Label Propagation and Graph Neural Networks

Austin R. Benson · Cornell University

GrAPL 2021: Workshop on Graphs, Architectures, Programming, and Learning



Joint work with Junteng Jia (Cornell)

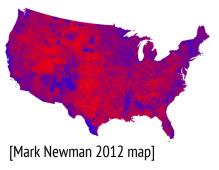
Graph data modeling complex systems are everywhere.



Societynodes are people edges are friendships



Financenodes are accounts
edges are transactions

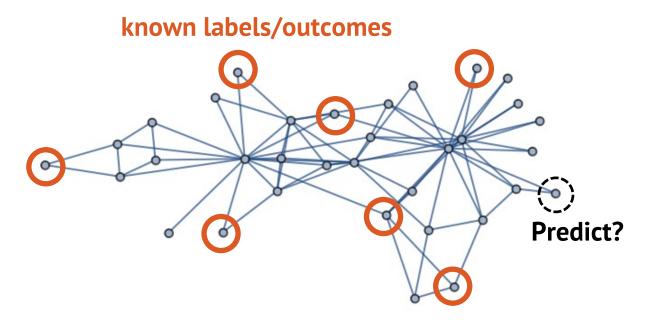


Elections nodes are regions edges are social / geo



Commerce nodes are products edges are copurchases

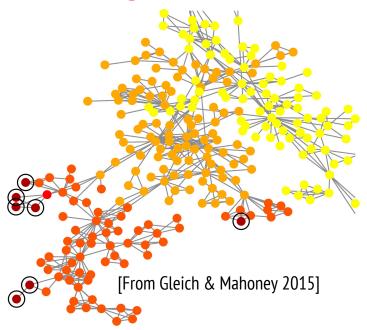
We often want to predict/estimate/construct/forecast attributes/labels/outcomes/clusters on nodes.



- Bad actors in financial transaction graphs [Weber+ 18, 19; Pareja+ 20]
- Gender in social networks
 [Peel 17; Altenburger-Ugander 18]
- Document classification in citation networks [Lu-Getoor 03; Kipf-Welling 17]
- Product categories from coreview/copurchase [Huang+ 20; Veldt+ 20]
- Election outcomes from social connections [Jia-Benson 21]
- Might have rich additional info on nodes (features)
 transaction history, user interests, document text, product ratings, demographics
- Graph-based semi-supervised learning, clustering, node prediction, relational learning, collective classification, community detection, ...

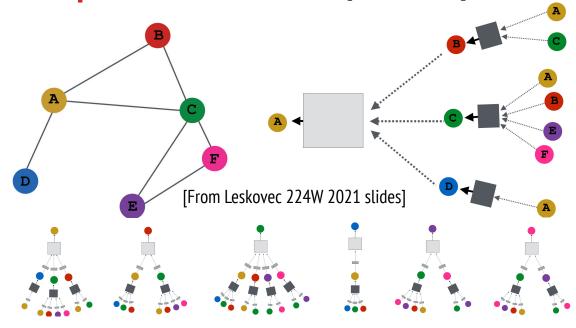
We will analyze two broad classes of algorithms.

1. Label Propagation [early 2000s]



- Propagate/spread/diffuse known values.
- Doesn't use features.

2. Graph Neural Networks [late 2010s]



- Combine neighbor features via neural nets.
- Train with known outcomes.
- Produces vector h_v for each node v.

Key questions.

- 1. When should each work well or poorly?
- 2. What are the computational tradeoffs?
- 3. How can we combine them?
- 4. What is the relationship between them?

The formal problem we are solving.

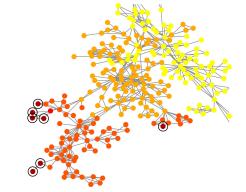
Problem input.

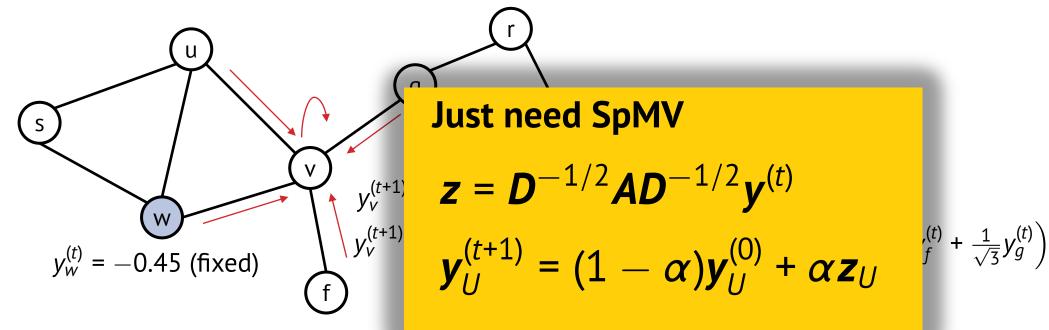
- Graph G = (V, E).
- |*V*| x *p* matrix *X* of node features.
- Subset $L \subset V$ of labeled nodes.
- Length-|L| vector y_L of outcomes on L (real-valued or categorical).

Problem output.

• Length-|U| vector y_U of real-valued outcomes on $U = V \setminus L$.

