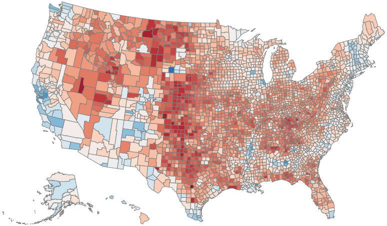
Modeling and Inferring Attributed Graphs

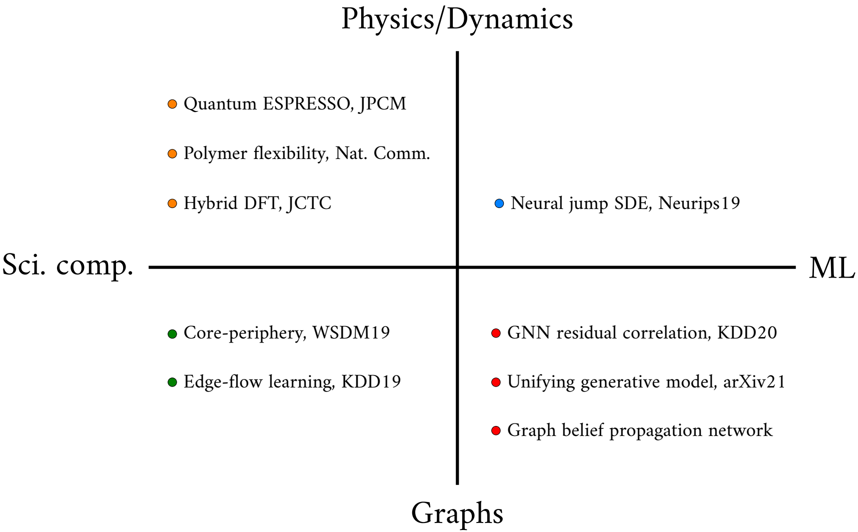


Junteng Jia

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

Ph.D. Thesis Defense – April 12, 2021

Research Overview



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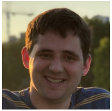
Physics/Dynamics

- Quantum ESPRESSO, JPCM
- Polymer flexibility, Nat. Comm.
- Hybrid DFT, JCTC
- Neural jump SDE, Neurips19

Sci. comp. ML

- Core-periphery, WSDM19
- Edge-flow learning, KDD19
- GNN residual correlation, KDD20
- Unifying generative model, arXiv21
- Graph belief propagation network



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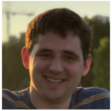


Graphs

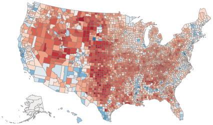
Graphs Data are Increasingly More Complex

Social Networks

nodes: people
edges: friendships

Finance

nodes: accounts
edges: transations



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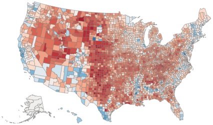

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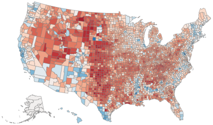

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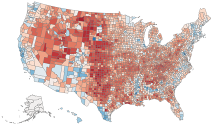

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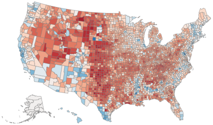

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- node attributes are oftentimes incomplete

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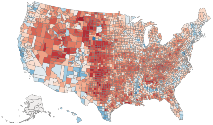

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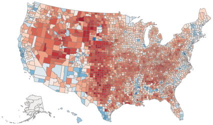

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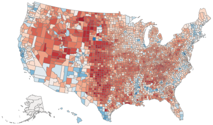

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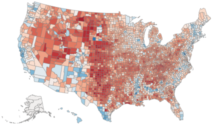

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- however, research often driven by improving on benchmark datasets
  - classification in citation/coauthor network [Lu-Getoor 03; Kipf-Welling 17; Shchur+ 18]

Regression vs Classification

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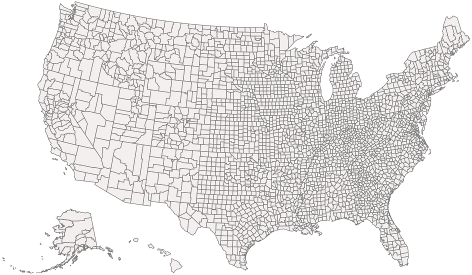
- Later, we extend to the classification setting
  Labels are discrete-valued like cat/dog, male/female ...

Node Label Prediction in Attributed Graphs

Motivating example — Predicting election from pollsters



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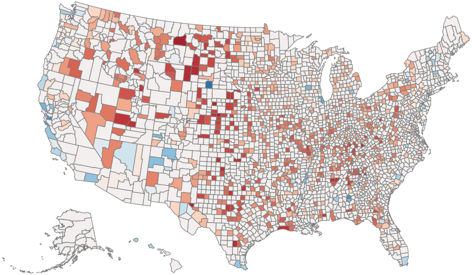

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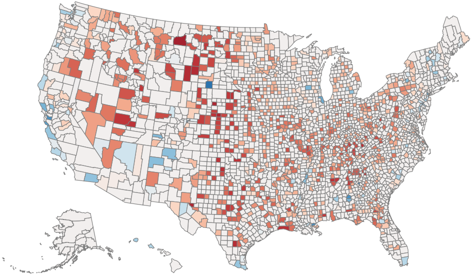

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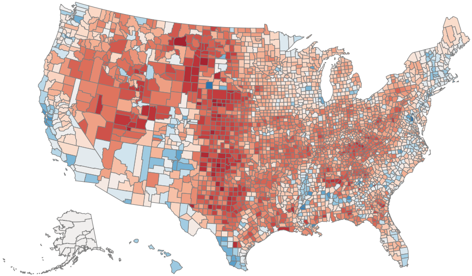

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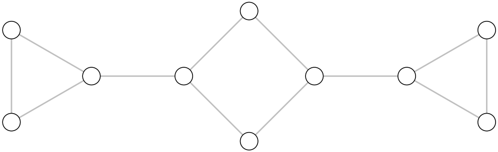

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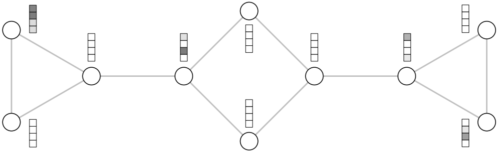

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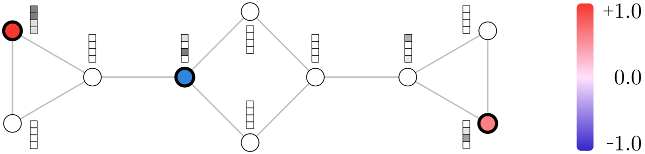

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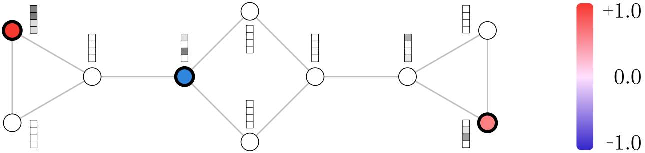

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- Problem output:
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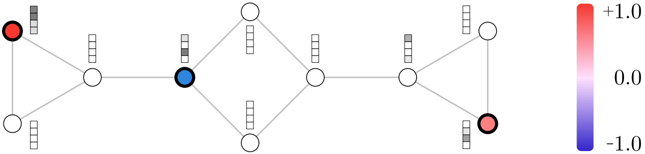
There are two Broad Classes of Methods

Label propagation is a transductive method [early 2000s]



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

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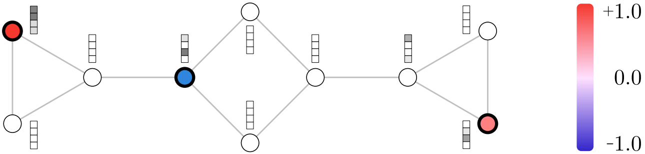

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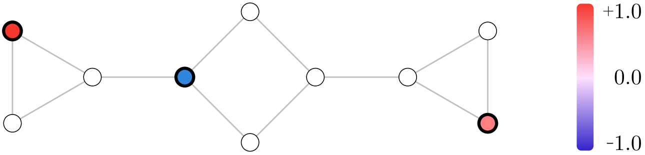

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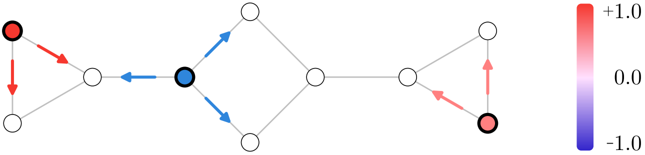

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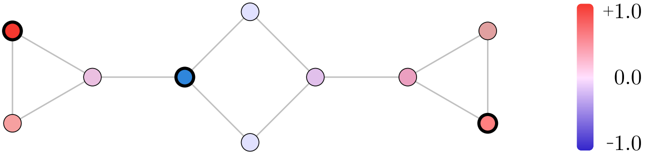

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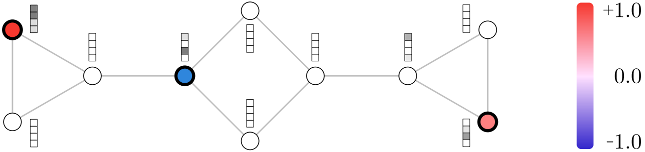

