On the Prediction Instability of Graph Neural Networks

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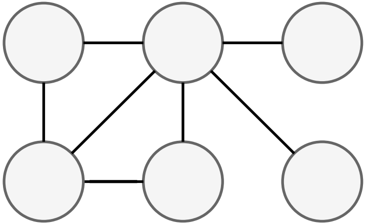
Prediction (in-)stability



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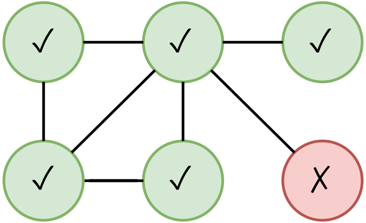

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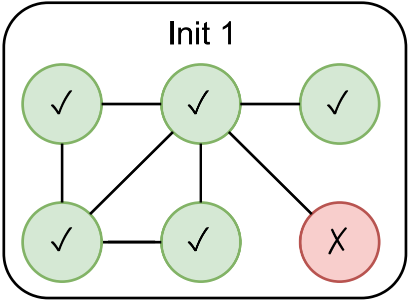

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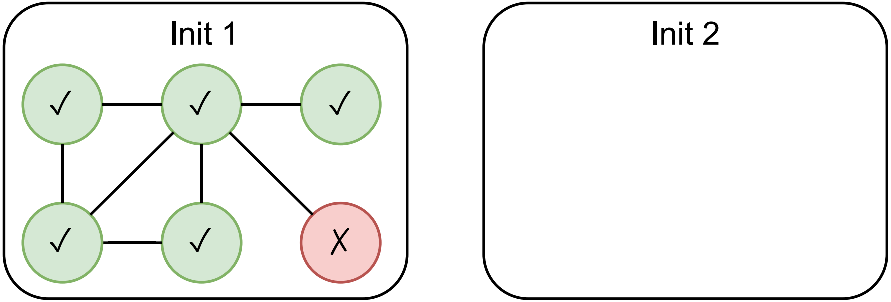

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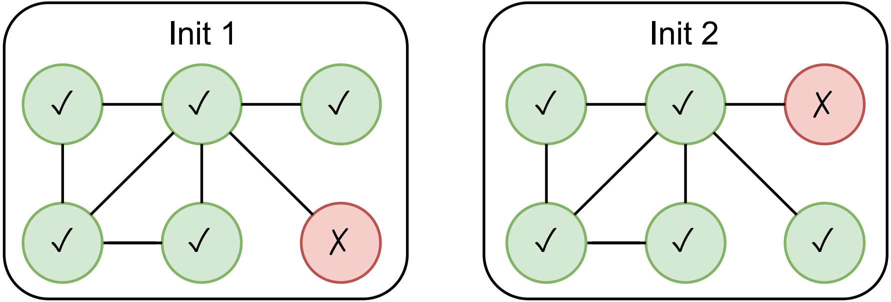

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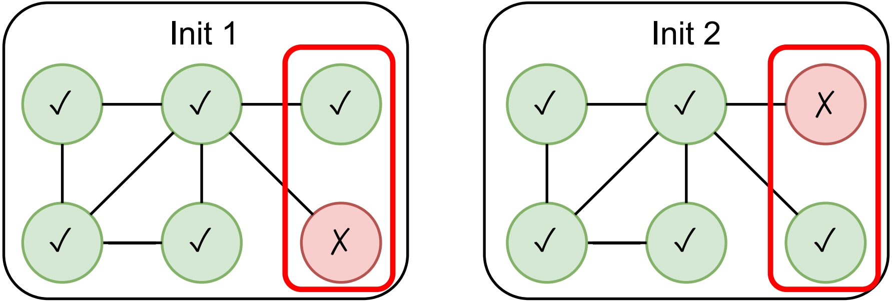

