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大规模图机器学习的可扩展性

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CONTENTS

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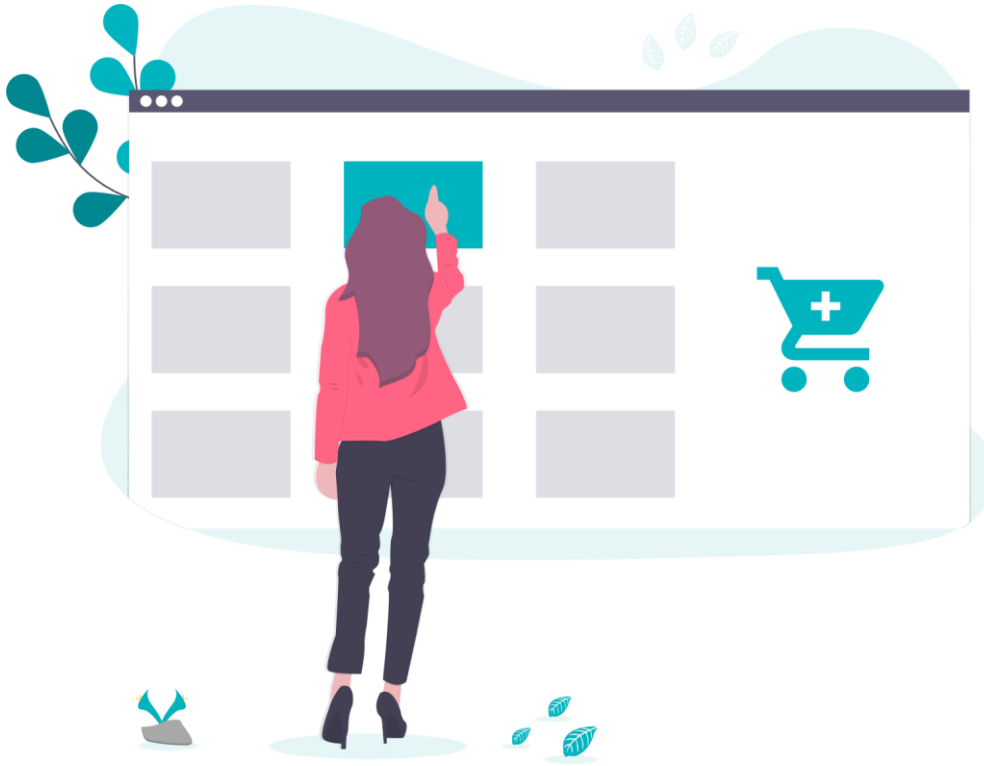
/01

Motivation篇

GNN的应用和局限



Applications of GNN

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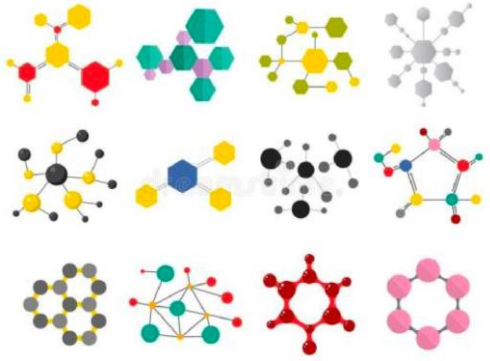
Many real-world data are graphs.

Social Network

Knowledge Graph



Drugs and New materials

- Graph Neural Network (GNN) has achieved great success in many graph-based applications.

- Compared with CNN, GNN has the ability to enhance its feature (or representation in each layer) with the adjacent nodes, and thus improve the model performance.

Low Scalability of GNN

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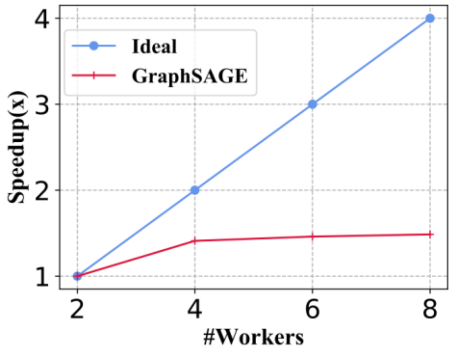
1. High Memory/Time Cost in Single Machine

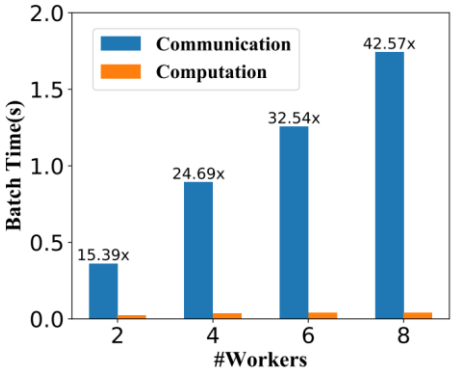
- Hard to load the feature and adjacent matrix due to limited GPU memory.
- The matrix multiplication is time-consuming.

2. High Communication Cost in Distributed Setting

- k-layer GNNs have to pull and aggregate the graph embedding of the k-hop neighbors of nodes in each batch training.
- The speedup is unsatisfactory due to the high communication cost.