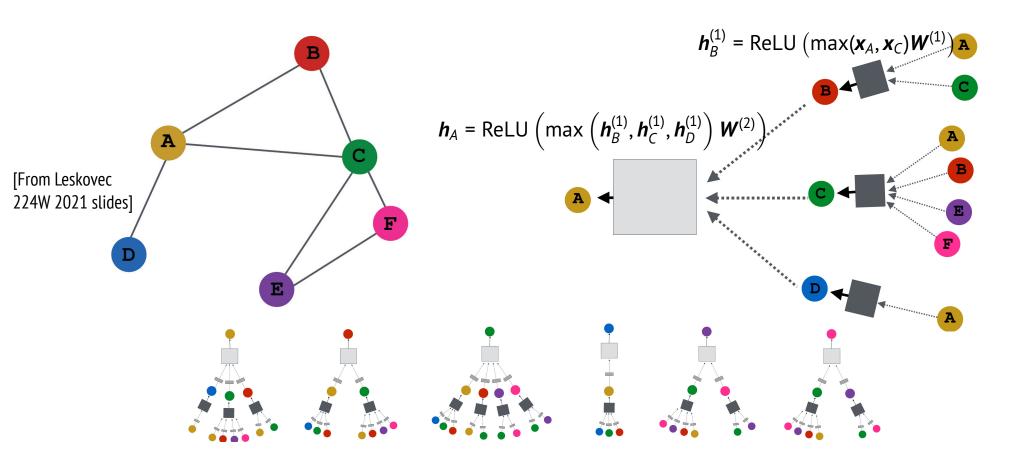
Label propagation is just neighbor averaging.





- At convergence, everyone is roughly the average over their neighbors \rightarrow smooth!
- Regression. Start with real values (0/mean at unknown) \rightarrow smoothed value for each node.

Graph neural networks aggregate features.



- Regression. Prediction at node $A = \langle \beta, h_A \rangle$.
- BIG optimization problem trained with labeled nodes and automatic differentiation.
- **DIFFICULT** to implement, parallelize, reproduce.







Hi

Graph Convolutional Neural Networks for Web-Scale

Recommender Systems Rex Ying*†, Ruining He*, Kaifeng Chen*†, Pong Eksombatchai*,

William L. Hamilton[†], Jure Leskovec*[†] kaifengchen,pong}@pinterest.com,{rexying,wleif,jure}@stanford.edu

cience Projects

ects List

My Projects

Add Project

Project Details

Complete this form to Edit or Archive a Project.

Project Title *:

Julia library for graph neural networks

computing. Recently, they have overnous

FASTGCN: FAST LEARNING WITH GRAPH CONVOL TIONAL NETWORKS VIA IMPORTANCE SAMPLING

Jie Chen*, Tengfei Ma*, Cao Xiao IBM Research

chenjie@us.ibm.com, Tengfei.Mal@ibm.com, cxiao@us.ibm.com



IMPROVING THE ACCURACY, SCALABILITY, AND PERFORMANCE OF GRAPH NEURAL NETWORKS WITH ROC

arameters



I don't know the details of how you're then simply taking the best output from seed".

For example, say your only hyperparam final loss, but there's also just a lot of n hyperparameter tuning might try 0.49, the "true" test accuracy much, simply re

Reducing Communication in Graph Neural Network Training

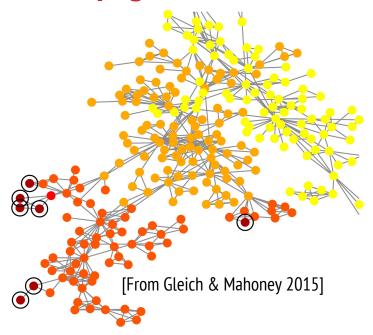
Alok Tripathy, Katherine Yelick, Aydın Buluç

* Electrical Engineering and Computer Sciences, University of California, Berkeley † Computational Research Division, Lawrence Berkeley National Laboratory

equivalent to rerunning your 10

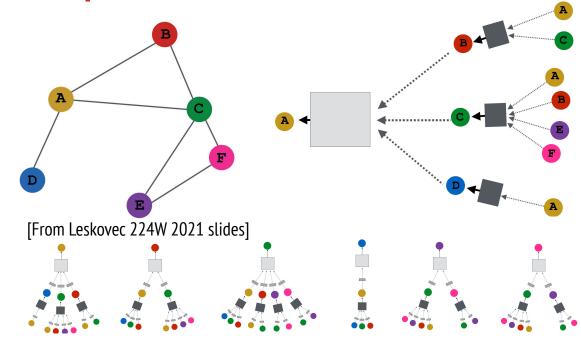
We will analyze two broad classes of algorithms.

1. Label Propagation [early 2000s]



- Strong modeling assumption: connected nodes have similar labels.
- Works because of homophily [McPherson+ 01]
 a.k.a. assortativity [Newman 02]
- Why not use additional info/features?
- **FAST** a few sparse matrix-vector products

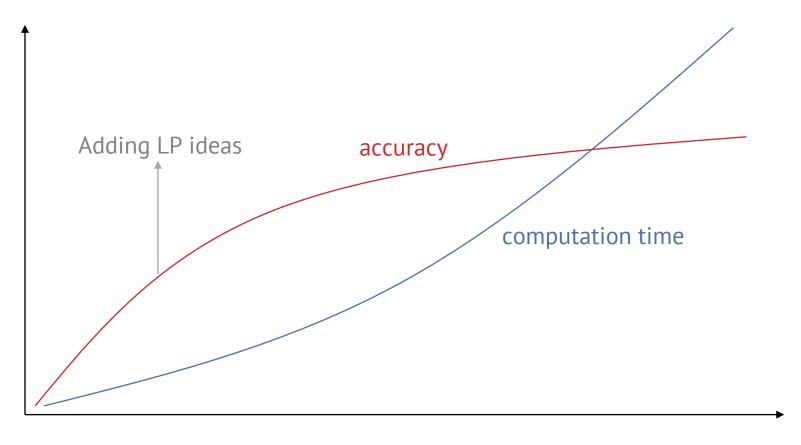
2. Graph Neural Networks [late 2010s]



- Strong modeling assumption: labels only depend on neighbor features
- Works because these features are sometimes very informative.
- Why not assume labels are correlated?
- **SLOW** many parameters, irregular computation

	Node features	Neighborhood features	Neighborhood labels
Supervised ML (like OLS)			
Label propagation			<u></u>
Graph neural networks	<u></u>		
Our work			

Also see *Collective Classification in Network Data* [Sen+ 08] for overview of similar ideas from early 2000s.



