ICML 2022

NAFS: A Simple yet Tough-to-beat Baseline for Graph Representation

Presented by

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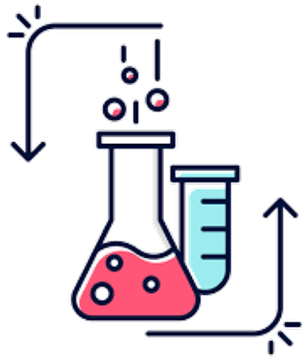
Outline

1. Motivation

2. Method



3. Experiment

4. Conclusion

Outline

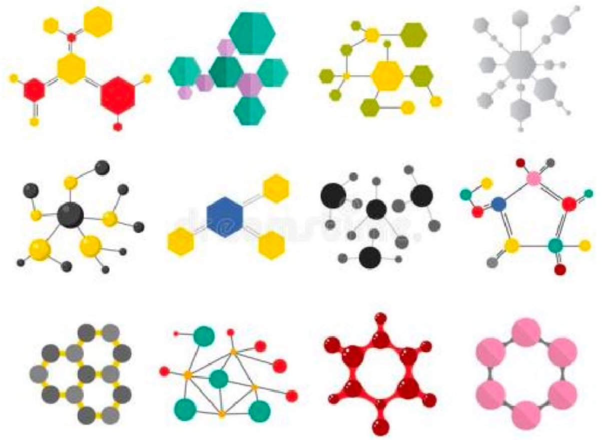
Motivation

Graph Representation Learning

Graph representation learning has been extensively applied in various application scenarios.

Social Network

Knowledge Graph



Drugs and New materials

- ➢ Traditional methods: Deep-Walk, Node2vec, LINE, etc.
  - Only graph structure can be used
- ➢ Graph Neural Network-based methods: GAE, VGAE, etc.
  - Both graph structure and node feature can be used
  - SOTA performance

Feature Smoothing in GNN

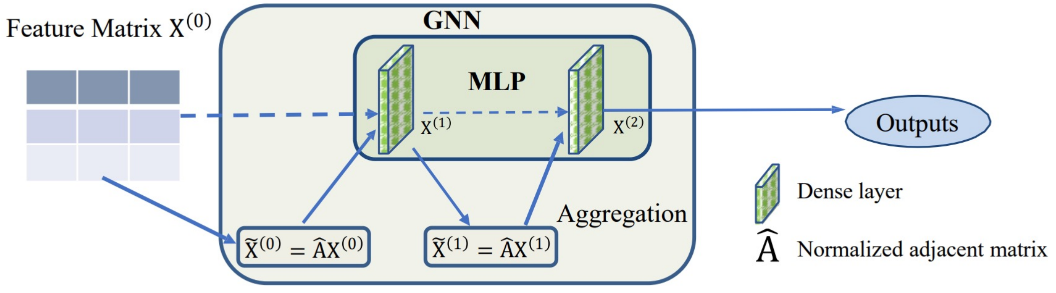
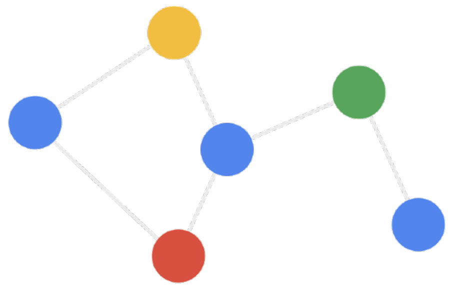

Feature Matrix $X^{(0)}$
GNN
MLP
$X^{(1)}$
$X^{(2)}$
Outputs
$\tilde{X}^{(0)} = \hat{A}X^{(0)}$
$\tilde{X}^{(1)} = \hat{A}X^{(1)}$
Aggregation
Dense layer
$\hat{A}$ Normalized adjacent matrix

Figure 1. The framework of a two-layer GCN models.



