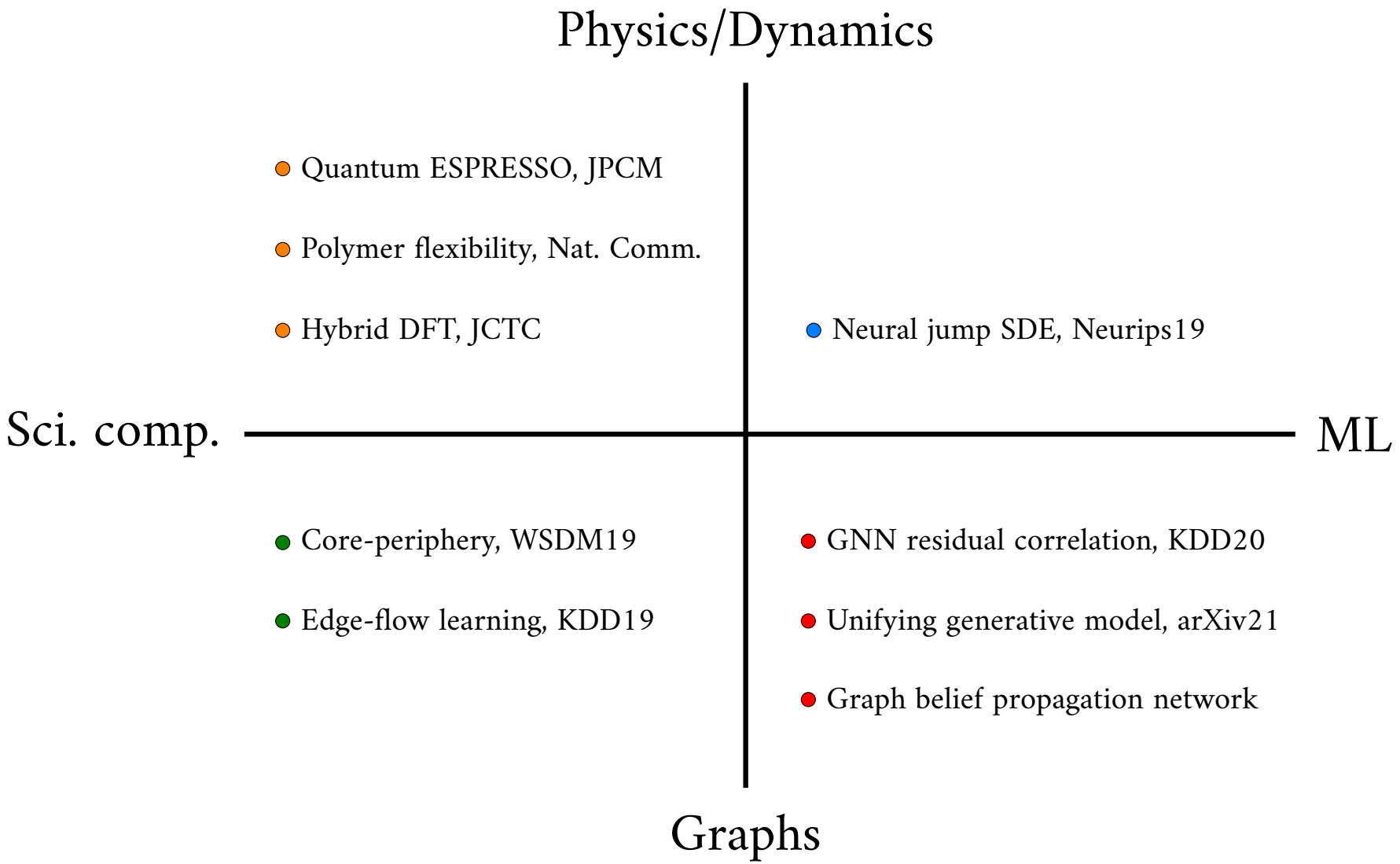


Junteng Jia

Department of Computer Science, Cornell University, Ithaca, NY 14853

Ph.D. Thesis Defense – April 12, 2021

Research Overview



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- Quantum ESPRESSO, JPCM
- Polymer flexibility, Nat. Comm.
- Hybrid DFT, JCTC
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Sci. comp. — ML

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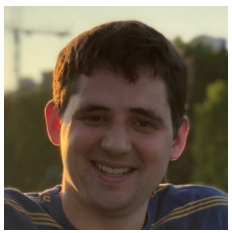
- Graph belief propagation network



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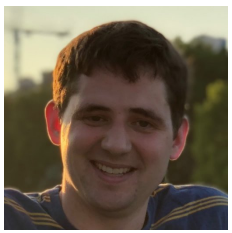

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Graphs Data are Increasingly More Complex

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nodes: people
edges: friendships

Finance

nodes: accounts
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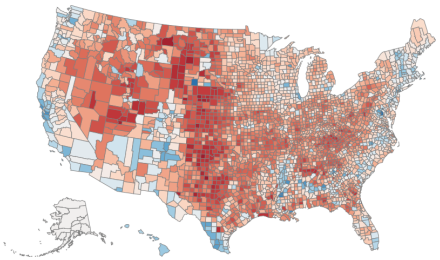

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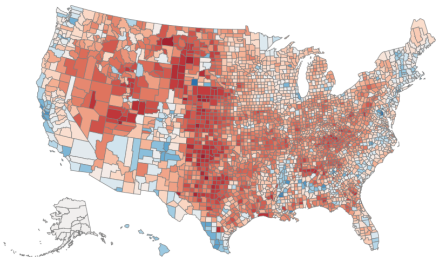

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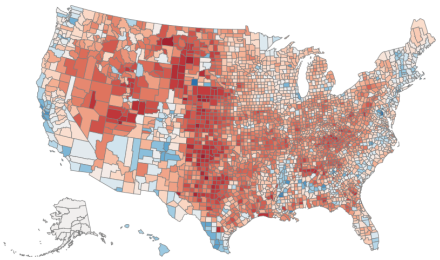

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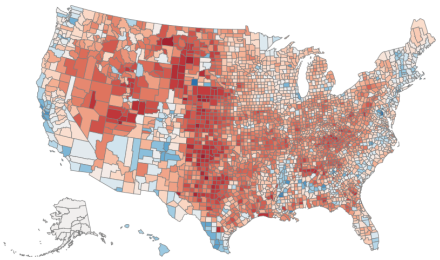

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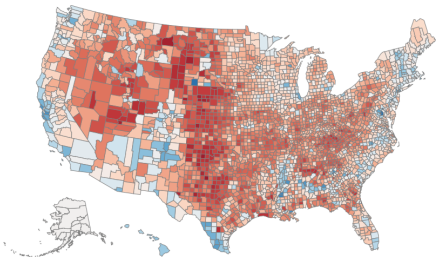

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- node attributes are oftentimes incomplete

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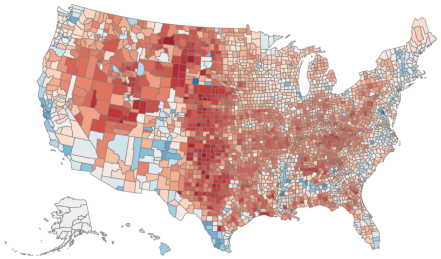

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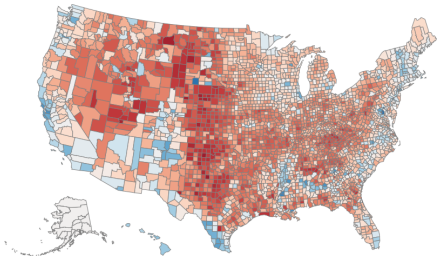

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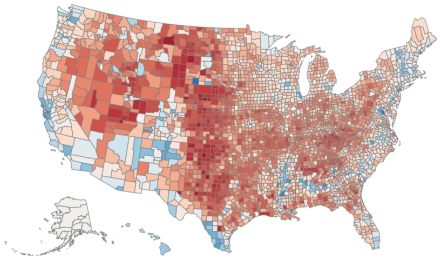

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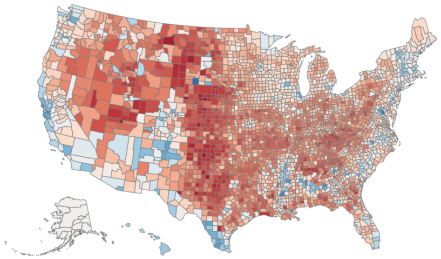

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- however, research often driven by improving on benchmark datasets
  - classification in citation/coauthor network [Lu-Getoor 03; Kipf-Welling 17; Shchur+ 18]

Regression vs Classification

- First, we develop theory (statistical models) on regression problems
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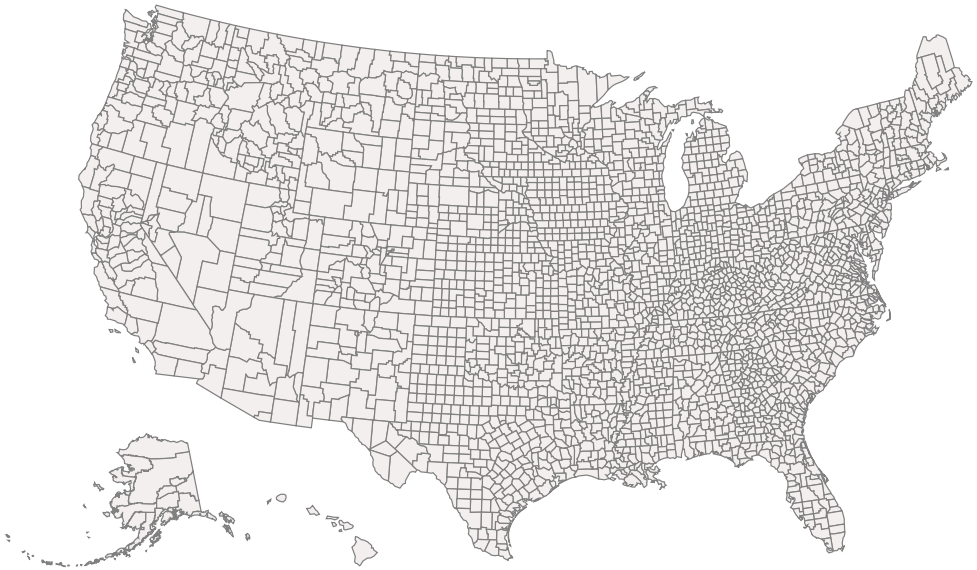
- Later, we extend to the classification setting
  Labels are discrete-valued like cat/dog, male/female ...

Node Label Prediction in Attributed Graphs

Motivating example — Predicting election from pollsters



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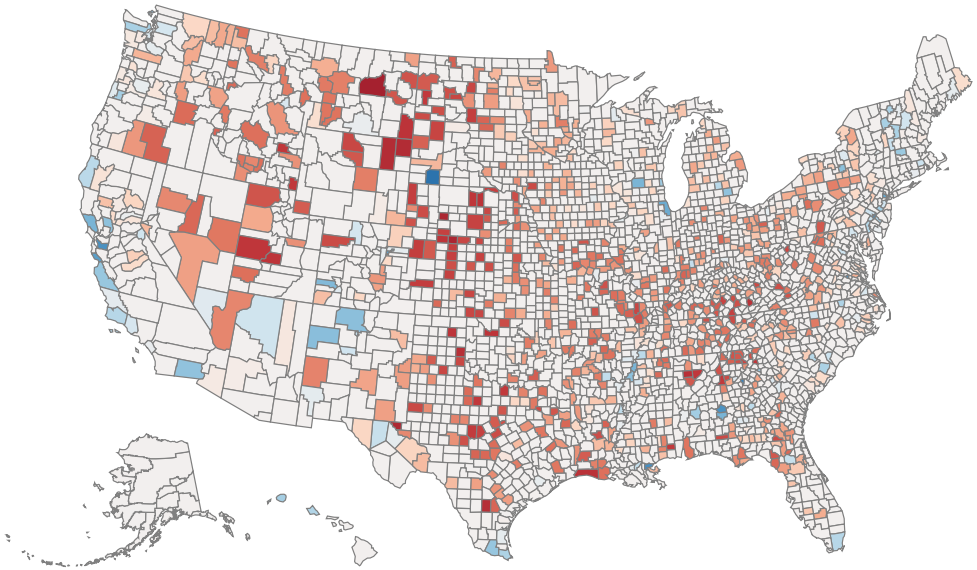

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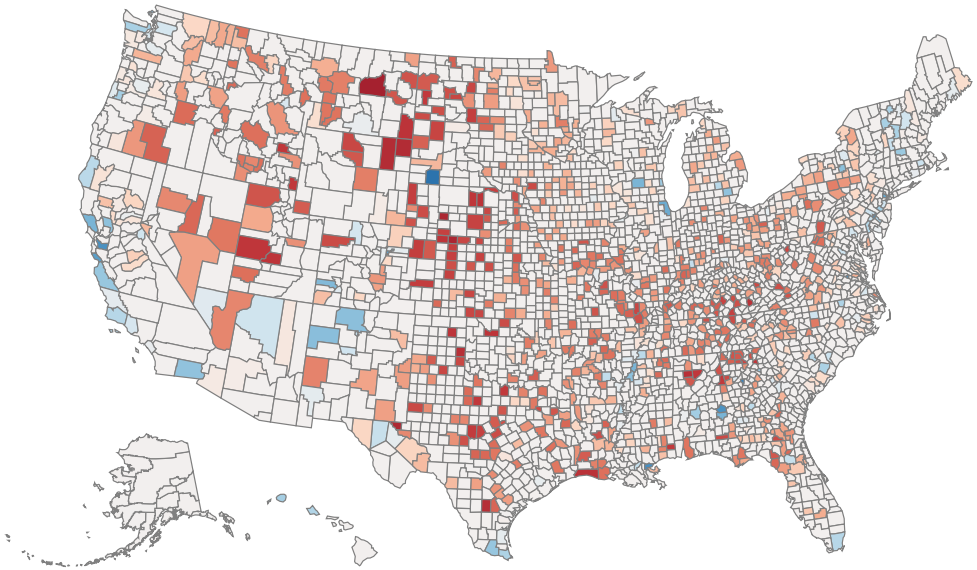

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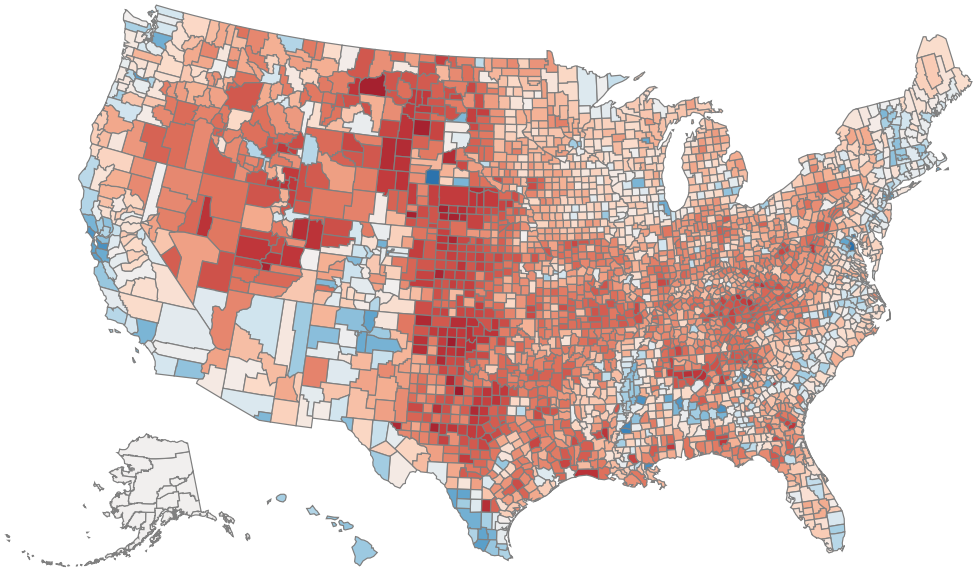

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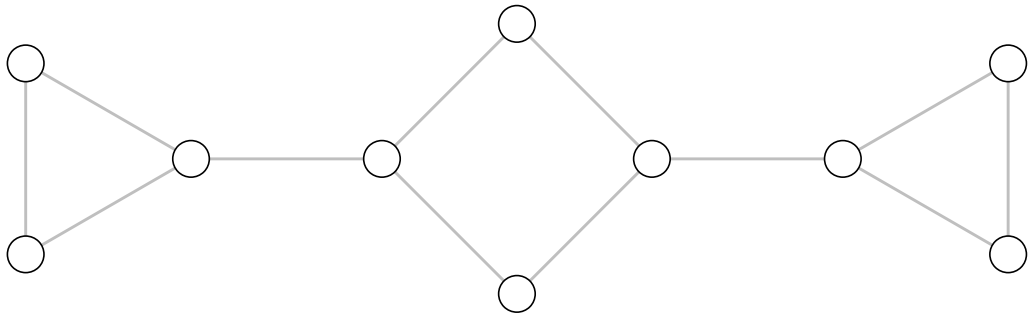

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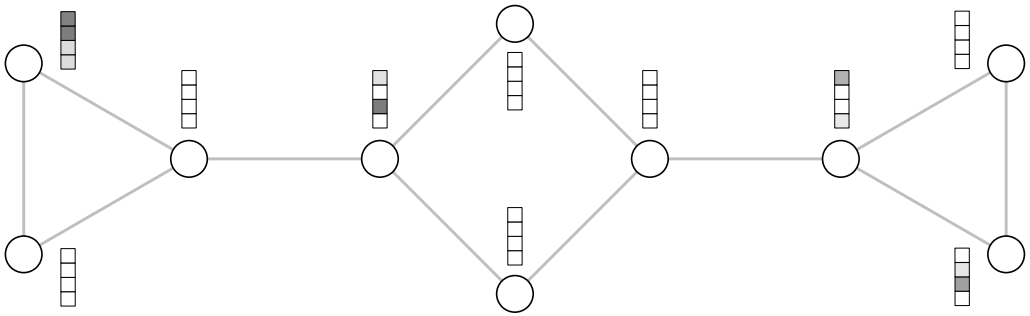

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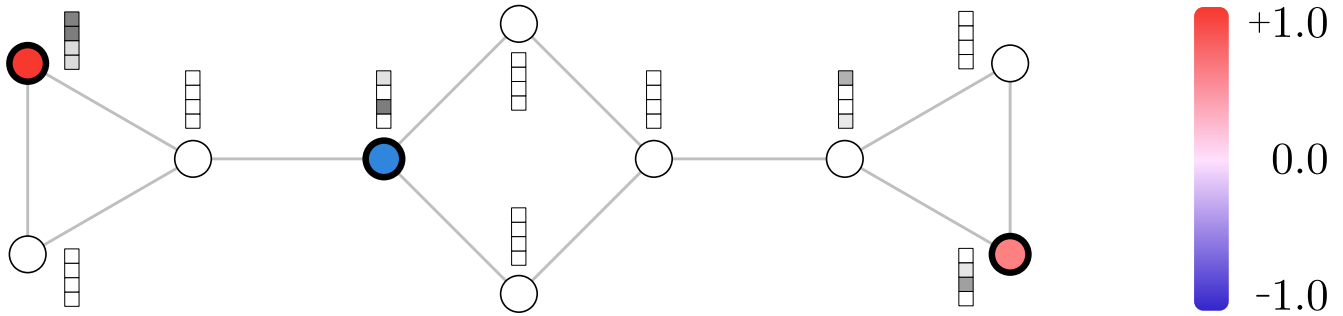

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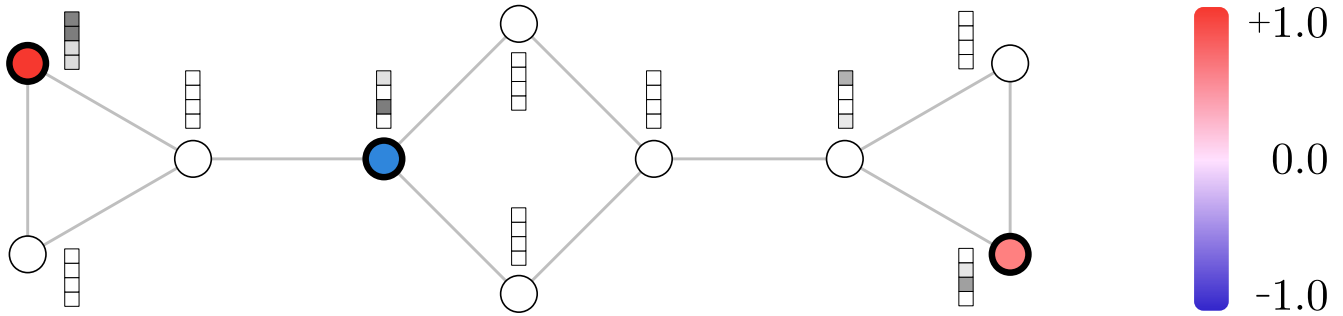

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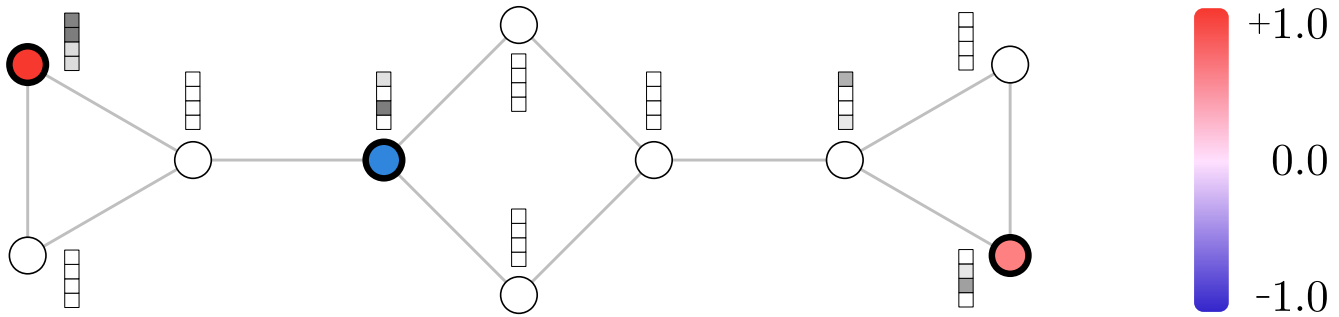
There are two Broad Classes of Methods

Label propagation is a transductive method [early 2000s]



[Zhu+ 03; Zhou+ 04; Wang-Zhang 06]

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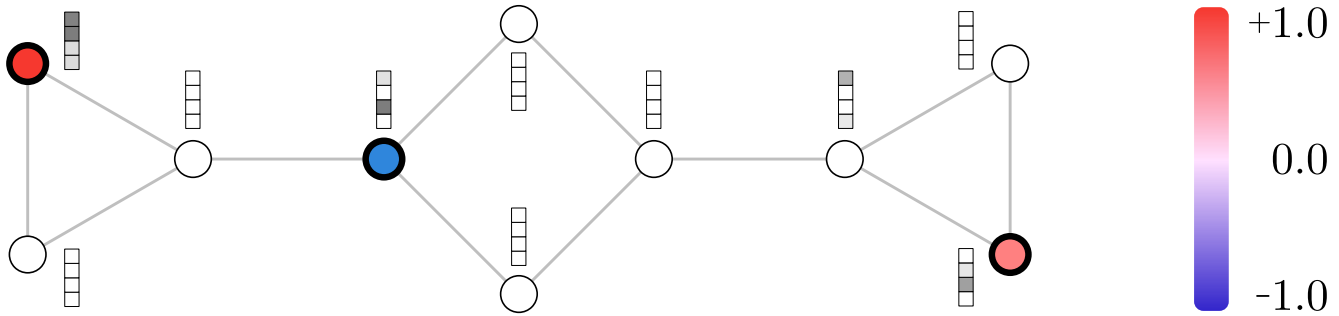

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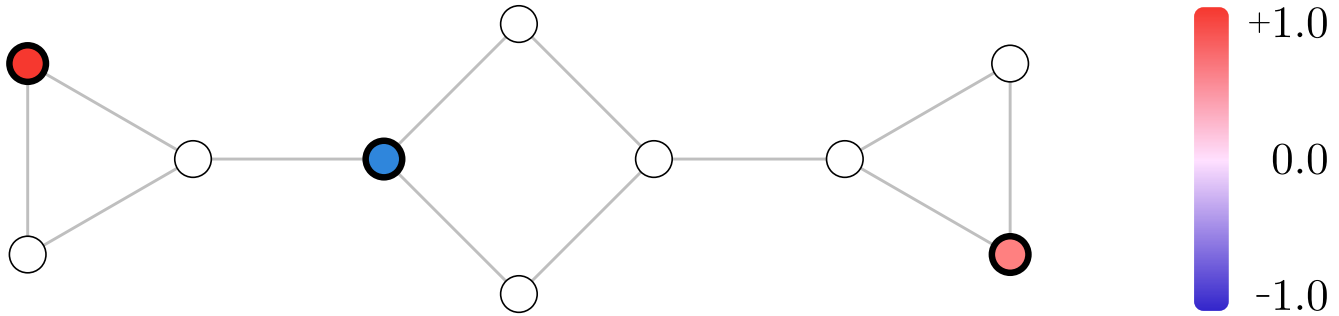

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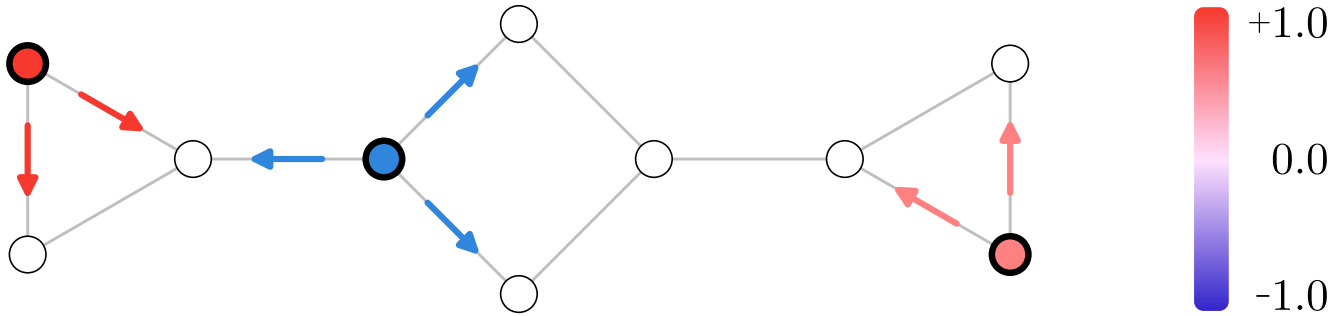

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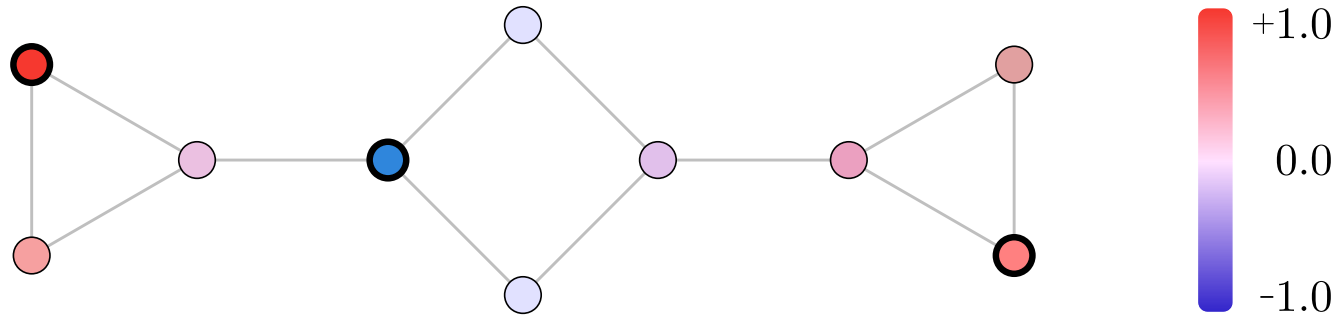

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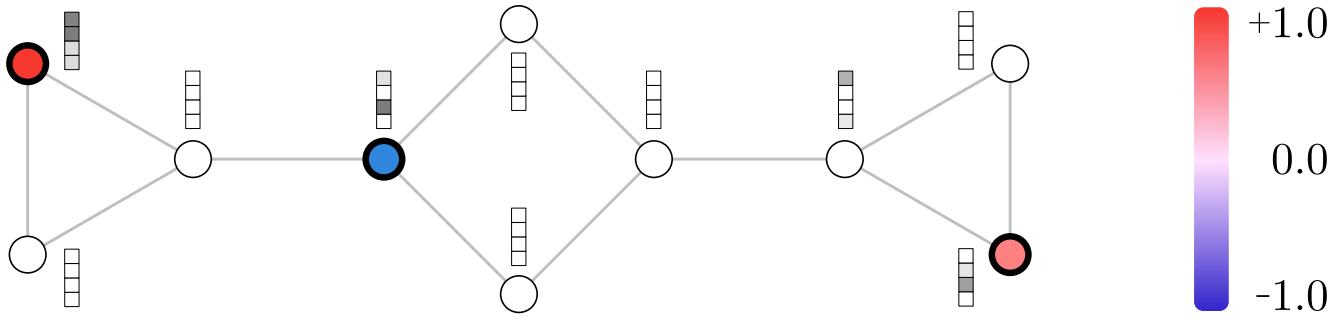

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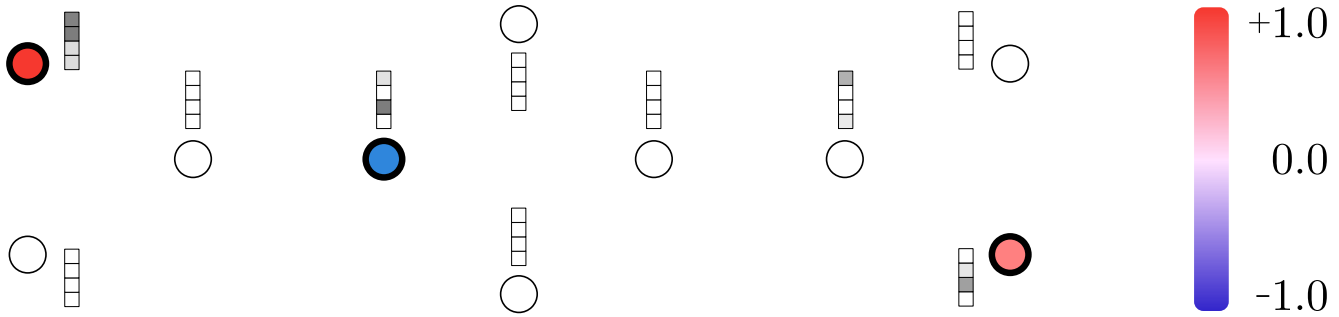