More use of node features → (bigger & fancier GNNs)

Leaderboard for ogbn-products

The classification accuracy on the test and validation sets. The higher, the better.

Package: >=1.1.1

Rank	Method	Test Accuracy	Validation Accuracy	Contact	References	#Params	Hardware	Date
1	MLP + C&S	0.8418 ± 0.0007	0.9147 ± 0.0009	Horace He (Cornell)	Paper, Code	96,247	GeForce RTX 2080 (11GB GPU)	Oct 27, 2020
2	Linear + C&S	0.8301 ± 0.0001	0.9134 ± 0.0001	Horace He (Cornell)	Paper, Code	10,763	GeForce RTX 2080 (11GB GPU)	Oct 27, 2020
3	UniMP	0.8256 ± 0.0031	0.9308 ± 0.0017	Yunsheng Shi (PGL team)	Paper, Code	1,475,605	Tesla V100 (32GB)	Sep 8, 2020
4	Plain Linear + C&S	0.8254 ± 0.0003	0.9103 ± 0.0001	Horace He (Cornell)	Paper, Code	4,747	GeForce RTX 2080 (11GB GPU)	Oct 27, 2020
5	DeeperGCN+FLAG	0.8193 ± 0.0031	0.9221 ± 0.0037	Kezhi Kong	Paper, Code	253,743	NVIDIA Tesla V100 (32GB GPU)	Oct 20, 2020



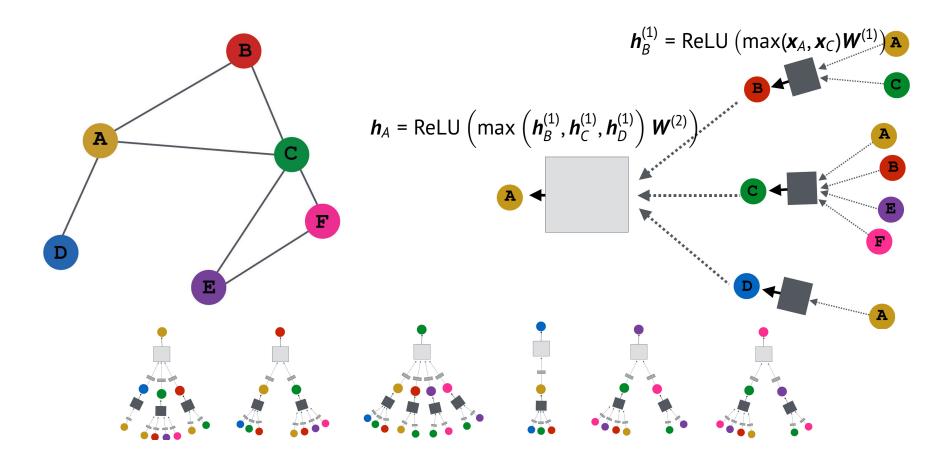
Joint work with Qian Huang, Horace He, Abhay Sing (Cornell) Ser-Nam Lim (Facebook)

Datasets	Classes	Nodes	Edges	Parameter Δ	Accuracy Δ	Time (s)
Arxiv	40	169,343	1,166,243	-84.90%	+0.37	12 (+90)
Products	47	2,449,029	61,859,140	-93.47%	+1.99	171 (+2959)
Cora	7	2,708	5,429	-98.37%	+1.28	< 1 (+7)
Citeseer	6	3,327	4,732	-89.68%	-0.70	< 1 (+7)
Pubmed	3	19,717	44,338	-96.00%	-0.29	< 1 (+14)
Email	42	1,005	25,571	-97.89%	+4.33	43 (+17)
Rice31	10	4,087	184,828	-99.02%	+1.39	39 (+12)
US County	2	3,234	12,717	-74.56%	+1.77	39 (+12)
wikiCS	10	11,701	216,123	-84.88%	+2.03	7 (+11)

Combining Label Propagation and Simple Models Out-performs Graph Neural Networks. Q. Huang et al., ICLR 2021.

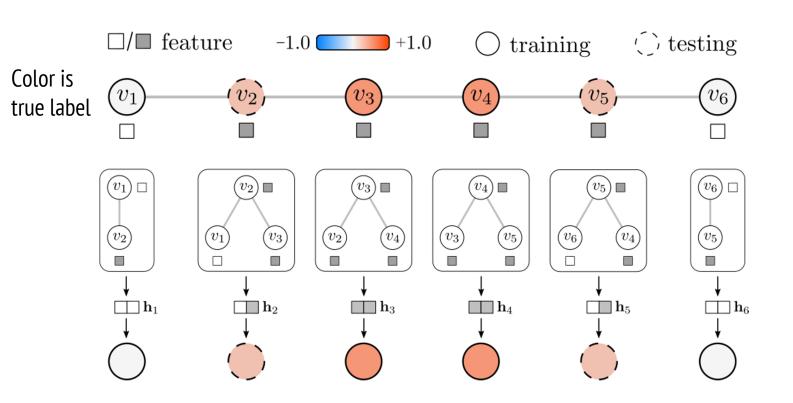
The core problem is that (traditional) GNNs make uncorrelated predictions.

Graph neural networks make uncorrelated predictions.