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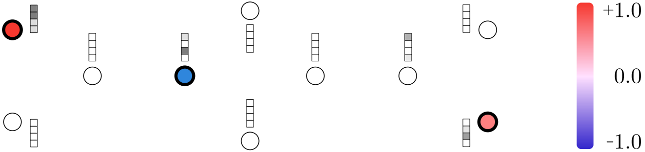

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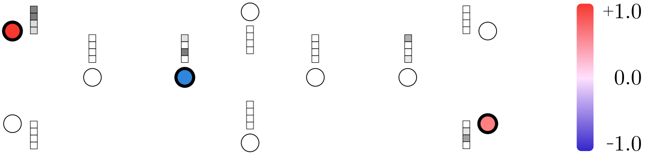

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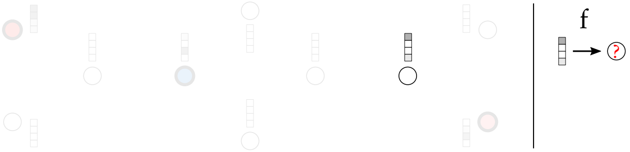

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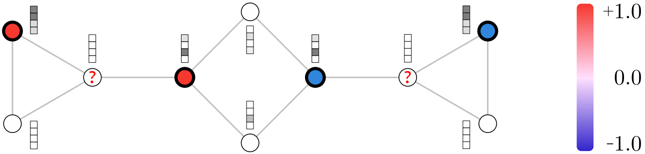

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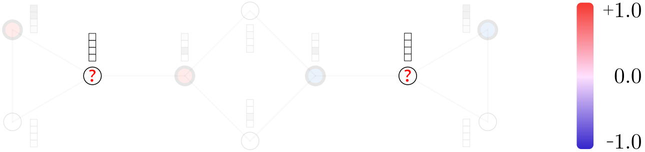

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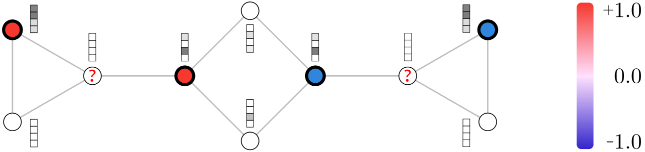

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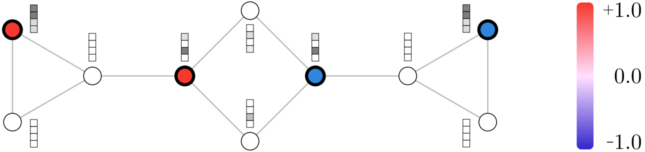

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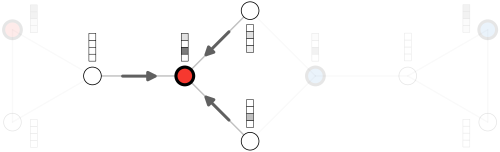

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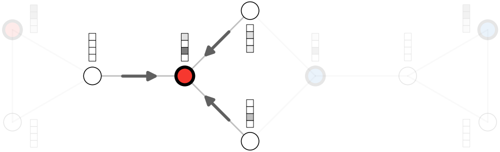

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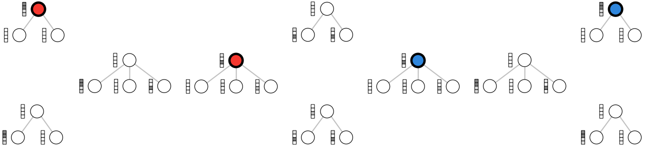

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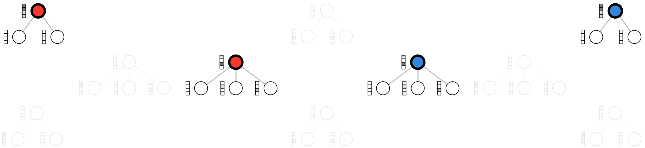

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[Kipf-Welling 16; Hamilton+ 17; Zhou+ 18; Velickovic+ 18; Xu+ 19; ∼10,000 papers in 5 years]

There are two Broad Classes of Methods

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

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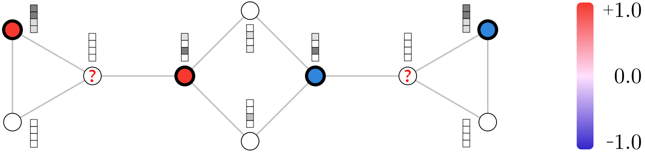

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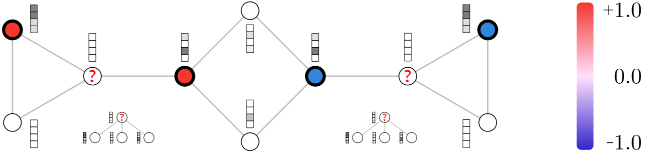

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  - vertices with the same subtrees are indistinguishable

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Combing GNN with Label Propagation

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

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???	●	●	●

Combing GNN with Label Propagation

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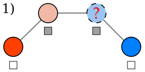
Combing GNN with Label Propagation

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

1)



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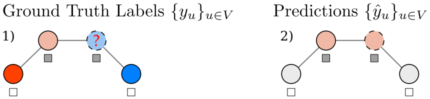

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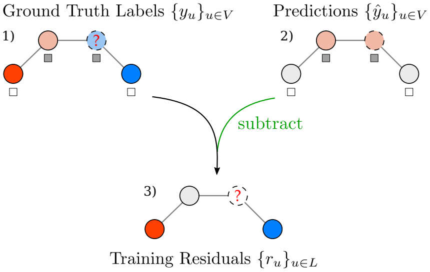

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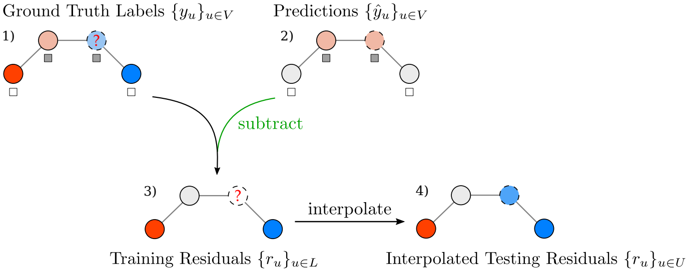

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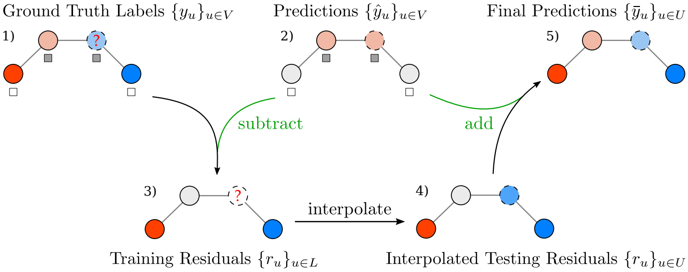

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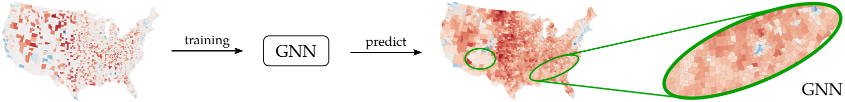
  - final prediction = inductive prediction + estimated residual

GNN/RP Works Super Well in Practice



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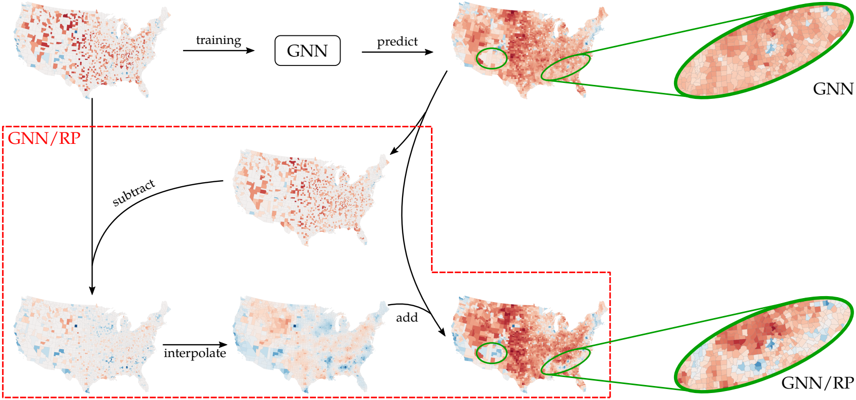

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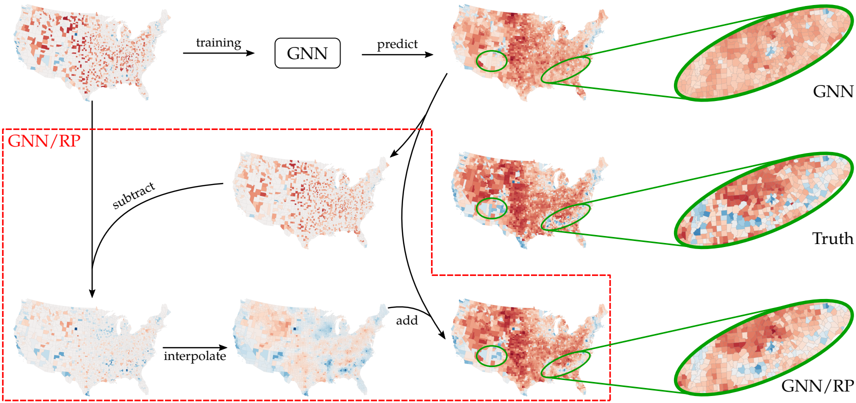