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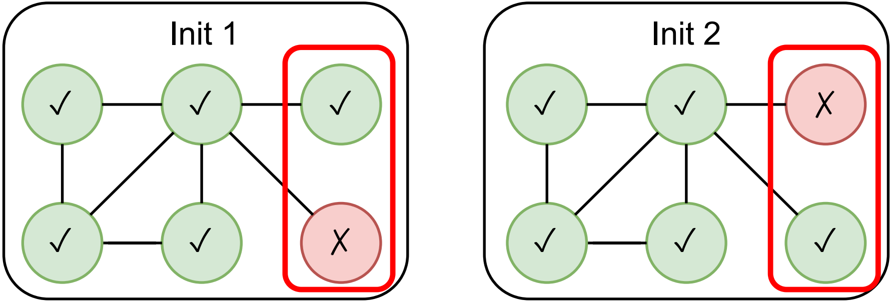
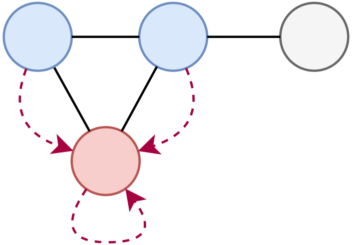


- Individual predictions rely on random factors

Graph Neural Networks (GNNs)



- Focus: Graph Convolutional Networks (GCN)[1] and Graph Attention Networks (GAT)[2]

[1] Kipf and Welling 2017.

[2] Veličković et al. 2018.

Context

- Fully reproducible training may be infeasible[3]
- Previous works mainly focus on large non-graph models[4]
- Work on graph models focused on older unsupervised methods with geometrical perspective[5]

[3] Zhuang et al. 2022.

[4] Summers and Dinneen 2021.

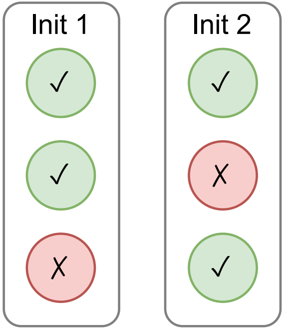
[5] Wang et al. 2022; Schumacher et al. 2021.

Outline

1. Introduction
2. Do GNNs exhibit significant prediction instability?
3. What is the influence of node properties?
4. What is the influence of hyperparameters?
5. Where do instabilities arise?
6. Summary

How to measure prediction instability

- Measure with disagreement: share of predictions that are different between two models



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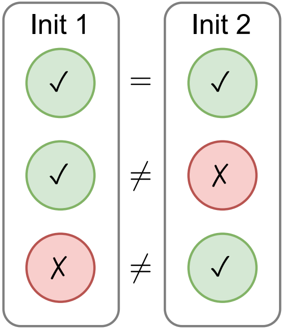

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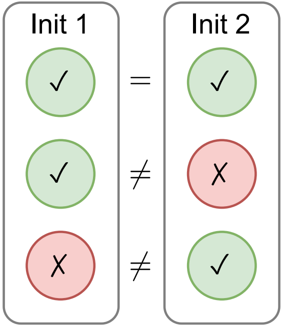
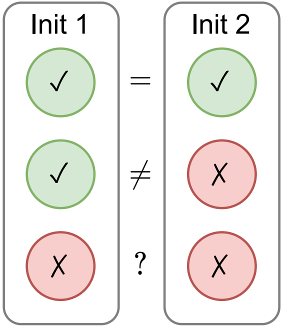


Disagreement $= \frac{2}{3}$

Error rate affects possible disagreement



Disagreement $\geq \frac{1}{3}$

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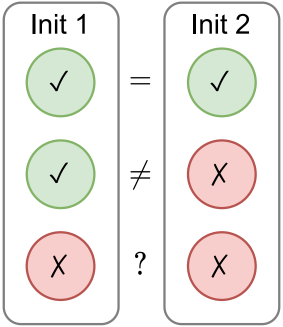