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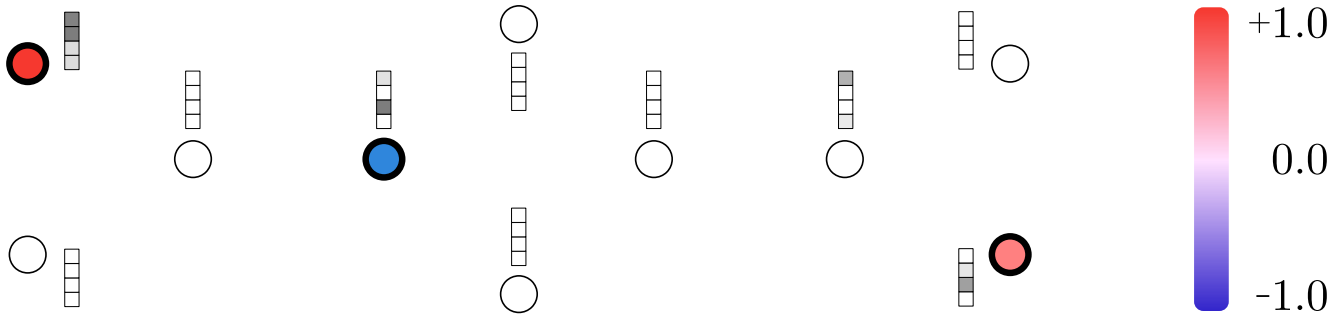

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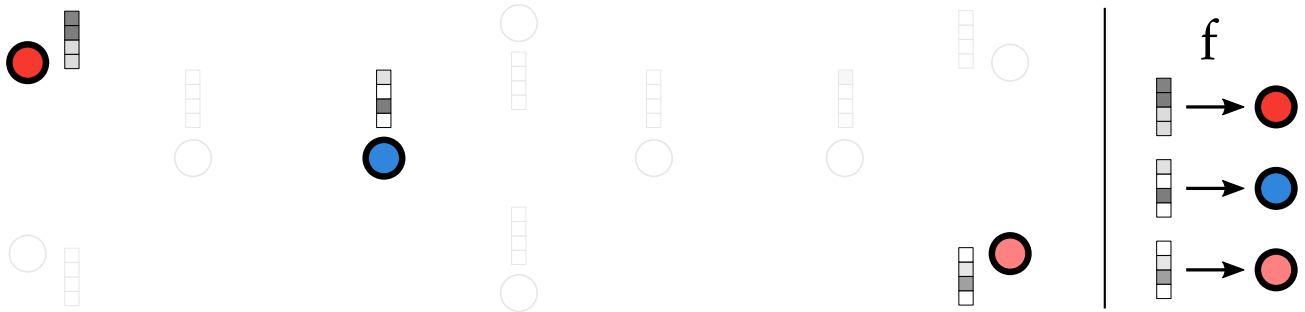

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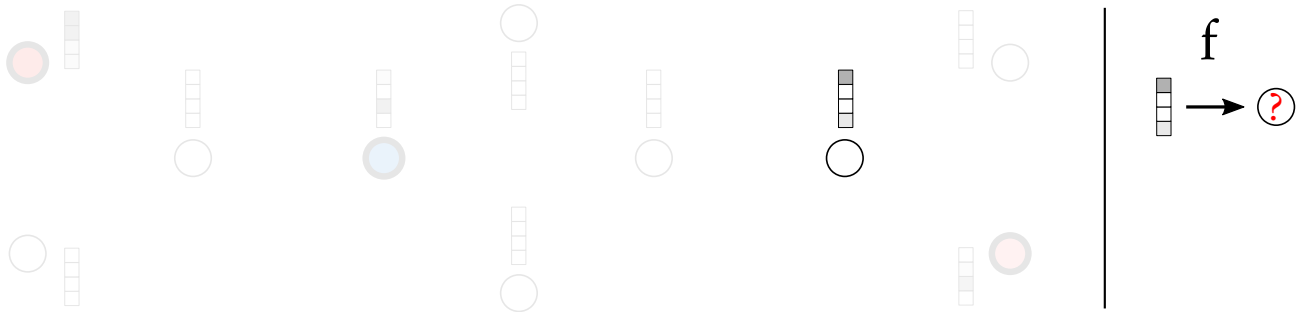

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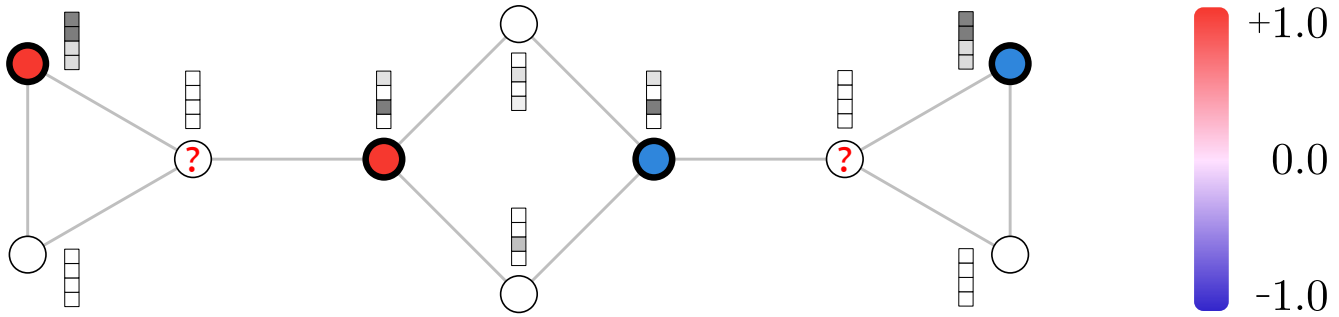

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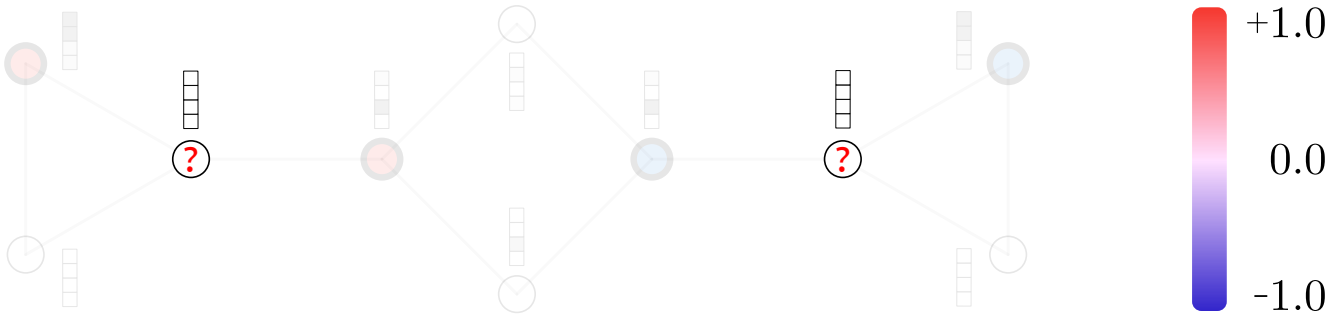

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  - ignore graph structure, treat data points as i.i.d. samples
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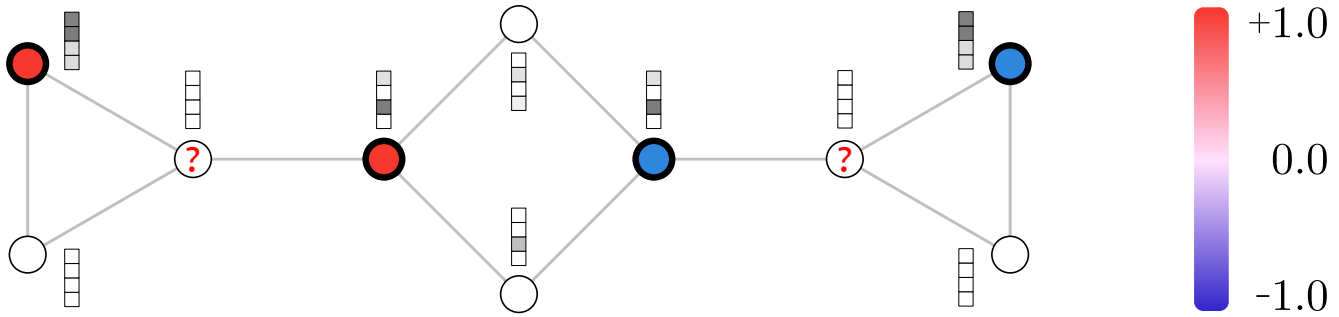
There are two Broad Classes of Methods

Inductive methods start with naive i.i.d. predictors



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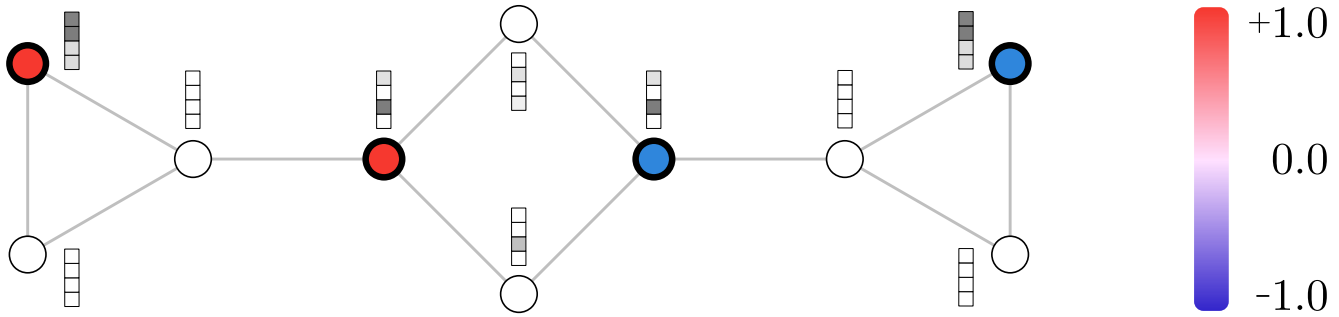
A more sophisticated inductive method is Graph Neural Networks [late 2010s]



- assumption: a label only depend on features in the neighborhood

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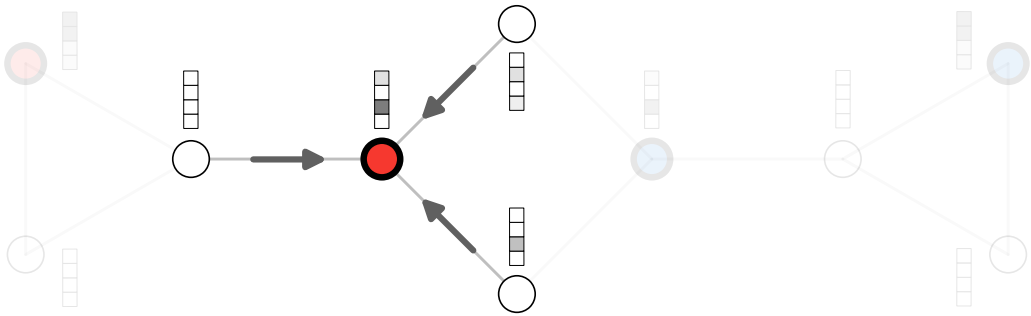

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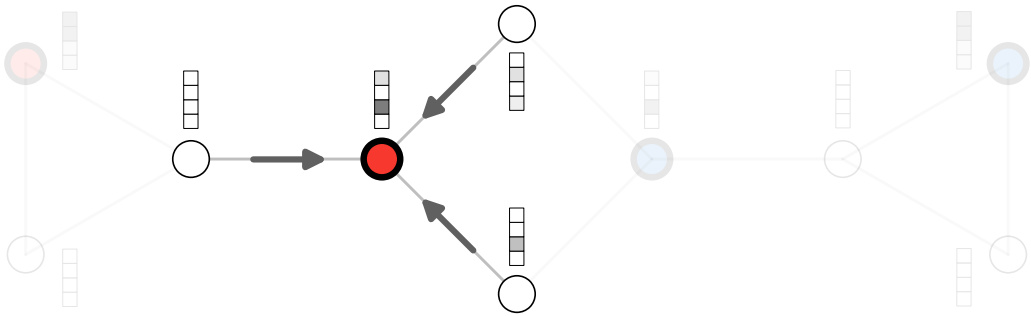

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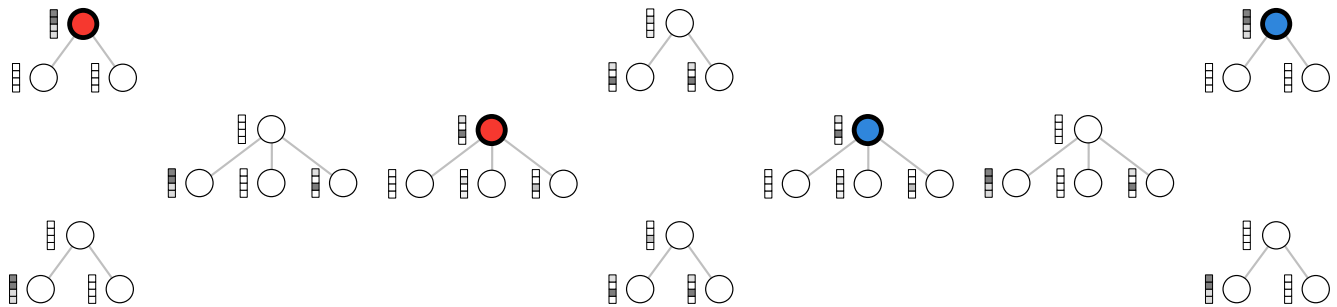

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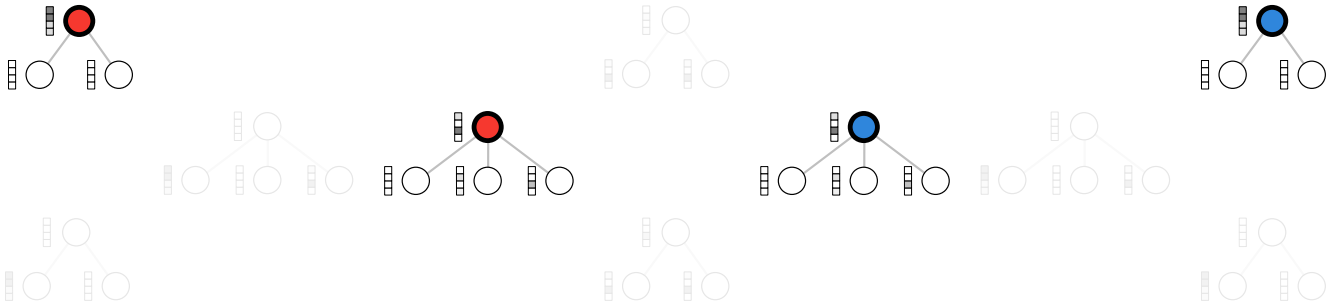

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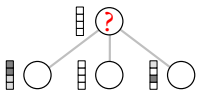

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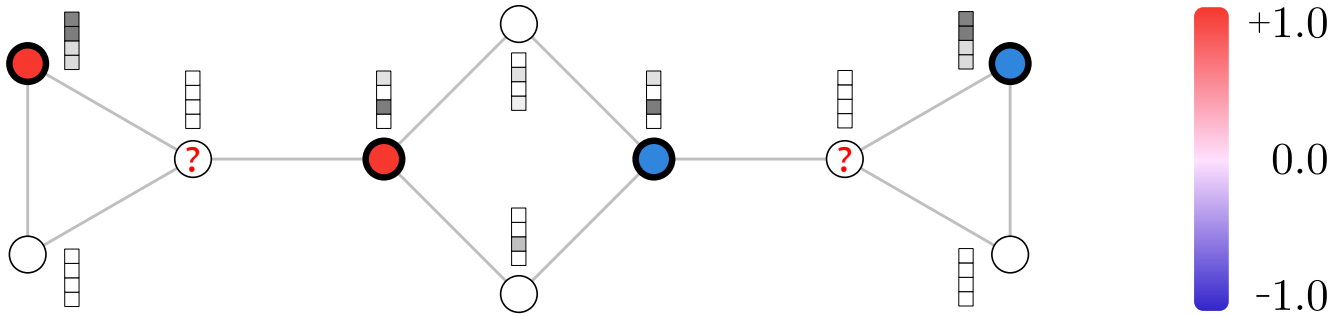

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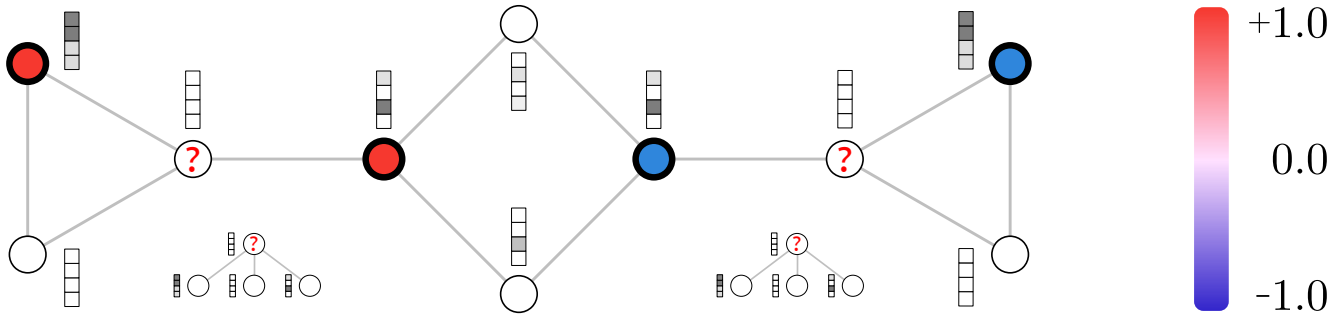

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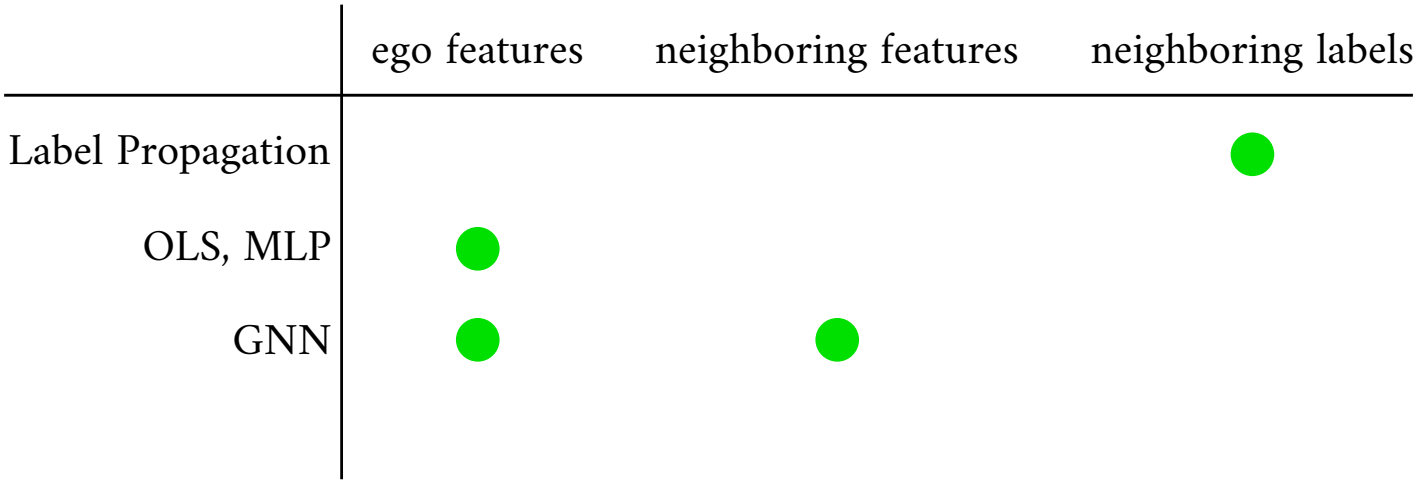
Combing GNN with Label Propagation



Combing GNN with Label Propagation

	ego features	neighboring features	neighboring labels
Label Propagation			●
OLS, MLP	●		
GNN	●	●	
???	●	●	●

Combing GNN with Label Propagation

Can we combine an inductive GNN with Label Propagation?

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- decompose outcomes as learnable from features and correlated residuals

$$y_u = f\left(\{\boldsymbol{x}_v\}_{v \in N_K(u)}\right) + r_u$$

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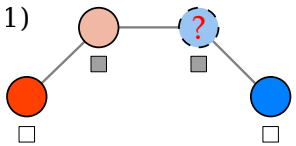
conceptually similar to boosting; the two "weak predictors" uses different inputs

Combing GNN with Label Propagation

Ground Truth Labels $\{y_u\}_{u \in V}$



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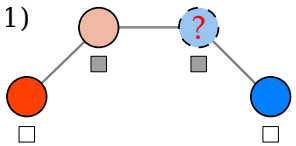
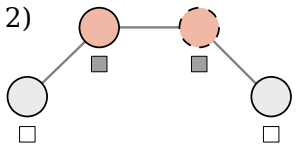


Predictions $\{\hat{y}_u\}_{u\in V}$



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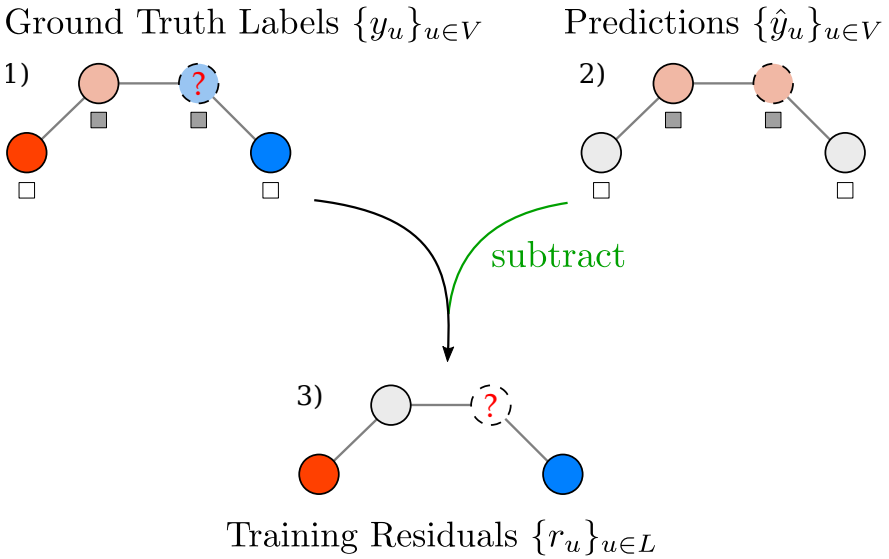

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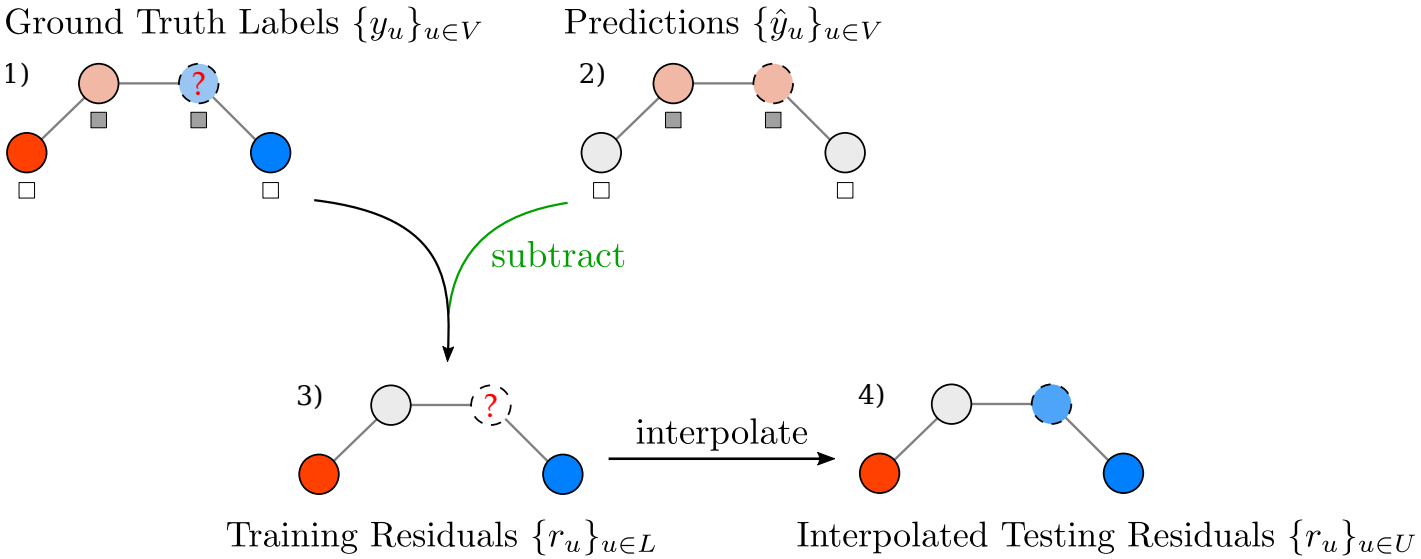

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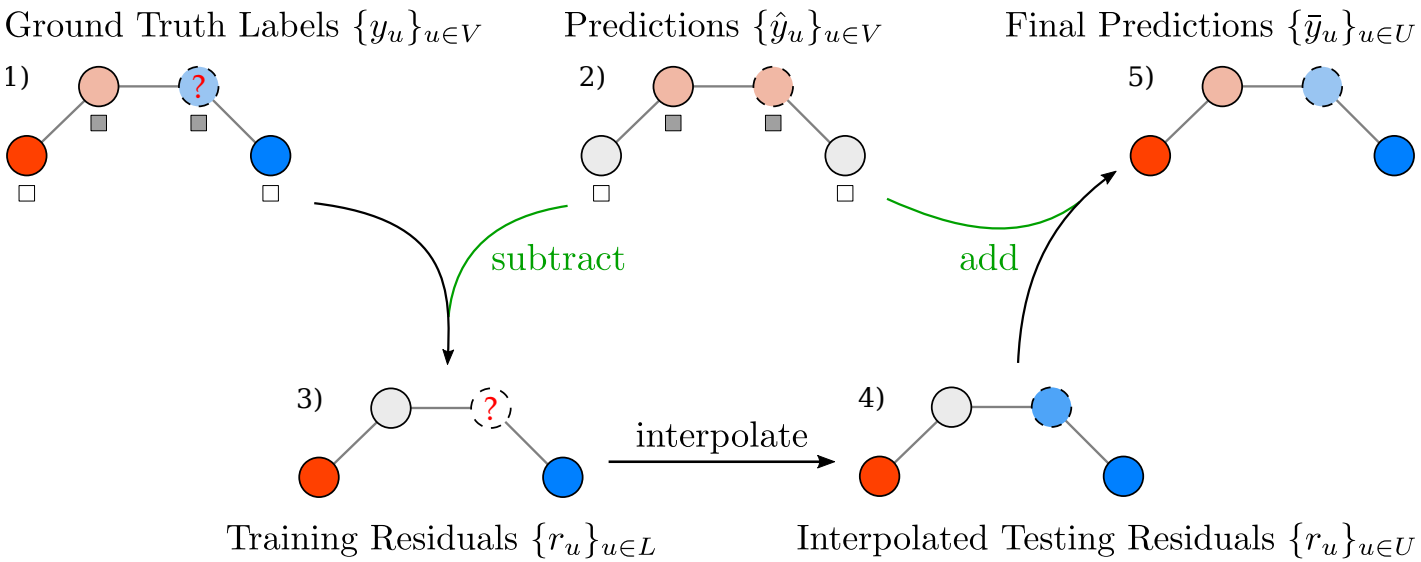

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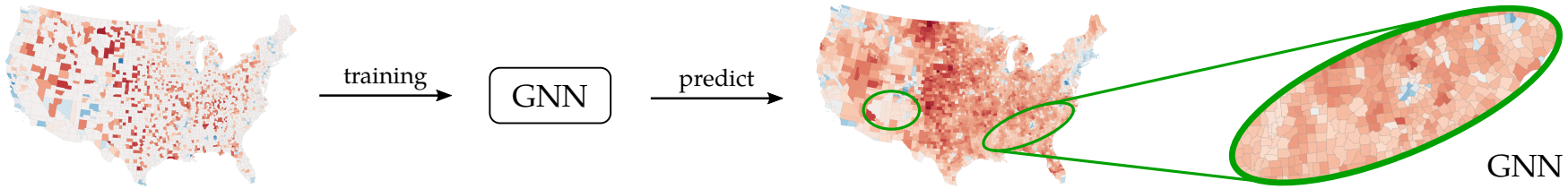
  - final prediction = inductive prediction + estimated residual