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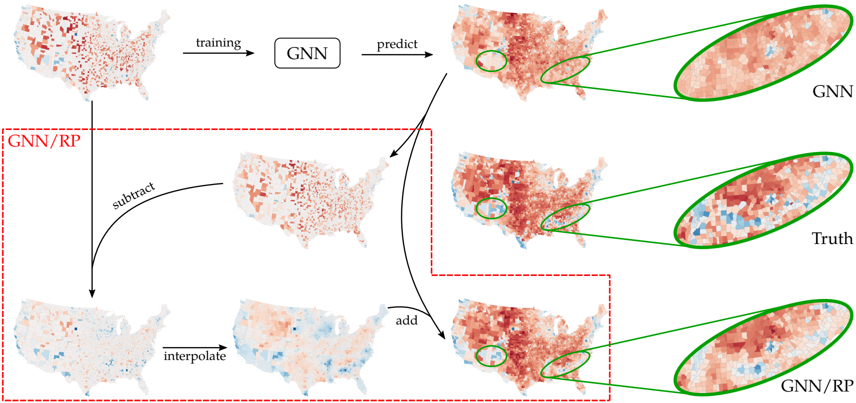

- coefficient of determination (R^2) increases from 0.51 to 0.69 on test set

RP Assumes Linearly Correlated Residuals

	ego features	neighboring features	neighboring labels
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Statistical Model for Node Attributes

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

Statistical Model for Node Attributes

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  - graph topology $G(V, E)$
  - features on all vertices, $\boldsymbol{X} = [\boldsymbol{x}_u]_{u \in V}$
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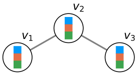
  - different observations gives different algorithms

Statistical Model for Node Attributes

Data Type | Corresponding Gaussian MRF | Learning Algorithm



graph data ($\mathbf{X}$, $\mathbf{y}$, G)

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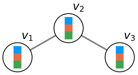

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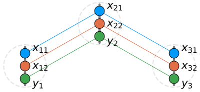

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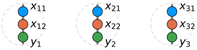

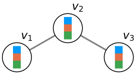

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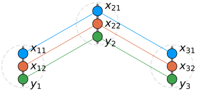

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linear regression

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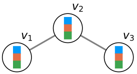

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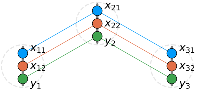

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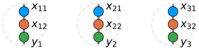

condition on **X**

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

linear regression

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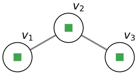
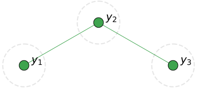
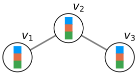


graph data (**y**, G)





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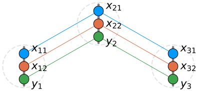

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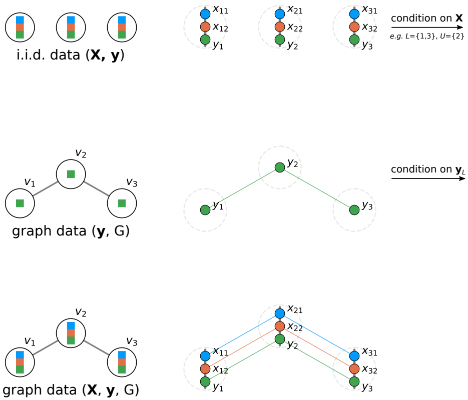


linear regression

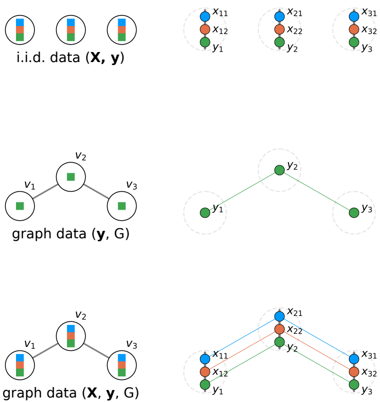
$E[\mathbf{y}_U|\mathbf{X}] = \mathbf{X}_U\beta \qquad \beta = (\mathbf{X}_L^\intercal\mathbf{X}_L)^{-1}\mathbf{X}_L^\intercal\mathbf{y}_L$

label propagation

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

Statistical Model for Node Attributes

Data Type | Corresponding Gaussian MRF | Learning Algorithm



condition on **X** → *e.g. L={1,3}, U={2}*

linear regression

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

condition on $\mathbf{y}_L$ →

label propagation

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

condition on **X** →

linear GCN

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

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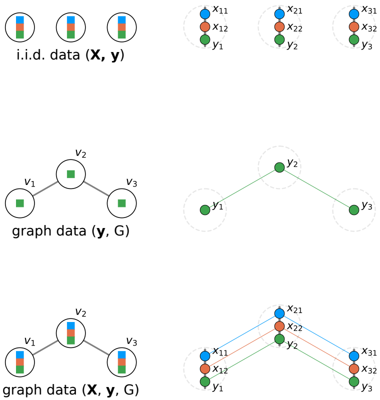


$\xrightarrow[\text{e.g. } L=\{1,3\},\ U=\{2\}]{\text{condition on } \mathbf{X}}$ linear regression

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

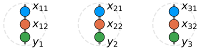
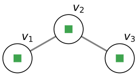
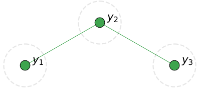
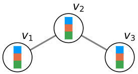
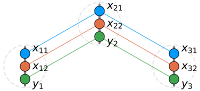
$\xrightarrow{\text{condition on } \mathbf{y}_L}$ label propagation

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

$\xrightarrow{\text{condition on } \mathbf{X}}$ *linear GCN* $\xrightarrow{\text{further condition on } \mathbf{y}_L}$ *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

Data Type	Corresponding Gaussian MRF		Learning Algorithm
 i.i.d. data (**X, y**)		condition on $\mathbf{X}$ → *e.g. L={1,3}, U={2}*	linear regression $E[\mathbf{y}_U \vert \mathbf{X}] = \mathbf{X}_U\beta \qquad \beta = (\mathbf{X}_L^\top \mathbf{X}_L)^{-1}\mathbf{X}_L^\top \mathbf{y}_L$
 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* $\xrightarrow{\text{further condition on } \mathbf{y}_L}$ *residual propagation* $E[\mathbf{y}_U \vert \mathbf{X}] = [(\mathbf{I}+\omega\mathbf{N})^{-1}\mathbf{X}\beta]_U \qquad E[\mathbf{y}_U \vert \mathbf{X}, \mathbf{y}_L] = \cdots$

Statistical Model for Node Attributes

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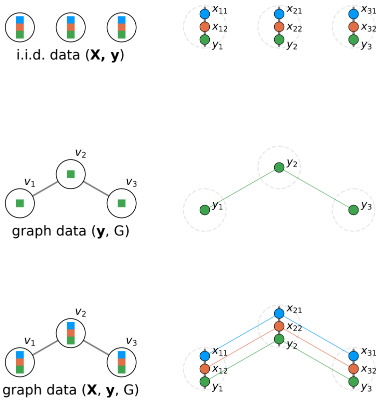

condition on **X** → *e.g.* $L=\{1,3\}$, $U=\{2\}$

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

↓ +nonlinearity

MLP

condition on $\mathbf{y}_L$ →

label propagation

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

condition on **X** →

linear GCN $\xrightarrow{\text{further condition on } \mathbf{y}_L}$ *residual propagation*

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

↓ 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.
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- Probability density function: $\rho(\boldsymbol{A}|\boldsymbol{H},\boldsymbol{h}) = \frac{e^{-\varphi(\boldsymbol{A}|\boldsymbol{H},\boldsymbol{h})}}{\int d\boldsymbol{A'}\ e^{-\varphi(\boldsymbol{A'}|\boldsymbol{H},\boldsymbol{h})}}$

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

Case 1. Linear Regression if no Edge Exists

This is a well-known result for standard linear models

- Gaussian MRF log-potential simplifies as:

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$$\rho(\boldsymbol{A}|\boldsymbol{H},\boldsymbol{h}) = \prod_{u=1}^{n} \frac{e^{-\frac{1}{2}\boldsymbol{a}_u^\intercal \boldsymbol{H} \boldsymbol{a}_u}}{\int d\boldsymbol{a}'_u \; e^{-\frac{1}{2}\boldsymbol{a}'^\intercal_u \boldsymbol{H} \boldsymbol{a}'_u}} = \prod_{u=1}^{n} \sqrt{\frac{\det(\boldsymbol{H})}{(2\pi)^{q+1}}} \cdot e^{-\frac{1}{2}\boldsymbol{a}_u^\intercal \boldsymbol{H} \boldsymbol{a}_u}$$

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

Case 2. Label Propagation if no Feature

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

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

In practice, ω or α can be tuned with cross-validation on the training set.