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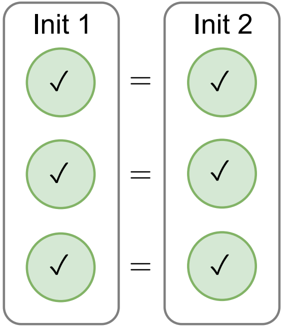
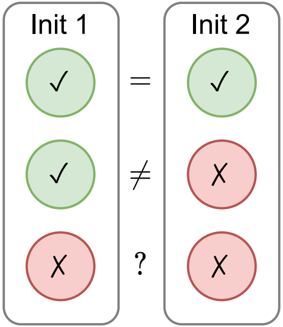


Disagreement $= \frac{0}{3}$

Error rate affects possible disagreement



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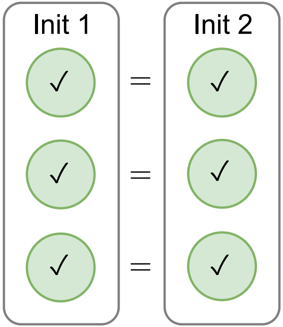

Disagreement $= \frac{0}{3}$

- Normalization possible but similar results

GNN predictions are significantly unstable

- Train 50 different initializations and compare pairwise

Dataset	Model	Accuracy	d	d_{norm}	d_{False}
CiteSeer	GAT				
	GCN				
Pubmed	GAT				
	GCN				
CS	GAT				
	GCN				
Physics	GAT				
	GCN				
Computers	GAT				
	GCN				
Photo	GAT				
	GCN				
WikiCS	GAT				
	GCN				

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Dataset	Model	Accuracy	d	d_{norm}	d_{False}
CiteSeer	GAT	69.0 ± 1.0			
	GCN	69.2 ± 0.7			
Pubmed	GAT	75.7 ± 0.6			
	GCN	76.8 ± 0.5			
CS	GAT	90.7 ± 0.5			
	GCN	90.7 ± 0.5			
Physics	GAT	92.0 ± 0.7			
	GCN	92.7 ± 0.3			
Computers	GAT	81.0 ± 1.5			
	GCN	81.2 ± 0.9			
Photo	GAT	90.3 ± 0.8			
	GCN	90.8 ± 0.5			
WikiCS	GAT	79.6 ± 0.3			
	GCN	79.4 ± 0.2			

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Dataset	Model	Accuracy	d	d_{norm}	d_{False}
CiteSeer	GAT	69.0 ± 1.0	10.5 ± 1.7		
	GCN	69.2 ± 0.7	7.1 ± 1.0		
Pubmed	GAT	75.7 ± 0.6	3.7 ± 1.4		
	GCN	76.8 ± 0.5	2.4 ± 0.7		
CS	GAT	90.7 ± 0.5	3.7 ± 0.5		
	GCN	90.7 ± 0.5	3.3 ± 0.6		
Physics	GAT	92.0 ± 0.7	3.8 ± 0.8		
	GCN	92.7 ± 0.3	1.6 ± 0.4		
Computers	GAT	81.0 ± 1.5	9.5 ± 2.2		
	GCN	81.2 ± 0.9	9.9 ± 1.9		
Photo	GAT	90.3 ± 0.8	4.4 ± 1.1		
	GCN	90.8 ± 0.5	3.7 ± 0.8		
WikiCS	GAT	79.6 ± 0.3	3.8 ± 0.5		
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- Train 50 different initializations and compare pairwise