GNN/RP Works Super Well in Practice



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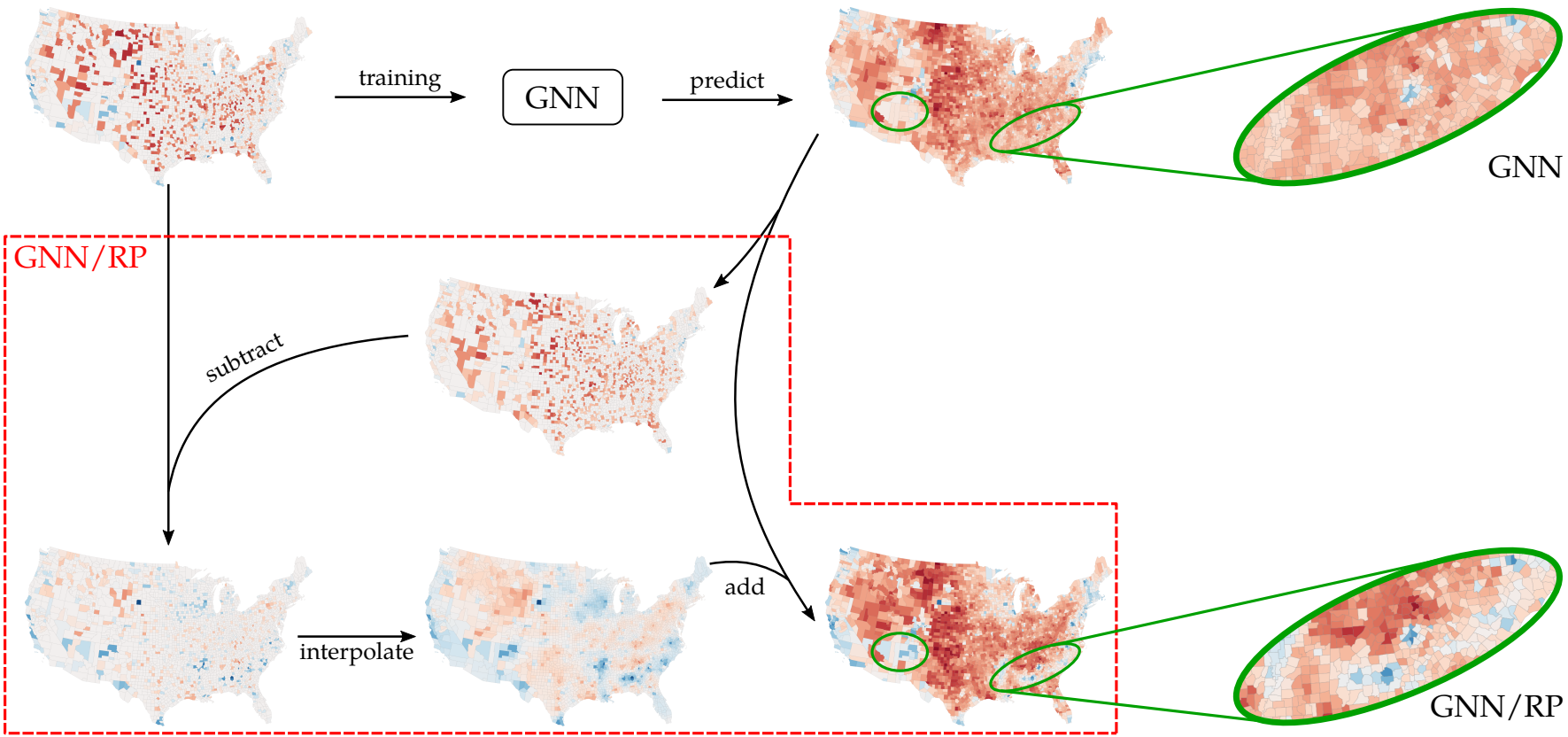

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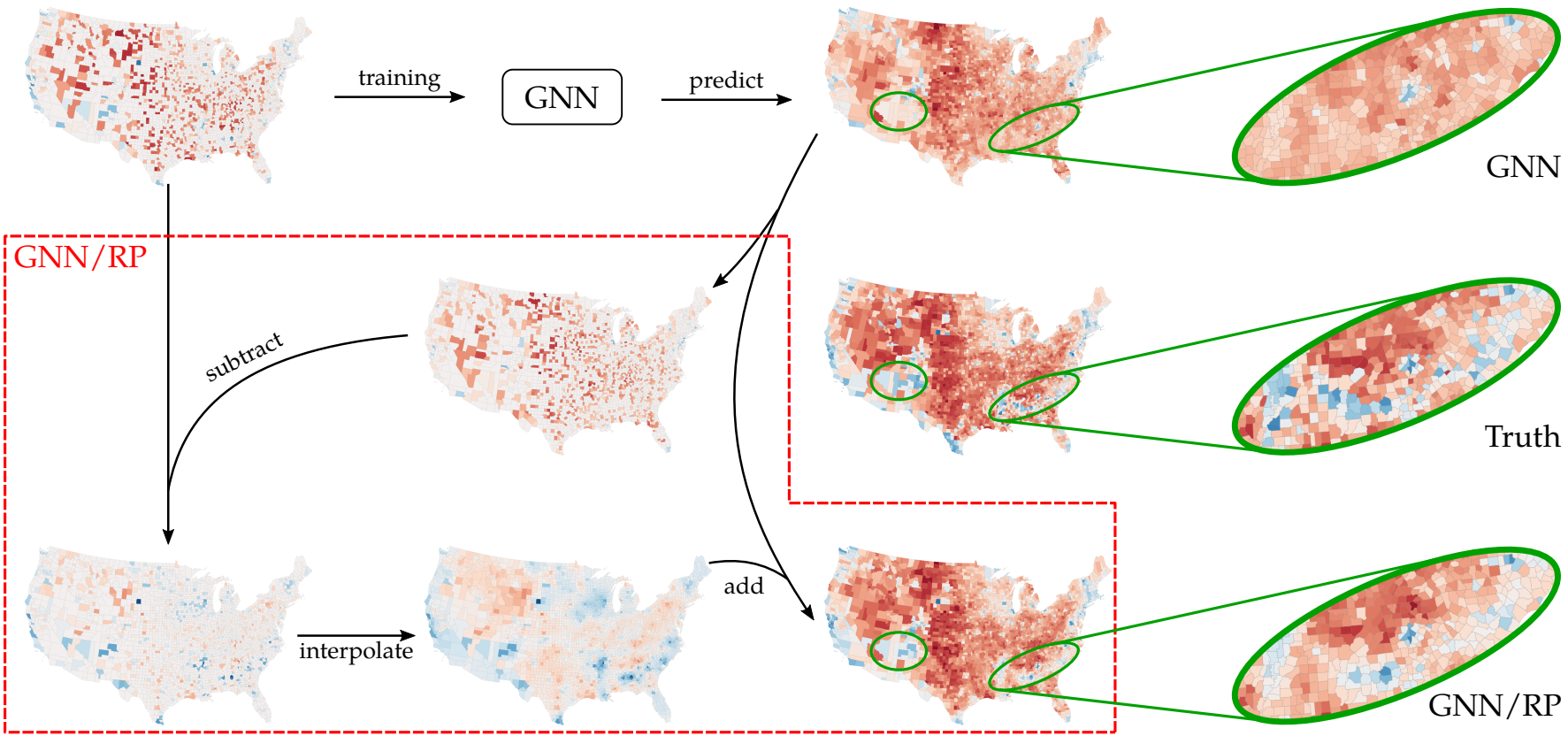

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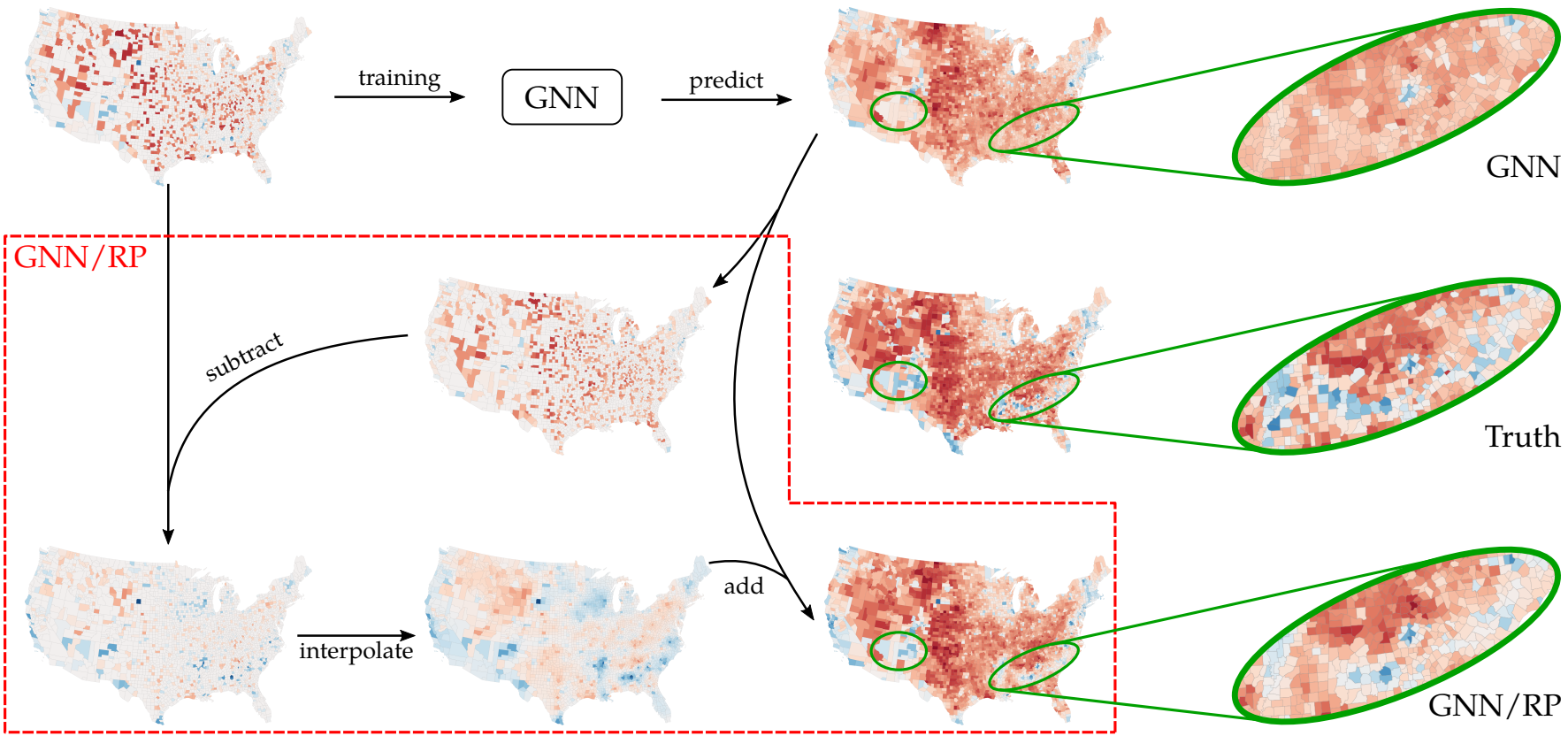

- coefficient of determination (R^2) increases from 0.51 to 0.69 on test set

RP Assumes Linearly Correlated Residuals

	ego features	neighboring features	neighboring labels
Label Propagation			●
OLS, MLP	●		
GNN	●	●	
GNN/RP	●	●	●

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$$\min_{\theta} \sum_{u \in L} (y_u - \hat{y}_u)^2, \quad \hat{y}_u = f(\boldsymbol{x}_u, \{\boldsymbol{x}_v : v \in N_K(u)\};\ \theta)$$

  corresponds to MLE assuming i.i.d. errors $\boldsymbol{y} = \hat{\boldsymbol{y}} + \boldsymbol{r},\ \boldsymbol{r} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{I})$

- residual propagation assumes correlated errors $\boldsymbol{r} \sim \mathcal{N}\left(\boldsymbol{0}, (\boldsymbol{I} - \alpha \boldsymbol{S})^{-1}\right)$
  - $\boldsymbol{S} = \boldsymbol{D}^{-1/2} \boldsymbol{W} \boldsymbol{D}^{-1/2}$ is the normalized adjacency matrix
  - residual propagation computes expectation of $\boldsymbol{r}_U$ conditioned on $\boldsymbol{r}_L$

Statistical Model for Node Attributes

Is there a common statistical framework that formalizes all three correlations?

Statistical Model for Node Attributes

- Problem input:
  - graph topology $G(V, E)$
  - features on all vertices, $\boldsymbol{X} = [\boldsymbol{x}_u]_{u \in V}$
  - labels on a subset of vertices $L \subset V$, training labels $\boldsymbol{y}_L = [y_u]_{u \in L}$
- Problem output:
  - labels on the rest of vertices $U \equiv V \backslash L$, testing labels $\boldsymbol{y}_U = [y_u]_{u \in U}$

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  - inference with conditional expectation $\boldsymbol{y}_U = E[\mathbf{y}_U | \texttt{observations}]$

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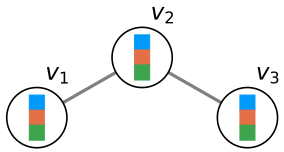
  - different observations gives different algorithms

Statistical Model for Node Attributes

Data Type	Corresponding Gaussian MRF	Learning Algorithm



graph data (**X**, **y**, G)

Statistical Model for Node Attributes

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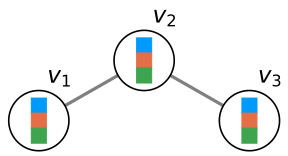
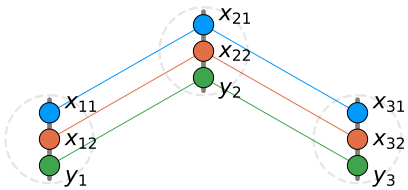


graph data (**X**, **y**, G)

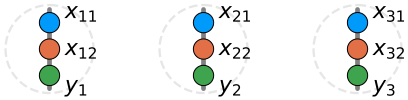


Statistical Model for Node Attributes

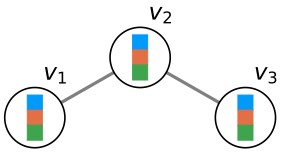
Data Type

i.i.d. data (**X, y**)

Corresponding Gaussian MRF



Learning Algorithm



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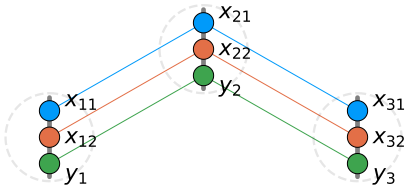


Statistical Model for Node Attributes

Data Type

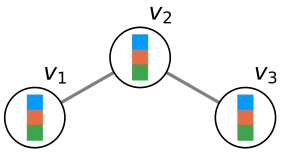
i.i.d. data (**X, y**)

Corresponding Gaussian MRF

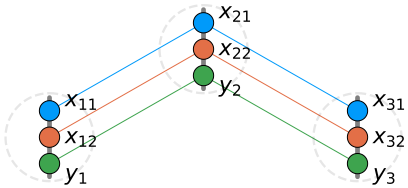
Learning Algorithm

linear regression

$E[\mathbf{y}_U|\mathbf{X}] = \mathbf{X}_U\beta$ $\beta = (\mathbf{X}_L^\top\mathbf{X}_L)^{-1}\mathbf{X}_L^\top\mathbf{y}_L$



graph data (**X**, **y**, G)



Statistical Model for Node Attributes

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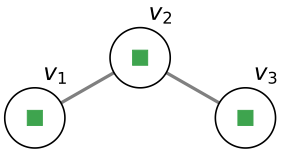
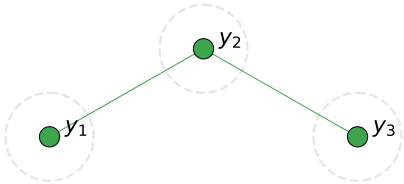
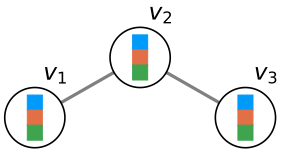
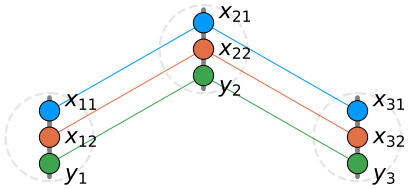
 i.i.d. data (**X, y**)		linear regression $E[\mathbf{y}_U \mid \mathbf{X}] = \mathbf{X}_U\beta$ $\beta = (\mathbf{X}_L^\top \mathbf{X}_L)^{-1}\mathbf{X}_L^\top \mathbf{y}_L$
 graph data (**y**, G)		
 graph data (**X**, **y**, G)		

Statistical Model for Node Attributes

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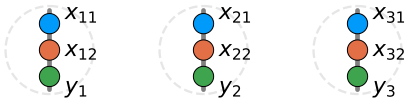
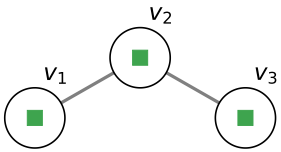
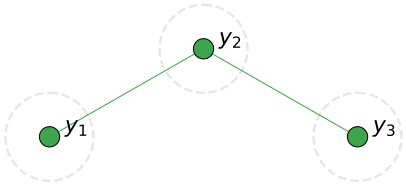
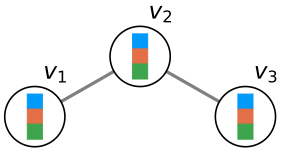
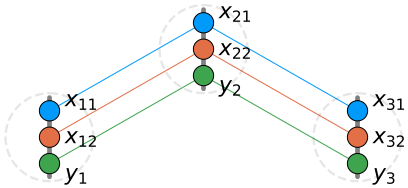
 i.i.d. data (**X, y**)		condition on $\mathbf{X}$ *e.g.* L={1,3}, U={2}	linear regression $E[\mathbf{y}_U \vert \mathbf{X}] = \mathbf{X}_U\beta$ $\quad \beta = (\mathbf{X}_L^\top \mathbf{X}_L)^{-1}\mathbf{X}_L^\top \mathbf{y}_L$
 graph data (**y**, G)		condition on $\mathbf{y}_L$	label propagation $E[\mathbf{y}_U \vert \mathbf{y}_L] = -(\mathbf{I} + \omega\mathbf{N})_{UU}^{-1}(\mathbf{I} + \omega\mathbf{N})_{UL}\mathbf{y}_L$
 graph data (**X**, **y**, G)			

Statistical Model for Node Attributes

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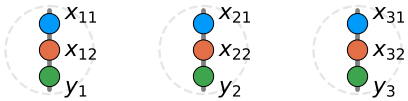
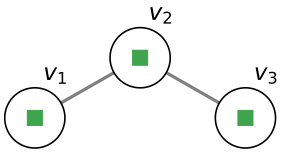
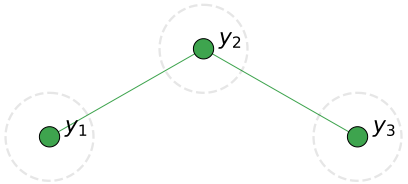
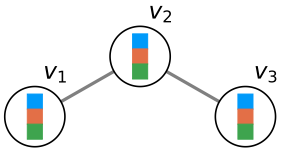
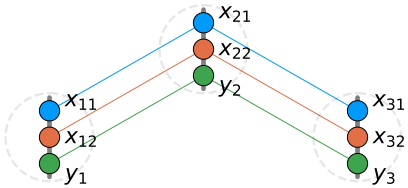
 i.i.d. data (**X, y**)		condition on $\mathbf{X}$ *e.g.* L={1,3}, U={2}	linear regression $E[\mathbf{y}_U \vert \mathbf{X}] = \mathbf{X}_U\beta$ $\quad \beta = (\mathbf{X}_L^\top \mathbf{X}_L)^{-1}\mathbf{X}_L^\top \mathbf{y}_L$
 graph data (**y**, G)		condition on $\mathbf{y}_L$	label propagation $E[\mathbf{y}_U \vert \mathbf{y}_L] = -(\mathbf{I}+\omega\mathbf{N})_{UU}^{-1}(\mathbf{I}+\omega\mathbf{N})_{UL}\mathbf{y}_L$
 graph data (**X**, **y**, G)		condition on $\mathbf{X}$	*linear GCN* $E[\mathbf{y}_U \vert \mathbf{X}] = [(\mathbf{I}+\omega\mathbf{N})^{-1}\mathbf{X}\beta]_U$

Statistical Model for Node Attributes

Data Type

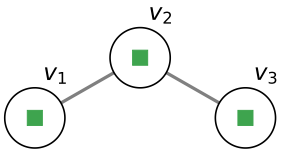
i.i.d. data (**X, y**)

Corresponding Gaussian MRF

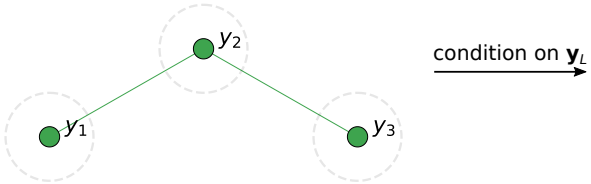
Learning Algorithm

linear regression

$E[\mathbf{y}_U|\mathbf{X}] = \mathbf{X}_U\beta \qquad \beta = (\mathbf{X}_L^\top\mathbf{X}_L)^{-1}\mathbf{X}_L^\top\mathbf{y}_L$

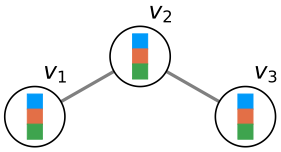


graph data (**y**, G)

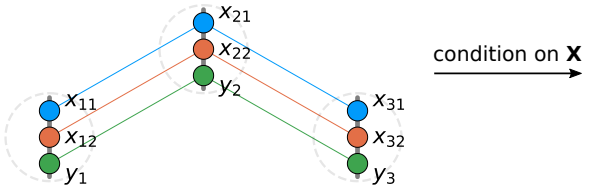


label propagation

$E[\mathbf{y}_U|\mathbf{y}_L] = -(\mathbf{I}+\omega\mathbf{N})_{UU}^{-1}(\mathbf{I}+\omega\mathbf{N})_{UL}\mathbf{y}_L$



graph data (**X**, **y**, G)



linear GCN —(further condition on $\mathbf{y}_L$)→ *residual propagation*

$E[\mathbf{y}_U|\mathbf{X}] = [(\mathbf{I}+\omega\mathbf{N})^{-1}\mathbf{X}\beta]_U$ $\qquad$ $E[\mathbf{y}_U|\mathbf{X},\mathbf{y}_L] = \cdots$

Statistical Model for Node Attributes

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i.i.d. data (**X, y**)

Corresponding Gaussian MRF

Learning Algorithm

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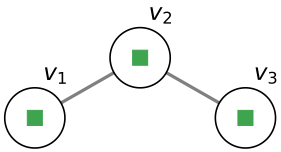
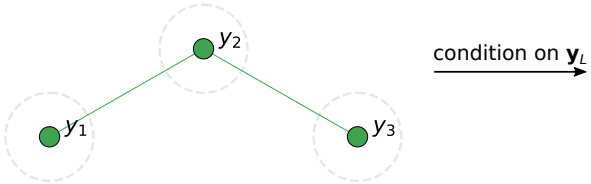


graph data (**y**, G)



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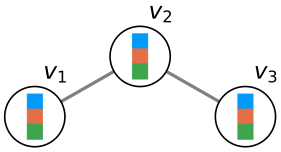
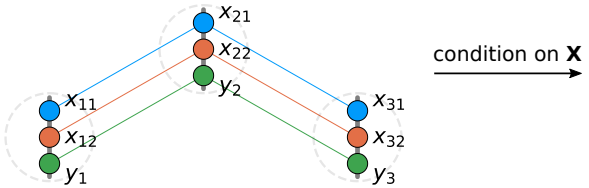
$E[\mathbf{y}_U|\mathbf{y}_L] = -(\mathbf{I}+\omega\mathbf{N})^{-1}_{UU}(\mathbf{I}+\omega\mathbf{N})_{UL}\mathbf{y}_L$



graph data (**X**, **y**, G)



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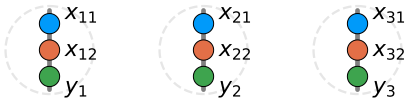
Statistical Model for Node Attributes

Data Type

i.i.d. data (**X, y**)

Corresponding Gaussian MRF



condition on $\mathbf{X}$

e.g. L={1,3}, U={2}

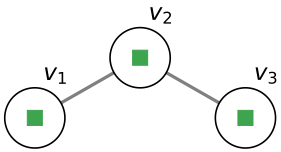
Learning Algorithm

linear regression

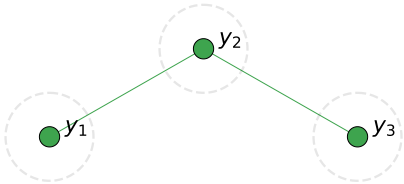
$E[\mathbf{y}_U|\mathbf{X}] = \mathbf{X}_U\beta \qquad \beta = (\mathbf{X}_L^\top\mathbf{X}_L)^{-1}\mathbf{X}_L^\top\mathbf{y}_L$

↓ +nonlinearity

MLP



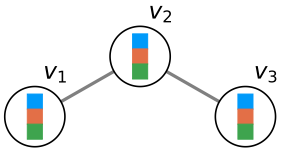
graph data (**y**, G)



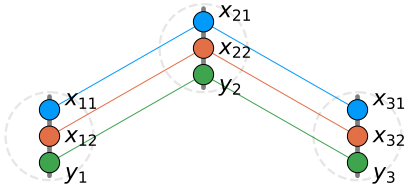
condition on $\mathbf{y}_L$

label propagation

$E[\mathbf{y}_U|\mathbf{y}_L] = -(\mathbf{I}+\omega\mathbf{N})_{UU}^{-1}(\mathbf{I}+\omega\mathbf{N})_{UL}\mathbf{y}_L$



graph data (**X**, **y**, G)



condition on $\mathbf{X}$

linear GCN → (further condition on $\mathbf{y}_L$) → *residual propagation*

$E[\mathbf{y}_U|\mathbf{X}] = [(\mathbf{I}+\omega\mathbf{N})^{-1}\mathbf{X}\beta]_U$

$E[\mathbf{y}_U|\mathbf{X}, \mathbf{y}_L] = \cdots$

↓ change filter

SGC (simple graph convolution)

↓ +nonlinearity

GCN (graph convolution network)

Statistical Model for Node Attributes

The joint distribution of all node attributes is a Gaussian MRF

- Real-valued attributes $\boldsymbol{a}_u = [\boldsymbol{x}_u; y_u] \in \mathbb{R}^{p+1}$ on each node u.
- $\boldsymbol{A}_i = i$th attribute over all nodes.
- $\boldsymbol{N} = \boldsymbol{I} - \boldsymbol{D}^{-1/2}\boldsymbol{W}\boldsymbol{D}^{-1/2}$ is the normalized Laplacian.

Statistical Model for Node Attributes

The joint distribution of all node attributes is a Gaussian MRF

- Real-valued attributes $\boldsymbol{a}_u = [\boldsymbol{x}_u; y_u] \in \mathbb{R}^{p+1}$ on each node u.
- $\boldsymbol{A}_i = i$th attribute over all nodes.
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This is a well-known result for standard linear models

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β is learned directly with OLS in a **discriminative** manner on the training nodes

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- Model parameters $\boldsymbol{H}, \boldsymbol{h}$ reduce to positive scalars:

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Computes expectation of $\mathbf{y}$ in the full model conditioned only on features

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$$= \underbrace{(\boldsymbol{I}_n + \omega \boldsymbol{N})^{-1} \boldsymbol{X}}_{\text{LP on features!}} \beta$$

$(\boldsymbol{I}_n + \omega \boldsymbol{N})^{-1} \boldsymbol{X}$ is the solution to label propagation for the features:

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$$= \underbrace{(\boldsymbol{I}_n + \omega \boldsymbol{N})^{-1} \boldsymbol{X}}_{\text{LP on features!}} \beta$$

$(\boldsymbol{I}_n + \omega \boldsymbol{N})^{-1}\boldsymbol{X}$ is the solution to label propagation for the features:

$$\boldsymbol{X}^{(k)} = \alpha \cdot \boldsymbol{S}\boldsymbol{X}^{(k-1)} + (1-\alpha) \cdot \boldsymbol{X}$$

Case 3. Linear Graph Convolution

Computes expectation of $\mathbf{y}$ in the full model conditioned only on features

- The joint distribution of all attributes is given by:

$$\mathrm{vec}(\mathbf{A}) \sim \mathcal{N}(\mathbf{0}, \mathbf{\Gamma}^{-1}), \quad \mathbf{\Gamma} = \boldsymbol{H} \otimes \boldsymbol{I}_n + \mathrm{diag}(\boldsymbol{h}) \otimes \boldsymbol{N}$$

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- Linear graph convolution (LGC)
  - use label propagation to smooth/preprocess features
  - just like linear regression, learn β with OLS on the training nodes

Case 3. Linear Graph Convolution

LGC [Jia-Benson 21]	$(1-\alpha)(\boldsymbol{I}+\alpha\boldsymbol{S}+\alpha^2\boldsymbol{S}^2+\ldots)\boldsymbol{X}\beta$	$\boldsymbol{S}=\boldsymbol{D}^{-1/2}\boldsymbol{W}\boldsymbol{D}^{-1/2}$
SGC [Wu+ 19]	$\tilde{\boldsymbol{S}}^K\boldsymbol{X}\beta$	$\tilde{\boldsymbol{S}}=(\boldsymbol{D}+\boldsymbol{I})^{-1/2}(\boldsymbol{W}+\boldsymbol{I})(\boldsymbol{D}+\boldsymbol{I})^{-1/2}$
GCN [Kipf-Welling 17]	$\sigma(\tilde{\boldsymbol{S}}\ldots\sigma(\tilde{\boldsymbol{S}}\boldsymbol{X}\boldsymbol{\Theta}^{(1)})\ldots\boldsymbol{\Theta}^{(K)})\beta$	

- connection to the graph convolutional network:
  - LGC sums decaying contributions from features on increasingly distant neighbors

Neumann expansion, $(\boldsymbol{I}+\omega\boldsymbol{N})^{-1}=\left(1-\frac{\omega}{1+\omega}\right)\left(\boldsymbol{I}-\frac{\omega}{1+\omega}\boldsymbol{S}\right)^{-1}=(1-\alpha)(\boldsymbol{I}+\alpha\boldsymbol{S}+\alpha^2\boldsymbol{S}^2+\ldots)$

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- LGC computes $E[\mathbf{y}_U|\boldsymbol{X}]$, **why not conditioning on $\mathbf{y}_L$ as well?**

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Case 4. Residual Propagation

- The conditional distribution of all labels conditioned on features:

$$\mathbf{y}|\mathbf{X} = \boldsymbol{X} \sim \mathcal{N}(\bar{\boldsymbol{y}}, \boldsymbol{\Gamma}_{PP}^{-1}), \quad \boldsymbol{\Gamma}_{PP} = H_{p+1,p+1}\boldsymbol{I}_n + h_{p+1}\boldsymbol{N}$$

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- Linear graph convolution with residual propagation (LGC/RP)
  - train LGC to predict both training nodes and testing nodes
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- Residual propagation post-processing is compatible with SGC, GCN, ...