- Use labels to find representation vectors h_A , h_B , h_C , h_D , h_E , and h_F and coefficients β .
- Given representations and coefficients, predictions are independent.
- Something strange? Compared to LP, use of labels is very implicit.
- Pervasive paradigm [Kipf-Welling 16; Hamilton+ 17; Zhou+ 18; ~10,000 papers in 5 years]

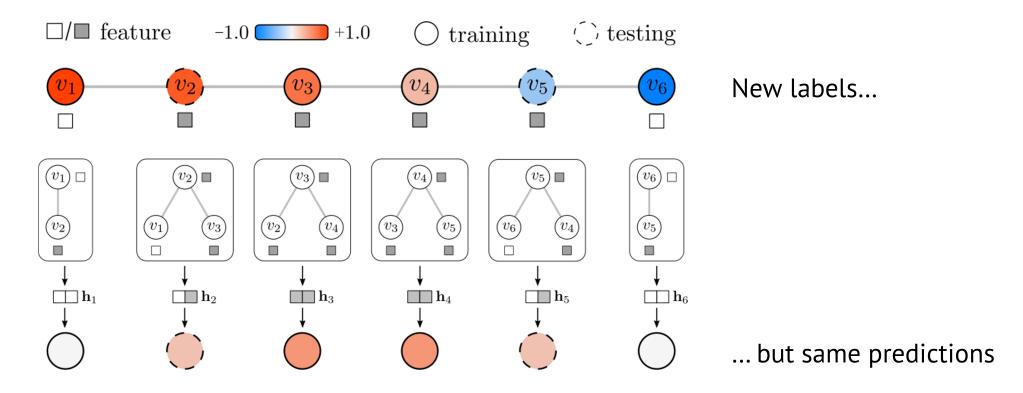
Graph neural networks make uncorrelated predictions.



- 1. Form local neighborhoods
- 2. Combine features to get a representation h_v at node v.
- 3. Predict outcome given representation (learn model params w/ training data)

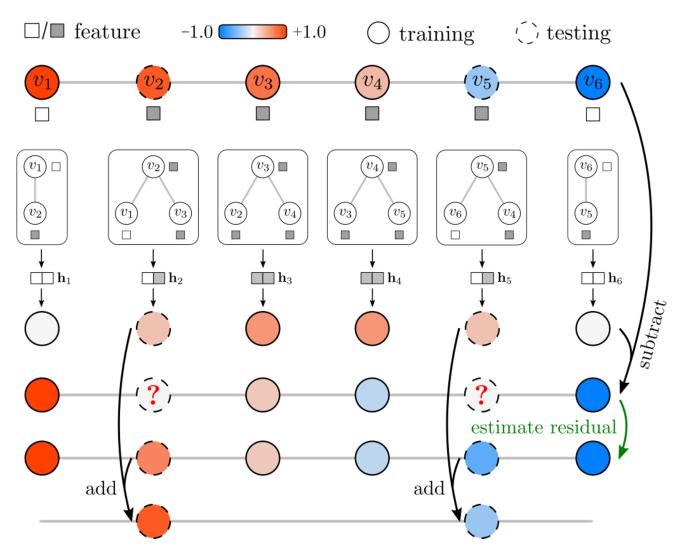
• If node features are overwhelmingly predictive, these uncorrelated predictions might be OK.

Uncorrelated GNN predictions can be catastrophic in simple cases when features are only mildly predictive.



- All we have done is change the label distribution!
- Big problem. Features are no longer super predictive.
- LP (ignoring features) would work much better.

We can correlate feature-based predictions by propagating residual errors.



Works with any GNN.

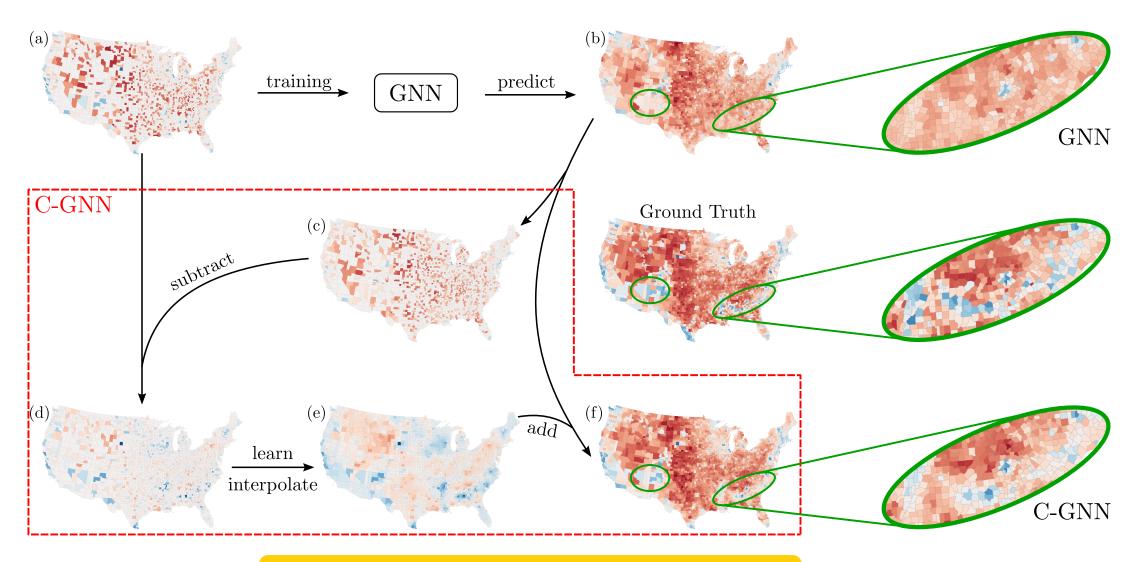
Just layer on top.

- 1. Standard GNN prediction.
- 2. Compute residual error.
- 3. Propagate residuals to estimate errors on test nodes.
- 4. Add residual to base prediction.

The residual propagation algorithm is simple.

- 1. Make a base prediction on each node with any method.
- 2. residual = true value base prediction (on labeled nodes)
- 3. Label propagation on residual \rightarrow smooth errors
- 4. Final prediction = smoothed residual + base prediction (= true value on labeled nodes)

Residual propagation works well in practice.



Out-of-sample R^2 0.51 \rightarrow 0.69.

Residual propagation works well in practice.