Speedup



Bottleneck

Low Flexibility of GNN

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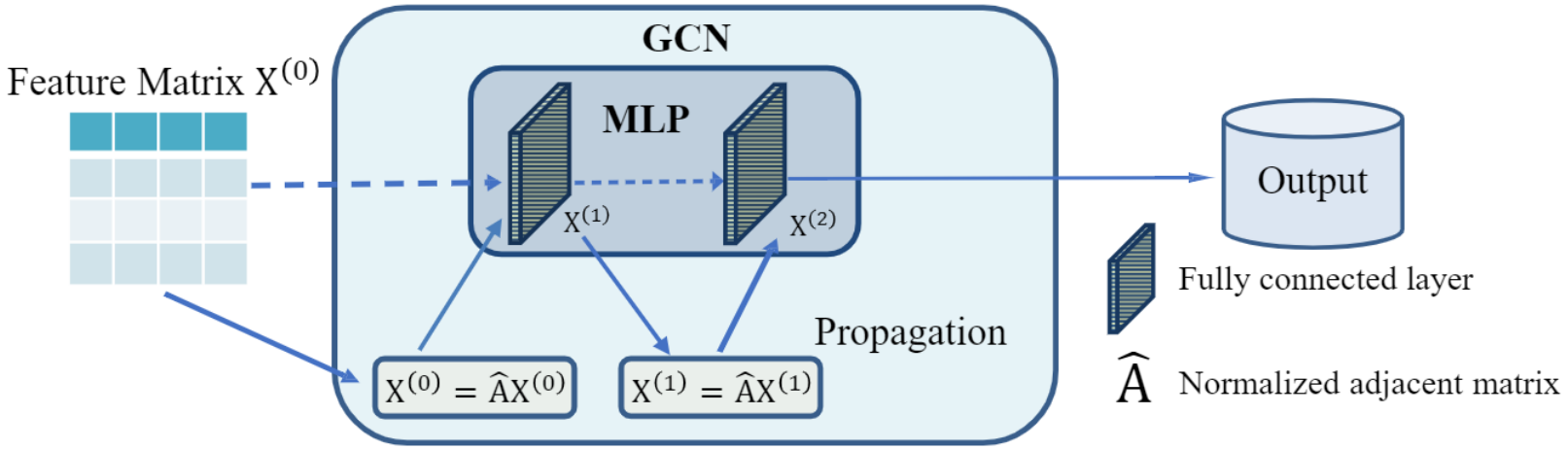
1. Restricting $D_p = D_t$



- GNN has two depth, the propagation depth D_p and transformation depth D_t
- We need large D_p for sparse graph and large D_t for large graph

Low Flexibility of GNN

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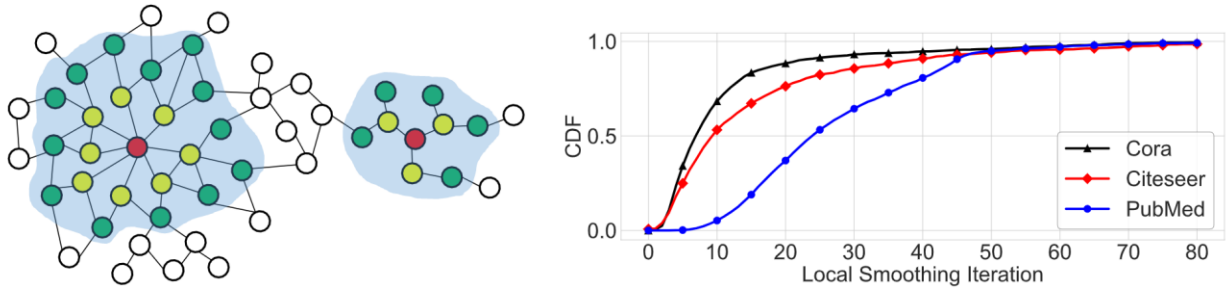
2. Inconsistent smoothing speed



(a) Two nodes with different local structures (b) The CDF of LSI in different graphs

Figure 1: (Left) The local graph structures for two nodes in different regions; the node in dense region has larger smoothed area within two iterations of propagation. (Right) The CDF of LSI in three citation networks.

- Smoothing speed in dense region is extremely faster than the sparse region and noise is introduced if we propagate so many times.
- Different nodes require different propagation steps.

Over-Smoothing issue

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- GNN smooths the representation of each node via aggregating its own representations and the ones of its neighbors.
- Suppose $\widetilde{\mathrm{D}}$ is the diagonal node degree matrix with self loops, and $\widehat{\mathrm{A}} = \widetilde{\mathrm{D}}^{r-1}\widetilde{\mathrm{A}}\widetilde{\mathrm{D}}^{-r}$ is the normalized adjacency matrix. By continually smoothing the node feature with infinite number of propagation in SGC, the final smoothed feature is

$$\mathrm{X}^{(\infty)} = \widehat{\mathrm{A}}^{\infty}\mathrm{X}, \qquad \widehat{\mathrm{A}}^{\infty}_{i,j} = \frac{(d_i+1)^r\left(d_j+1\right)^{1-r}}{2m+n}$$

The final feature is over-smoothed and unable to capture the full graph structure information since it only relates with the node degrees of target nodes and source nodes.

An example of over-smoothing

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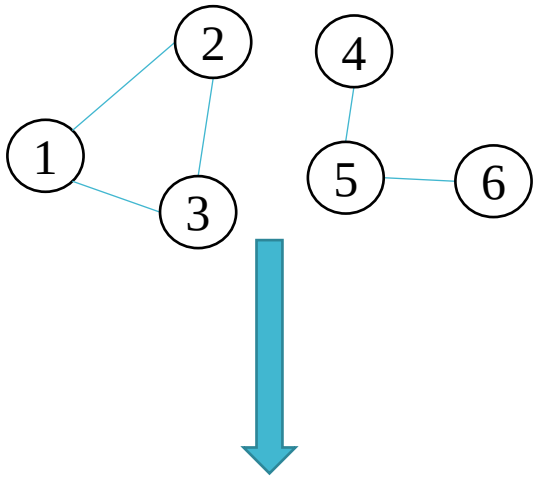
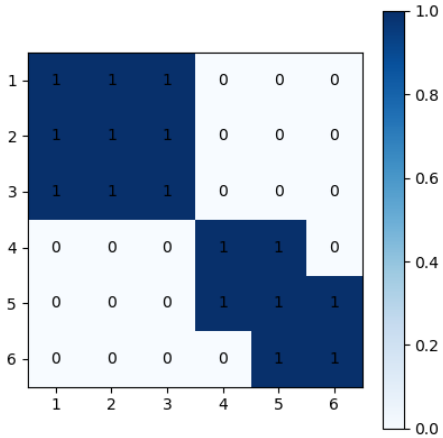


$$\lim_{k\to\infty}(\tilde{\mathbf{D}}^{-1}\tilde{\mathbf{A}})^k_{i,j} = \frac{d_j+1}{2m+n}$$