Node embedding

Degree Matrix

Node embedding

$$\mathbf{X}^{(l+1)} = \delta\left(\widetilde{\mathbf{D}}^{-\frac{1}{2}}\widetilde{\mathbf{A}}\widetilde{\mathbf{D}}^{-\frac{1}{2}}\mathbf{X}^{(l)}\mathbf{W}^{(l)}\right)$$

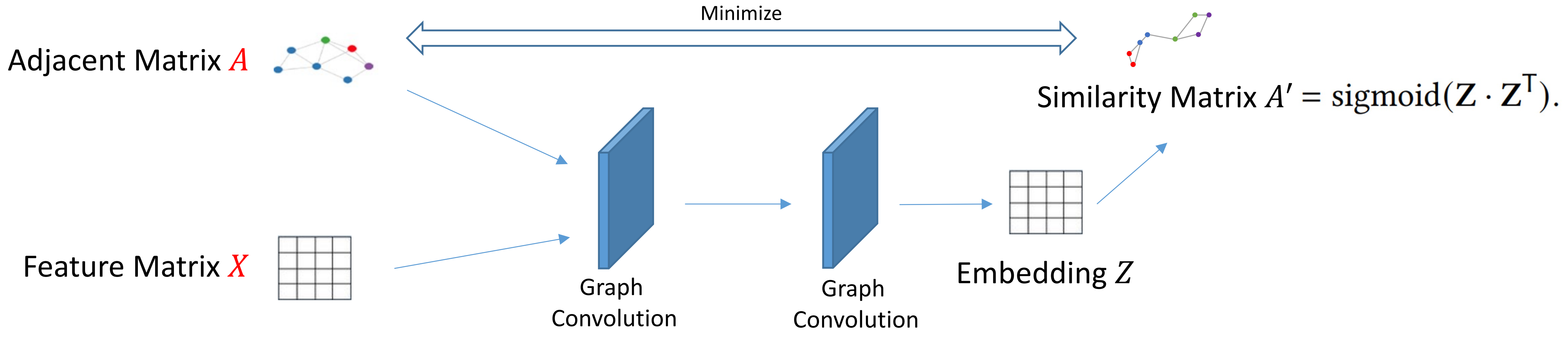
Adjacency Matrix

Model parameter

- Each GCN layer as contains two operations: feature aggregation and nonlinear transformation. Some works argue that the entanglement of feature aggregation and nonlinear transformation might harm both the performance and robustness of GNN.
- GNN will degenerate to MLP if $\hat{A}$ is the identity matrix, which is equivalent to removing the feature aggregation process in each GCN layer.

Graph Neural Networks

Graph Auto-Encoder (GAE)



- GNN-based graph representation learning has attracted intensive interest by combining knowledge from both graph structure and node features.

- Most GNN-based representation learning methods are designed based on GAE.

Drawbacks

Drawbacks of current methods

1) **Low Scalability**

They can not scale well to large graphs due to the expensive computation cost and high memory usage.

- Repeatedly perform the computationally expensive and recursive feature smoothing
- Introduce high memory usage by storing the dense-form adjacency matrix on GPU.

2) **Shallow Architecture**

The performance decreases as the layers become deeper.

- Information Propogation: Shallow architecture can not involve the full graph information due a few propagations.
- Nonlinear Transformation: The expressive power is low due to a few nonlinear transformation.

Observation

- **Over-Smoothing Issue**

When applying $\hat{\mathrm{A}} = \widetilde{\mathrm{D}}^{r-1}\widetilde{\mathrm{A}}\widetilde{\mathrm{D}}^{-r}$ as adjacency matrix $\hat{\mathrm{A}}$, the stationary state follows

$$\hat{\mathrm{A}}^{\infty}_{i,j} = \frac{(d_i+1)^r (d_j+1)^{1-r}}{2m+n}, \tag{3}$$

After infinite times of aggregation, the influence from node v_i to v_j is only determined by the degrees of them.

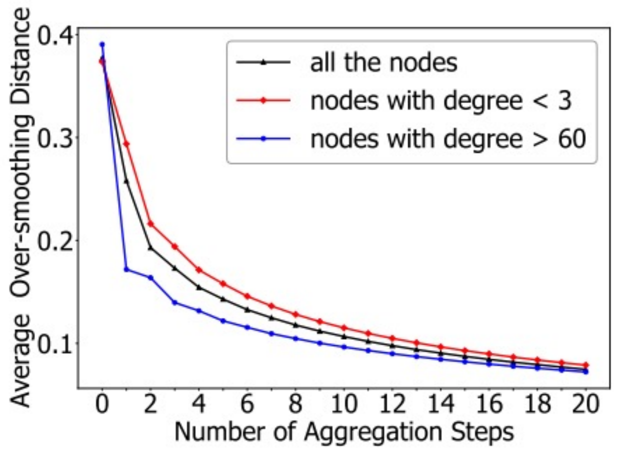
- **Over-Smoothing Distance**

Definition 1 (Over-smoothing Distance). *The Over-smoothing Distance $D_i(k)$ parameterized by node i and smoothing step k is defined as*

$$D_i(k) = Dis([\hat{\mathbf{A}}^k\mathbf{X}]_i, [\hat{\mathbf{A}}^{\infty}\mathbf{X}]_i), \tag{4}$$

A smaller value indicates that the node is closer to the stationary state, i.e., closer to over-smoothing.