 R^2 on county-level demographics predictions.

vote share $0.51 \rightarrow 0.69$

income $0.75 \rightarrow 0.81$

education level $0.70 \rightarrow 0.72$

unemployment level $0.55 \rightarrow 0.75$

 R^2 on traffic predictions.

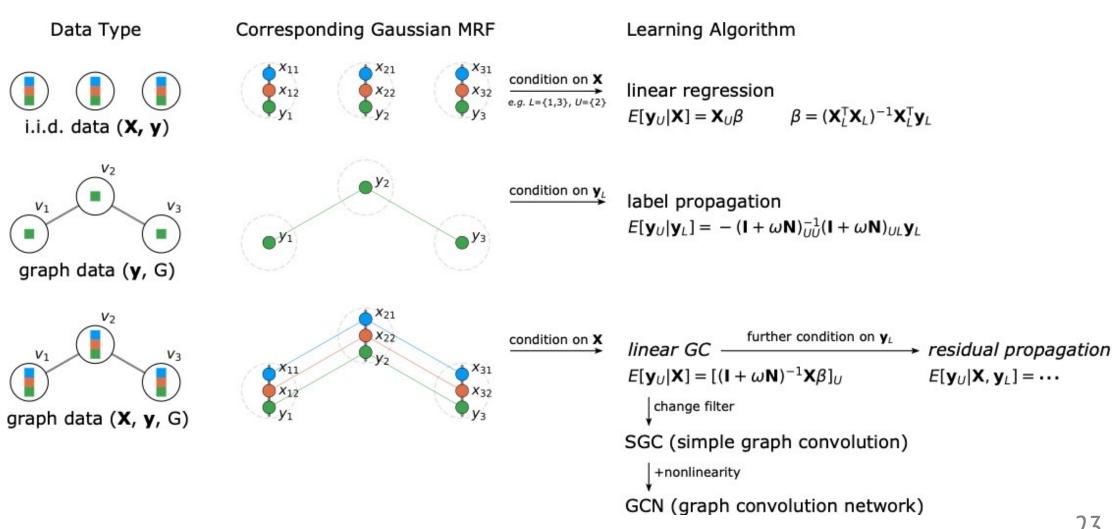
Anaheim $0.76 \rightarrow 0.81$

Chicago $0.68 \rightarrow 0.72$

Why does this work?

Do we need the NN in GNNs?

We developed a random model for attributes on nodes, where statistical inference leads to GNN/LP algorithms.



Our model is based on smooth random attributes.

- Random real-valued attribute vectors $\mathbf{a}_{u} = [\mathbf{x}_{u}; y_{u}]$ on each node u.
- $A_i = i$ th attribute over all nodes.
- $N = I D^{-1/2} WD^{-1/2}$ is the normalized Laplacian.
- Gaussian MRF random attribute model

$$\phi(\mathbf{A}|\mathbf{H},\mathbf{h}) = \frac{1}{2} \sum_{u=1}^{n} \mathbf{A}_{u}^{\mathsf{T}} \mathbf{H} \mathbf{a}_{u} + \frac{1}{2} \sum_{i=1}^{p+1} \mathbf{h}_{i} \mathbf{A}_{i}^{\mathsf{T}} \mathbf{N} \mathbf{A}_{i}, \quad \mathbf{H} \in \mathbb{R}^{(p+1) \times (p+1)} \text{ spd}, \quad \mathbf{0} \leq \mathbf{h} \in \mathbb{R}^{(p+1)}$$

$$= \sum_{(u,v) \in E} (A_{ui}/\sqrt{d_{u}} - A_{vi}/\sqrt{d_{v}})^{2}$$

$$\rho(\mathbf{A} = \mathbf{A}|\mathbf{H}, \mathbf{h}) = \frac{e^{-\phi(\mathbf{A}|\mathbf{H}, \mathbf{h})}}{\int d\mathbf{A}' \ e^{-\phi(\mathbf{A}'|\mathbf{H}, \mathbf{h})}}$$
 Smoother attributes are more likely (homophily / assortativity)

$$\text{vec}(\mathbf{A}) \sim \mathcal{N}(\mathbf{0}, \mathbf{\Gamma}^{-1}), \quad \mathbf{\Gamma} = \mathbf{H} \otimes \mathbf{I}_n + \text{diag}(\mathbf{h}) \otimes \mathbf{N}$$
 Just a multivariate normal random variable in the end

Graph learning is now just statistical inference.

1. Ignore graph, condition on features \rightarrow linear regression.

$$E[\mathbf{y}|\mathbf{X} = \mathbf{X}] = \mathbf{X}^{\mathsf{T}}\boldsymbol{\beta} \longrightarrow \min_{\boldsymbol{\beta}} ||\mathbf{X}_{L}\boldsymbol{\beta} - \mathbf{y}_{L}||_{2}^{2} \longrightarrow \mathbf{X}_{U}\hat{\boldsymbol{\beta}}$$
(classical derivation of linear models)

2. Ignore features, condition on graph, labels \rightarrow label prop.

$$E[\mathbf{y}_{U}|\mathbf{y}_{L} = \mathbf{y}_{L}, \mathbf{G}] = -(\mathbf{I}_{n} + \omega \mathbf{N})_{UU}^{-1} (\mathbf{I}_{n} + \omega \mathbf{N})_{UL} \mathbf{y}_{L}, \quad \omega = h/H$$
label prop
Smoothing amount ~ homophily * variance