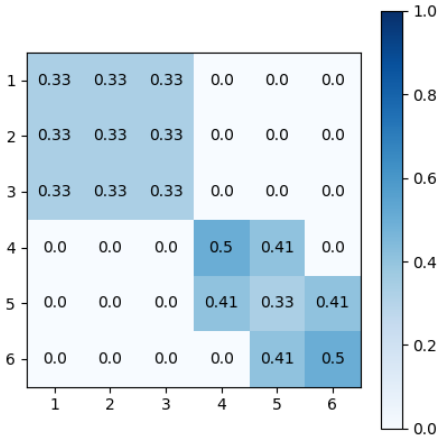
$$\lim_{k\to\infty}(\tilde{\mathbf{A}}\tilde{\mathbf{D}}^{-1})^k_{i,j} = \frac{d_i+1}{2m+n}$$

$$\lim_{k\to\infty}(\tilde{\mathbf{D}}^{-1/2}\tilde{\mathbf{A}}\tilde{\mathbf{D}}^{-1/2})^k_{i,j} = \frac{\sqrt{(d_i+1)(d_j+1)}}{2m+n}$$

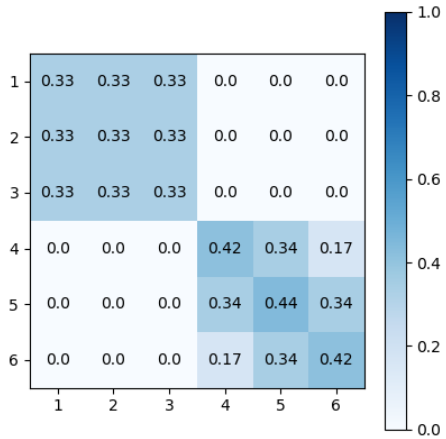
where $n = |V|$, $m = |E|$ *and* $d_i = \sum_j \mathbf{A}_{ij}$.



A

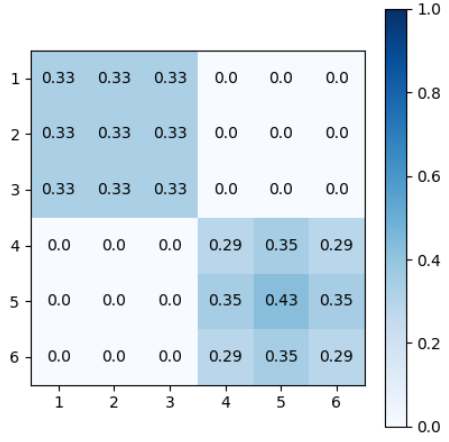


$\left(\widetilde{D}^{-1/2}A\widetilde{D}^{-1/2}\right)^1$



$\left(\widetilde{D}^{-1/2}A\widetilde{D}^{-1/2}\right)^2$

...



$\left(\widetilde{D}^{-1/2}A\widetilde{D}^{-1/2}\right)^{26}$

limitations

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1. Over-smoothing

- Deep GNN faces the over-smoothing problem that the node representation is less discriminative.

2. Under-smoothing

- Each node in a k-layer GNN can only capture the node attribute and node dependency information in its k-hop neighbors. For sparse graphs, lots of valuable information in unlabeled nodes is ignored when we use shallow architecture.

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/02 Related Works篇

Scalable GNNs

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1. Sampling

- Graph-wise sampling: Cluster-GCN, GraphSAINT
- Layer-wise sampling: Fast-GCN, AS-GCN
- Node-wise sampling: GraphSAGE, VR-GCN

2. Model decoupling

- SGC
- SIGN
- GBP
- S2GC

Our method focuses on the second type since it is more efficient and scalable.

SGC(ICML 19)