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$$\begin{aligned} E[\mathbf{y}_U | \mathbf{y}_L = \boldsymbol{y}_L] = -\mathbf{\Gamma}_{UU}^{-1}\mathbf{\Gamma}_{UL}\boldsymbol{y}_L &= -(H\boldsymbol{I}_n + h\boldsymbol{N})_{UU}^{-1}(H\boldsymbol{I}_n + h\boldsymbol{N})_{UL}\boldsymbol{y}_L \\ &= -(\boldsymbol{I}_n + \omega\boldsymbol{N})_{UU}^{-1}(\boldsymbol{I}_n + \omega\boldsymbol{N})_{UL}\boldsymbol{y}_L \end{aligned}$$

$\omega = h/H$;

In practice, ω or α can be tuned with cross-validation on the training set.

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$$\boldsymbol{y}_U^{(k)} = \left[\alpha \cdot \boldsymbol{S}\boldsymbol{y}^{(k-1)} + (1-\alpha) \cdot \hat{\boldsymbol{y}}\right]_U; \quad \boldsymbol{y}_L^{(k)} = \boldsymbol{y}_L$$

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$\alpha = \omega/(1+\omega) \in (0,1)$ controls smoothing level

In practice, ω or α can be tuned with cross-validation on the training set.

Case 2. Label Propagation if no Feature

- 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

- 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

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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]	$(1-\alpha)(\boldsymbol{I}+\alpha\boldsymbol{S}+\alpha^2\boldsymbol{S}^2+\dots)\boldsymbol{X}\beta$	$\boldsymbol{S}=\boldsymbol{D}^{-1/2}\boldsymbol{W}\boldsymbol{D}^{-1/2}$
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]	$\sigma(\tilde{\boldsymbol{S}}\dots\sigma(\tilde{\boldsymbol{S}}\boldsymbol{X}\boldsymbol{\Theta}^{(1)})\dots\boldsymbol{\Theta}^{(K)})\beta$	

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

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

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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)

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- Linear graph convolution with residual propagation (LGC/RP)
  - train LGC to predict both training nodes and testing nodes
  - run LP to interpolate from training residuals $\boldsymbol{r}_L$ to testing residuals $\boldsymbol{r}_U$
  - add interpolated testing residuals $\boldsymbol{r}_U$ to initial predictions $\bar{\boldsymbol{y}}_U$ as corrections

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  with the conditional mean given by: $\bar{\boldsymbol{y}} = (\boldsymbol{I}_n + \omega \boldsymbol{N})^{-1}\boldsymbol{X}\beta$

- Further conditioning on $\mathbf{y}_L = \boldsymbol{y}_L$

$$E[\boldsymbol{y}_U|\mathbf{X} = \boldsymbol{X}, \mathbf{y}_L = \boldsymbol{y}_L] = \bar{\boldsymbol{y}}_U + \underbrace{(\boldsymbol{I} + \omega\boldsymbol{N})_{UU}^{-1}(\boldsymbol{I} + \omega\boldsymbol{N})_{UL}(\bar{\boldsymbol{y}}_L - \boldsymbol{y}_L)}_{\text{constrained LP from training residuals}}$$

- Linear graph convolution with residual propagation (LGC/RP)
  - train LGC to predict both training nodes and testing nodes
  - run LP to interpolate from training residuals $\boldsymbol{r}_L$ to testing residuals $\boldsymbol{r}_U$
  - add interpolated testing residuals $\boldsymbol{r}_U$ to initial predictions $\bar{\boldsymbol{y}}_U$ as corrections

- 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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- Inductive/RP always outperforms LP and the inductive base predictor

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Our Model Connects a lot of Dots

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

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  - formalizes three types of correlations that are helpful for learning node labels

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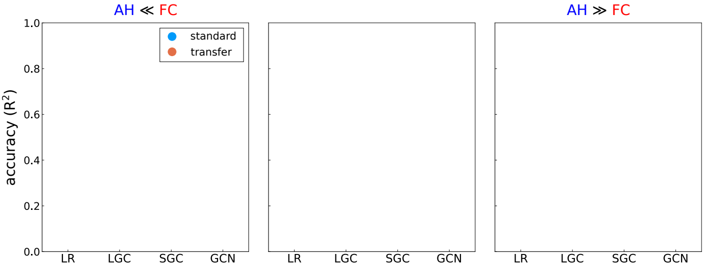
  - we can use LGC to interpret empirical datasets

We can Sample Data to Test Algorithms

Transfer learning experiments on inductive methods



- standard: 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.

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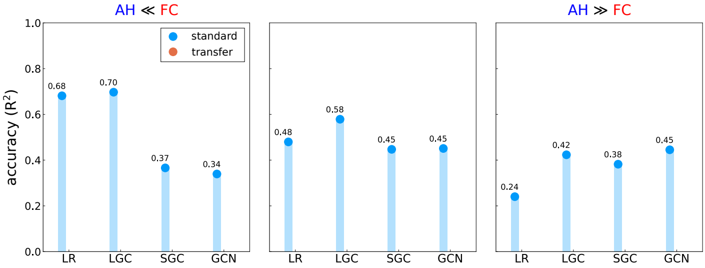

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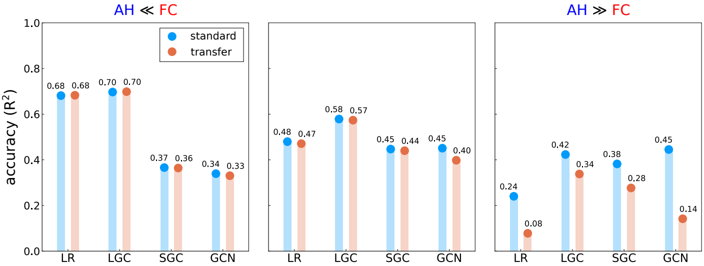

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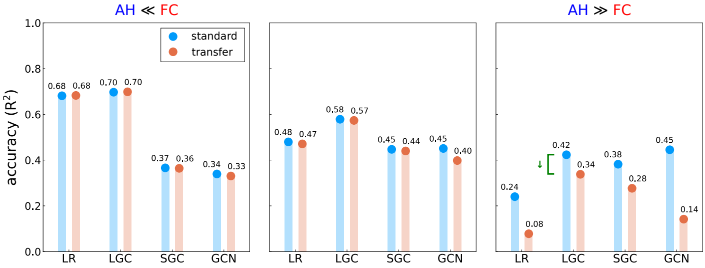

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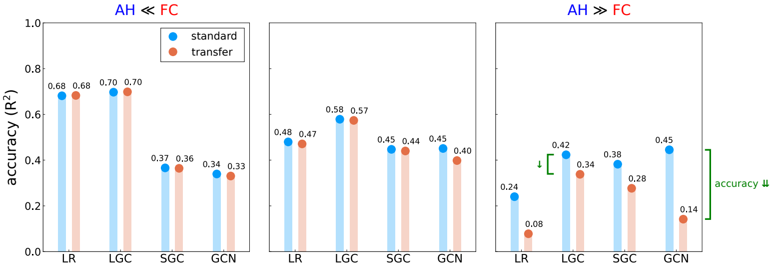

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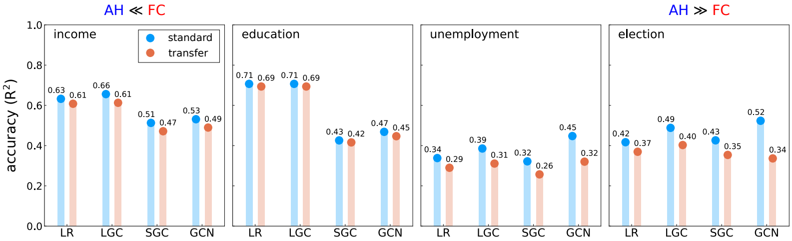

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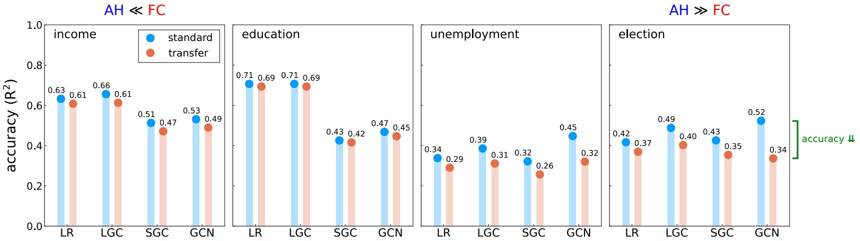

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Our Model Helps Understand Smoothing

- 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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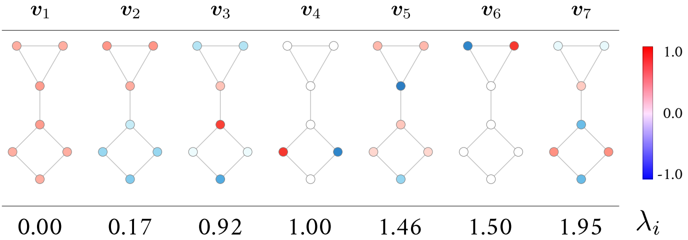