Dataset	Model	Accuracy	d	d_{norm}	d_{False}
CiteSeer	GAT	69.0 ± 1.0	10.5 ± 1.7	15.4 ± 2.5	
	GCN	69.2 ± 0.7	7.1 ± 1.0	10.3 ± 1.6	
Pubmed	GAT	75.7 ± 0.6	3.7 ± 1.4	6.4 ± 2.7	
	GCN	76.8 ± 0.5	2.4 ± 0.7	4.1 ± 1.4	
CS	GAT	90.7 ± 0.5	3.7 ± 0.5	17.3 ± 2.0	
	GCN	90.7 ± 0.5	3.3 ± 0.6	15.4 ± 2.7	
Physics	GAT	92.0 ± 0.7	3.8 ± 0.8	19.7 ± 4.2	
	GCN	92.7 ± 0.3	1.6 ± 0.4	8.6 ± 2.7	
Computers	GAT	81.0 ± 1.5	9.5 ± 2.2	21.6 ± 5.6	
	GCN	81.2 ± 0.9	9.9 ± 1.9	24.2 ± 4.9	
Photo	GAT	90.3 ± 0.8	4.4 ± 1.1	18.9 ± 4.9	
	GCN	90.8 ± 0.5	3.7 ± 0.8	17.5 ± 3.7	
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- Train 50 different initializations and compare pairwise

Dataset	Model	Accuracy	d	d_{norm}	d_{False}
CiteSeer	GAT	69.0 ± 1.0	10.5 ± 1.7	15.4 ± 2.5	22.3 ± 3.8
	GCN	69.2 ± 0.7	7.1 ± 1.0	10.3 ± 1.6	15.1 ± 2.4
Pubmed	GAT	75.7 ± 0.6	3.7 ± 1.4	6.4 ± 2.7	8.0 ± 3.3
	GCN	76.8 ± 0.5	2.4 ± 0.7	4.1 ± 1.4	5.6 ± 2.2
CS	GAT	90.7 ± 0.5	3.7 ± 0.5	17.3 ± 2.0	22.0 ± 3.6
	GCN	90.7 ± 0.5	3.3 ± 0.6	15.4 ± 2.7	19.9 ± 4.1
Physics	GAT	92.0 ± 0.7	3.8 ± 0.8	19.7 ± 4.2	25.7 ± 6.4
	GCN	92.7 ± 0.3	1.6 ± 0.4	8.6 ± 2.7	12.2 ± 4.3
Computers	GAT	81.0 ± 1.5	9.5 ± 2.2	21.6 ± 5.6	29.6 ± 7.3
	GCN	81.2 ± 0.9	9.9 ± 1.9	24.2 ± 4.9	31.9 ± 6.0
Photo	GAT	90.3 ± 0.8	4.4 ± 1.1	18.9 ± 4.9	26.0 ± 6.9
	GCN	90.8 ± 0.5	3.7 ± 0.8	17.5 ± 3.7	24.1 ± 5.5
WikiCS	GAT	79.6 ± 0.3	3.8 ± 0.5	8.6 ± 1.3	11.7 ± 1.8
	GCN	79.4 ± 0.2	3.3 ± 0.4	7.6 ± 1.0	10.1 ± 1.4

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Photo	GAT	90.3 ± 0.8	4.4 ± 1.1	18.9 ± 4.9	26.0 ± 6.9
	GCN	90.8 ± 0.5	3.7 ± 0.8	17.5 ± 3.7	24.1 ± 5.5
WikiCS	GAT	79.6 ± 0.3	3.8 ± 0.5	8.6 ± 1.3	11.7 ± 1.8
	GCN	79.4 ± 0.2	3.3 ± 0.4	7.6 ± 1.0	10.1 ± 1.4

Outline

Setup

- Centrality, clustering etc. could influence stability
- PageRank, clustering coefficient, k-core, class label