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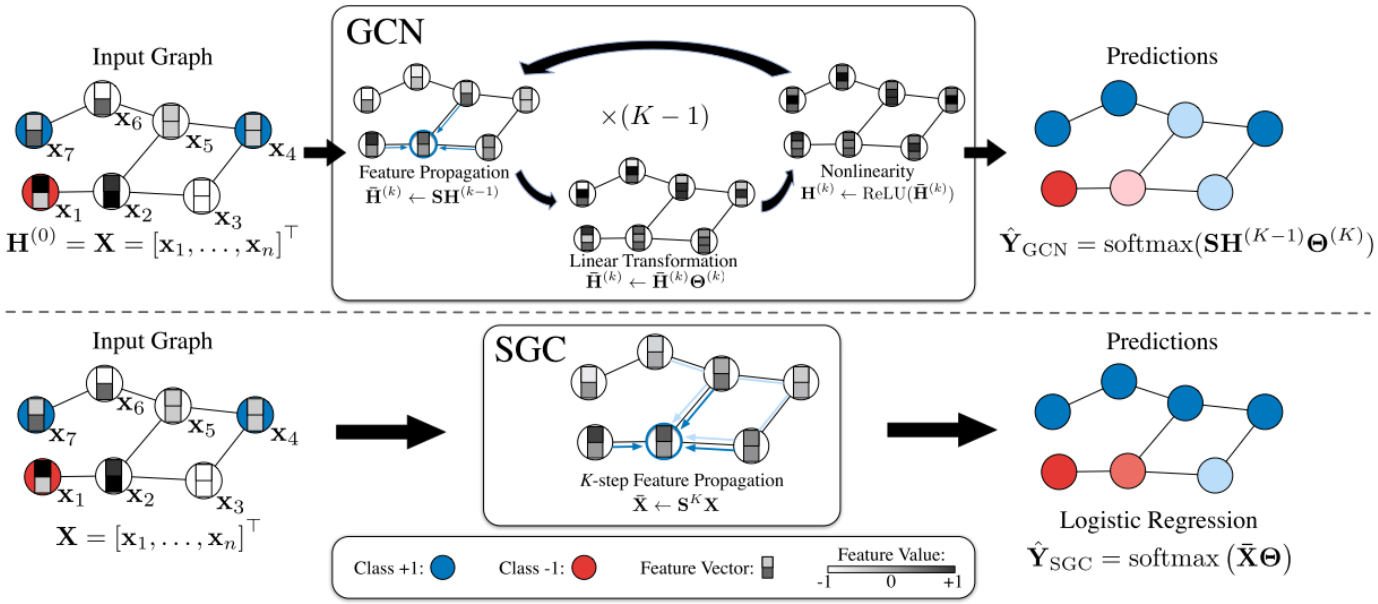

Figure 1. Schematic layout of a GCN v.s. a SGC. *Top row:* The GCN transforms the feature vectors repeatedly throughout K layers and then applies a linear classifier on the final representation. *Bottom row:* the SGC reduces the entire procedure to a simple feature propagation step followed by standard logistic regression.

- SGC firstly propagates the feature to high order and then keeping a small number of transformation.
- It faces over-smoothing issue when the propagation step is large.

SIGN

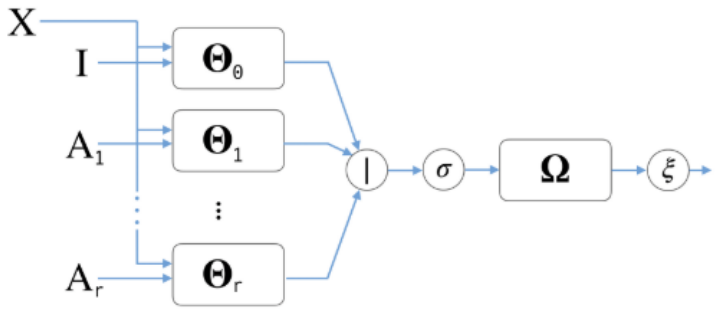

Figure 1: The *SIGN* architecture for r generic graph filtering operators. $\mathbf{\Theta}_k$ represents the k-th dense layer transforming node-wise features downstream the application of operator k, $|$ is the concatenation operation and $\mathbf{\Omega}$ refers to the dense layer used to compute final predictions.

SIGN further improve SGC by adding more diffusion operators, such as PageRank-based and triangle-based adjacency matrices.

- No flexibility: some node needs less receptive field while other nodes need more. SIGN simply concatenate the global and local representation, ignoring the personalization of each node.

DAGNN(KDD 20)

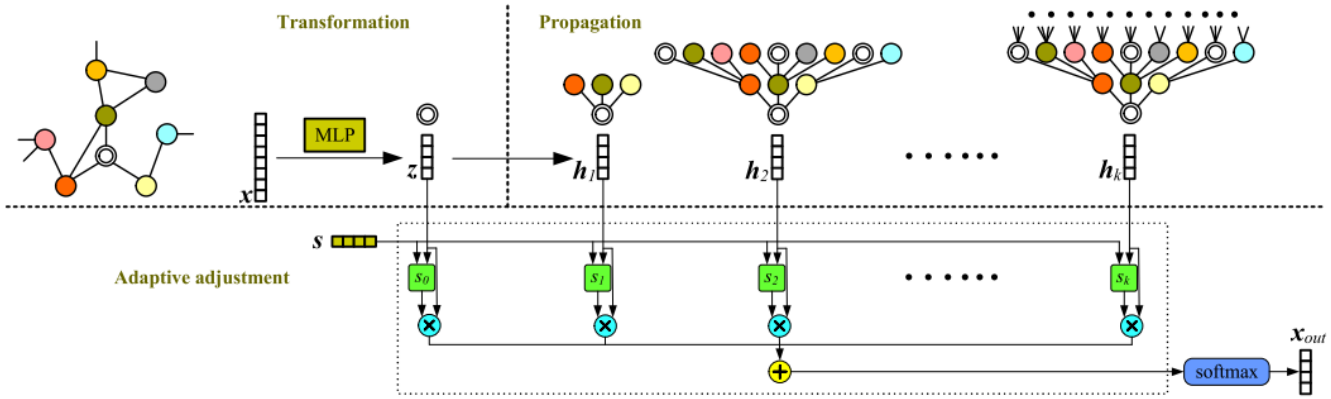

Figure 5: An illustration of the proposed Deep Adaptive Graph Neural Network (DAGNN) . For clarity, we show the pipeline to generate the prediction for one node. Notation letters are consistent with Eq.(8) but bold lowercase versions are applied to denote representation vectors. s is the projection vector that computes retainment scores for representations generating from various receptive fields. s_0, s_1, s_2, and s_k represent the retainment scores of z, h_1, h_2, and h_k, respectively.

It can be seen as a type of label propagation since it just weighted ensemble the outputs of each propagated MLP predictions.