The Derived Algorithms Perform Super Well

Dataset	Outcome	LP	LR	LGC (α)	SGC (K)	GCN (K)	LGC/RP	SGC/RP	GCN/RP
U.S.	income	0.40	0.63	0.66 (0.46)	0.51 (1.0)	0.53 (1.3)	**0.69**	0.55	0.55
	education	0.31	**0.71**	**0.71** (0.00)	0.43 (1.0)	0.47 (1.0)	**0.71**	0.46	0.48
	unemployment	0.47	0.34	0.39 (0.59)	0.32 (1.3)	0.45 (2.5)	**0.54**	0.52	0.53
	election	0.52	0.42	0.49 (0.68)	0.43 (1.1)	0.52 (2.1)	**0.64**	0.61	0.61
CDC	airT	0.95	0.85	0.86 (0.78)	0.86 (2.6)	0.95 (3.0)	0.96	**0.97**	**0.97**
	landT	0.89	0.81	0.81 (0.09)	0.79 (1.0)	0.91 (2.4)	0.90	0.93	**0.93**
	precipitation	0.89	0.59	0.61 (0.93)	0.61 (2.3)	0.79 (3.0)	0.89	**0.90**	**0.90**
	sunlight	0.96	0.75	0.81 (0.97)	0.80 (3.0)	0.90 (3.0)	0.96	**0.97**	**0.97**
	pm2.5	0.96	0.21	0.27 (0.99)	0.23 (2.7)	0.78 (3.0)	0.96	0.96	**0.97**
London	income	0.46	**0.85**	**0.85** (0.00)	0.64 (1.0)	0.63 (1.0)	**0.85**	0.65	0.64
	education	0.65	0.81	0.83 (0.40)	0.74 (1.6)	0.79 (1.4)	**0.86**	0.77	0.79
	age	0.65	0.73	0.73 (0.17)	0.66 (1.2)	0.70 (1.7)	**0.75**	0.72	0.72
	election	0.67	0.73	0.81 (0.74)	0.74 (2.0)	0.76 (2.1)	**0.85**	0.78	0.78
Twitch	days	0.08	0.58	0.59 (0.67)	0.22 (1.4)	0.26 (1.7)	**0.60**	0.23	0.26

30% training; hyperparameter α, K tuned with cross-validation on training nodes

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- LGC consistently outperforms SGC on all datasets (explain from graph filtering later)

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	landT	0.89	0.81	0.81 (0.09)	0.79 (1.0)	0.91 (2.4)	0.90	0.93	**0.93**
	precipitation	0.89	0.59	0.61 (0.93)	0.61 (2.3)	0.79 (3.0)	0.89	**0.90**	**0.90**
	sunlight	0.96	0.75	0.81 (0.97)	0.80 (3.0)	0.90 (3.0)	0.96	**0.97**	**0.97**
	pm2.5	0.96	0.21	0.27 (0.99)	0.23 (2.7)	0.78 (3.0)	0.96	0.96	**0.97**
London	income	0.46	**0.85**	**0.85** (0.00)	0.64 (1.0)	0.63 (1.0)	**0.85**	0.65	0.64
	education	0.65	0.81	0.83 (0.40)	0.74 (1.6)	0.79 (1.4)	**0.86**	0.77	0.79
	age	0.65	0.73	0.73 (0.17)	0.66 (1.2)	0.70 (1.7)	**0.75**	0.72	0.72
	election	0.67	0.73	0.81 (0.74)	0.74 (2.0)	0.76 (2.1)	**0.85**	0.78	0.78
Twitch	days	0.08	0.58	0.59 (0.67)	0.22 (1.4)	0.26 (1.7)	**0.60**	0.23	0.26

- LGC consistently outperforms SGC on all datasets (explain from graph filtering later)
- Inductive/RP always outperforms LP and the inductive base predictor

30% training; hyperparameter α, K tuned with cross-validation on training nodes

Our Model Connects a lot of Dots

	ego features	neighboring features	neighboring labels
Label Propagation			●
OLS, MLP	●		
GNN	●	●	
GNN/RP	●	●	●

- Our generative model,

Our Model Connects a lot of Dots

	ego features	neighboring features	neighboring labels
Label Propagation			●
OLS, MLP	●		
GNN	●	●	
GNN/RP	●	●	●

- Our generative model,
  - formalizes three types of correlations that are helpful for learning node labels

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	ego features	neighboring features	neighboring labels
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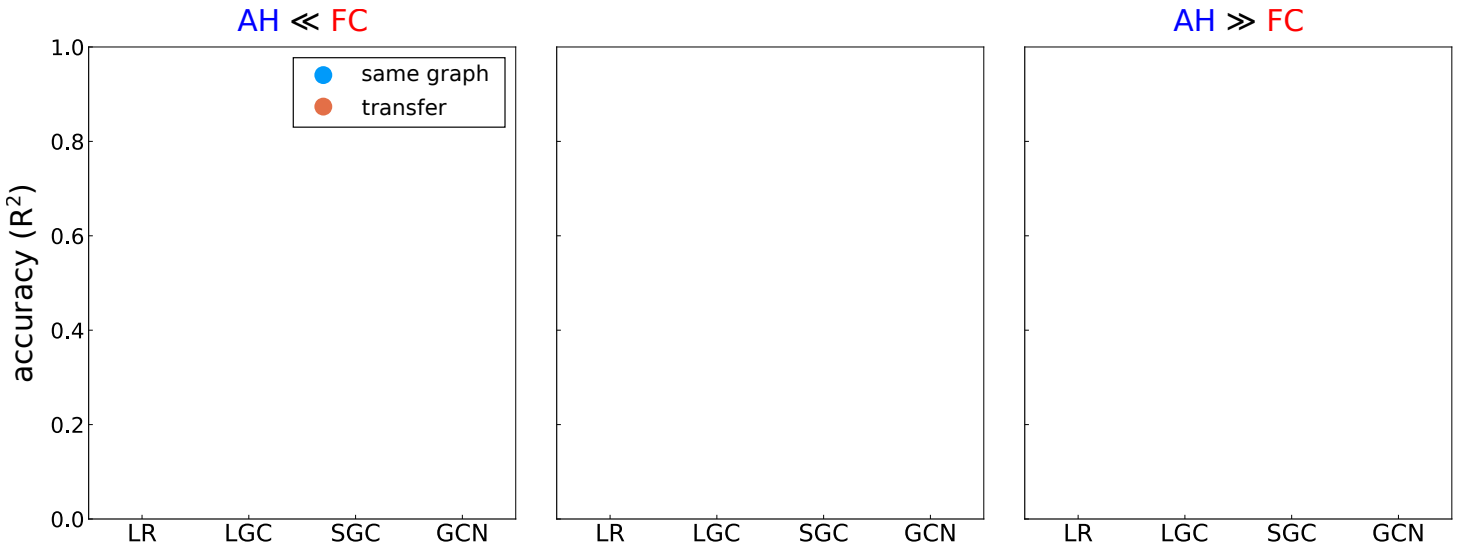
  - How are SGC and LGC different? our model helps understand smoothing
  - we can use LGC to interpret empirical datasets

We can Sample Data to Test Algorithms

Transfer learning experiments on inductive methods

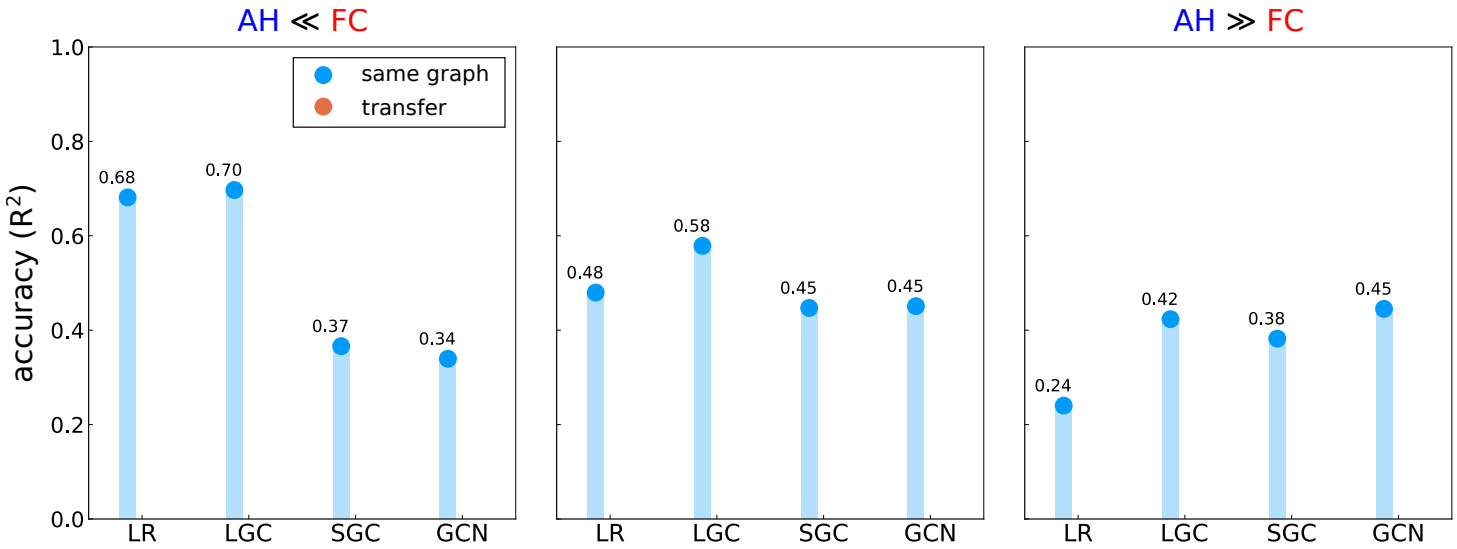


- same graph: sample one attributed graphs G_1, train and test on different vertices

The real-world dataset we consider here is the election data from 2012/2016.

We can Sample Data to Test Algorithms

Transfer learning experiments on inductive methods



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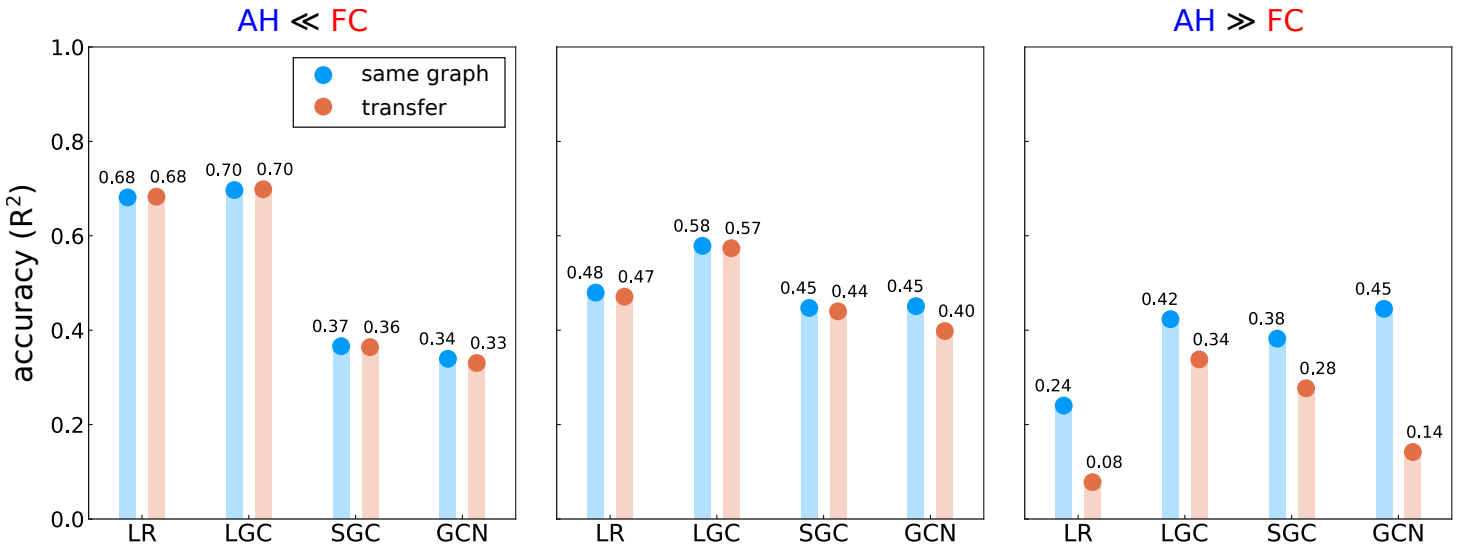

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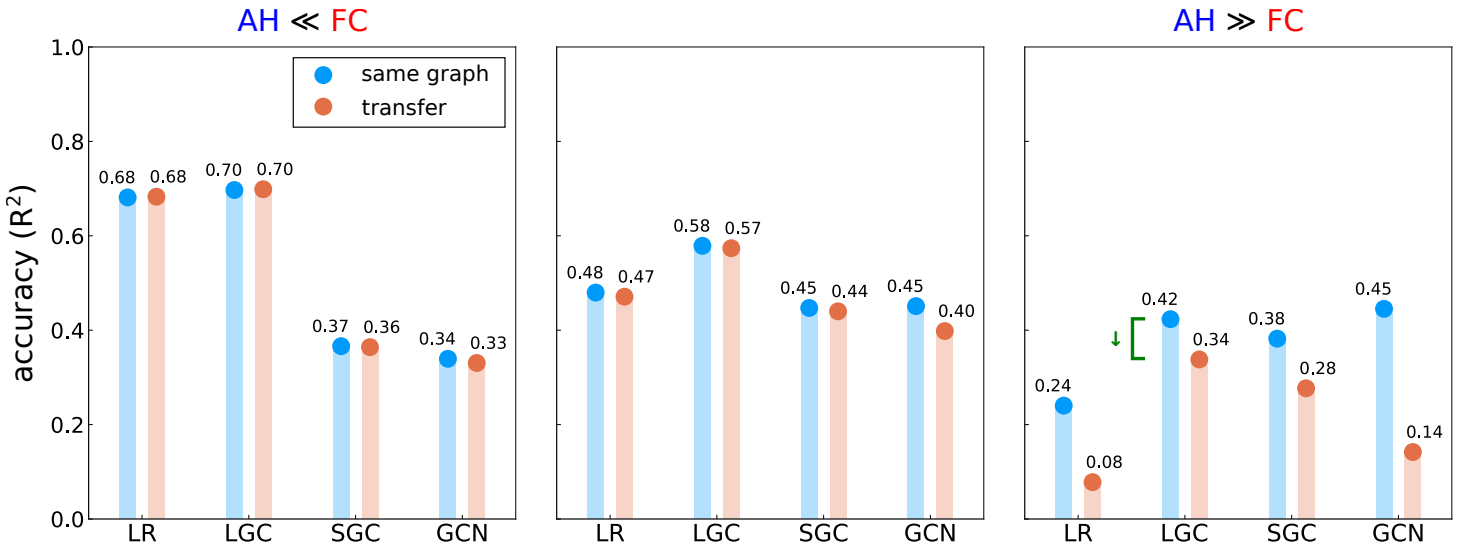

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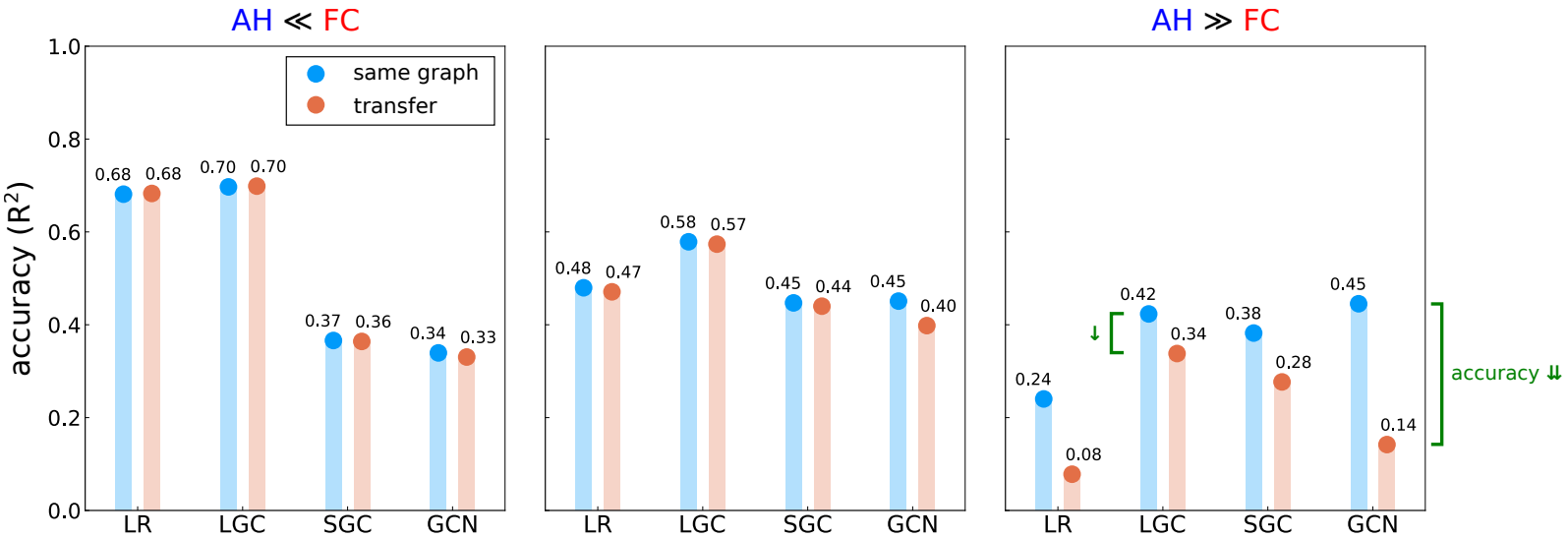

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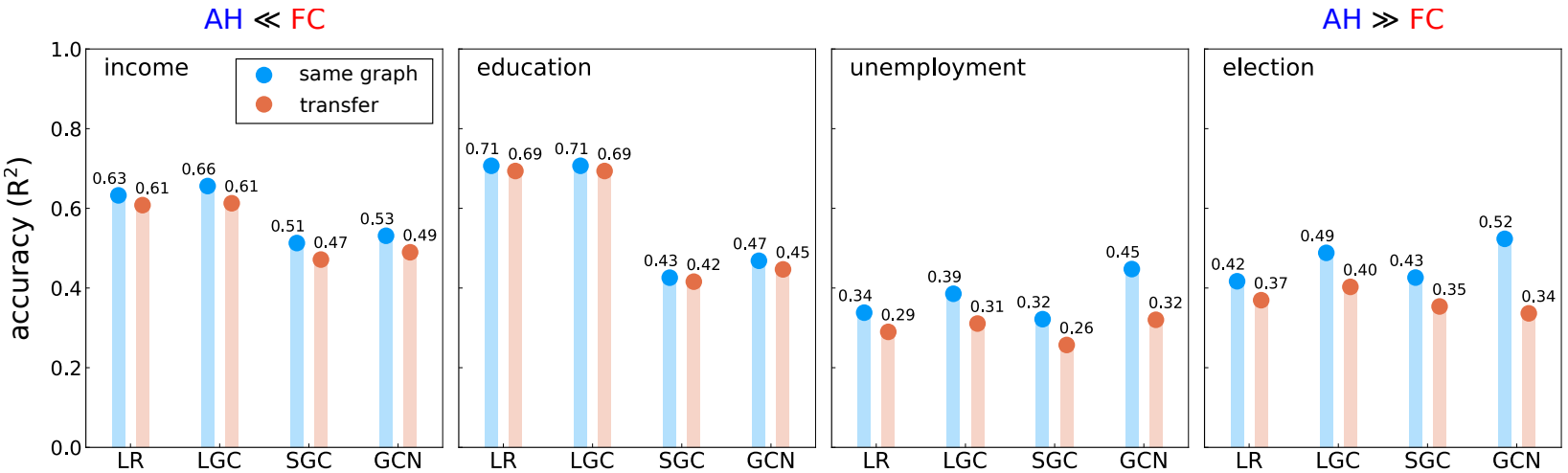
Transfer learning experiments on inductive methods



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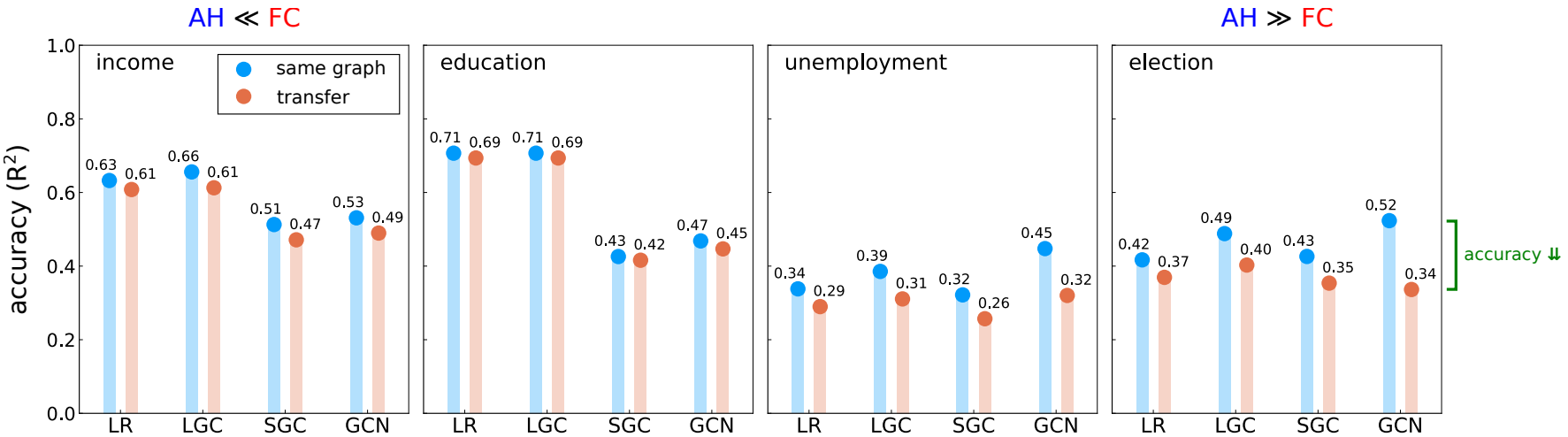

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The real-world dataset we consider here is the election data from 2012/2016.

Our Model Helps Understand Smoothing

- Spectral graph theory measures smoothness with eigenvectors of $\boldsymbol{N} = \boldsymbol{V}\boldsymbol{\Lambda}\boldsymbol{V}^\intercal$.

[Ortega+ 2018; Li+ 2018; Li+ 2019]

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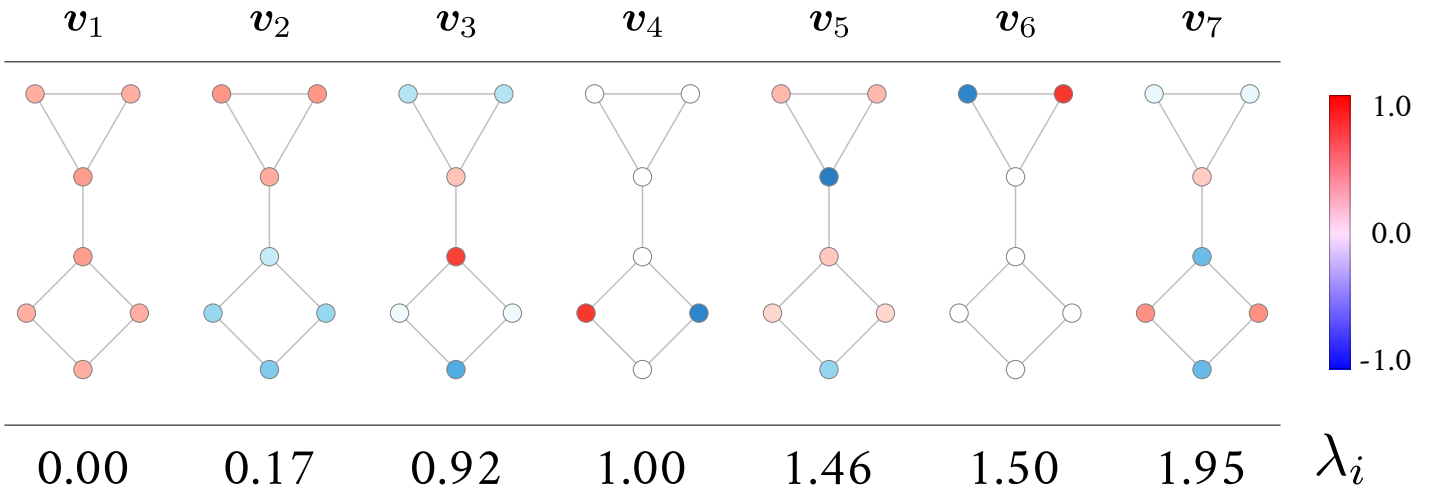

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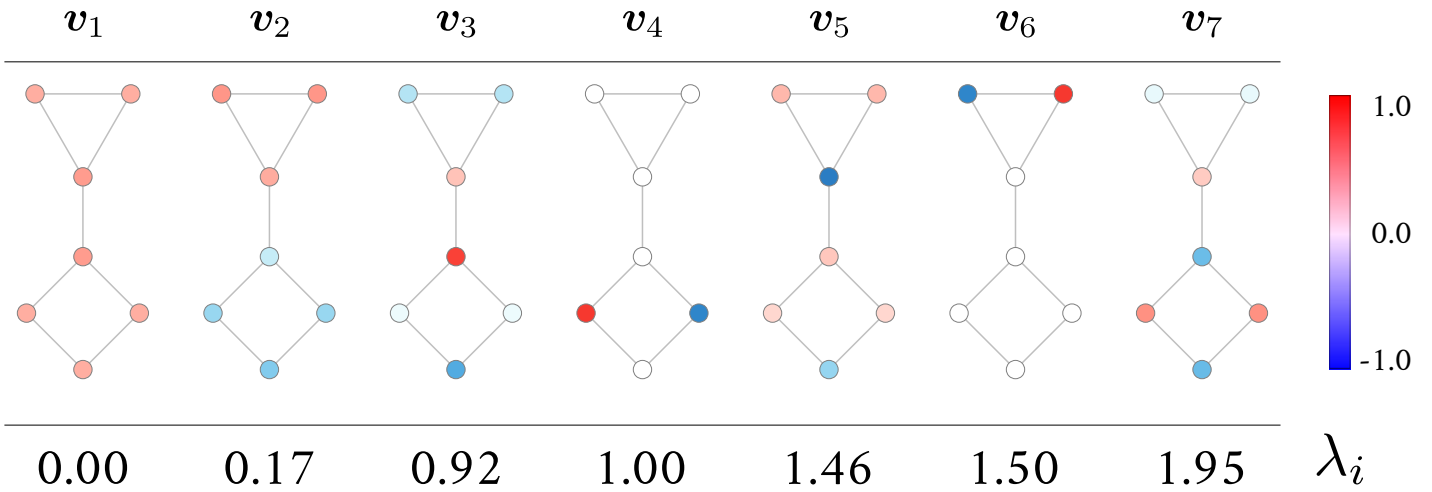

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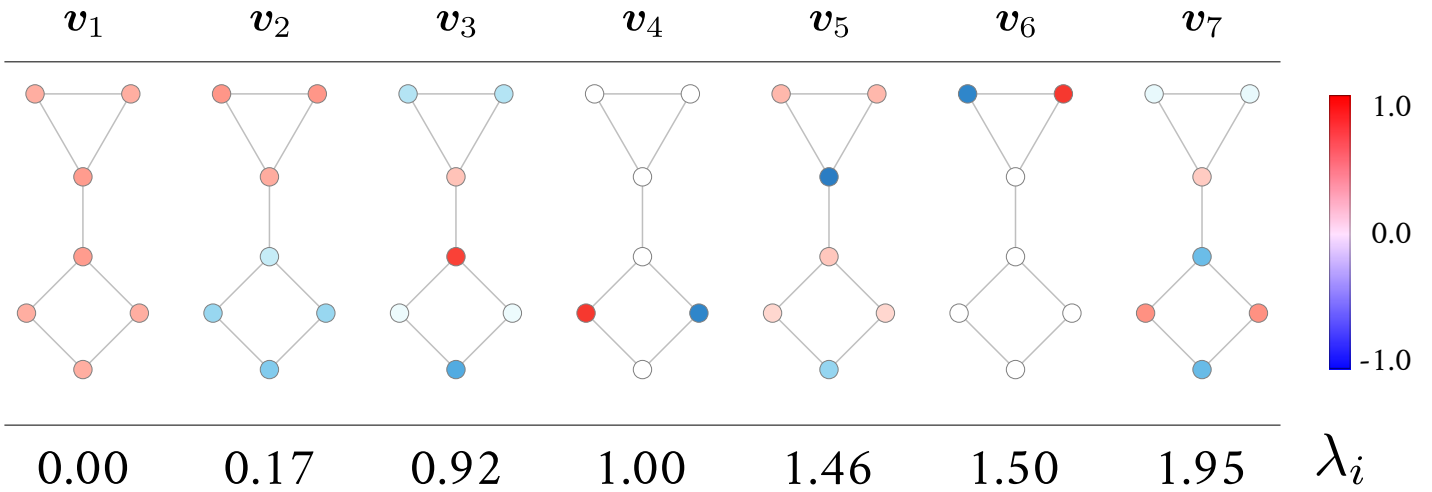

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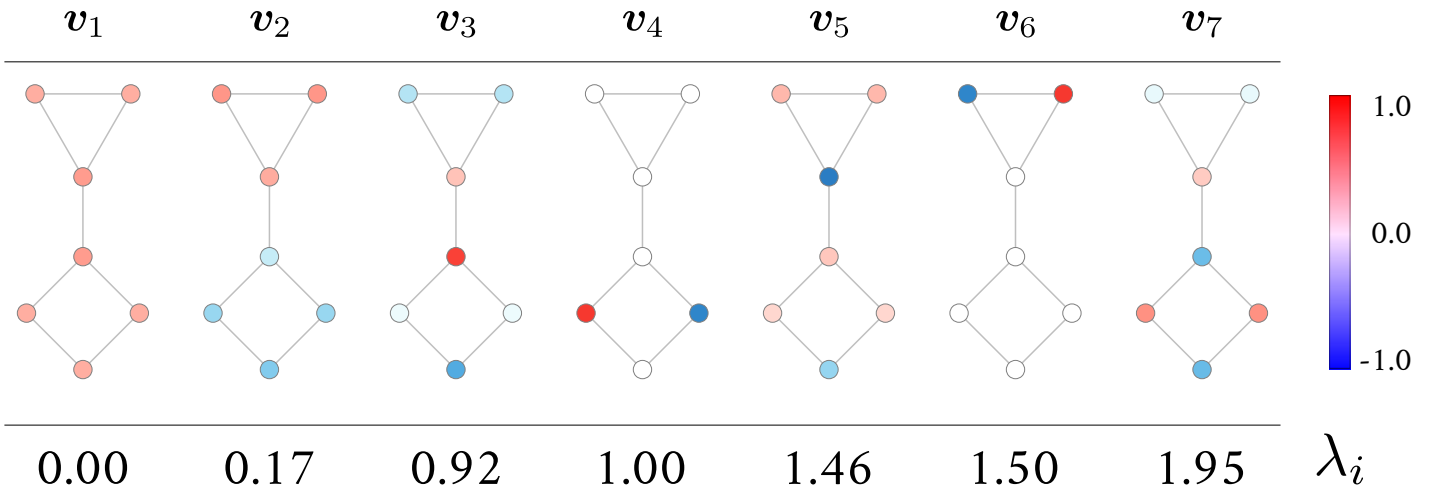