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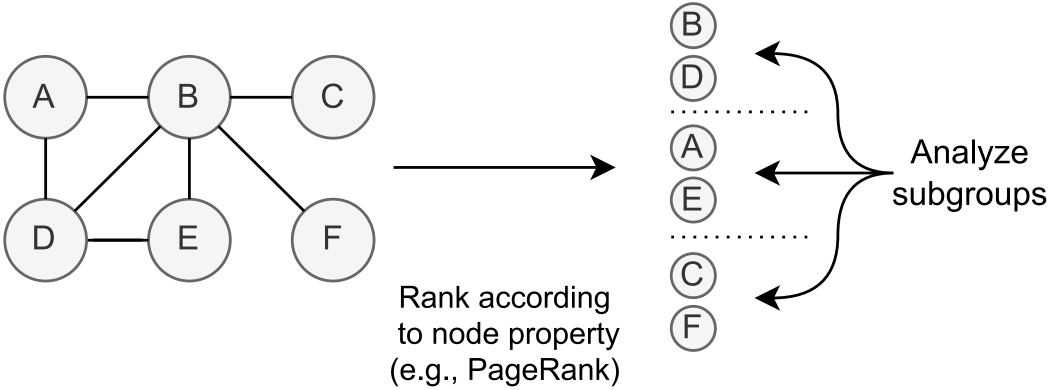
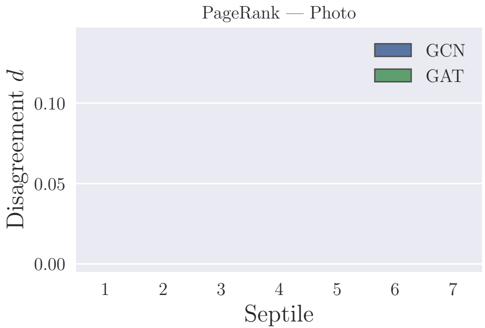


Results: PageRank



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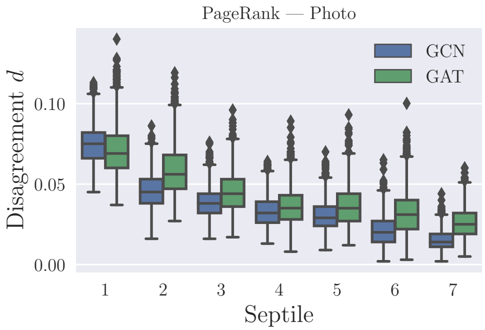
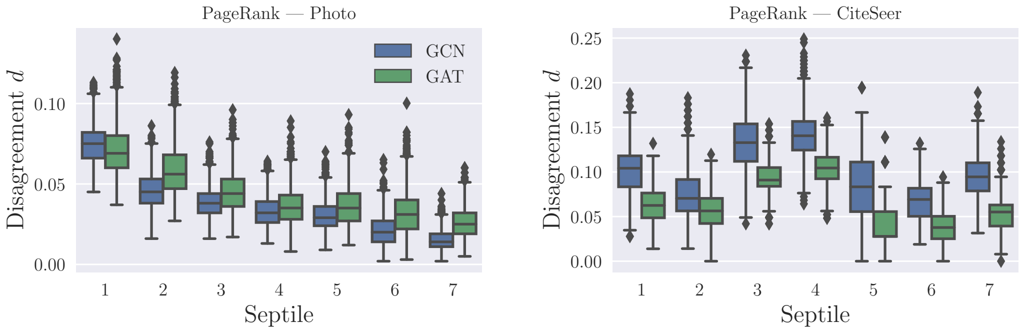