3. Ignore labels, condition on features + graph \rightarrow linearized GNN.

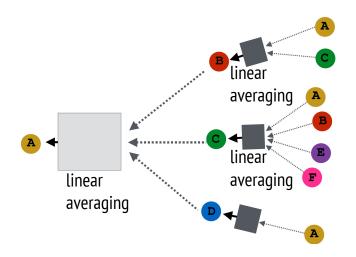
$$E[\mathbf{y}|\mathbf{X} = \mathbf{X}, \mathbf{G}] = (\mathbf{I}_n + \omega \mathbf{N})^{-1} \mathbf{X} \boldsymbol{\beta} \longrightarrow \min_{\boldsymbol{\beta}} \|[(\mathbf{I}_n + \omega \mathbf{N})^{-1} \mathbf{X}]_L \boldsymbol{\beta} - \mathbf{y}_L\|_2 \longrightarrow [(\mathbf{I}_n + \omega \mathbf{N})^{-1} \mathbf{X}]_U \hat{\boldsymbol{\beta}}$$
label prop
on features

4. Condition on features + labels + graph \rightarrow linearized GNN + residual prop. $E[\mathbf{y}_{U}|\mathbf{X}=\mathbf{X},\mathbf{y}_{L}=\mathbf{y}_{L},\mathbf{G}]=\bar{\mathbf{y}}_{U}+(\mathbf{I}+\omega\mathbf{N})_{UU}^{-1}(\mathbf{I}+\omega\mathbf{N})_{UL}(\bar{\mathbf{y}}_{L}-\mathbf{y}_{L}),\ \bar{\mathbf{y}}=(\mathbf{I}_{n}+\omega\mathbf{N})^{-1}\mathbf{X}\hat{\boldsymbol{\beta}}$ label prop residual prop (on features)

Linear graph convolutions are linearized GNNs that come from the conditioning on features.

Linear graph convolution (LGC).

- 1. Run LP on each feature → smoothed features.
- Ordinary least squares on these preprocessed, smoothed features.



Linear graph convolutions are linearized GNNs that come from the conditioning on features.

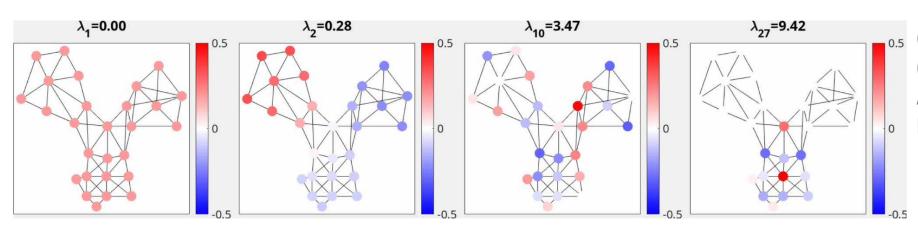
```
Linear Graph Convolution (LGC) (1-\alpha) \left(I+\alpha S+\alpha^2 S^2+...\right) X\beta S=D^{-1/2}WD^{-1/2} [Jia-Benson 21] Simplified Graph Convolution (SGC) \tilde{S}^K X\beta \tilde{S}=(D+I)^{-1/2}(W+I)(D+I)^{-1/2} [Wu+ 19] Graph Convolution Network (GCN) \sigma(\tilde{S} ... \sigma(\tilde{S} X \Theta^{(1)}) ... \Theta^{(K)})\beta [Kipf-Welling 17]
```

- α is continuous, while K is discrete.
- Does nonlinearity help?
- Does extra parameterization of each "propagation step" in GCN help?
- SGC as $K \rightarrow \infty$ is nonsensical.

Dataset	Outcome	LP	LR	LGC (α)	SGC (<i>K</i>)	GCN (<i>K</i>)	LGC/RP	SGC/RP	GCN/RP
	income	0.40	0.63	0.66 (0.46)	0.51 (1.0)	0.53 (1.3)	0.69	0.55	0.55
U.S.	education	0.31	0.71	0.71 (0.00)	0.43 (1.0)	0.47 (1.0)	0.71	0.46	0.48
0.3.	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
	airT	0.95	0.85	0.86 (0.78)	0.86 (2.6)	0.95 (3.0)	0.96	0.97	0.97
CDC	landT	0.89	0.81	0.81 (0.09)	0.79 (1.0)	0.91 (2.4)	0.90	0.93	0.93
CDC	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
	income	0.46	0.85	0.85 (0.00)	0.64 (1.0)	0.63 (1.0)	0.85	0.65	0.64
London	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

```
function LGC_params(S, X, y, L; \alpha=0.9, num_iters=10)
         X_{smooth} = copy(X)
 2
         for _ in 1:num_iters
 3
              X_{smooth} = (1 - \alpha) * X + \alpha * S * X_{smooth}
 4
 5
         end
          return X_smooth, X_smooth[L, :] \ y[L]
 6
 7
     end
 8
 9
     function residual_prop(S, y, \bar{y}, U; \alpha=0.9, num_iters=10)
10
         r = y - \bar{y}
11
         r[U] = 0
         for _ in 1:num_iters
12
13
              z = S * r
              r[U] = \alpha * z[U]
14
15
         end
16
          return r
17
     end
18
19
     function LGC_RP_prediction(
         S, # normalized adjacency D^{-1/2} A D^{-1/2}
20
21
         X, # n x d feature matrix for n nodes
         U, # indices of unlabeled nodes
22
23
              # indices of labeled nodes
24
         y, # n x 1 label vector (zero on y[U])
25
         X_{smooth}, \hat{\beta} = LGC_{params}(S, X, y, L)
26
         \bar{y} = X_smooth * \hat{\beta}
27
          r = residual\_prop(S, y, \bar{y}, L)
28
          return ȳ[U] + c[U]
29
30
     end
```

Our model helps us understand smoothing.