- The MLP prediction and the label propagation can not be decoupled and DAGNN is trained in an end-to-end manner. Correspondingly, the scalability is limited.
- One global vector is adopted to train the weight of different propagated label, such process may be hard to train.

/03 Method篇

NDLS(NeurIPS 2021, Spotlight)

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Problem: how to control the smoothness in a node dependent way ?

Definition Local-Smoothing Iteration(LSI, parameterized by ϵ) is defined as

$$K(i,\epsilon) = \min\left\{k: \left\|\tilde{I}_i - I(k)_i\right\|_2 < \epsilon\right\},$$

Where ϵ is an arbitrary small constant with $\epsilon > 0$,

$$I(k)_{i,j} = \frac{\partial \widehat{\mathrm{X}}_{ih}^{(k)}}{\partial \widehat{\mathrm{X}}_{jh}^{(0)}}, \forall h \in \{1,2,\cdots,f\}, \text{and } \tilde{I} = I(\infty).$$

Node Dependent Local Smoothing

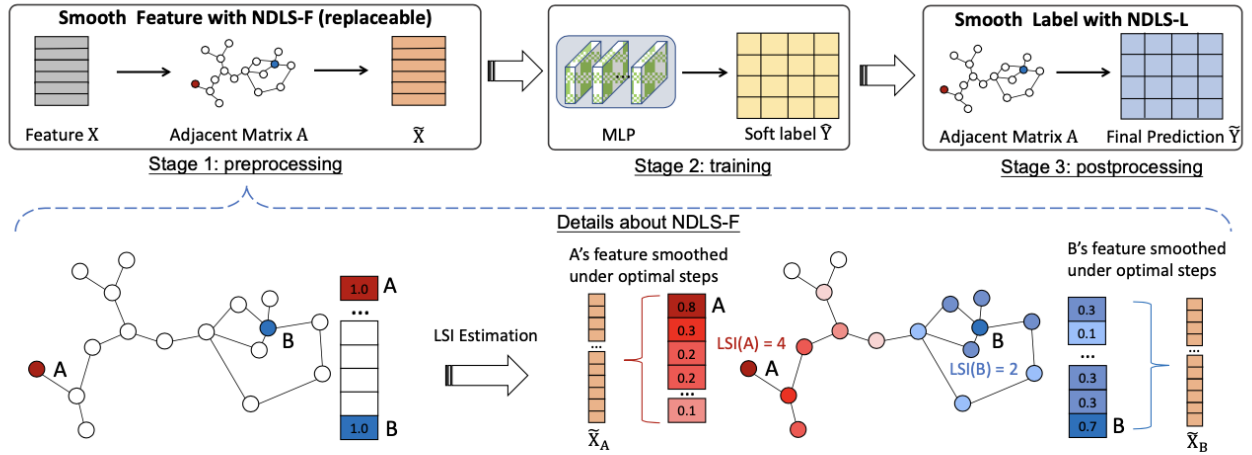

Figure 2: Overview of the proposed NDLS method, containing 1) feature smoothing with NDLS (NDLS-F); 2) model training with smoothed features; 3) label smoothing with NDLS (NDLS-L). NDLS-F and NDLS-L are pre-processing and post-processing steps, respectively.

Node Dependent Propagation → P(NDLS-F)-T-P(NDLS-L) ← Node Dependent Propagation

All ML models (MLP, LR, XGB, ect.) can be applied

Method

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Vector Form

$$\widetilde{\mathbf{X}}_i(\epsilon) = \frac{1}{K(i,\epsilon)+1} \sum_{k=0}^{K(i,\epsilon)} \mathbf{X}_i^{(k)}.$$

NDLS-F

$$\widetilde{\mathbf{Y}}_i(\epsilon) = \frac{1}{K(i,\epsilon)+1} \sum_{k=0}^{K(i,\epsilon)} \hat{\mathbf{Y}}_i^{(k)}.$$

NDLS-L

Matrix Form

$$\widetilde{\mathbf{X}}(\epsilon) = \sum_{k=0}^{\max_i K(i,\epsilon)} \mathbf{M}^{(k)}\mathbf{X}^{(k)}, \qquad \mathbf{M^{(k)}}_{ij} = \begin{cases} \frac{1}{K(i,\epsilon)+1}, & i=j \quad and \quad k \le K(i,\epsilon) \\ 0, & \text{otherwise} \end{cases}$$

T

$$\widetilde{\mathbf{Y}}(\epsilon) = \sum_{k=0}^{\max_i K(i,\epsilon)} \mathbf{M}^{(k)}\hat{\mathbf{Y}}^{(k)},$$

Table 1: Algorithm analysis for existing scalable GNNs. n, m, c, and f are the number of nodes, edges, classes, and feature dimensions, respectively. b is the batch size, and k refers to the number of sampled nodes. L corresponds to the number of times we aggregate features, K is the number of layers in MLP classifiers. For the coupled GNNs, we always have $K = L$.