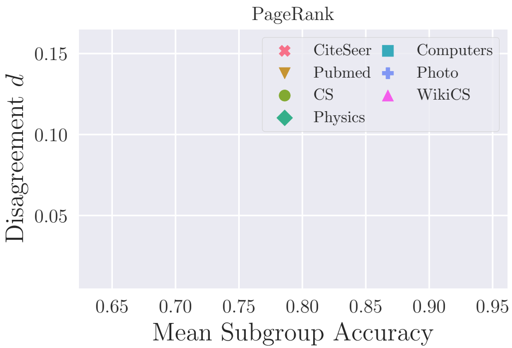
- Central nodes are more stable

Results: PageRank



- Central nodes are more stable
- Less clear effects for other properties

Error Rate and Disagreement are correlated



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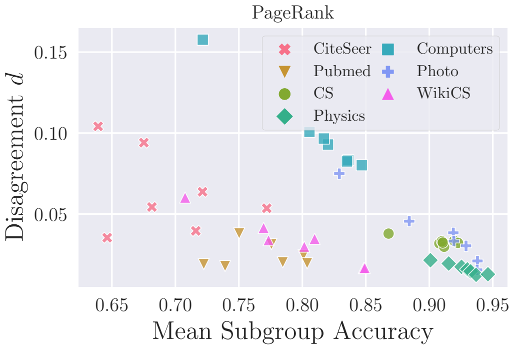
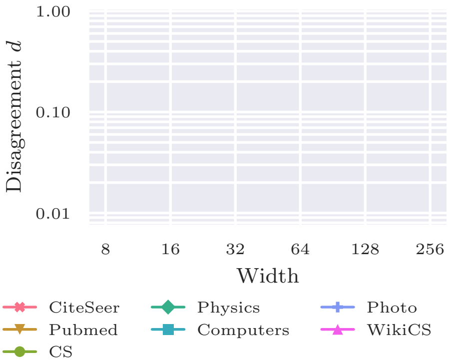


- Central nodes are more stably predicted
- Normalized disagreement explains this effect

Outline

Influence of hyperparameters

- Change configuration of model along one axis, e.g., width



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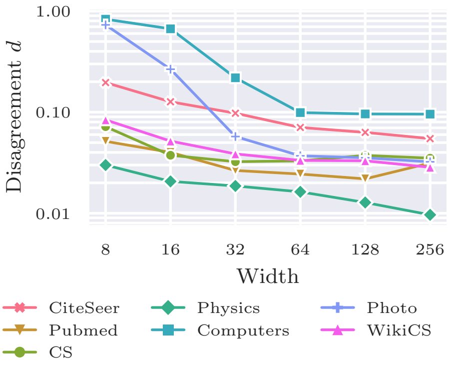

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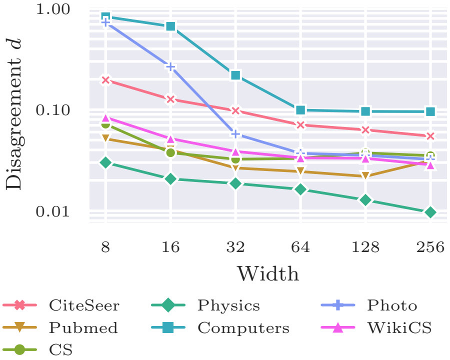

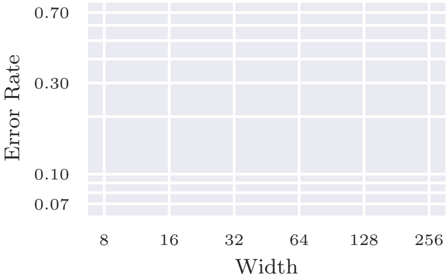

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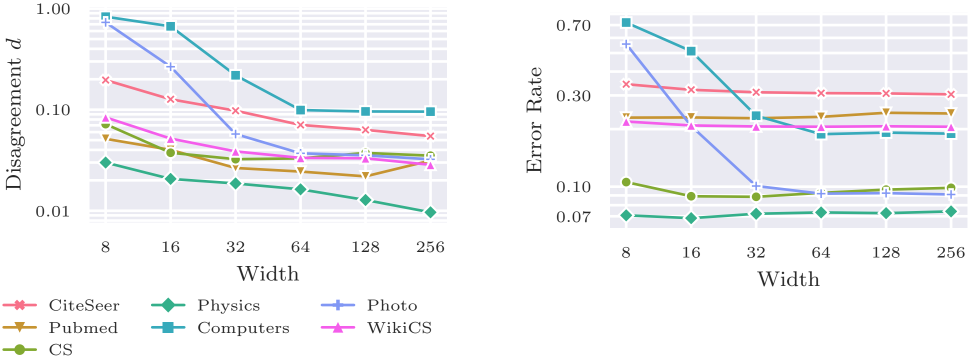