Graph Signal Processing: Overview, Challenges and Applications, Ortega et al., Proc. IEEE, 2018.

$$\mathbf{N} = \mathbf{V} \mathbf{\Lambda} \mathbf{V}^{\mathsf{T}}$$
, feature $\mathbf{f} = \sum_{i=1}^{n} c_i v_i$

LGC
$$f \rightarrow \sum_{i=1}^{n} \frac{1}{(1 + \omega \lambda_i)} c_i v_i$$

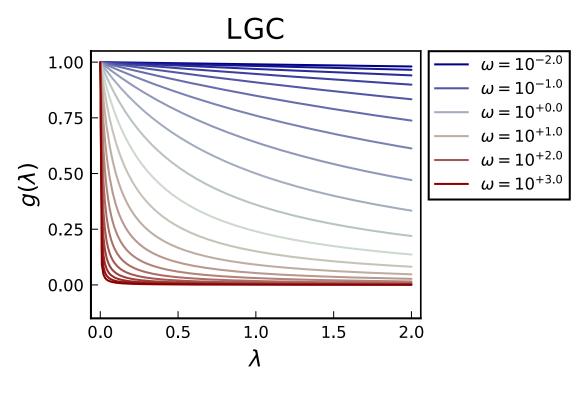
SGC
$$f o \sum_{i=1}^{n} (1 - d/(d+1)\lambda_i)^K c_i v_i$$

Low-pass on $[0, \infty)$, continuous parameterization.

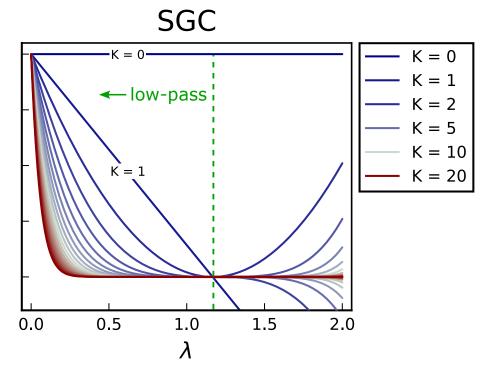
Low-pass on [0, (d + 1)/d], discrete parameterization.

Encouraging smoothness.

Our model helps us understand smoothing.

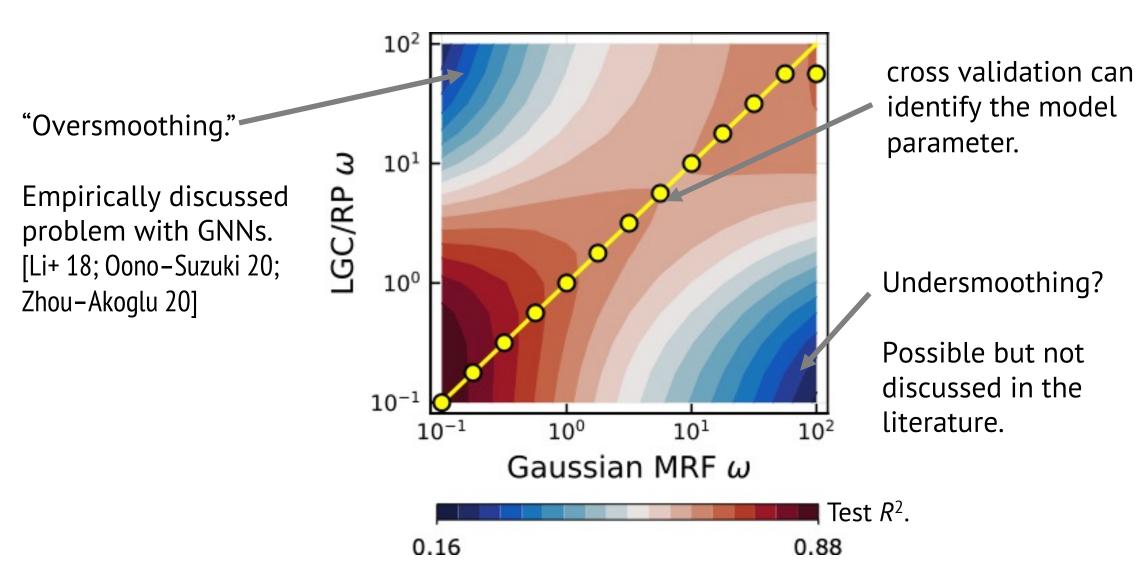


$$f = \sum_{i=1}^{n} c_i v_i \rightarrow \sum_{i=1}^{n} \frac{1}{(1 + \omega \lambda_i)} c_i v_i$$



$$\boldsymbol{f} = \sum_{i=1}^{n} c_{i} v_{i} \rightarrow \sum_{i=1}^{n} (1 - d/(d+1)\lambda_{i})^{K} c_{i} v_{i}$$

Our model helps us understand smoothing.



We can also evaluate on our generative model.

_	h_0	$LP\left(lpha ight)$	LR	LGC (α)	SGC (K)	GCN (<i>K</i>)	LGC/RP (α)	SGC/RP (K, α)	GCN/RP (K, α)
Low homophily.	1	0.19 (0.79)	0.68	0.70 (0.28)	0.37 (1.8)	0.34 (1.7)	0.73 (0.29)	0.40 (1.8, 0.21)	0.37 (1.7, 0.21)
	10	0.43 (0.95)	0.48	0.58 (0.57)	0.45 (2.1)	0.45 (2.0)	0.68 (0.56)	0.56 (2.1, 0.46)	0.54 (2.0, 0.43)
High homophily.	100	0.59 (0.99)	0.24	0.42 (0.85)	0.38 (2.3)	0.45 (2.5)	0.64 (0.85)	0.63 (2.3, 0.81)	0.62 (2.5, 0.79)

- GCN more expressive but prone to overfitting.
- More homophily \rightarrow larger K, α
- Adding residual prop never hurts!
- GCN better with more homophily?
 "memorizing" neighborhood features (zero training error)
 + smoothness in data → better out-of-sample prediction

Our model provides a nice setup for inductive learning.