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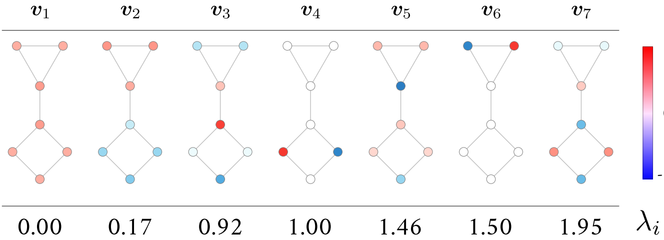

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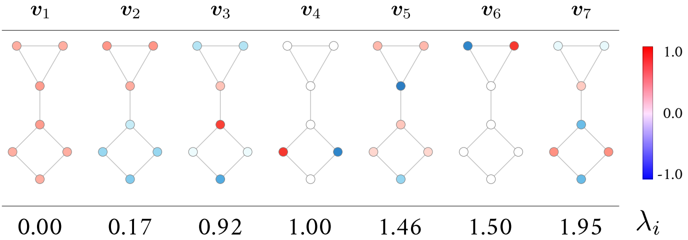

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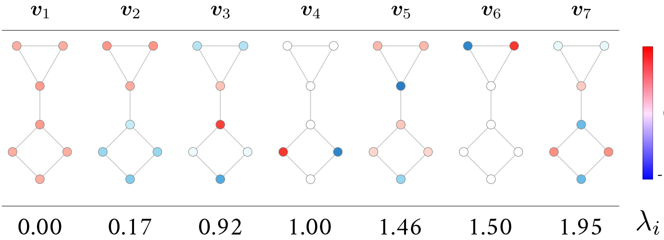

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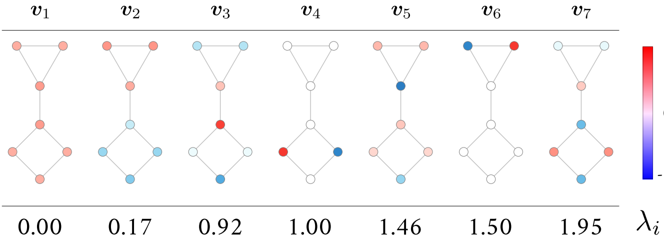

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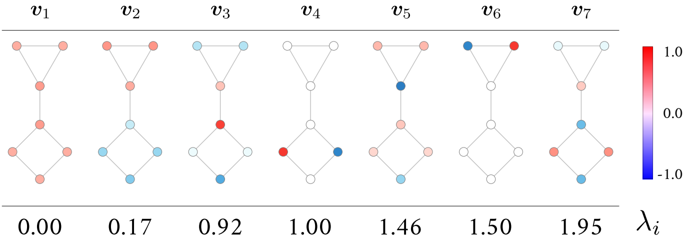

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LGC :

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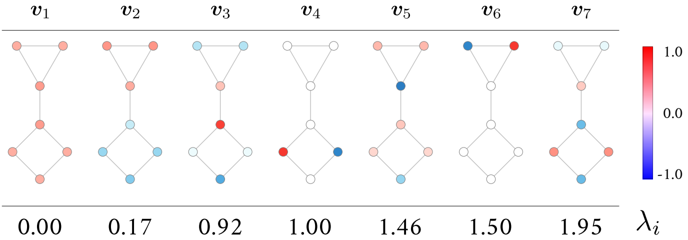

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SGC : $$\tilde{\boldsymbol{S}}^K \boldsymbol{f} = \sum_i c_i \boldsymbol{v}_i \;\; (1 - {}^{d}\!/\!{}_{(d+1)} \lambda_i)^K$$

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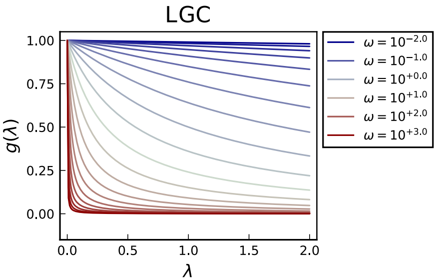

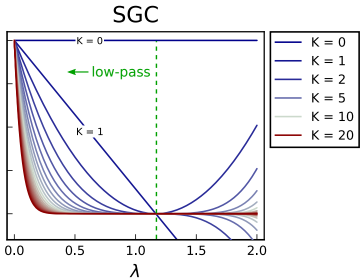

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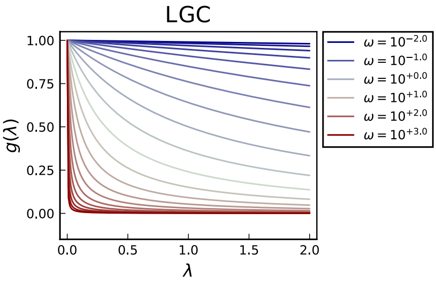

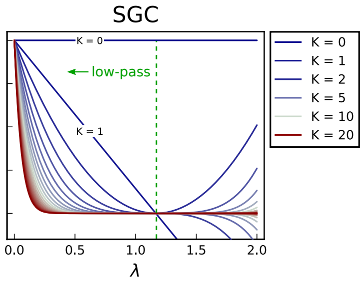

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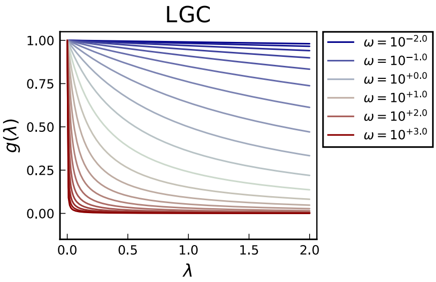
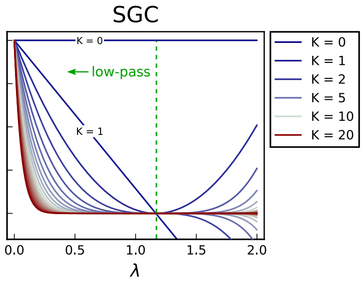
- LGC is a low-pass filter on the entire eigenspectrum $[0, 2]$





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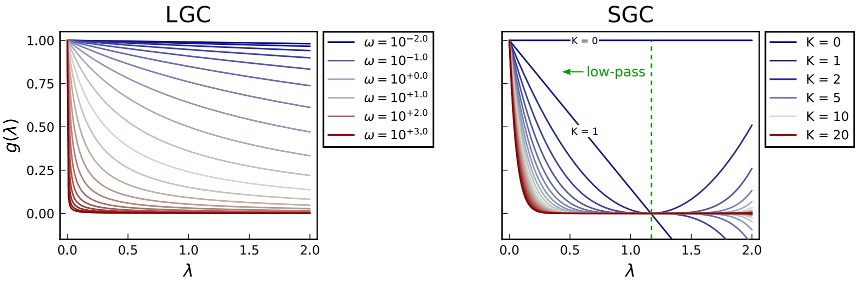
Our Model Helps Understand Smoothing



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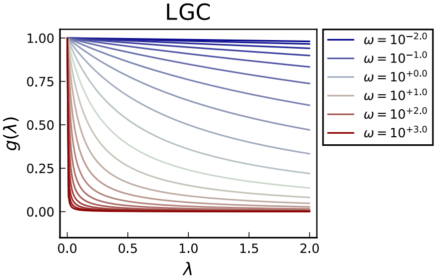

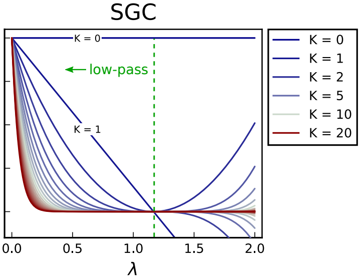

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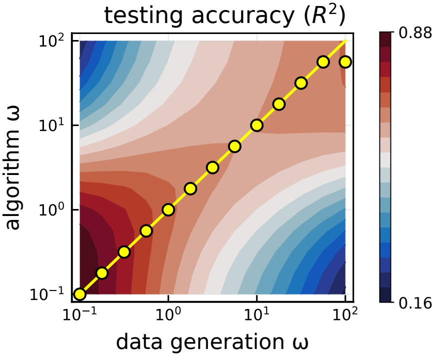

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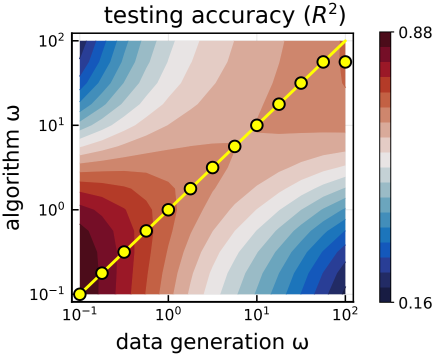

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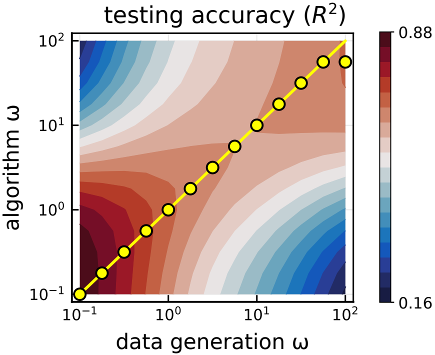