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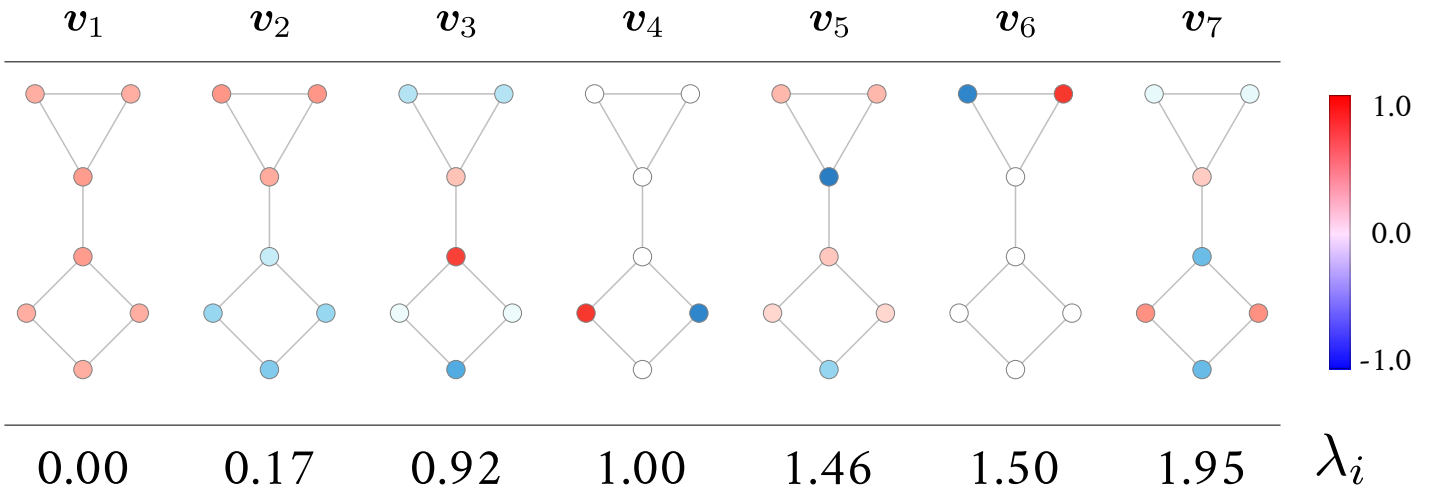

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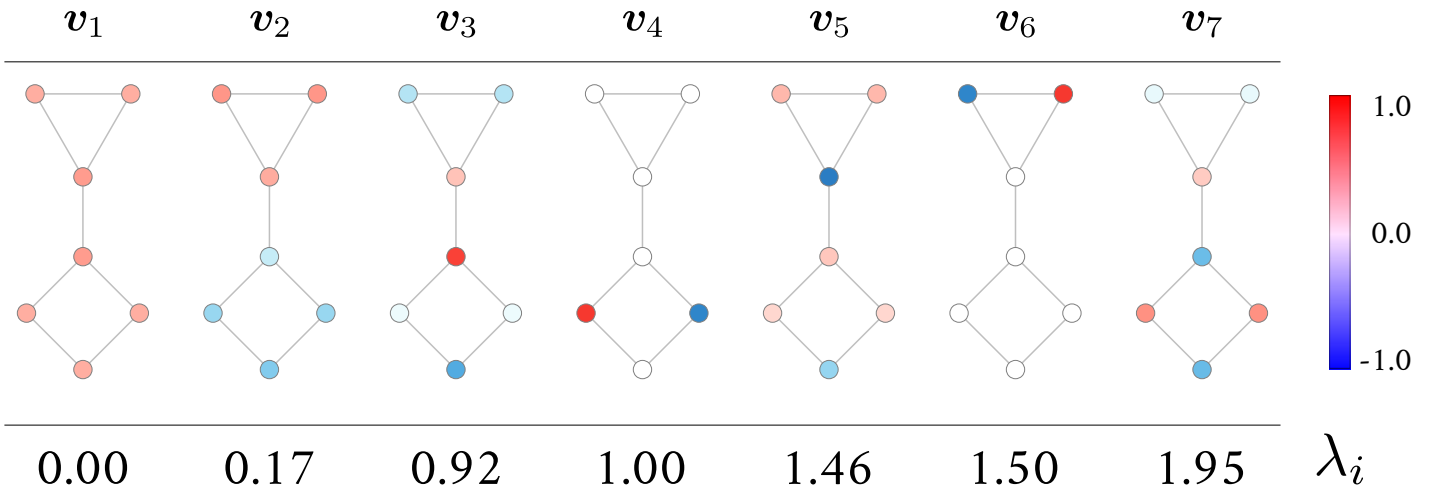

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LGC :
$$(\boldsymbol{I} + \omega \boldsymbol{N})^{-1}\boldsymbol{f} = \sum_i c_i \boldsymbol{v}_i \ \ (1 + \omega\lambda_i)^{-1}$$

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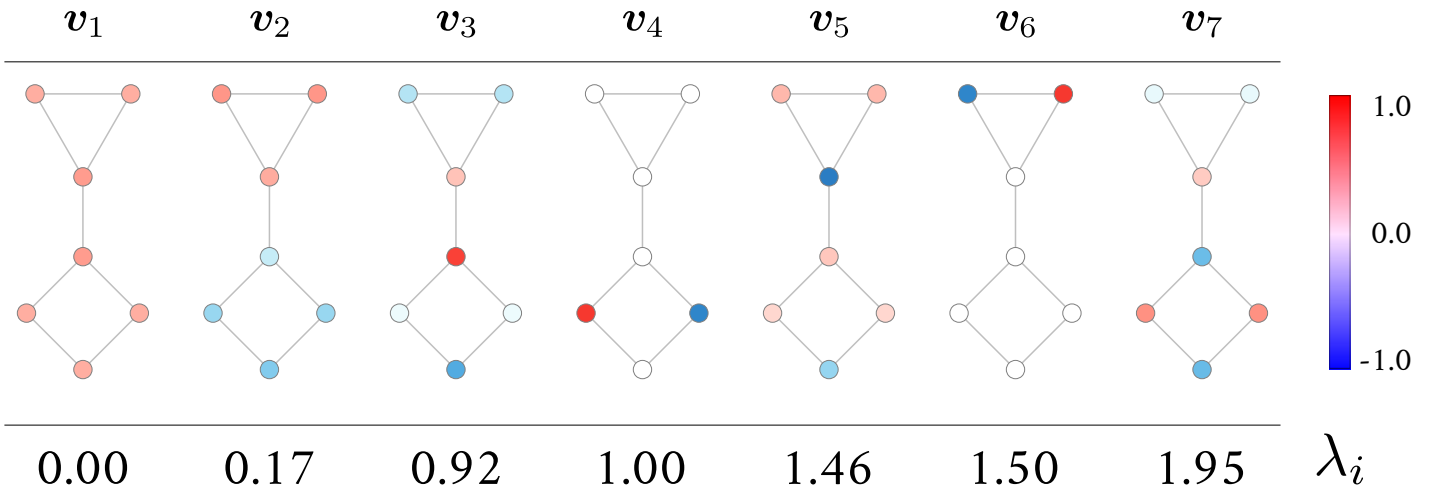

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SGC :
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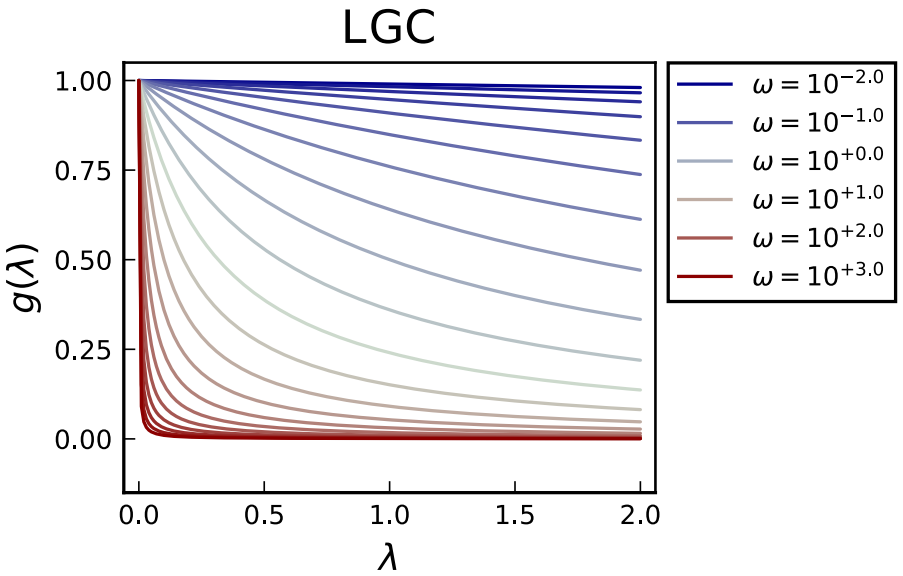

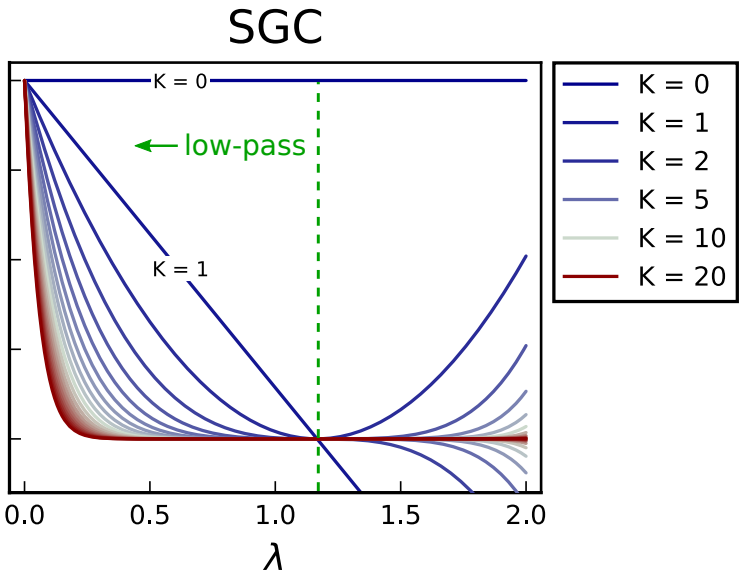

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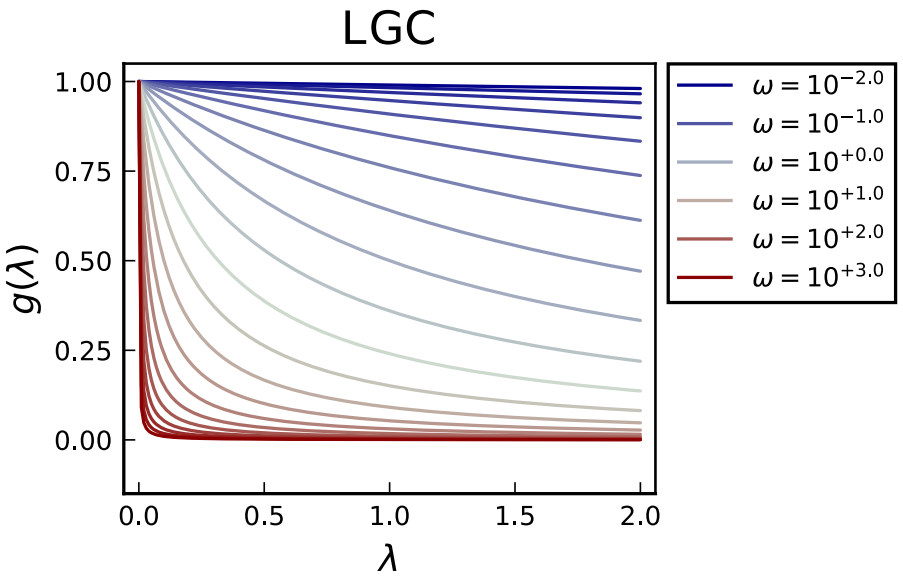

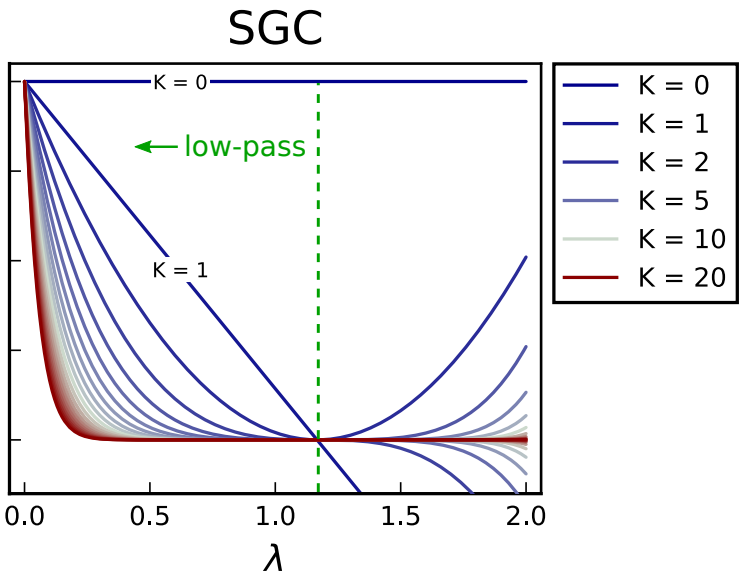

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- LGC is a low-pass filter on the entire eigenspectrum $[0, 2]$

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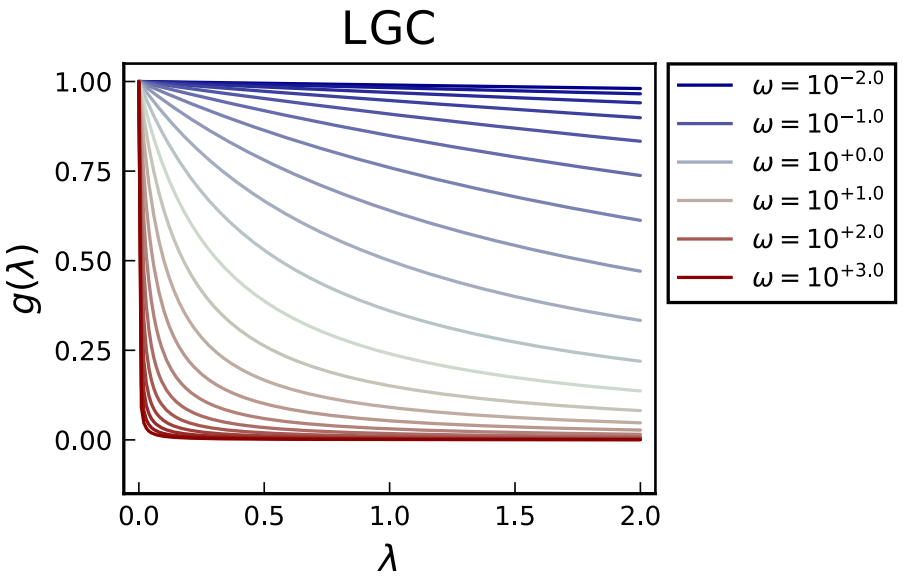

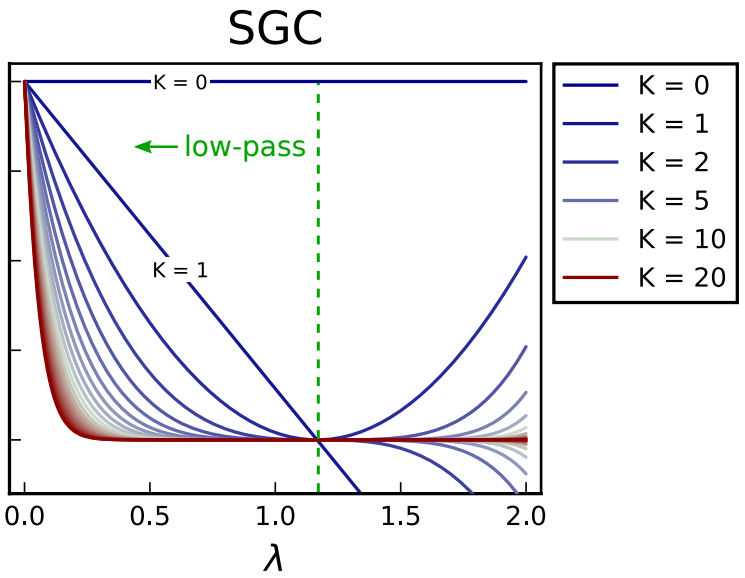

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- LGC is a low-pass filter on the entire eigenspectrum $[0, 2]$
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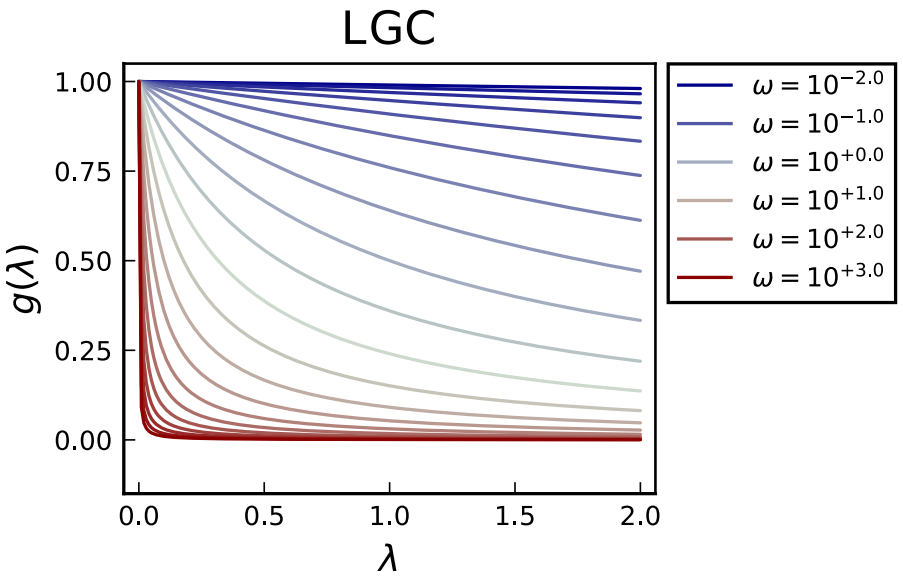

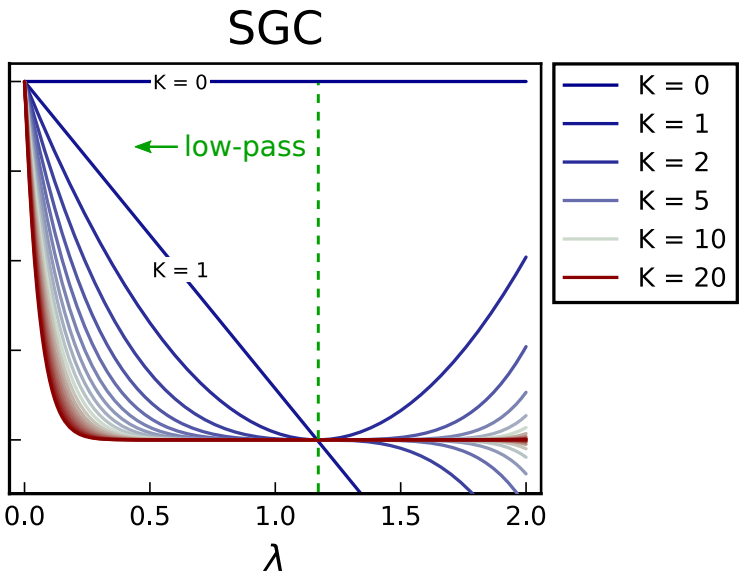

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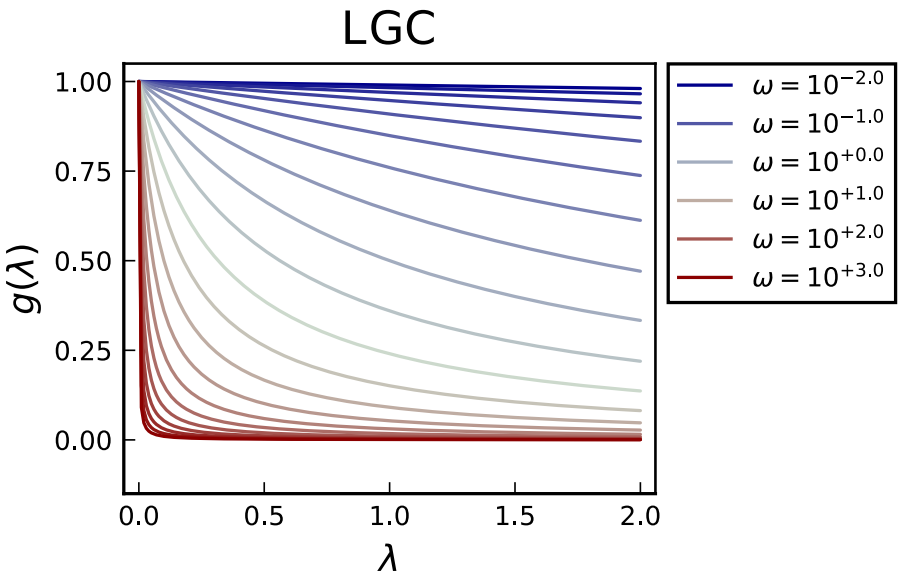

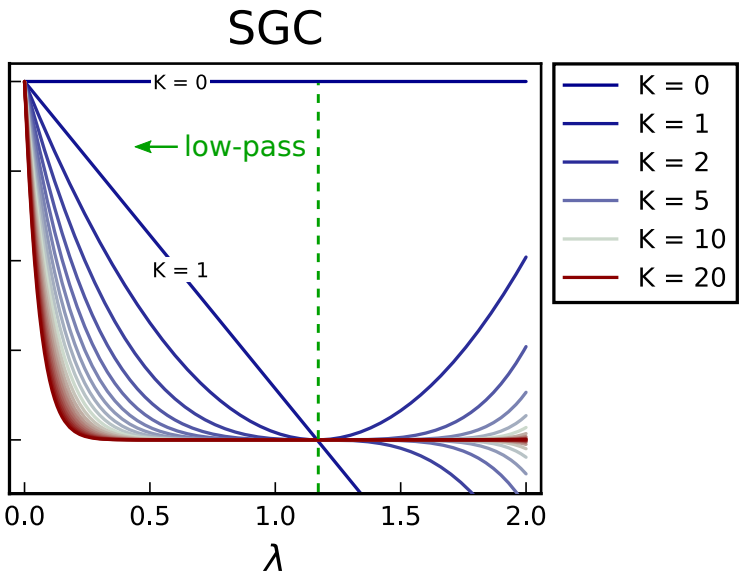

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- LGC is a low-pass filter on the entire eigenspectrum $[0, 2]$
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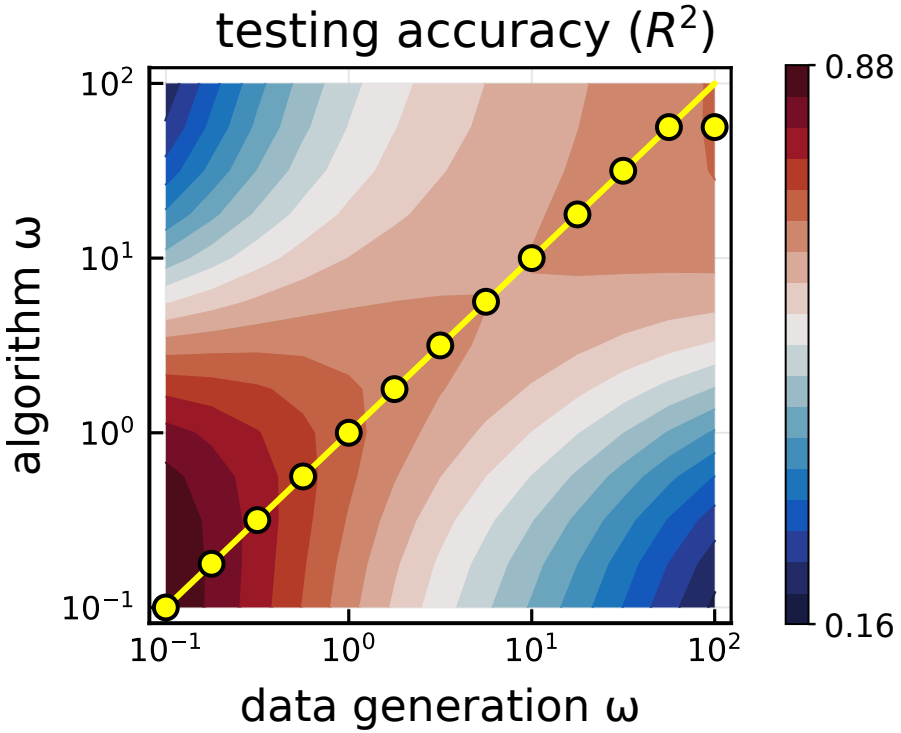
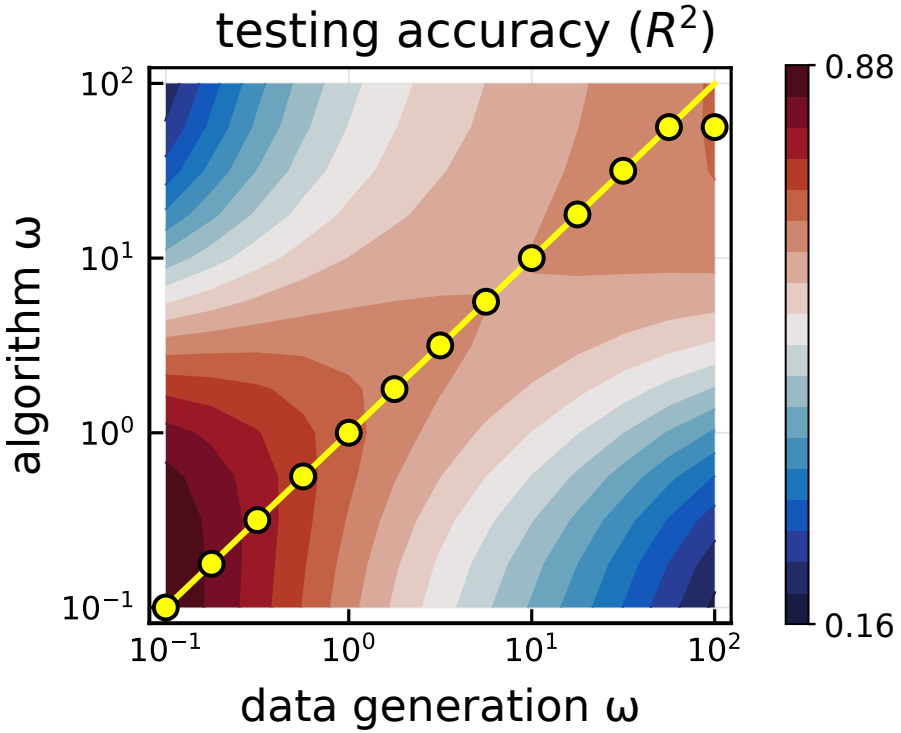


- Sample datasets from our generative model, with different $\omega = h/H$

Our Model Helps Understand Smoothing



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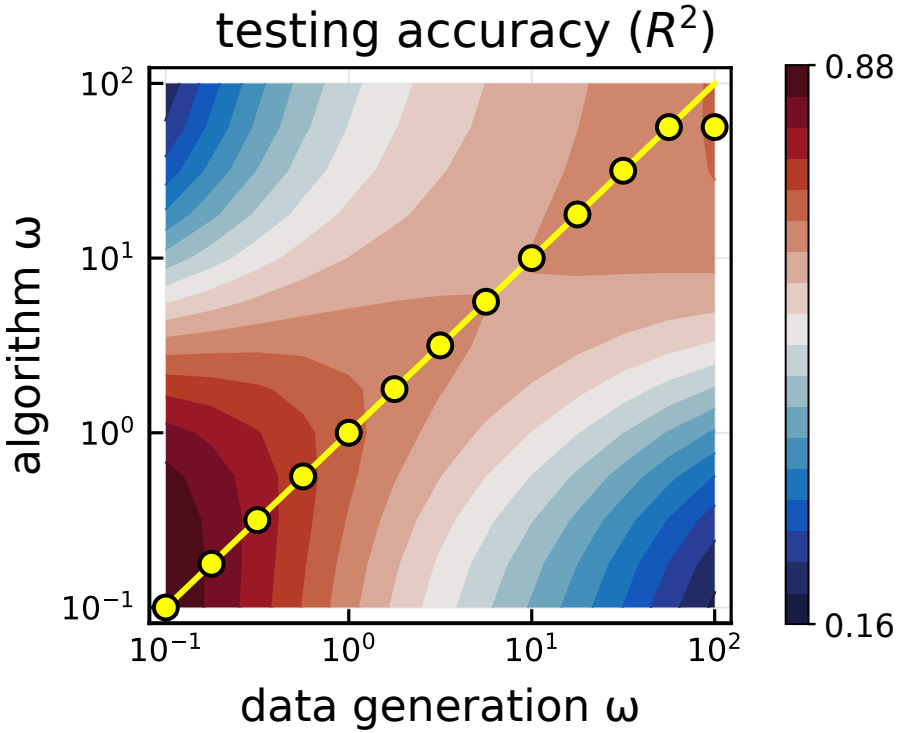

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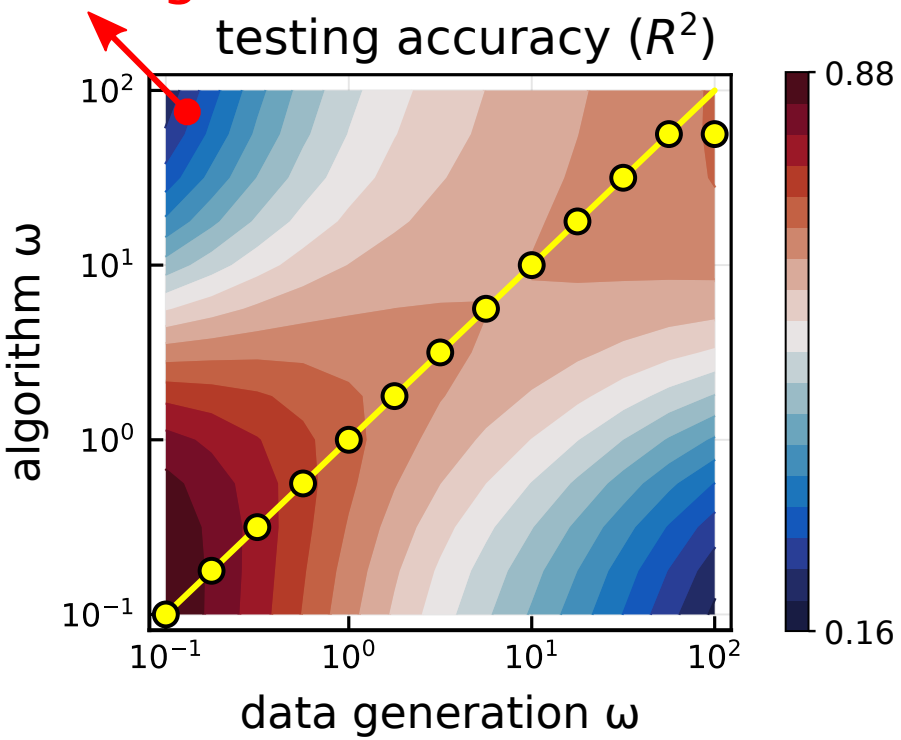