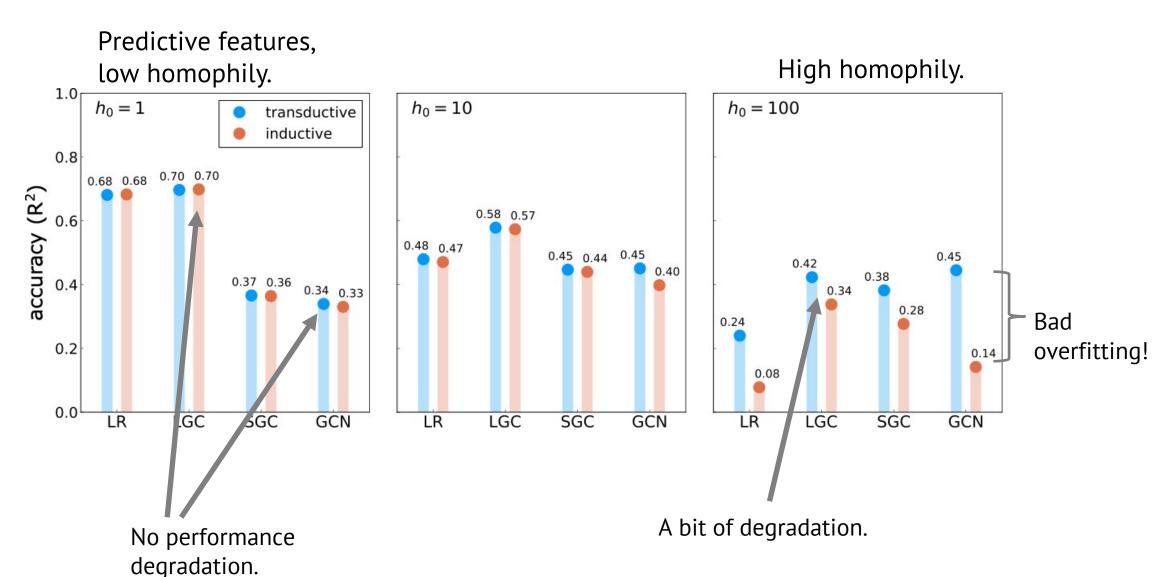
Problem input.

- Graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$.
- $|V_1| \times p$ matrix X_1 and $|V_2| \times p$ matrix X_2 of node features (same features)
- Subset $L_1 \subset V$ of labeled nodes.
- Length- $|L_1|$ vector \mathbf{y}_{L_1} of outcomes on L_1 .

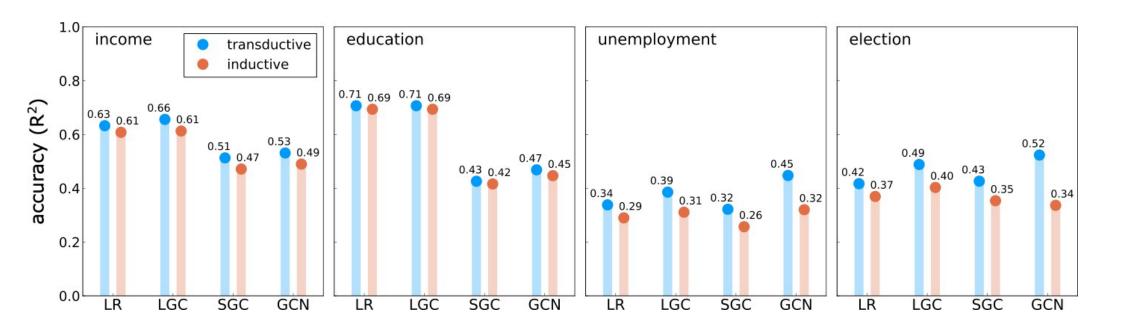
Problem output.

• Length- $|V_2|$ vector **y**of outcomes on nodes V_2 .

Our model provides a nice setup for inductive learning.



Our model provides a nice setup for inductive learning.



- Graph G_1 from 2012 election data.
- Graph G_2 from 2016 election data.

Major takeaway. Label propagation is a powerful tool.

- 1. LP can be applied to residuals (correlated errors).
- 2. LP can be applied to features (smoothing / de-noising).
- 3. While traditionally seen as separate ideas, LP and basic GNN ideas can be derived from a common model and combined effectively.
- 4. LP is scalable and easy to program. Just big SpMVs!
- 5. Linear models are often superior to nonlinear ones (GNNs) in practice... you just need to find the right one.

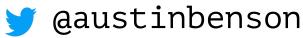
$$\mathbf{y}_{U}^{\mathsf{LGC/RP}} = [(\mathbf{I}_{n} + \omega \mathbf{N})^{-1} \mathbf{X} \boldsymbol{\beta}]_{U} - (\mathbf{I} + \omega \mathbf{N})_{UU}^{-1} (\mathbf{I} + \omega \mathbf{N})_{UL} (\mathbf{y}_{L} - [(\mathbf{I}_{n} + \omega \mathbf{N})^{-1} \mathbf{X} \boldsymbol{\beta}]_{L})$$

There are lots of open research directions.

- 1. Theory or more principled approaches for classification?
- 2. More formal understanding of computational tradeoffs?
- 3. Similar ideas for other graph problems? link prediction, random walk prediction, graph classification, ...
- 4. Generative models to explain other GNN ideas? attention, GraphSAGE, skip connections, ...

Label Propagation and Graph Neural Networks

THANKS! Austin R. Benson
http://cs.cornell.edu/~arb





A Unifying Generative Model for Graph Learning Algorithms: Label Propagation, Graph Convolutions, and Combinations. Junteng Jia and Austin R. Benson. arXiv:2101.07730, 2021.



Residual Correlation in Graph Neural Network Regression. Junteng Jia and Austin R. Benson. Proc. of KDD, 2020.

🙀 julia https://github.com/000Justin000/gnn-residual-correlation

Combining Label Propagation and Simple Models Out-performs Graph Neural Networks. Qian Huang, Horace He, Abhay Singh, Ser-Nam Lim, and Austin R. Benson. Proc. of ICLR, 2021.





https://github.com/CUAI/CorrectAndSmooth