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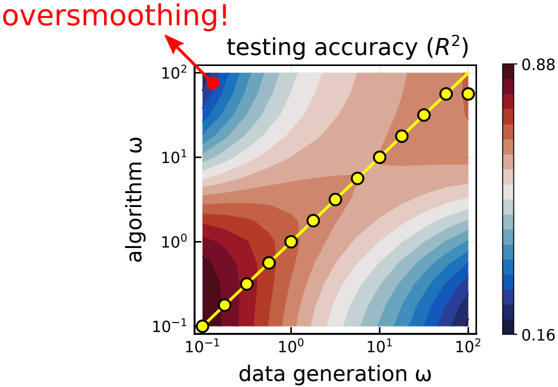

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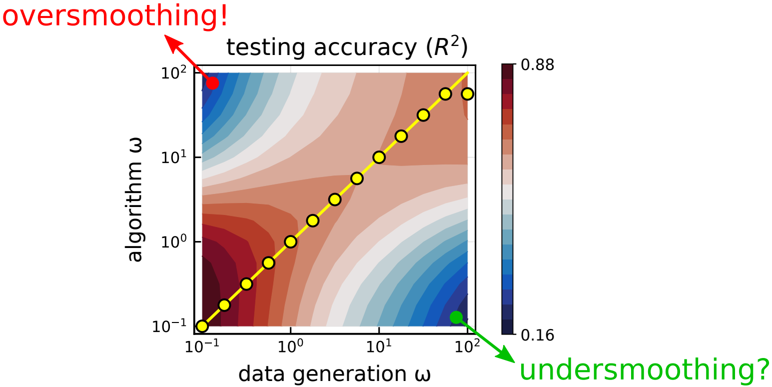

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We can use LGC to Interpret Empirical Data

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?

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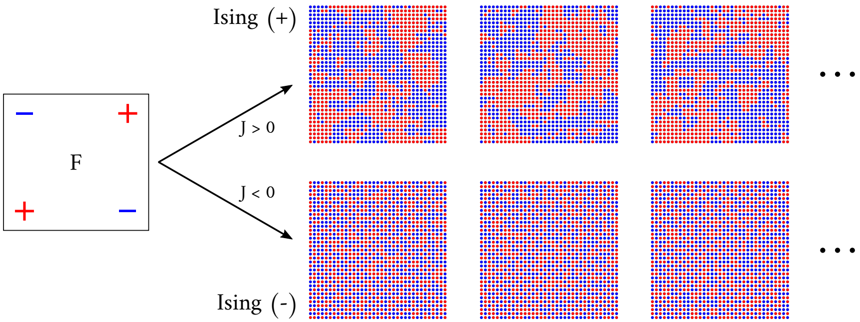
What if labels aren't Poistively Correlated?



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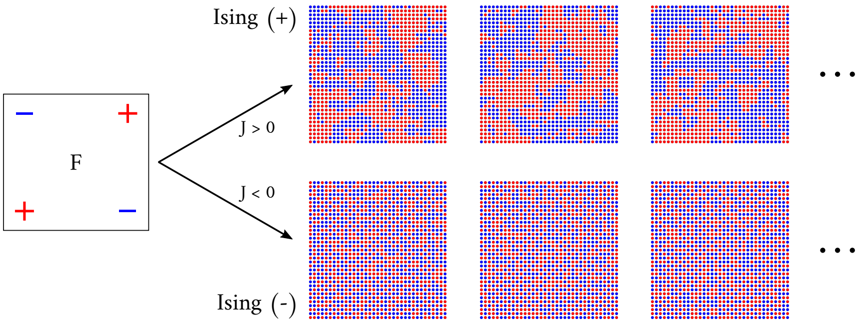

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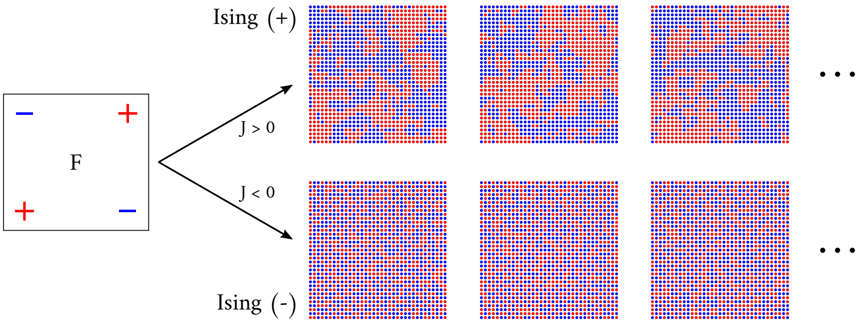

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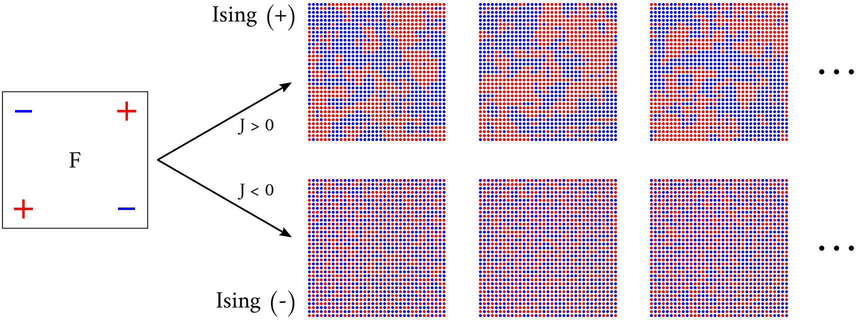

- Sometimes labels can be negatively correlated among neigbors.
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- Residuals are negatively correlated among neighbors as well.

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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$$\alpha^*, \beta^* = \arg\max_{\alpha,\beta} \left[\log|\boldsymbol{\Gamma}| - \log|\boldsymbol{\Gamma}_{UU}| - \boldsymbol{r}_L^\intercal(\boldsymbol{\Gamma}_{LL} - \boldsymbol{\Gamma}_{LU}\boldsymbol{\Gamma}_{UU}^{-1}\boldsymbol{\Gamma}_{UL})\boldsymbol{r}_L\right]$$

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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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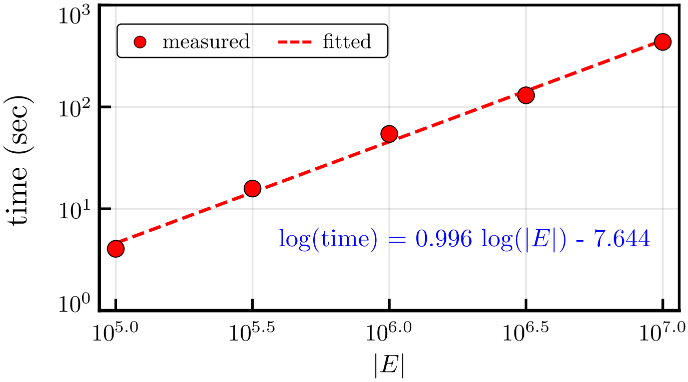
- Estimate gradient with stochastic trace estimator & CG solver

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

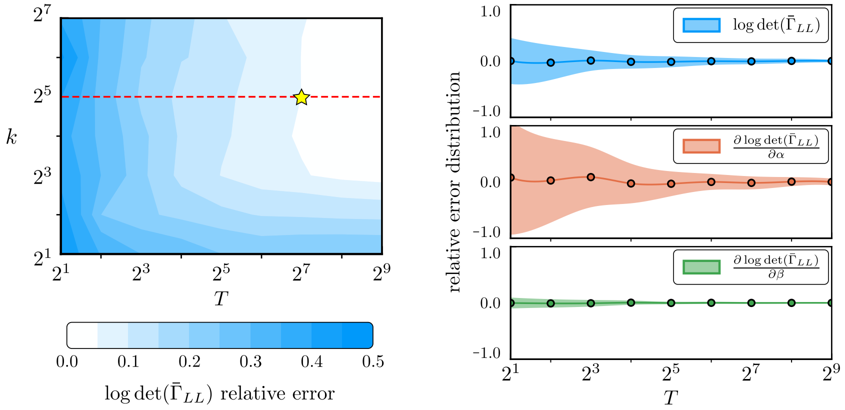
[Ubaru+ 2017; Gardner+ 2018]

Stochastic Estimation is Efficient



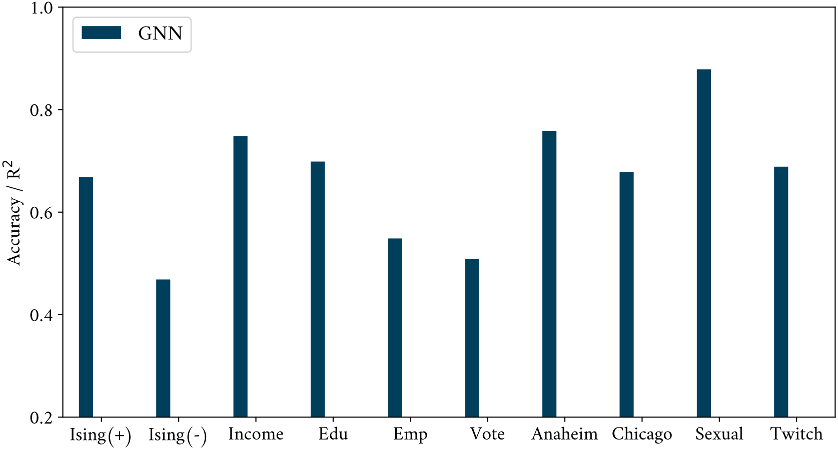
- Stochastic trace estimator cost $\mathcal{O}(|E|)$, linear in the # of edges