Type	Method	Preprocessing and postprocessing	Training	Inference	Memory
Node-wise sampling	GraphSAGE	-	$\mathcal{O}(k^L nf^2)$	$\mathcal{O}(k^L nf^2)$	$\mathcal{O}(bk^L f + Lf^2)$
Layer-wise sampling	FastGCN	-	$\mathcal{O}(kLnf^2)$	$\mathcal{O}(kLnf^2)$	$\mathcal{O}(bkLf + Lf^2)$
Graph-wise sampling	Cluster-GCN	$\mathcal{O}(m)$	$\mathcal{O}(Lmf + Lnf^2)$	$\mathcal{O}(Lmf + Lnf^2)$	$\mathcal{O}(bLf + Lf^2)$
Linear model	SGC	$\mathcal{O}(Lmf)$	$\mathcal{O}(nf^2)$	$\mathcal{O}(nf^2)$	$\mathcal{O}(bf + f^2)$
	S^2GC	$\mathcal{O}(Lmf)$	$\mathcal{O}(nf^2)$	$\mathcal{O}(nf^2)$	$\mathcal{O}(bf + f^2)$
	SIGN	$\mathcal{O}(Lmf)$	$\mathcal{O}(Knf^2)$	$\mathcal{O}(Knf^2)$	$\mathcal{O}(bLf + Kf^2)$
	GBP	$\mathcal{O}(Lnf + L\frac{\sqrt{m \lg n}}{\varepsilon})$	$\mathcal{O}(Knf^2)$	$\mathcal{O}(Knf^2)$	$\mathcal{O}(bf + Kf^2)$
Linear model	NDLS	$\mathcal{O}(Lmf + Lmc)$	$\mathcal{O}(Knf^2)$	$\mathcal{O}(Knf^2)$	$\mathcal{O}(bf + Kf^2)$

NDLS has a smaller or competitive training and inference complexity comparing with other scalable GNNs.

What influences LSIs?

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Theorem 3.1. *Given feature smoothing* $\mathbf{X}^{(k)} = \hat{\mathbf{A}}^k\mathbf{X}$ *with* $\hat{\mathbf{A}} = \tilde{\mathbf{D}}^{-1}\tilde{\mathbf{A}}$, *we have*

$$K(i,\epsilon) \leq \log_{\lambda_2}\left(\epsilon\sqrt{\frac{\tilde{d}_i}{2m+n}}\right),$$

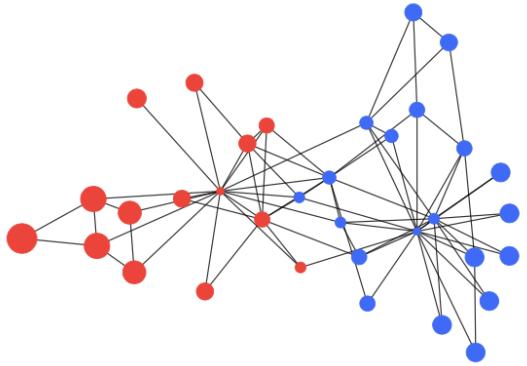
where λ_2 *is the second largest eigenvalue of* $\hat{\mathbf{A}}$, $\tilde{d}_i$ *denotes the degree of node* v_i *plus 1 (i.e.,* $\tilde{d}_i = d_i + 1$*), and* m, n *denote the number of edges and nodes respectively.*

Positively related with

- The scale of graph(m, n)
- The sparsity of graph (λ_2)

Negatively related with

- The node degree (d_i)



(b) The visualization of LSI

- Adjacent nodes have similar LSIs
- Nodes with a super-node as neighbors (or neighbor's neighbors) may have small LSIs

Theorem 3.2. *For any nodes* i *in a graph* $\mathcal{G}$,

$$K(i,\epsilon) \leq \max\{K(j,\epsilon), j \in N(i)\} + 1,$$

where $N(i)$ *is the set of node* v_i*'s neighbours.*

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/04 Experiment篇

Setups

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➢ Datasets

Table 2: Overview of datasets and task types (T/I represents Transductive/Inductive).

Dataset	#Nodes	#Features	#Edges	#Classes	#Train/Val/Test	Type	Description
Cora	2,708	1,433	5,429	7	140/500/1,000	T	citation network
Citeseer	3,327	3,703	4,732	6	120/500/1,000	T	citation network
Pubmed	19,717	500	44,338	3	60/500/1,000	T	citation network
Industry	1,000,000	64	1,434,382	253	5K/10K/30K	T	short-form video network
ogbn-papers100M	111,059,956	128	1,615,685,872	172	1,207K/125K/214K	T	citation network
Flickr	89,250	500	899,756	7	44K/22K/22K	I	image network
Reddit	232,965	602	11,606,919	41	155K/23K/54K	I	social network

➢ Baselines

1. **Decoupled GNNs:** APPNP, AP-GCN, PPRGo, DAGNN
2. **Coupled GNNs**: GCN, GAT, JK-Net
3. **Linear Models**: MLP, SGC, SIGN, S2GC, GBP

https://github.com/zwt233/NDLS

Accuracy and Efficiency Comparison

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Table 3: Results of transductive settings. OOM means "out of memory".

Type	Models	Cora	Citeseer	PubMed	Industry	ogbn-papers100M
Coupled	GCN	81.8±0.5	70.8±0.5	79.3±0.7	45.9±0.4	OOM
	GAT	83.0±0.7	72.5±0.7	79.0±0.3	46.8±0.7	OOM
	JK-Net	81.8±0.5	70.7±0.7	78.8±0.7	47.2±0.3	OOM
Decoupled	APPNP	83.3±0.5	71.8±0.5	80.1±0.2	46.7±0.6	OOM
	AP-GCN	83.4±0.3	71.3±0.5	79.7±0.3	46.9±0.7	OOM
	PPRGo	82.4±0.2	71.3±0.5	80.0±0.4	46.6±0.5	OOM
	DAGNN (Gate)	84.4±0.5	73.3±0.6	80.5±0.5	47.1±0.6	OOM
	DAGNN (NDLS-L)*	84.4±0.6	73.6±0.7	80.9±0.5	47.2±0.7	OOM
Linear	MLP	61.1±0.6	61.8±0.8	72.7±0.6	41.3±0.8	47.2±0.3
	SGC	81.0±0.2	71.3±0.5	78.9±0.5	45.2±0.3	63.2±0.2
	SIGN	82.1±0.3	72.4±0.8	79.5±0.5	46.3±0.5	64.2±0.2
	S^2GC	82.7±0.3	73.0±0.2	79.9±0.3	46.6±0.6	64.7±0.3
	GBP	83.9±0.7	72.9±0.5	80.6±0.4	46.9±0.7	65.2±0.3
Linear	NDLS-F+MLP*	84.1±0.6	73.5±0.5	81.1±0.6	47.5±0.7	65.3±0.5
	MLP+NDLS-L*	83.9±0.6	73.1±0.8	81.1±0.6	46.9±0.7	64.6±0.4
	SGC+NDLS-L*	84.2±0.2	73.4±0.5	81.1±0.4	47.1±0.6	64.9±0.3
	NDLS*	**84.6±0.5**	**73.7±0.6**	**81.4±0.4**	**47.7±0.5**	**65.6±0.3**