Observation



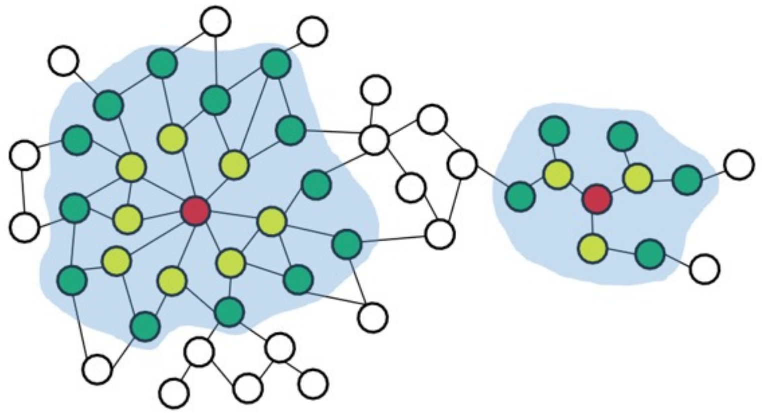


Figure 2. The diverse smoothing speed across nodes with different degrees. Nodes with larger degree have larger smoothing speed.

- Many previous works propose to decouple the feature smoothing and feature transformation in each GCN layer.

- Nodes with high degrees should have relatively small smoothing steps than nodes with low degrees. **Node-adaptive feature smoothing** must be adopted to satisfy each node's diverse needs of smoothing level.

Outline

Method

Node-Adaptive Feature Smoothing

- **Feature Smoothing:**
  We define the **smoothing weight** so that the smoothing operation can be performed in a node-adaptive manner.

Definition 2 (Smoothing Weight). *The Smoothing Weight $w_i(k)$ parameterized by node v_i and smoothing step k is defined with the softmax value of $\{D_i(0), D_i(1), \cdots, D_i(K)\}$:*

$$w_i(k) = e^{D_i(k)} / \sum_{l=0}^{K} e^{D_i(l)}, \qquad (5)$$

where K is the maximal smoothing step.

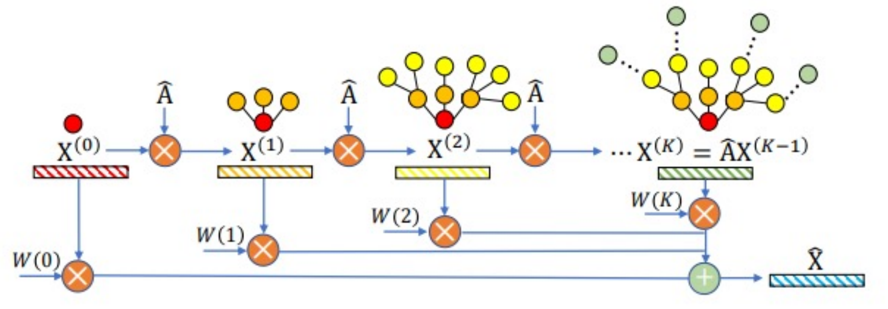


Figure 3. An overview of node-adaptive feature smoothing.

$$D_i(k) = ||[\hat{\mathbf{A}}^k\mathbf{X}]_i - [\hat{\mathbf{A}}^\infty\mathbf{X}]_i||_2$$

- **Feature Ensemble:**

  Different smoothing operators actually act as different knowledge extractors.

  we vary the value of r in the normalized adjacency matrix

$$\hat{\mathbf{A}}_r = \tilde{\mathbf{D}}^{r-1}\tilde{\mathbf{A}}\tilde{\mathbf{D}}^{-r}$$

Firstly perform the feature smoothing operation to generate corresponding smoothed features $\{\hat{\mathbf{X}}^{(1)}, \hat{\mathbf{X}}^{(2)}, ..., \hat{\mathbf{X}}^{(T)}\}$

Then, we combine them with concatenating, mean pooling, or max pooling, etc.