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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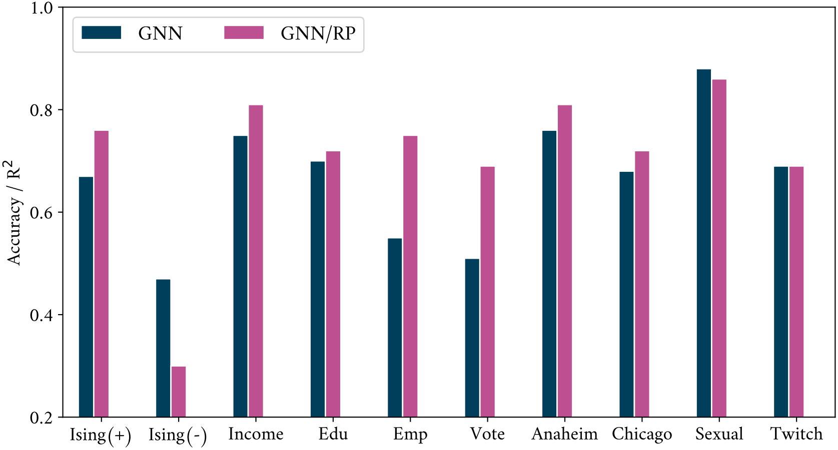

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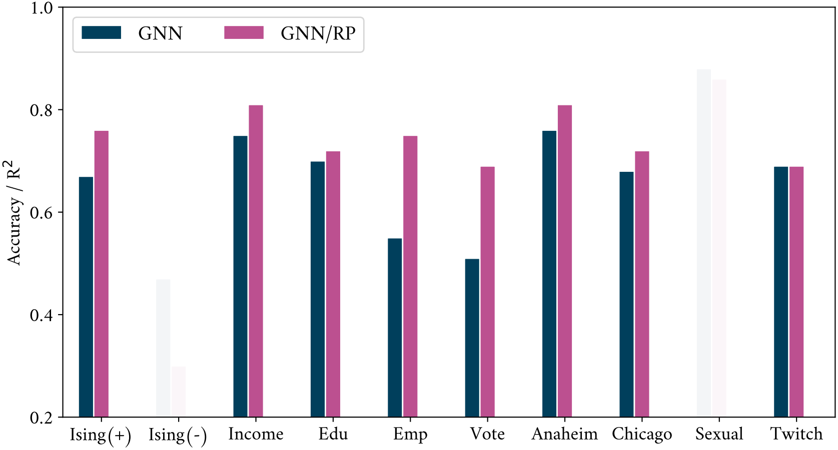

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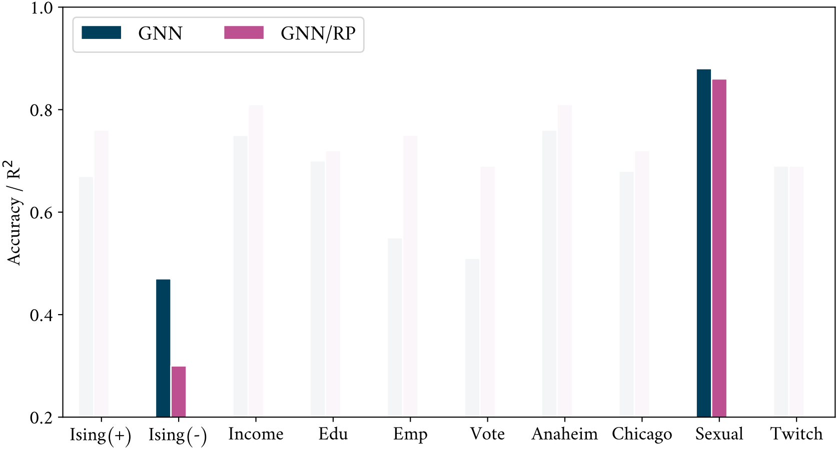

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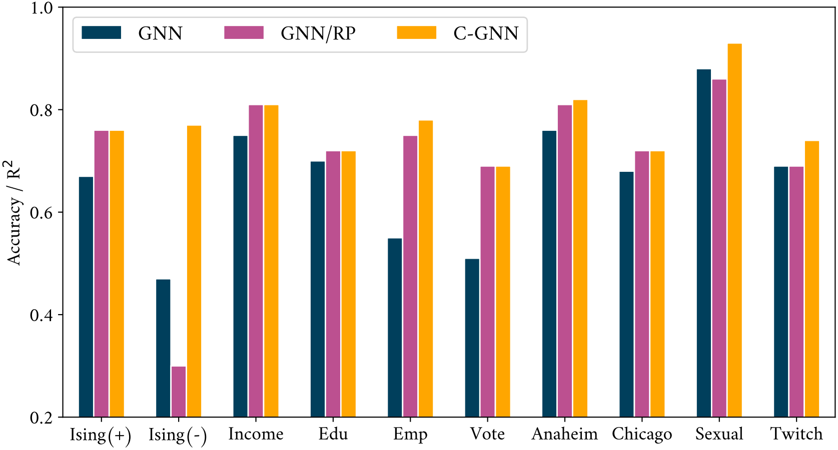

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- C-GNN performs the best on all datasets

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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$$P(\boldsymbol{y}) = \frac{\varphi(\boldsymbol{y})}{\sum_{\boldsymbol{y}'} \varphi(\boldsymbol{y}')}, \quad \varphi(\boldsymbol{y}) = \prod_{u \in V} h(y_u) \prod_{(u,v) \in E} H(y_u, y_v)$$

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which is just another pairwise MRF.

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

Learning algo from Probabilistic Inference

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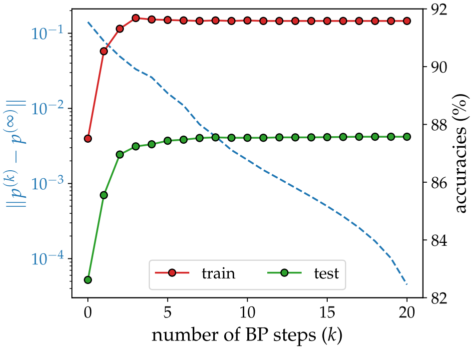
- Or we can compute $P(y_u|\boldsymbol{X}, \boldsymbol{y}_L)$:

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

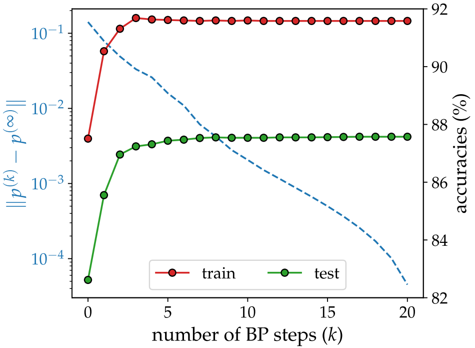
$$P(\boldsymbol{y}_U|\boldsymbol{X}, \boldsymbol{y}_L) \cong \prod_{u \in U} \left(f_\theta(y_u; \boldsymbol{x}_u) \prod_{\substack{u \in U, v \in L, \\ (u,v) \in E}} H_{uv}(y_u, y_v) \right) \prod_{\substack{u,v \in U, \\ (u,v) \in E}} H_{uv}(y_u, y_v)$$

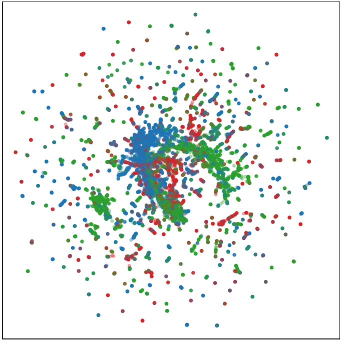
GBPN Case Study on PubMed Dataset



- Belief propagation converge quickly on real-world dataset

GBPN Case Study on PubMed Dataset





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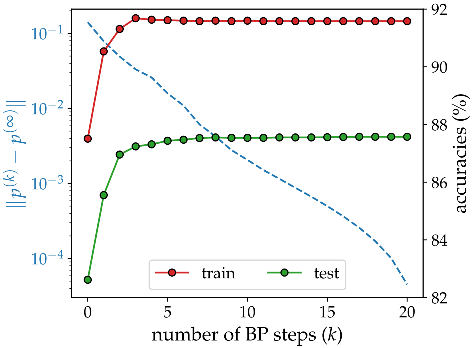