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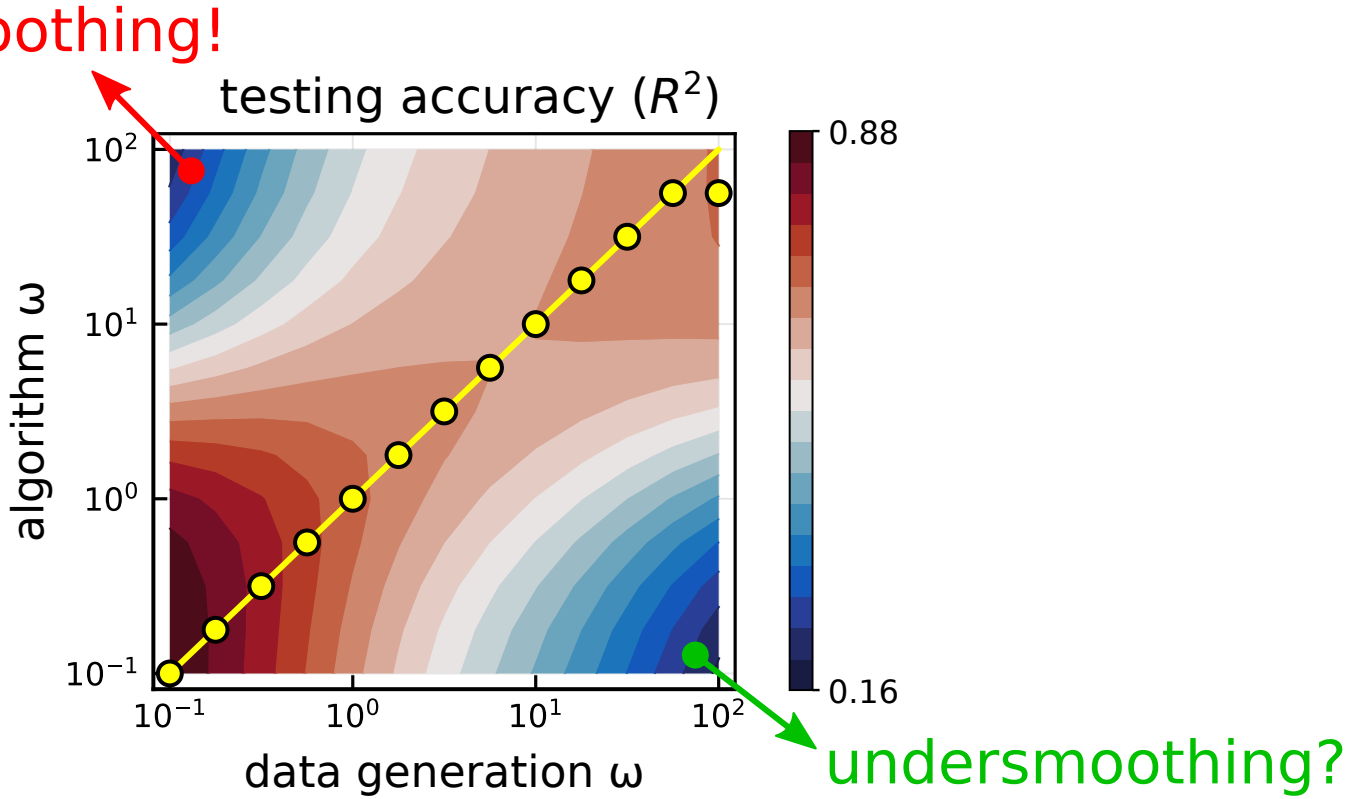

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We can use LGC to Interpret Empirical Data

year	sh050m	sh100m	sh500m	income	migration	birth	death	education	unemployment
2012	0.06	-0.42	0.24	0.22	0.16	-0.13	0.04	-0.90	-0.38
2016	-0.02	-0.38	0.22	0.70	0.21	-0.13	0.51	-1.53	-0.39

sh050m/sh100m/sh500m: shares of friends within 50/100/500 miles; features normalized to zero mean & unit variance

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- GOP leaning counties tend to have:
  - lower education levels, and higher income; this trend is stronger in 2016 than 2012
  - lower birth rate, and higher death rate $\rightarrow$ older population
  - lower unemployment rate, and higher migration rate $\rightarrow$ manufacturing hubs?
  - lower sh100m, and higher sh500m $\rightarrow$ rural areas?

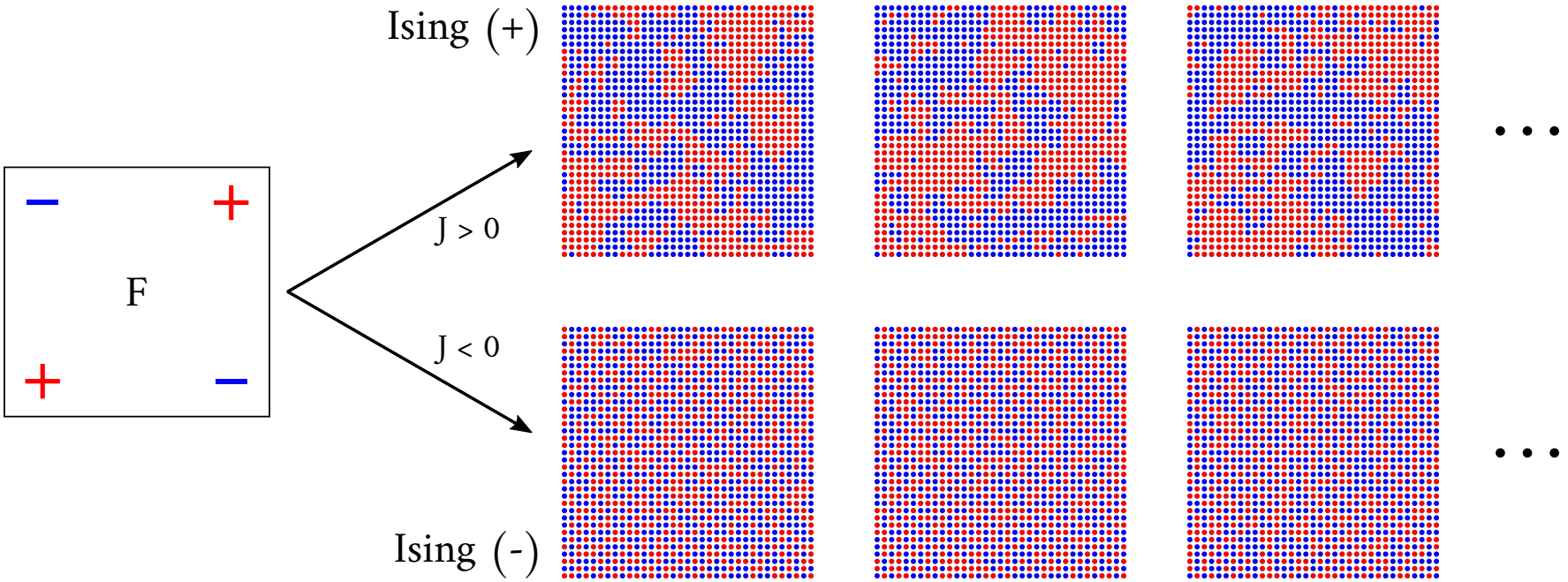
sh050m/sh100m/sh500m: shares of friends within 50/100/500 miles; features normalized to zero mean & unit variance

Where do we go from here?

- What if the labels are not positively correlated? (e.g. heterophily graphs)

- What if the labels are categorical variables? (node classification setting)

What if labels aren't Poistively Correlated?



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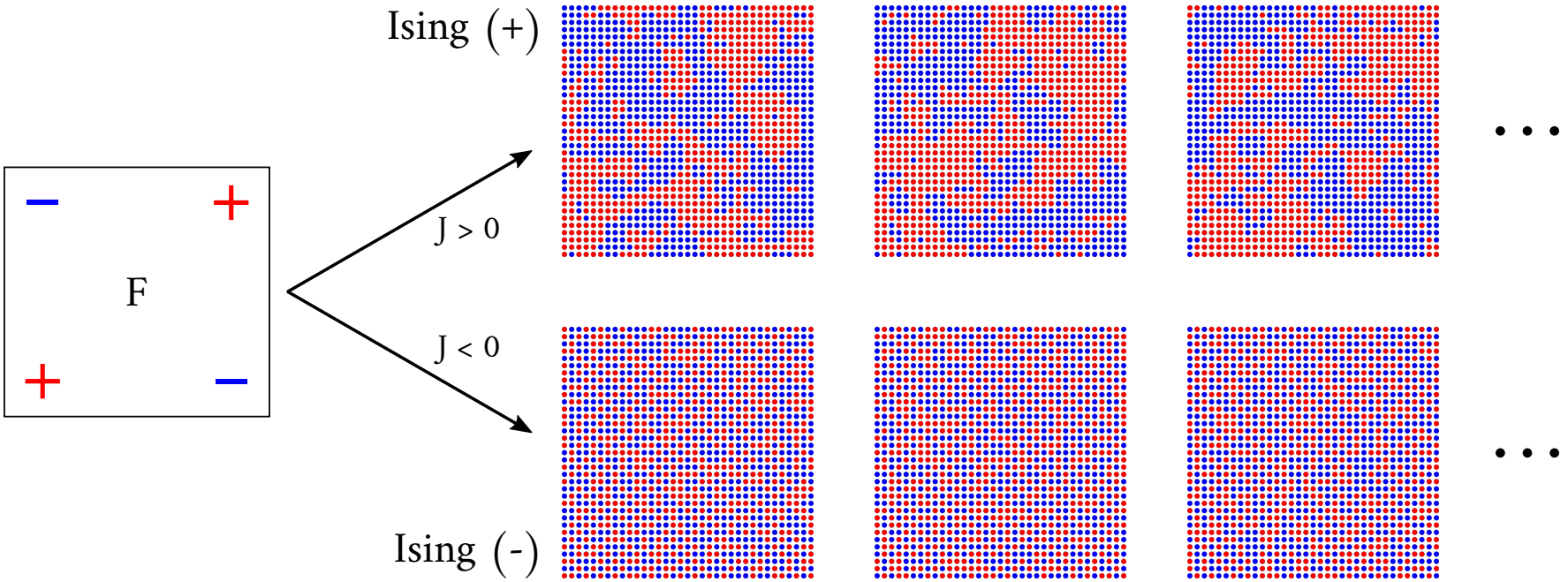

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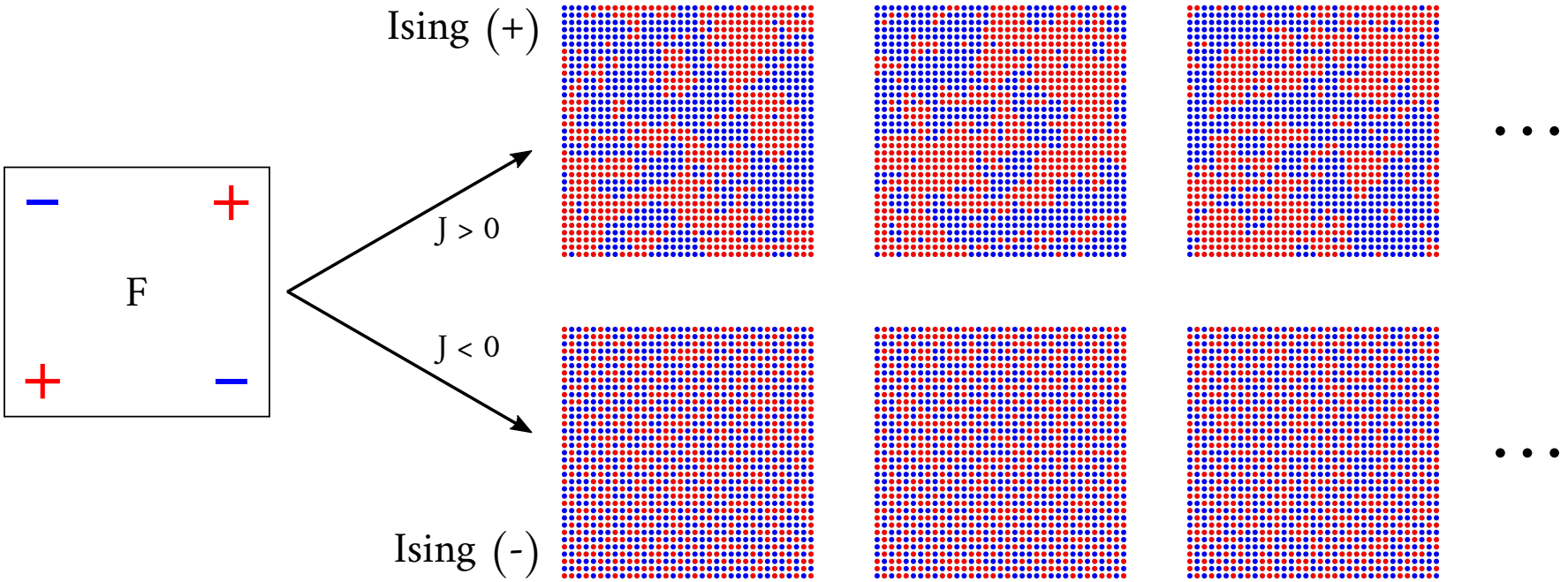

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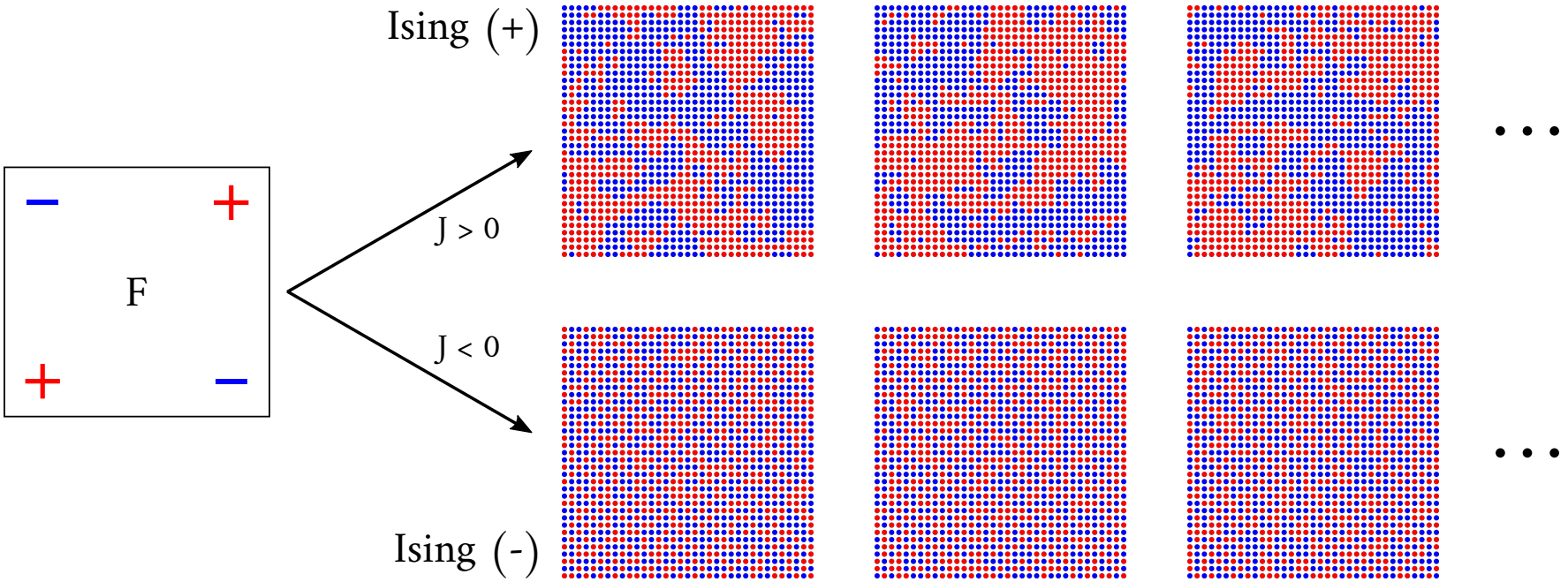

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- Residuals are negatively correlated among neighbors as well.

We can learn the Correlation Directly

- Model the residual with a multivariate Gaussian:

$$\mathbf{r} \sim \mathcal{N}(\mathbf{0}, \mathbf{\Gamma}^{-1}), \quad \mathbf{\Gamma} = \beta(\boldsymbol{I} - \alpha \boldsymbol{S}), \quad \boldsymbol{S} = \boldsymbol{D}^{-1/2} \boldsymbol{W} \boldsymbol{D}^{-1/2}$$

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- How do we determine the parameter α?
  - learn the optimal α, β with **maximum marginal likelihood**

We can learn the Correlation Directly

- Learn model by maximizing marginal likelihood of training residuals $\boldsymbol{r}_L$

[Ubaru+ 2017; Gardner+ 2018]

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- Estimate $\log|\boldsymbol{\Gamma}|$ with stochastic trace estimator & Lanczos quadrature

$$\log|\boldsymbol{\Gamma}| = \mathtt{tr}(\log\boldsymbol{\Gamma}) \approx \frac{1}{T}\sum_{t=1}^{T} \boldsymbol{z}_t^\intercal(\log\boldsymbol{\Gamma})\boldsymbol{z}_t = \frac{1}{T}\sum_{t=1}^{T}\sum_{i=1}^{n} \mu_{ti}^2 \log\lambda_i(\boldsymbol{\Gamma})$$

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  - $\boldsymbol{z}_t$ random Gaussian trial vectors with unit-variance
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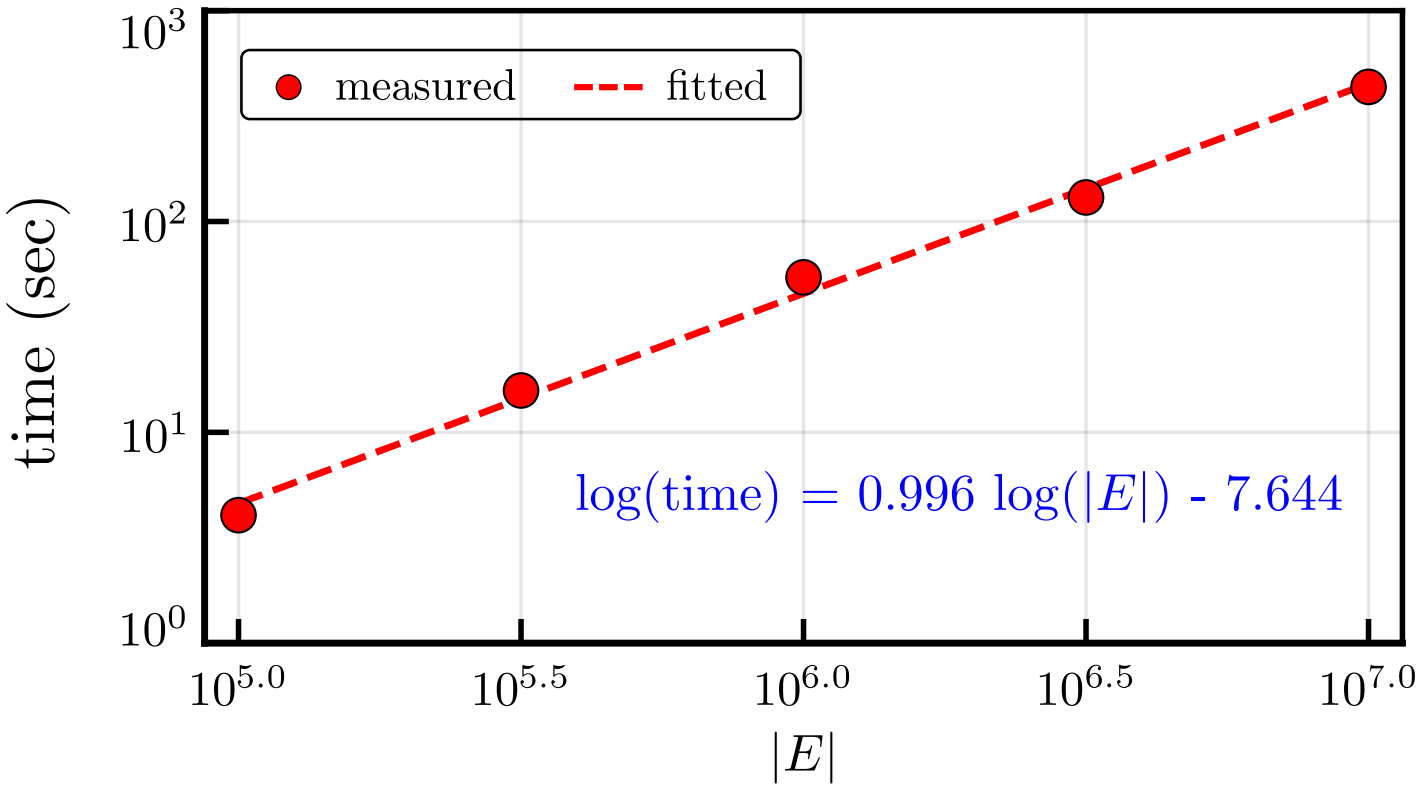
- Estimate gradient with stochastic trace estimator & CG solver

$$\frac{\partial\log|\boldsymbol{\Gamma}|}{\partial\alpha} \approx \frac{1}{T}\sum_{t=1}^{T}(\boldsymbol{\Gamma}^{-1}\boldsymbol{z}_t)^\intercal\left(\frac{\partial\boldsymbol{\Gamma}}{\partial\alpha}\boldsymbol{z}_t\right)$$

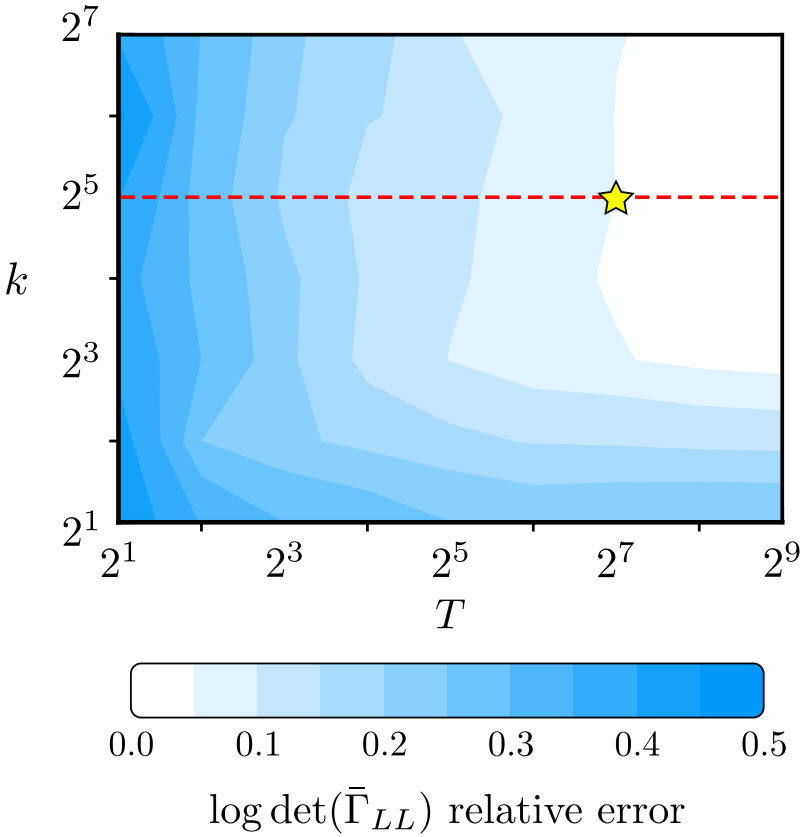
[Ubaru+ 2017; Gardner+ 2018]

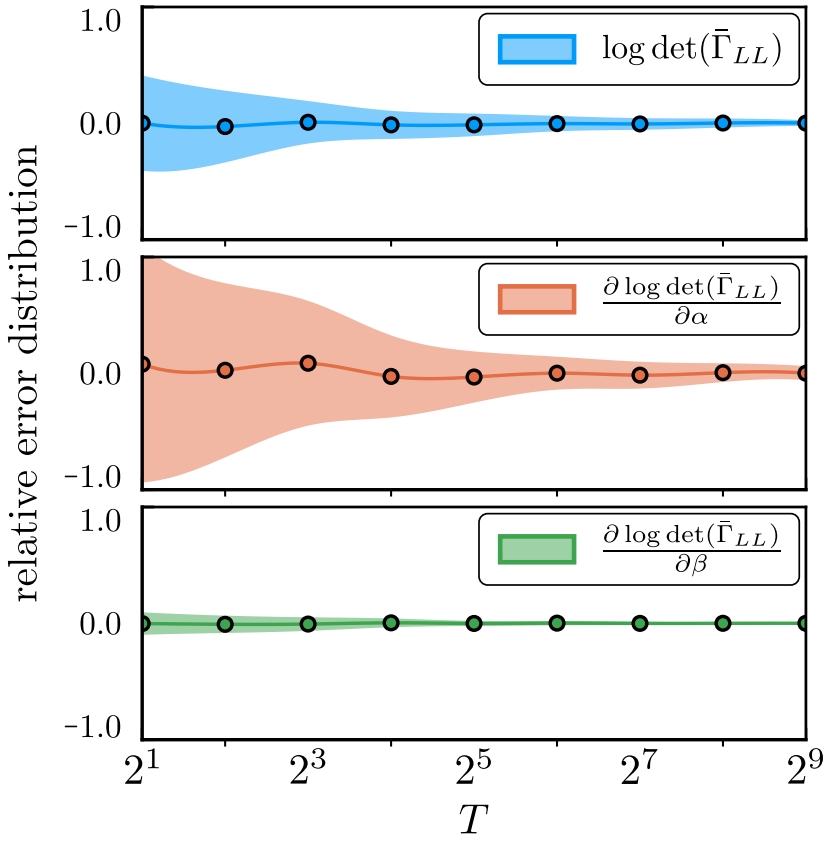
Stochastic Estimation is Efficient



- Stochastic trace estimator cost $\mathcal{O}(|E|)$, linear in the # of edges

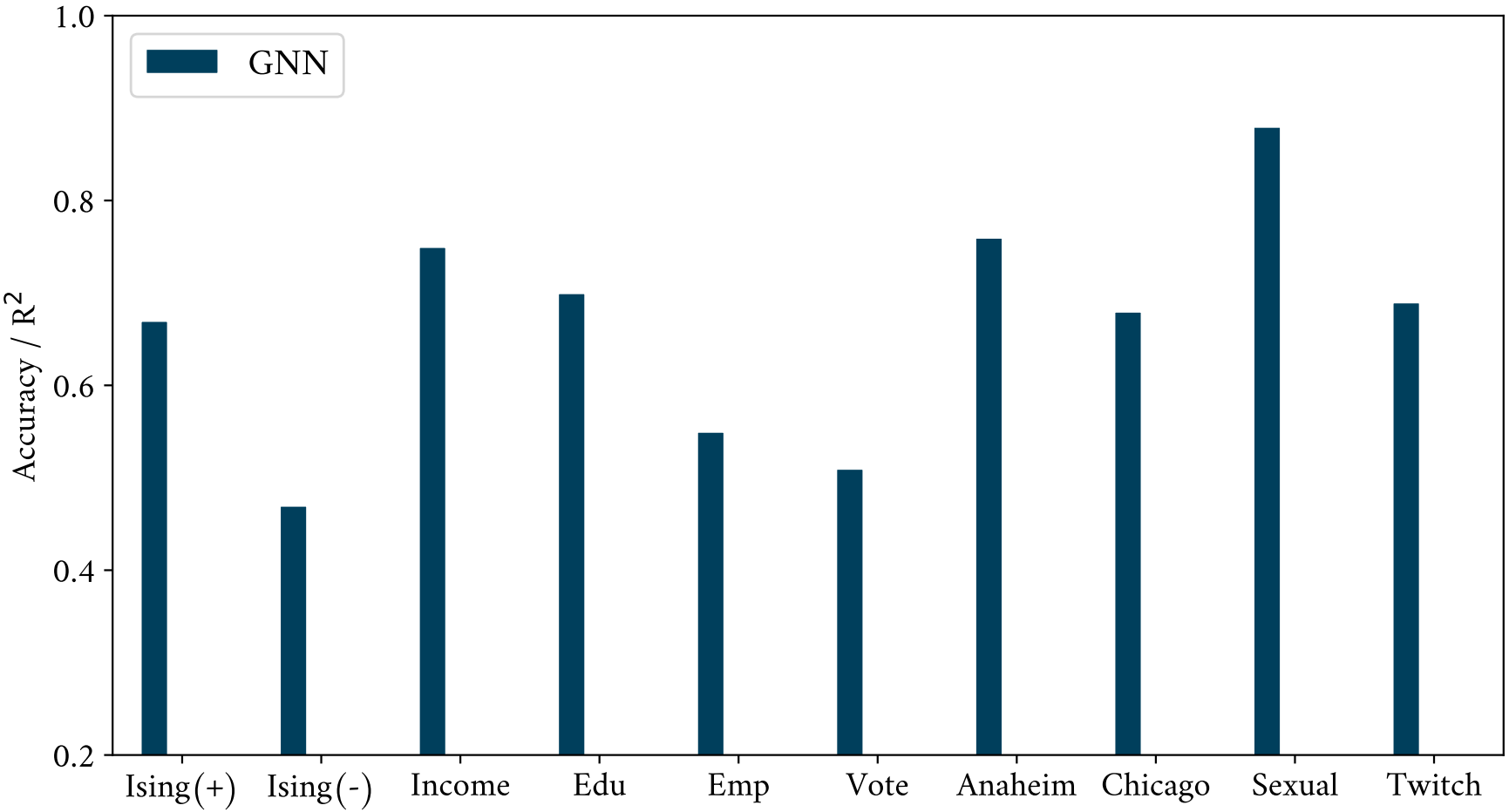
Stochastic Estimation is Accurate





- Stochastic trace estimator gives accurate results
  - a small number of CG iterations, Gaussian trial vectors; $< 5\%$ error
  - unbiased estimation of gradient optimize with SGD