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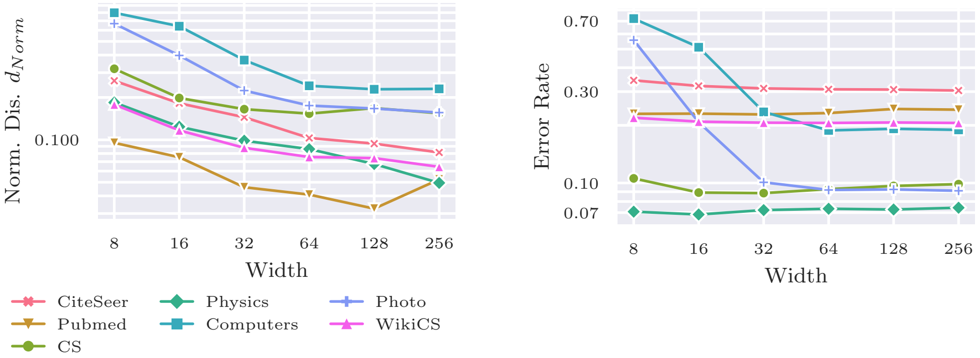
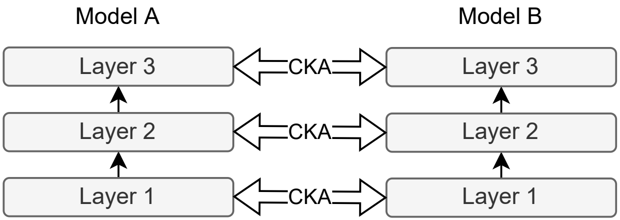


Outline

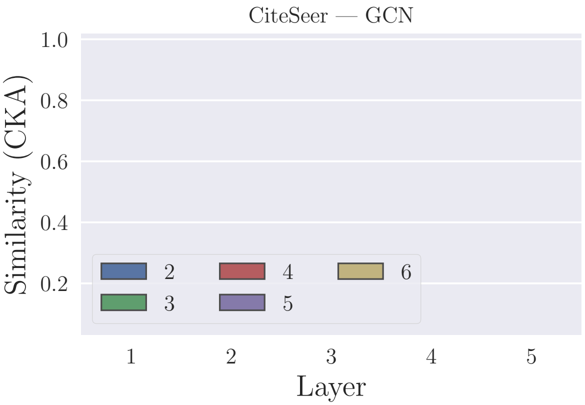
Where do instabilities arise?



- Compare representations of layers over varying depth with Centered Kernel Alignment (CKA)[6]

[6] Kornblith et al. 2019.

Where do instabilities arise?



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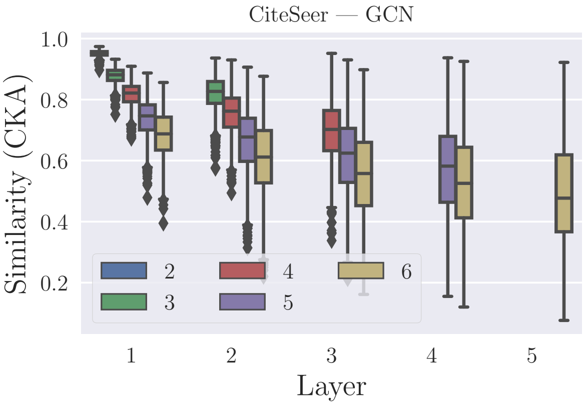

- Deep layers and deep models are less stable

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Summary

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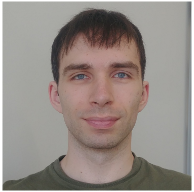
- Deep neural networks are not stable: GCN and GAT are no exception
- Data properties influence stability
- Selecting good hyperparameters can positively influence stability
- Internal representations mirror instability of predictions



Max Klabunde

Florian Lemmerich

Github: mklabunde/gnn-prediction-instability

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