Models	Flickr	Reddit
GraphSAGE	50.1±1.3	95.4±0.0
FastGCN	50.4±0.1	93.7±0.0
ClusterGCN	48.1±0.5	95.7±0.0
GraphSAINT	51.1±0.1	96.6±0.1
NDLS-F+MLP*	51.9±0.2	96.6±0.1
GraphSAGE+NDLS-L*	51.5±0.4	96.3±0.0
NDLS*	**52.6±0.4**	**96.8±0.1**

Table 4: Results of inductive settings.

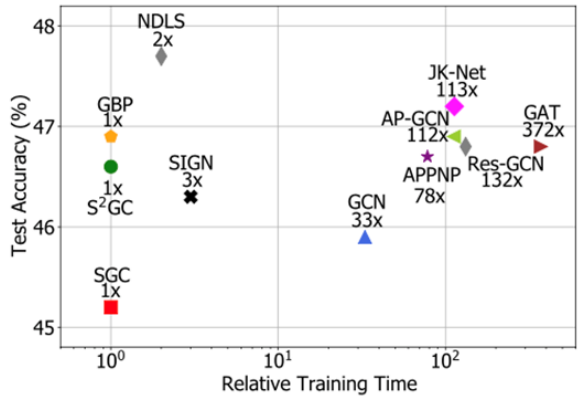
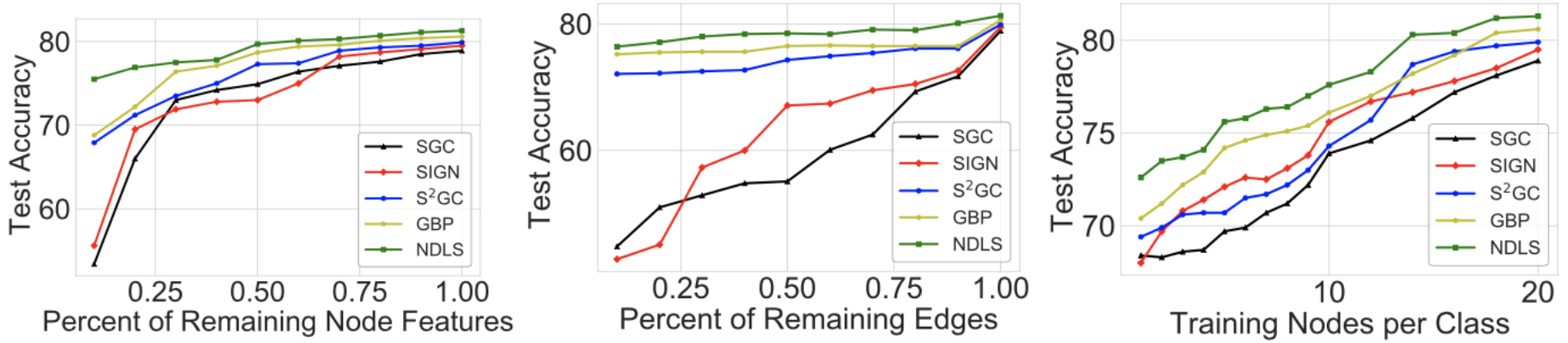


Figure 3: Performance along with training time on the Industry dataset.

- MLP with FS or LS achieve competitive performance.
- LS can be cooperated and improve the current model, such as SGC and DAGNN.
- Both FS and LS contributes to the performance.
- NDLS can get the best tradeoff between training time and test accuracy.

Other Experiments



(a) Feature Sparsity (b) Edge Sparsity (c) Label Sparsity

Figure 4: Test accuracy on PubMed dataset under different levels of feature, edge and label sparsity.

NDLS performs well and robustly on sparse graphs.

Table 1: Results of different base models on PubMed.

Base Models	Models	Accuracy	Gain
MLP	Base	72.7±0.6	-
	+ NDLS-F	81.1±0.6	+ 8.4
	+ NDLS-L	81.1±0.6	+ 8.4
	+ NDLS (both)	**81.4±0.4**	+ 8.7
RF	Base	74.4±0.2	-
	+ NDLS-F	80.3±0.1	+ 5.9
	+ NDLS-L	80.0±0.2	+ 5.6
	+ NDLS (both)	**80.5±0.4**	+ 6.1
XGB	Base	74.1±0.2	-
	+ NDLS-F	81.0±0.3	+ 6.9
	+ NDLS-L	79.8±0.2	+ 5.7
	+ NDLS (both)	**81.6±0.3**	+ 7.5

NDLS works with tree based models.