C-GNN Performs well on Heterophily Graphs



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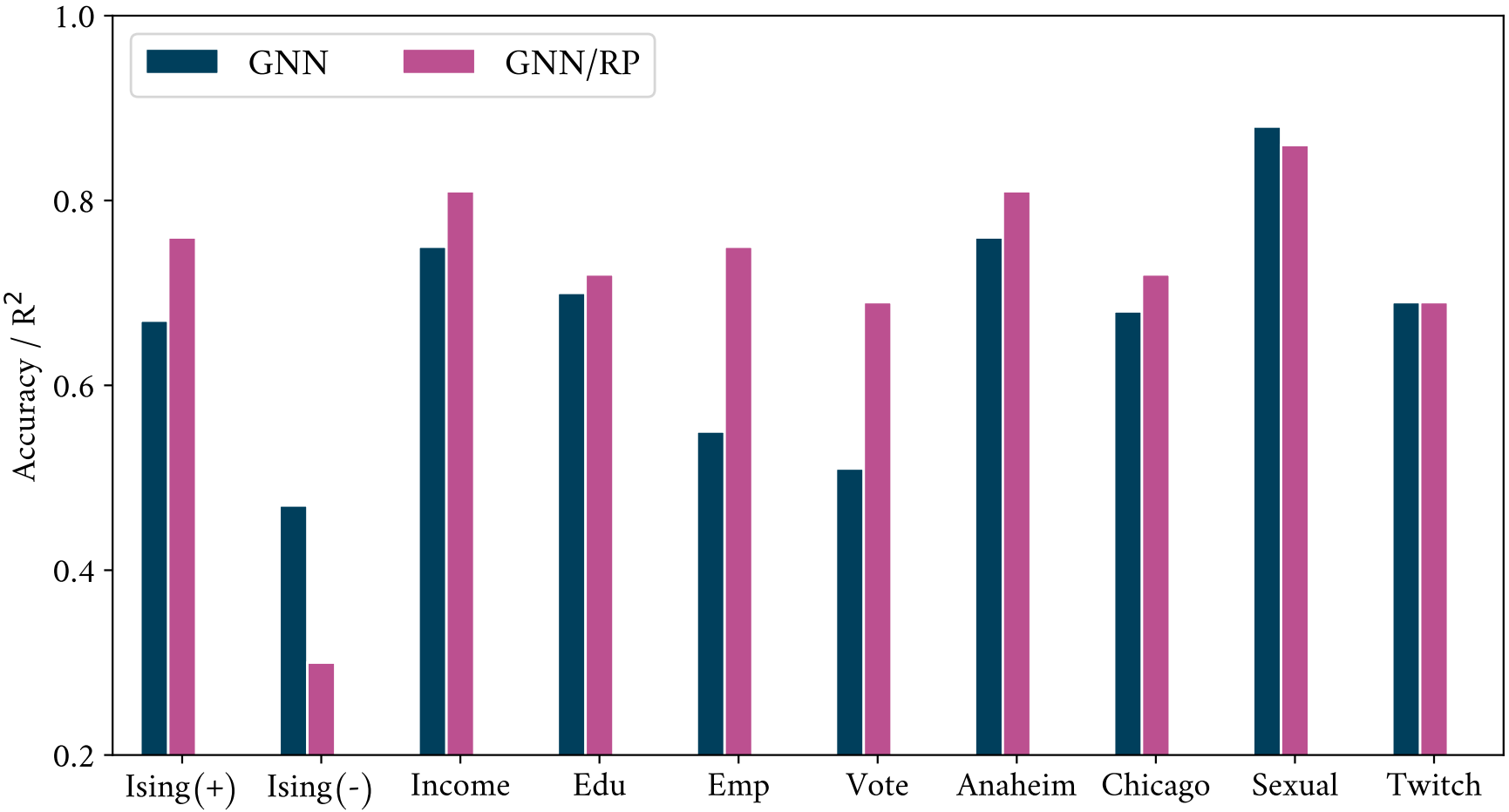

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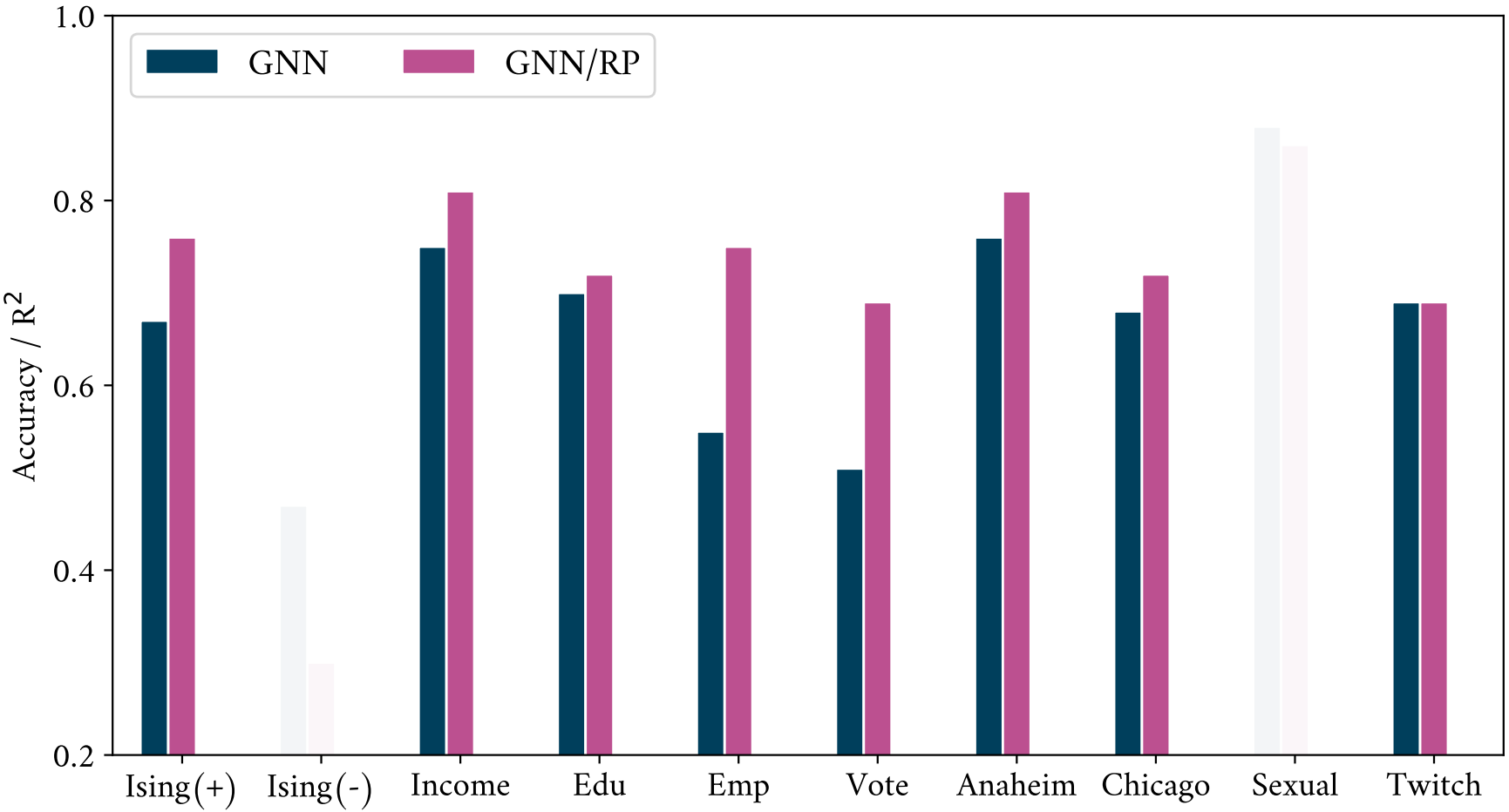

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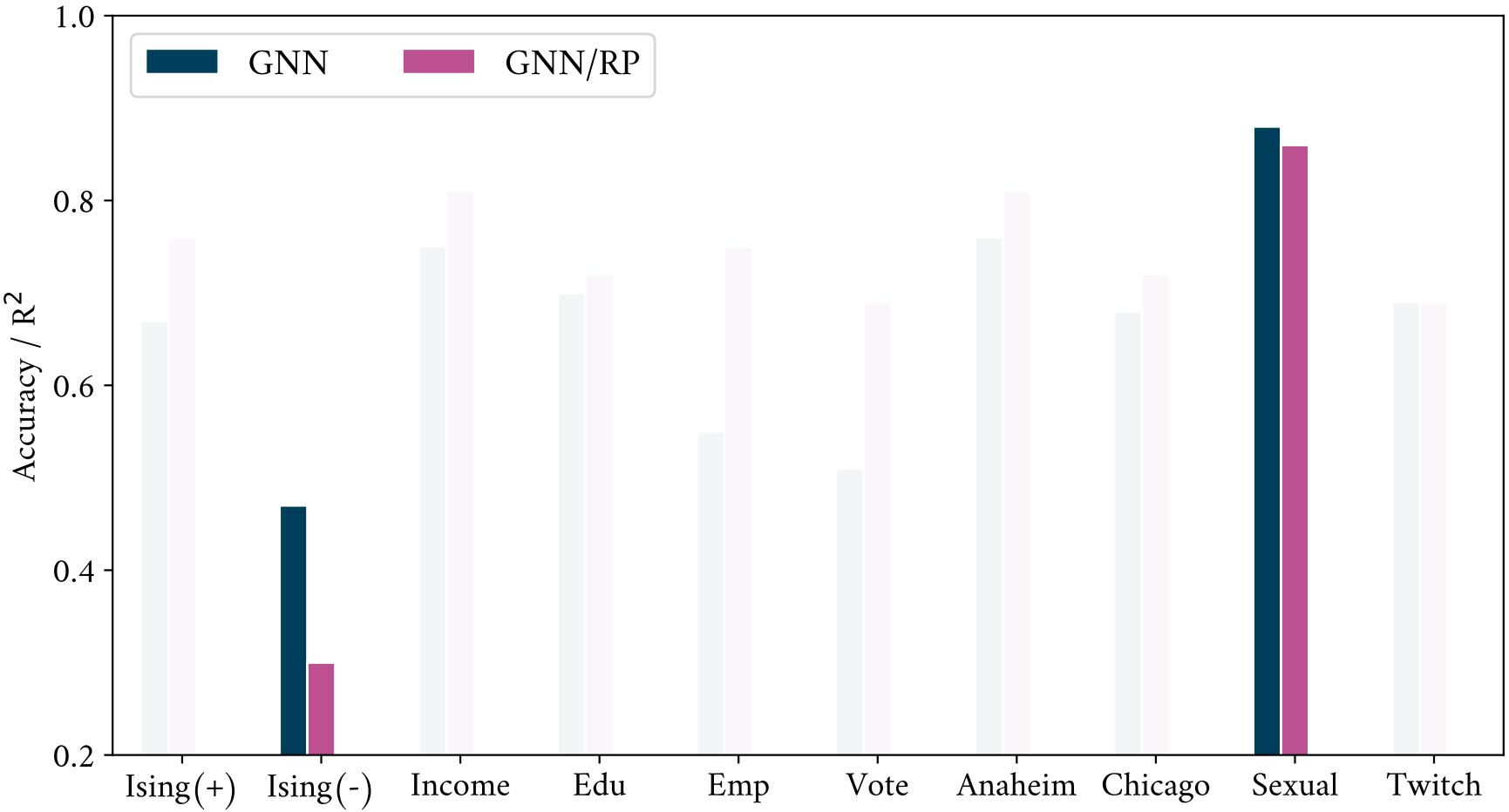

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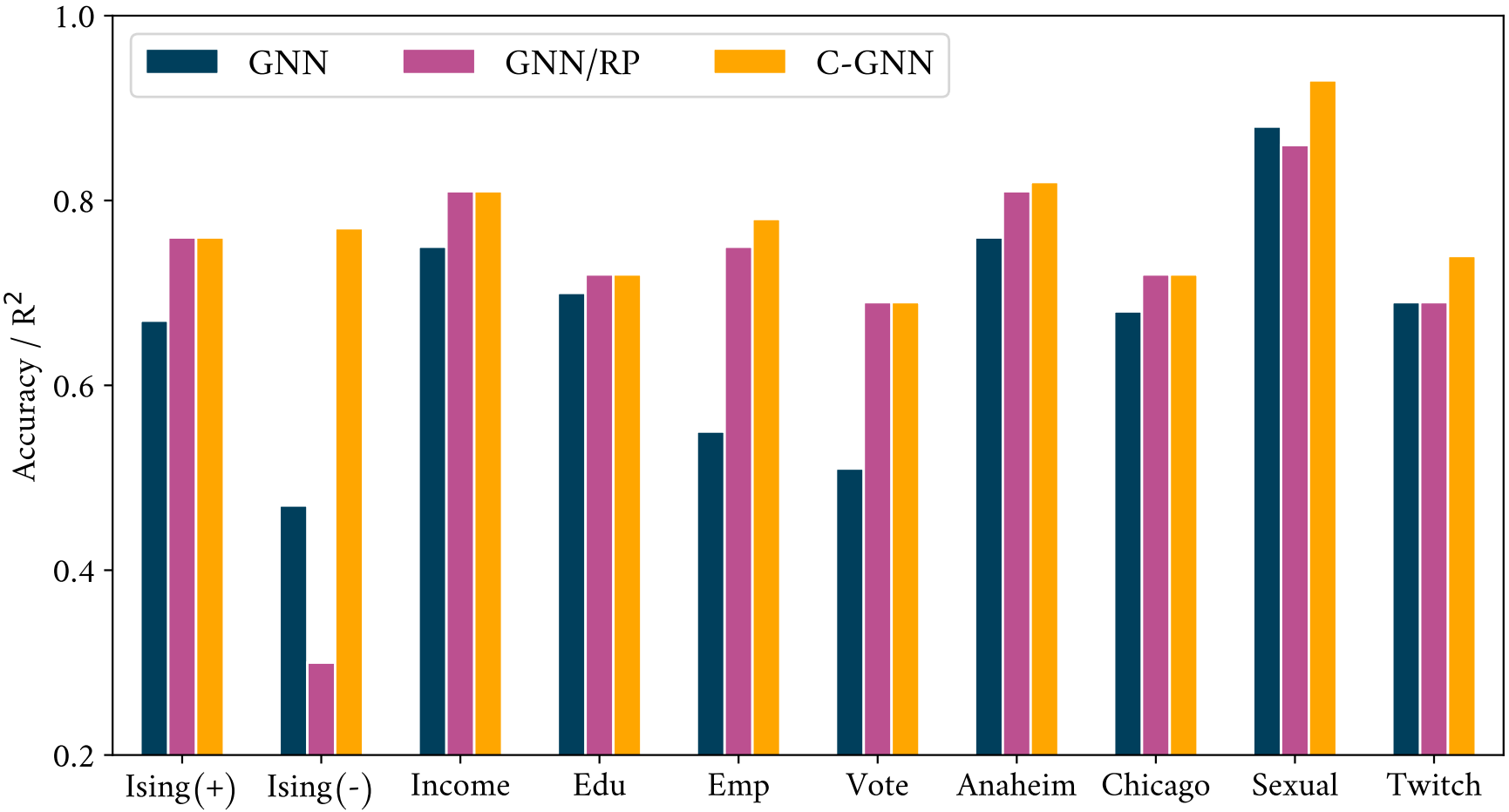

- GNN/RP outperforms GNN on homophily graphs; underperforms if heterophily
- C-GNN performs the best on all datasets

Where do we go from here?

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A Statistical Model for Attributed Graphs

- Consider a two-step process for generating node attributes:

$\boldsymbol{h} \in \mathbb{R}^c$, $\boldsymbol{H} \in \mathbb{R}^{c \times c}$ are model parameters with all positive entries

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which is just another pairwise MRF.

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Learning algo from Probabilistic Inference

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- Since $P(\boldsymbol{x}_u|y_u), \boldsymbol{h}, \boldsymbol{H}$ are unkonwn, we need to learn from data

Learning algo from Probabilistic Inference

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- Probabilistic inference: compute $P(y_u|\boldsymbol{X})$ with **belief propagation**
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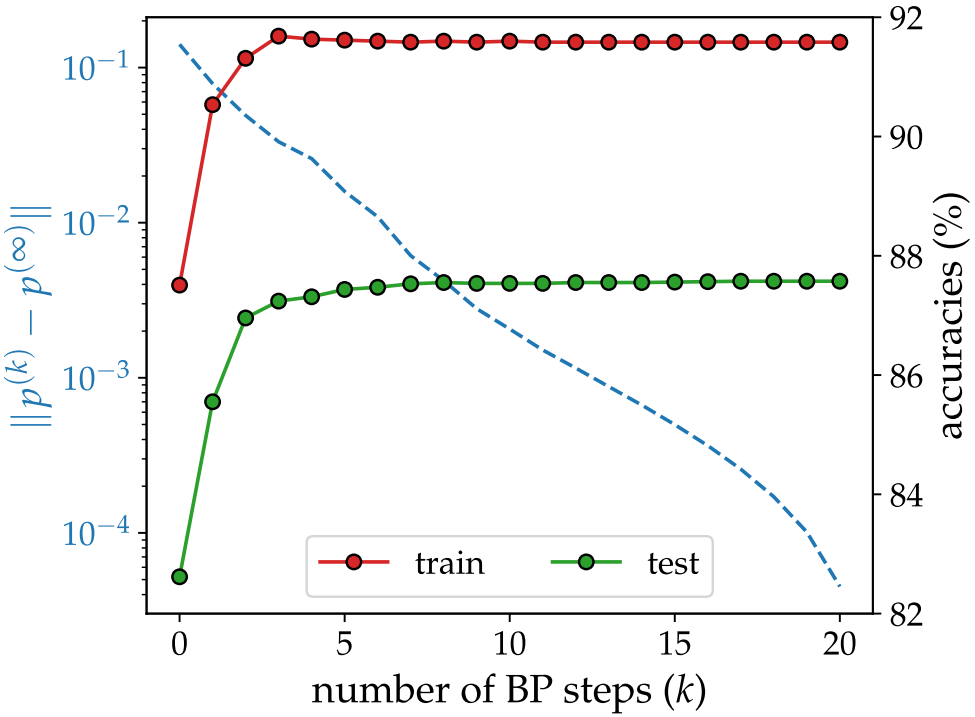
- After training, we can infer unknown labels directly $P(y_u|\boldsymbol{X})$.
- Or we can compute $P(y_u|\boldsymbol{X}, \boldsymbol{y}_L)$:

  further conditioning on $\boldsymbol{y}_L$, resulting in a pairwise MRF on $G[U]$

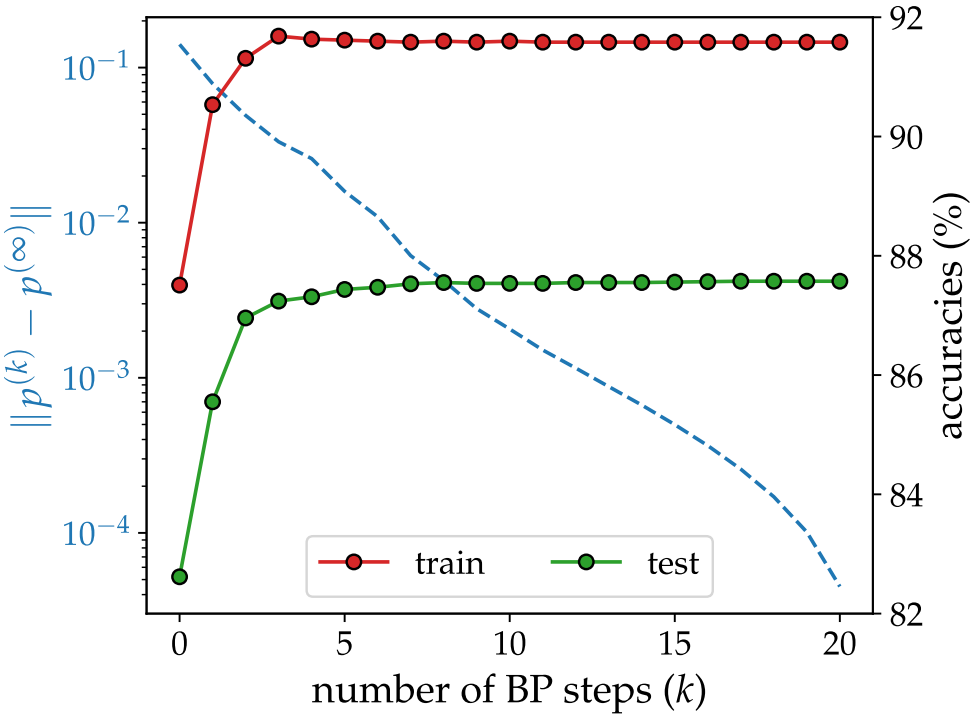
$$P(\boldsymbol{y}_U|\boldsymbol{X}, \boldsymbol{y}_L) \cong \prod_{u \in U} \left(f_\theta(y_u; \boldsymbol{x}_u) \prod_{\substack{u \in U, v \in L, \\ (u,v) \in E}} H_{uv}(y_u, y_v) \right) \prod_{\substack{u, v \in U, \\ (u,v) \in E}} H_{uv}(y_u, y_v)$$

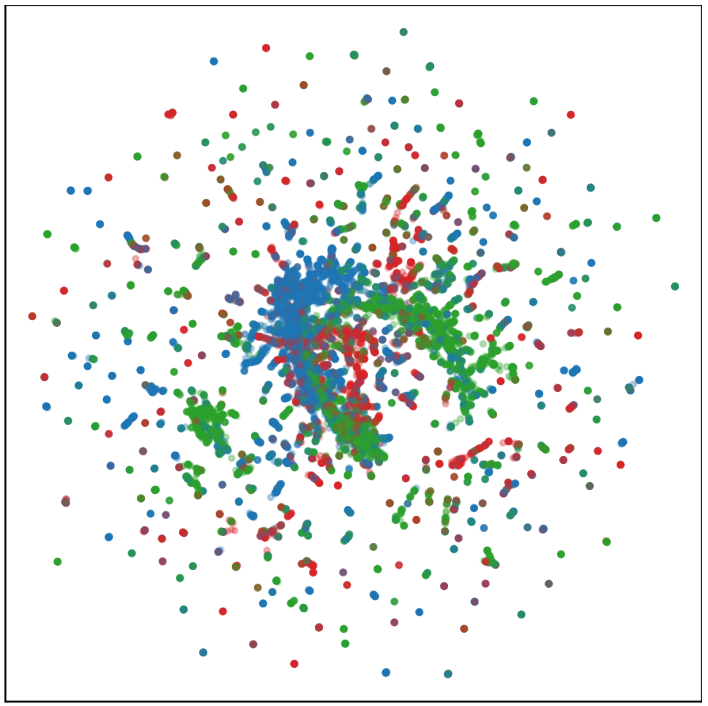
GBPN Case Study on PubMed Dataset



- Belief propagation converge quickly on real-world dataset

GBPN Case Study on PubMed Dataset





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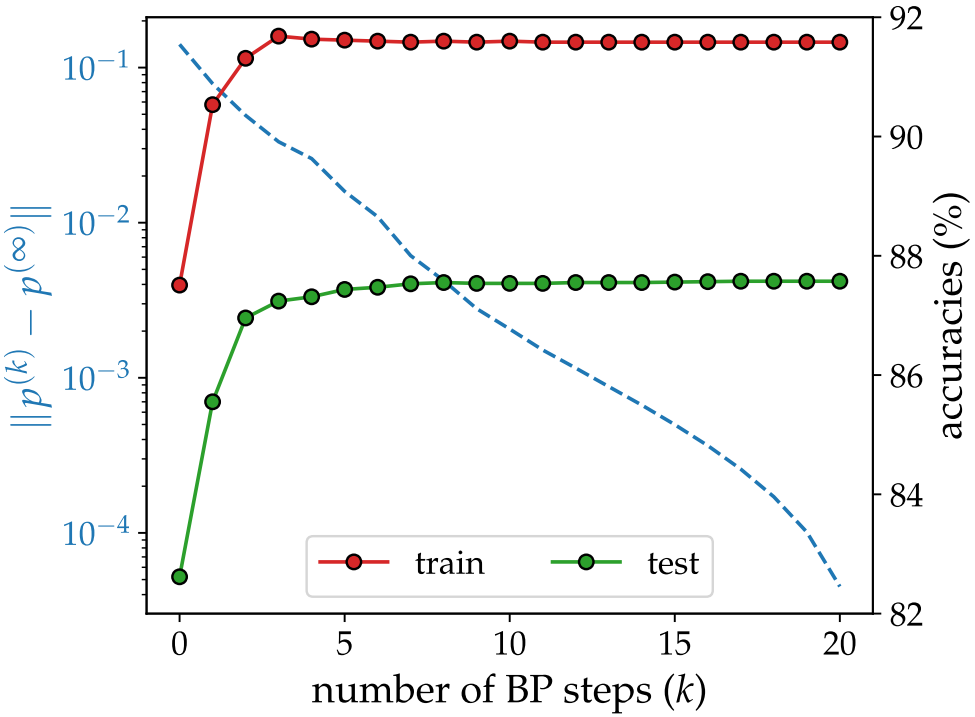

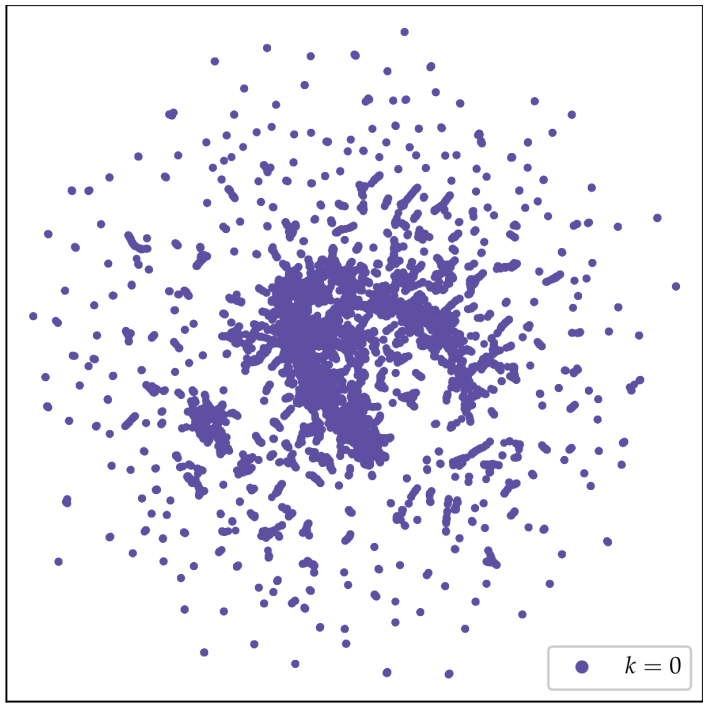

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- GBPN is interpretable (node correctly predicted by GBPN after k steps)

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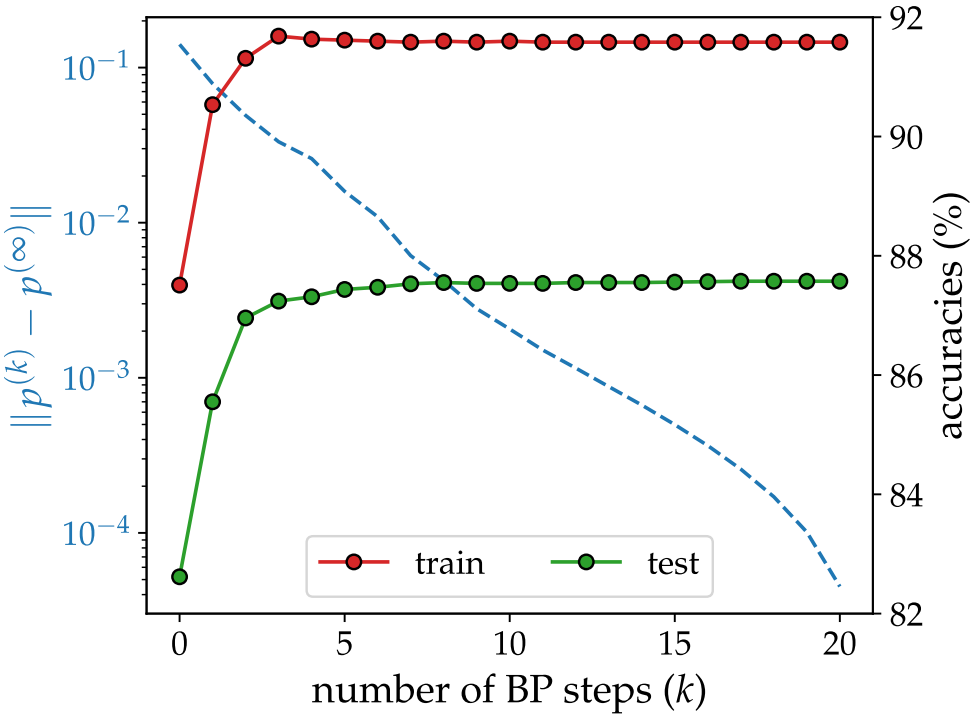