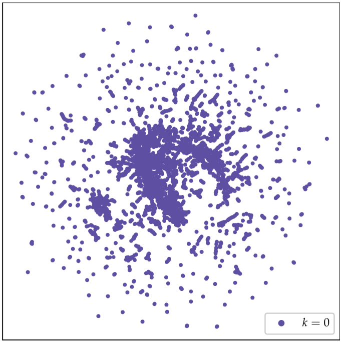

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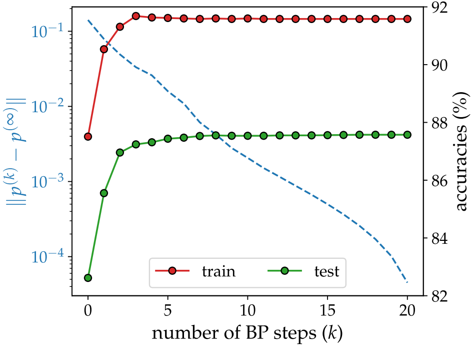

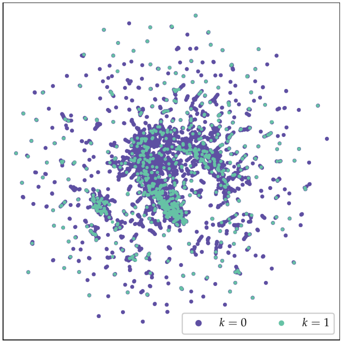

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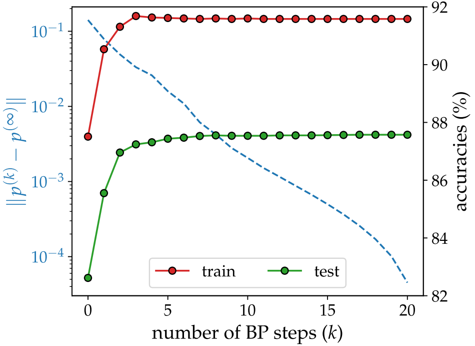

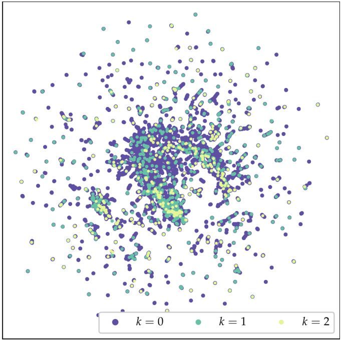

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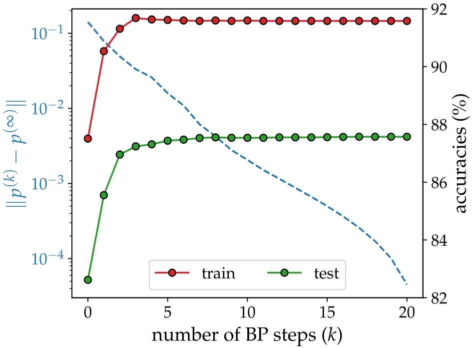

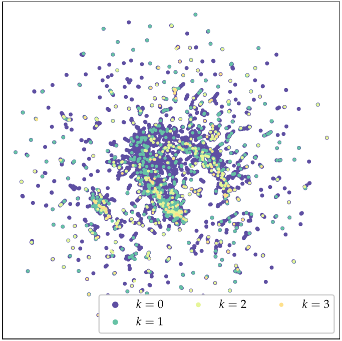

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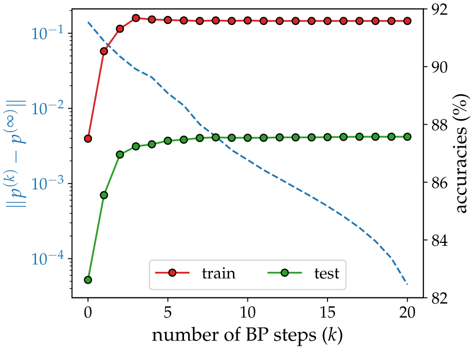

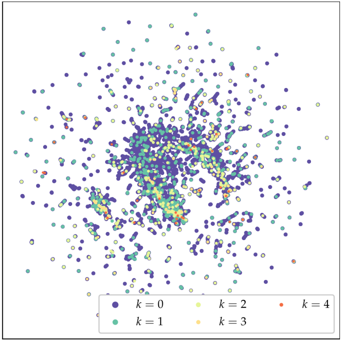

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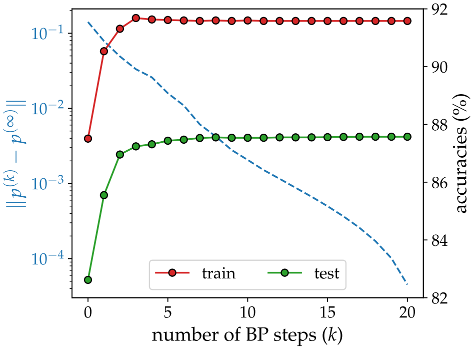

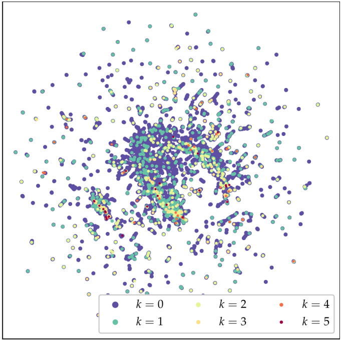

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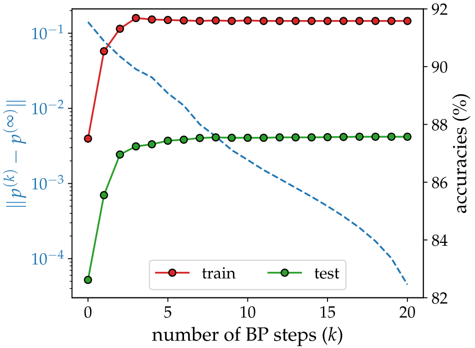

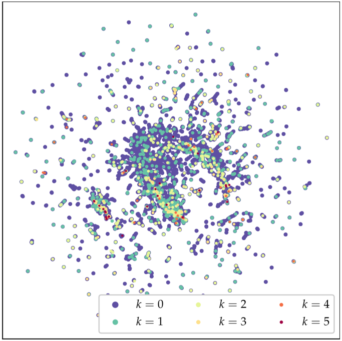

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  first get easy examples right, then iteratively correct harder examples with neighbors

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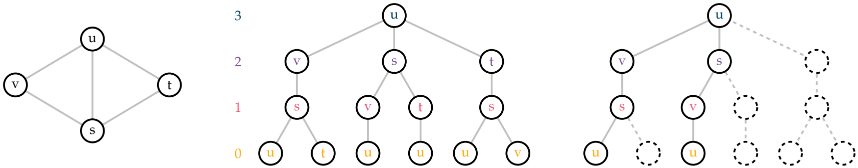
- GBPN is not only more interpretable, but also more accurate

Performance on Large-scale Datasets



- We design a subsampling algorithm for mini-batch training

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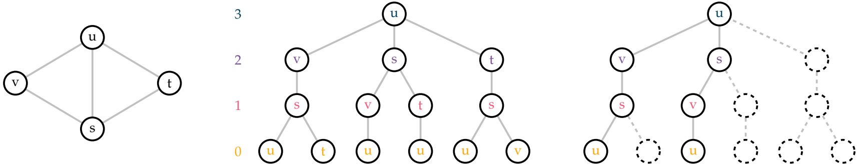

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Chase	61.1 ± 0.3	77.5 ± 0.5	74.6 ± 0.8	83.0 ± 0.5	**86.2** ± 0.5
arXiv	54.6 ± 0.3	**70.4** ± 0.3	**70.4** ± 0.2	69.4 ± 1.1	70.1 ± 0.1
Products	61.5 ± 0.2	78.1 ± 0.2	76.8 ± 0.0	**81.4** ± 0.4	81.2 ± 0.1

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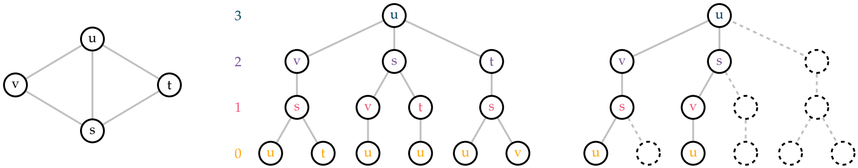

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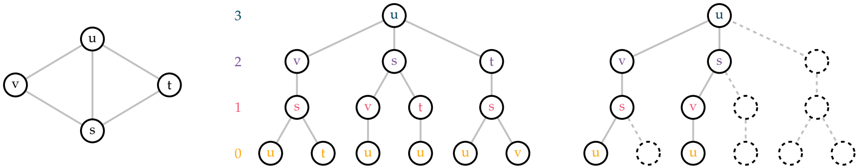

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- GBPN(T) outperforms GBPN(I) by a noticable margin on some dataset

Conclusions

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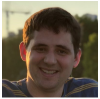
- My thesis proposed a generative model that accounts for three different types of correlations in attributed graphs. It unifies existing algorithms and motivates new ones with the state-of-the-art performance.
- Our model successfully generalizes to non-homophily graphs and node classification setting.

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**
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- **Find me at . . .**
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  - Personal website: https://000justin000.github.io

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