Interpretability

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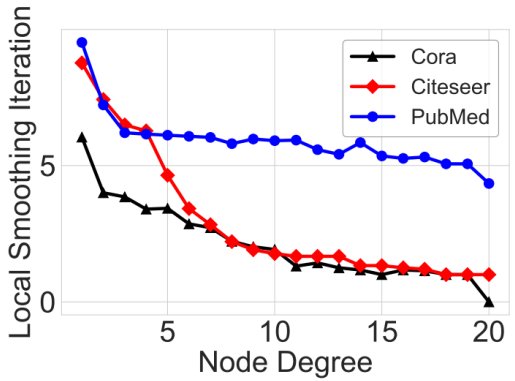
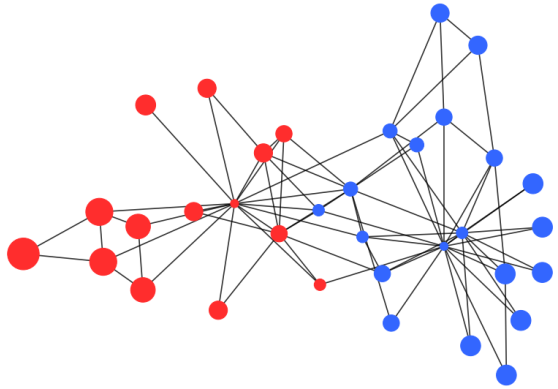


(a) LSI along with the node degree



(b) The visualization of LSI

Figure 5: (Left) LSI distribution along with the node degree in three citation networks. (Right) The visualization of LSI in Zachary's karate club network. Nodes with larger radius have larger LSIs.

Theorem 3.1. *Given feature smoothing* $\mathbf{X}^{(k)} = \hat{\mathbf{A}}^k\mathbf{X}$ *with* $\hat{\mathbf{A}} = \tilde{\mathbf{D}}^{-1}\tilde{\mathbf{A}}$*, we have*

$$K(i,\epsilon) \leq \log_{\lambda_2}\left(\epsilon\sqrt{\frac{\tilde{d}_i}{2m+n}}\right), \tag{5}$$

where λ_2 *is the second largest eigenvalue of* $\hat{\mathbf{A}}$*,* $\tilde{d}_i$ *denotes the degree of node* v_i *plus 1 (i.e.,* $\tilde{d}_i = d_i + 1$*), and* m*,* n *denote the number of edges and nodes respectively.*

Theorem 3.2. *For any nodes* i *in a graph* $\mathcal{G}$*,*

$$K(i,\epsilon) \leq \max\{K(j,\epsilon), j \in N(i)\} + 1, \tag{6}$$

where $N(i)$ *is the set of node* v_i*'s neighbours.*

- Nodes with a higher degree have a smaller LSI (**Theorem 3.1**)
- Adjacent nodes have similar LSIs (**Theorem 3.2**)
- Nodes with a super-node as neighbors (or neighbor's neighbors) may have small LSIs (**Theorem 3.2**)

Implementation

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Table 6: URLs of baseline codes.

Type	Baselines	URLs
Coupled	GCN	https://github.com/rusty1s/pytorch_geometric
	GAT	https://github.com/rusty1s/pytorch_geometric
Decoupled	APPNP	https://github.com/rusty1s/pytorch_geometric
	PPRGo	https://github.com/TUM-DAML/pprgo_pytorch
	AP-GCN	https://github.com/spindro/AP-GCN
	DAGNN	https://github.com/divelab/DeeperGNN
Sampling	GraphSAGE	https://github.com/williamleif/GraphSAGE
	GraphSAINT	https://github.com/GraphSAINT/GraphSAINT
	FastGCN	https://github.com/matenure/FastGCN
	Cluster-GCN	https://github.com/benedekrozemberczki/ClusterGCN
Linear	SGC	https://github.com/Tiiiger/SGC
	SIGN	https://github.com/twitter-research/sign
	S^2GC	https://github.com/allenhaozhu/SSGC
	GBP	https://github.com/chennnM/GBP
	NDLS	https://github.com/zwt233/NDLS

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/05 Conclusion篇

Conclusion

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Advantages

1. Deep

- NDLS is able to go very deep without the over-smoothing issue

2. Scalable

- MLP (or tree-based model) is easy for distributed learning (no feature pulling communication)

3. Efficient

- MLP (or tree-based model) is simple and acquires less computation cost compared with GNNs

4. Flexible

- NDLS can be applied to any ML models

Applications

1. Sparse Graph

- NDLS can help to propagate the graph information of sparse graph by increasing the propagation steps.

2. Large Graph

- NDLS is scalable in distributed settings for extremely large graph in industrial production environment.

PKU-DAIR实验室

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北京大学数据与智能实验室(Data and Intelligence Research Lab at Peking University)：
实验室由北京大学计算机系长江学者特聘教授崔斌老师带领，多年来主要在人工智能、大数据等领域进行前沿研究，在理论和技术创新以及系统研发上取得多项成果，已在国际顶级学术会议和期刊发表学术论文100余篇。

开源项目：实验室围绕机器学习系统已经展开了多方面的研究工作，包括机器学习/深度学习系统优化、 AutoML、图机器学习、AI4DB等，发布了多个开源项目：

黑盒优化系统OpenBox
https://github.com/PKU-DAIR/open-box

OpenBox

自动化机器学习系统MindWare
https://github.com/PKU-DAIR/mindware

MindWare
TOOLS FOR DATA INTELLIGENCE

分布式深度学习系统河图（Hetu）
https://github.com/PKU-DAIR/hetu

Hetu 河图

分布式机器学习平台Angel
https://github.com/Angel-ML

Angel

欢迎感兴趣的同学联系实习或交流问题！

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企业合作:
2017年，课题组与腾讯公司成立北京大学-腾讯协同创新实验室，深度合作并开源了分布式机器学习平台Angel。另外，实验室还与阿里巴巴、苹果、百度、快手、中兴通讯等多家知名企业开展项目合作和前沿探索，解决实际问题，进行科研成果的转化落地。

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Thanks