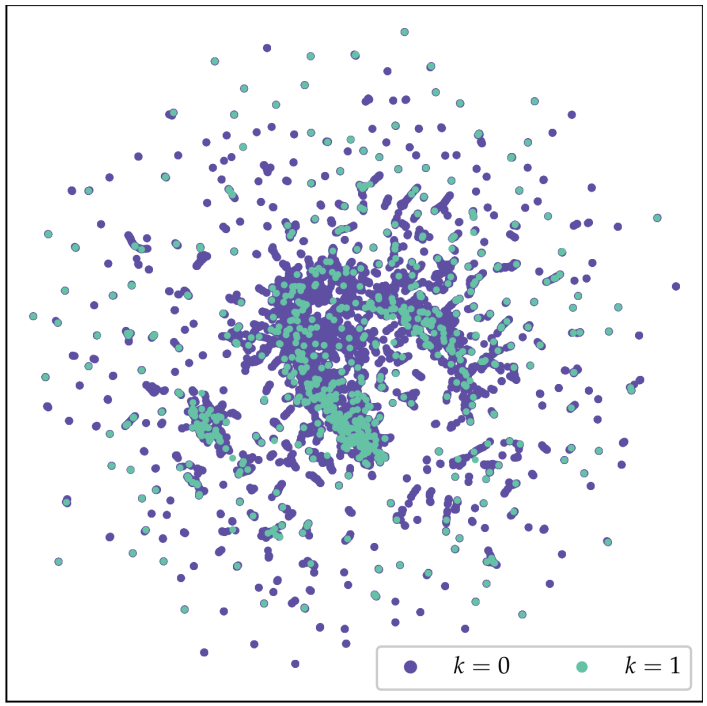

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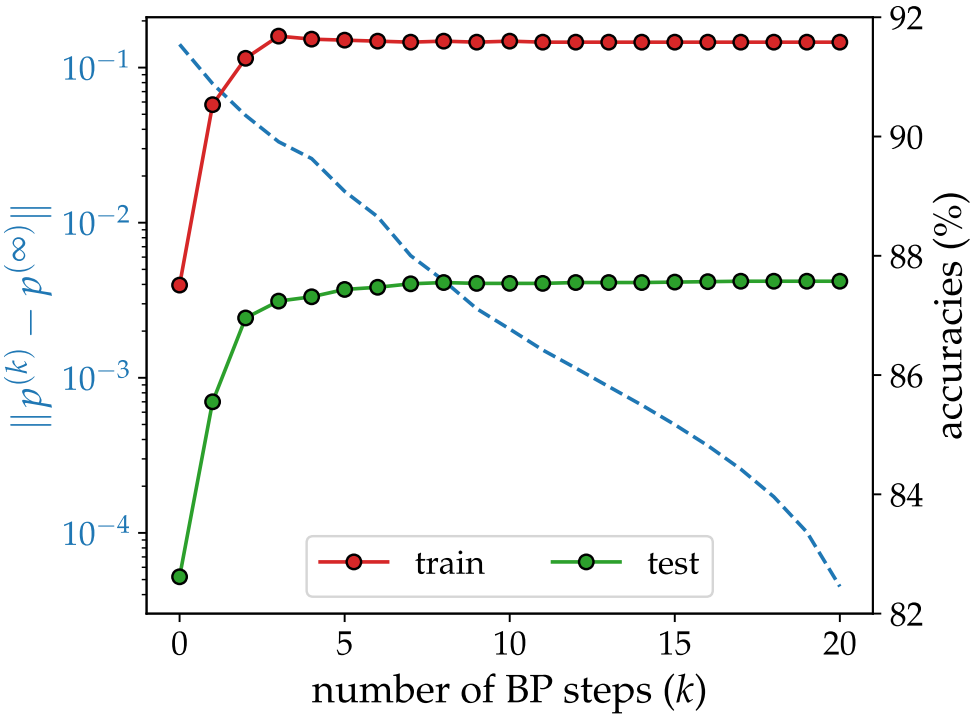

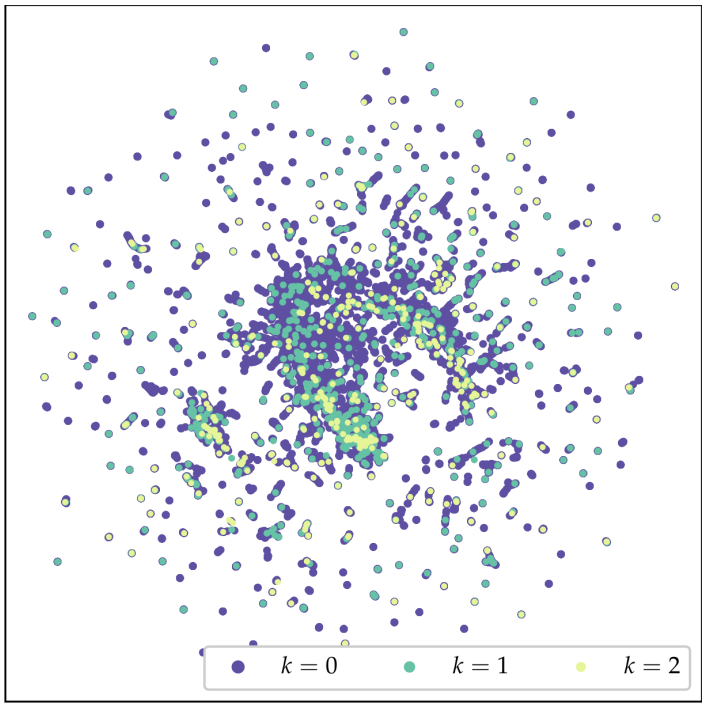

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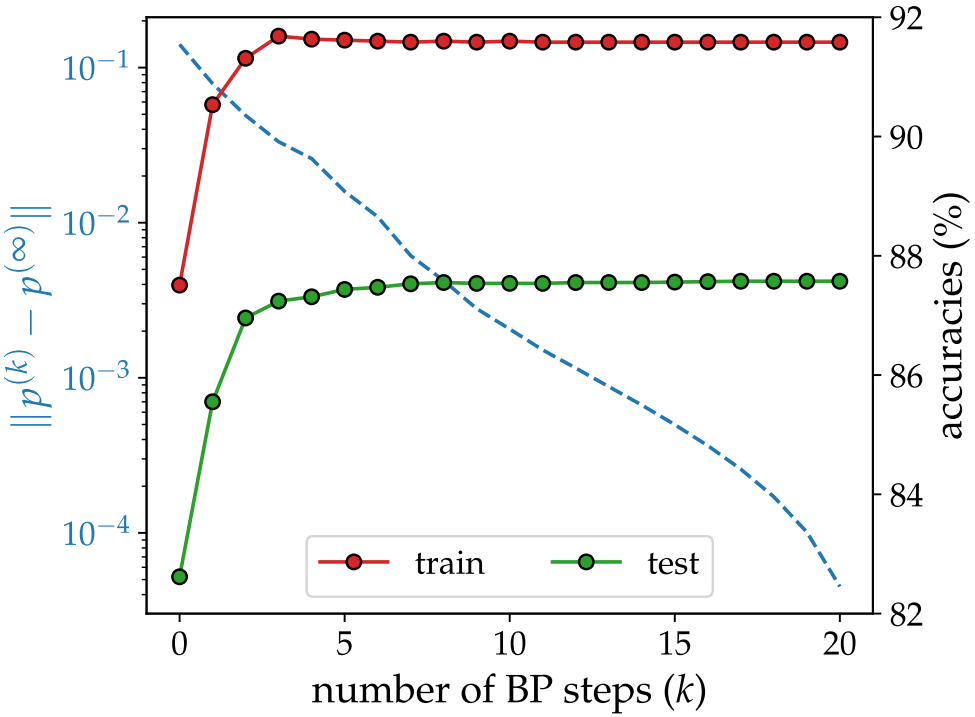

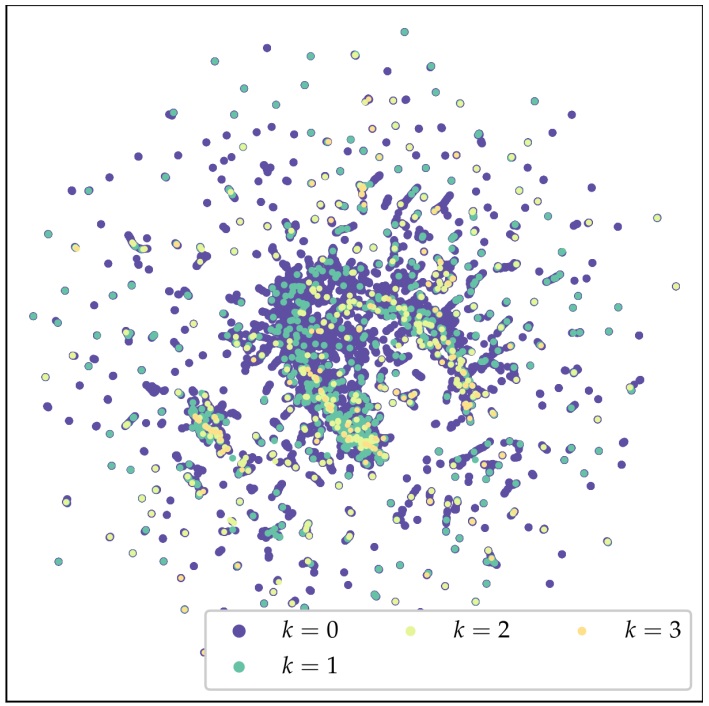

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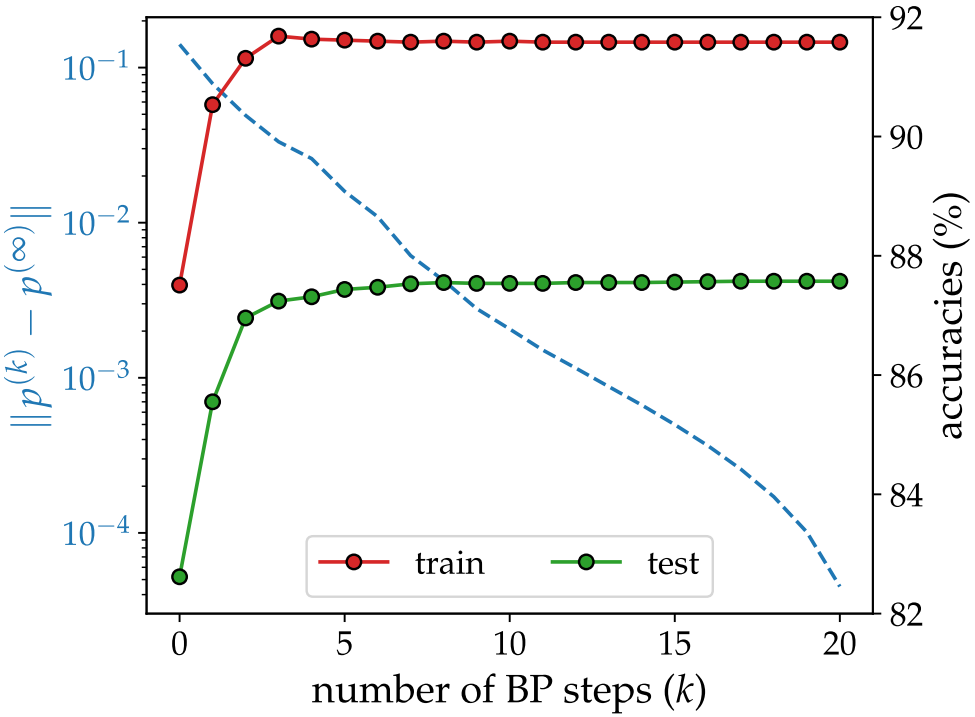

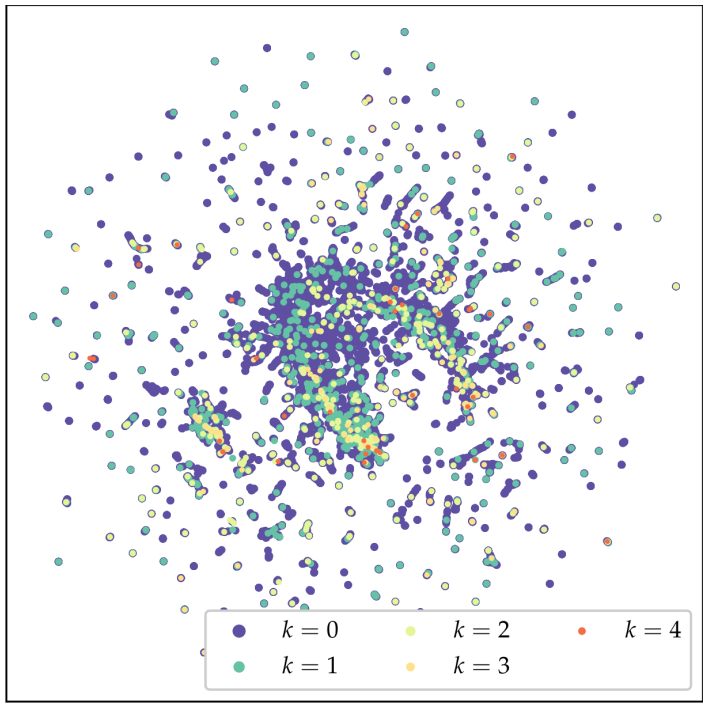

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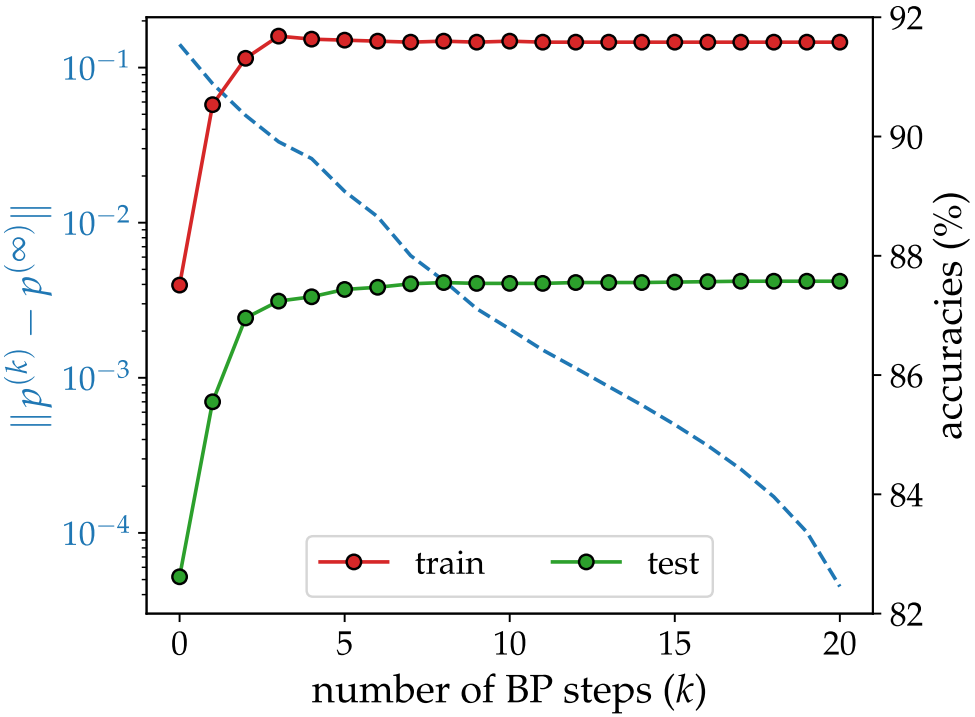

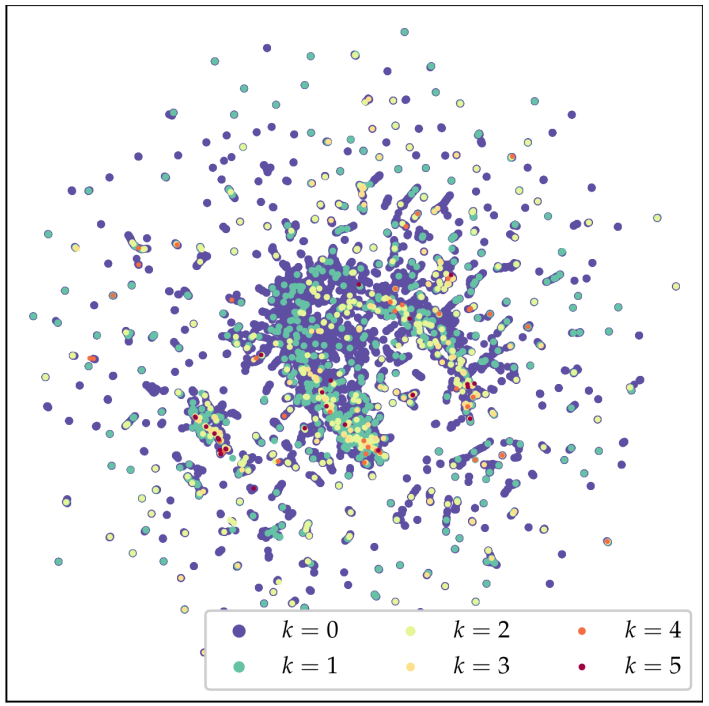

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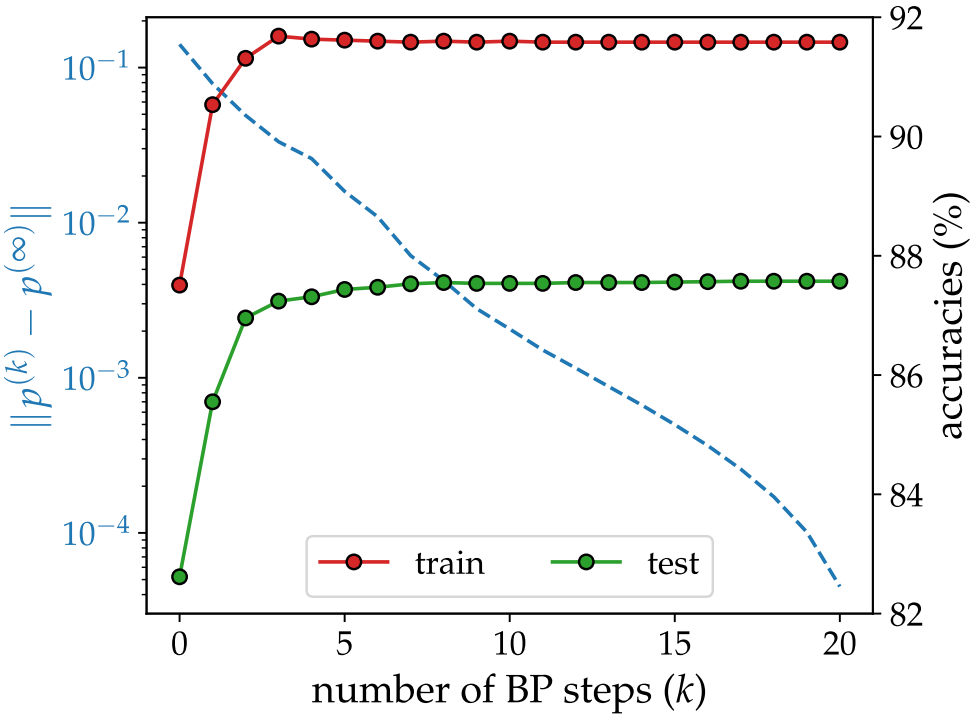

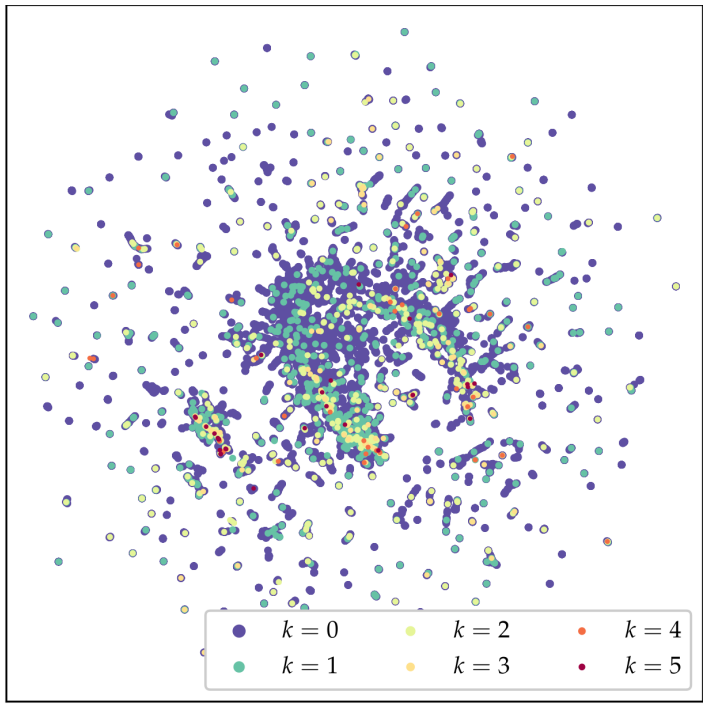

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  first get easy examples right, then iteratively correct harder examples with neighbors

Performance on Benchmark Datasets

dataset	MLP	SGC	GCN	GraphSAGE	GAT	GBPN(I)	GBPN(T)
County	89.8 ± 0.6	88.2 ± 0.7	87.9 ± 0.7	**90.9** ± 0.5	90.5 ± 0.4	90.1 ± 0.7	90.4 ± 0.8
Sexual	73.9 ± 1.4	76.1 ± 1.4	83.7 ± 1.1	93.0 ± 0.9	93.7 ± 0.9	97.0 ± 0.5	**97.1** ± 0.5
Cora	72.4 ± 1.1	**87.1** ± 0.7	**87.1** ± 0.7	**87.1** ± 0.8	86.7 ± 0.7	84.8 ± 0.8	84.8 ± 0.8
CiteSeer	70.5 ± 0.9	72.9 ± 1.1	73.4 ± 0.9	73.1 ± 0.8	72.5 ± 0.8	**73.9** ± 0.7	73.7 ± 0.7
PubMed	86.6 ± 0.4	86.9 ± 0.3	87.0 ± 0.3	87.8 ± 0.3	88.0 ± 0.2	**88.2** ± 0.3	**88.2** ± 0.3
CS	94.1 ± 0.2	93.1 ± 0.2	93.1 ± 0.3	93.6 ± 0.3	94.3 ± 0.3	**95.4** ± 0.1	**95.4** ± 0.2
Physics	95.8 ± 0.2	96.1 ± 0.1	96.1 ± 0.1	96.2 ± 0.2	96.4 ± 0.1	**96.8** ± 0.1	**96.8** ± 0.1

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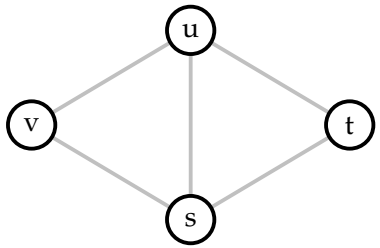
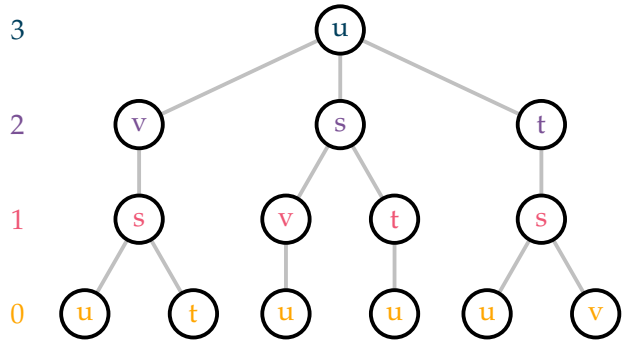
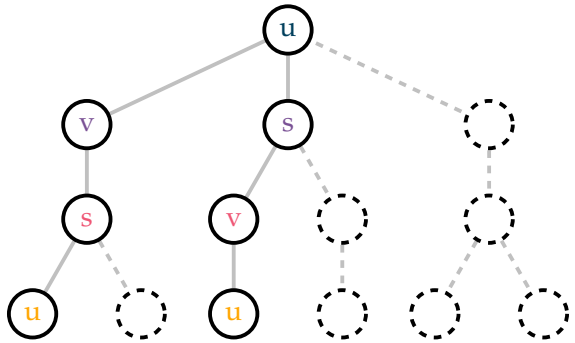
- GBPN is not only more interpretable, but also more accurate

Performance on Large-scale Datasets

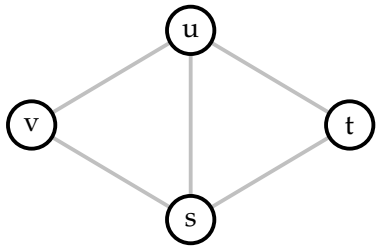


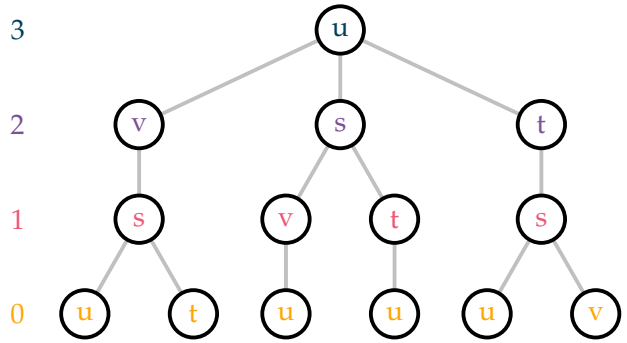


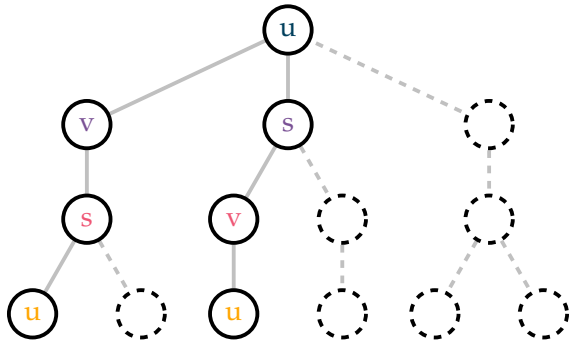


- We design a subsampling algorithm for mini-batch training

Performance on Large-scale Datasets







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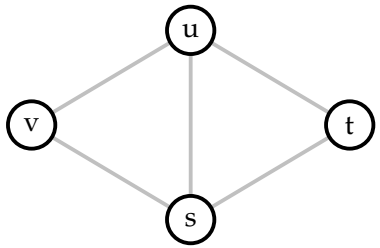
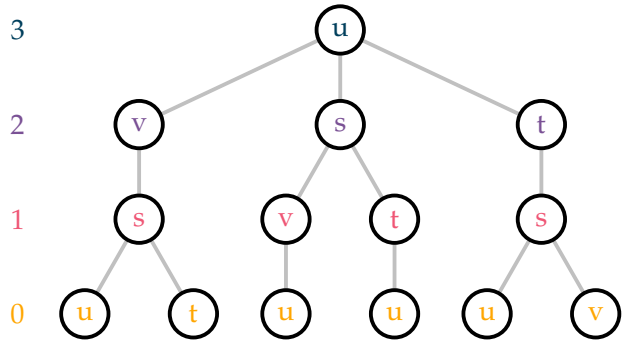
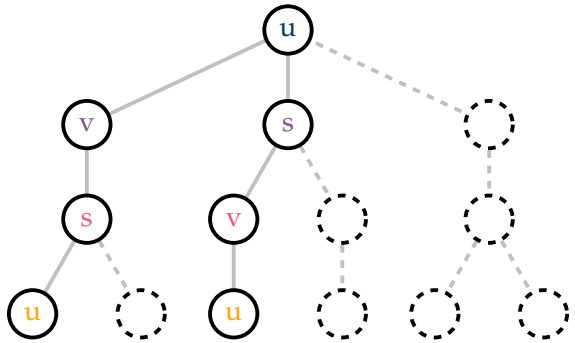
Performance on Large-scale Datasets







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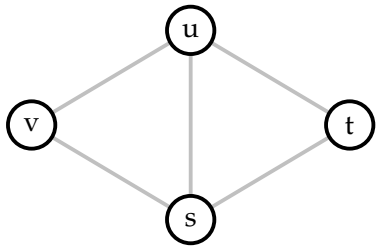
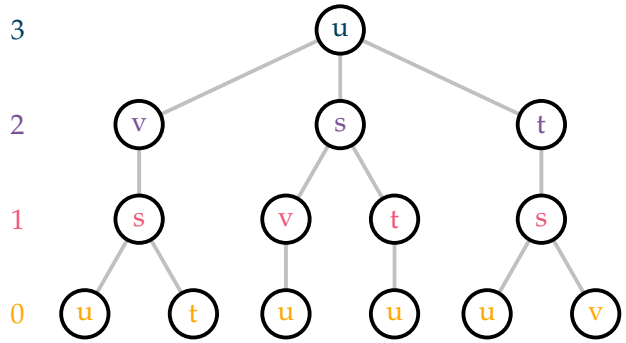
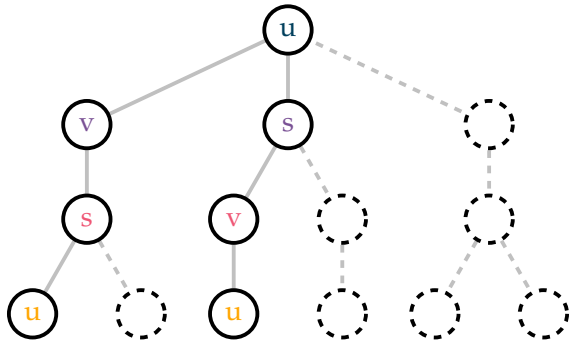
- GBPN outperforms baselines overall

Performance on Large-scale Datasets







dataset	MLP	GraphSAGE	GAT	GBPN(I)	GBPN(T)
Elliptic	98.2 ± 0.2	**98.4** ± 0.2	98.2 ± 0.3	**98.4** ± 0.1	**98.4** ± 0.2
Chase	61.1 ± 0.3	77.5 ± 0.5	74.6 ± 0.8	83.0 ± 0.5	**86.2** ± 0.5
arXiv	54.6 ± 0.3	**70.4** ± 0.3	**70.4** ± 0.2	69.4 ± 1.1	70.1 ± 0.1
Products	61.5 ± 0.2	78.1 ± 0.2	76.8 ± 0.0	**81.4** ± 0.4	81.2 ± 0.1

- We design a subsampling algorithm for mini-batch training
- GBPN outperforms baselines overall
- GBPN(T) outperforms GBPN(I) by a noticable margin on some dataset

Conclusions

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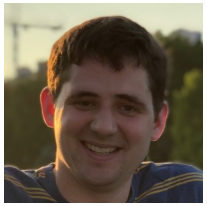
Conclusions

- One key aspect of semi-supervised node regression is to leverage feature correlation and attribute homophily.
- My thesis proposed a generative model that accounts for three different types of correlations in attributed graphs. It unifies existing algorithms and motivates new ones with the state-of-the-art performance.
- Our model successfully generalization to non-homophily graphs and node classification setting.

Acknowledgments

- **Committee Members**
  - Prof. Austin Benson
  - Prof. David Bindel
  - Prof. Jon Kleinberg



- **Collaborators**
  - Prof. Michael Schaub
  - Prof. Santiago Segarra


- **Supportors**
  - Parents & Family
  - Friends & Stacey

My Research

- **Modeling and Inferring Attributed Graphs**
  - Residual Correlation in Graph Neural Network Regression,
    Junteng Jia, Austin R. Benson, KDD2020,
    https://github.com/000Justin000/gnn-residual-correlation
  - A Unifying Generative Model for Graph Learning Algorithms,
    Junteng Jia, Austin R. Benson, arXiv2021,
    https://github.com/000Justin000/GaussianMRF
  - Graph Belief Propagation Networks,
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  - Personal website: https://000justin000.github.io

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