Theoretical Analysis

Theorem 2. *For any node i in graph $\mathcal{G}$, there always exists*

$$D_i(k) \le \lambda_2^k \sqrt{\frac{\sum_{j=1}^{n}(\tilde{d}_j ||\mathbf{X}_j||_2^2)}{\tilde{d}_i}}, \tag{10}$$

where $\tilde{d}_i = d_i + 1$, $\tilde{d}_j = d_j + 1$, $||\mathbf{X}_j||_2$ denotes the two-norm of the initial feature of node j, and $0 < \lambda_2 < 1$ denotes the second largest eigenvalue of the normalized adjacency matrix $\hat{\mathbf{A}}$.

- Nodes with smaller degrees may have larger $D_i(k)$
- For the nodes with smaller degrees, its result of weighted average depends more equally on all itself, its near neighbors, and its distant neighbors.
- The Aggregation Weight of the node in a sparser graph (λ_2 is positively relative with the sparsity of a graph) decays slower as k increases.

$$\begin{aligned} ||\hat{\mathbf{X}}_i - [\hat{\mathbf{A}}^\infty \mathbf{X}]_i||_2 &\ge \frac{\epsilon^2}{\lim_{K\to\infty}\sum_{k=0}^{K} D_i(k)} \\ &\ge \frac{\epsilon^2}{\frac{1}{1-\lambda_2}\sqrt{\frac{cdx}{\tilde{d}_i}}} > 0 \end{aligned}. \tag{19}$$

- Even K goes to infinity, we can prevent the node representations from reaching the stationary state.

Comparison with Existing GNNs

- **Deep Structural Information**

  By assigning each node with personalized smoothing weights, NAFS can gather deep structural information without encountering the over-smoothing issue.

- **Efficiency**

  Compared with GAE and its variants, our proposed NAFS does not have any trainable parameters, giving it a significant advantage in efficiency.

- **Memory Cost**

  NAFS only requires to store the sparse adjacency matrix and the smoothed features, and thus the memory cost is $O(m + nf)$, which grows linearly with graph size in typical real-world graphs.

Outline

Experiments

End-to-end Comparison

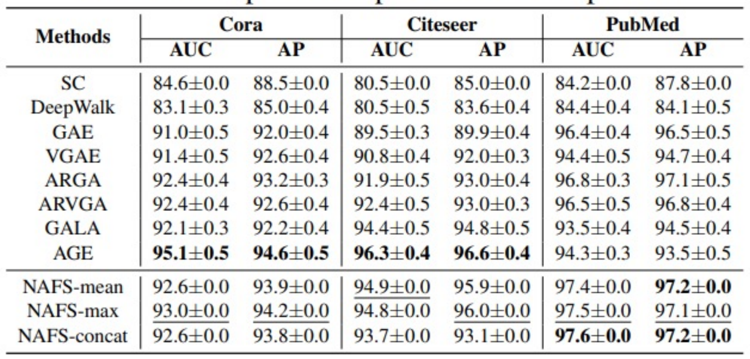


Table 1. Link prediction performance comparison.

Methods	Cora		Citeseer		PubMed	
	AUC	AP	AUC	AP	AUC	AP
SC	84.6±0.0	88.5±0.0	80.5±0.0	85.0±0.0	84.2±0.0	87.8±0.0
DeepWalk	83.1±0.3	85.0±0.4	80.5±0.5	83.6±0.4	84.4±0.4	84.1±0.5
GAE	91.0±0.5	92.0±0.4	89.5±0.3	89.9±0.4	96.4±0.4	96.5±0.5
VGAE	91.4±0.5	92.6±0.4	90.8±0.4	92.0±0.3	94.4±0.5	94.7±0.4
ARGA	92.4±0.4	93.2±0.3	91.9±0.5	93.0±0.4	96.8±0.3	97.1±0.5
ARVGA	92.4±0.4	92.6±0.4	92.4±0.5	93.0±0.3	96.5±0.5	96.8±0.4
GALA	92.1±0.3	92.2±0.4	94.4±0.5	94.8±0.5	93.5±0.4	94.5±0.4
AGE	**95.1±0.5**	**94.6±0.5**	**96.3±0.4**	**96.6±0.4**	94.3±0.3	93.5±0.5
NAFS-mean	92.6±0.0	93.9±0.0	94.9±0.0	95.9±0.0	97.4±0.0	**97.2±0.0**
NAFS-max	93.0±0.0	94.2±0.0	94.8±0.0	96.0±0.0	97.5±0.0	97.1±0.0
NAFS-concat	92.6±0.0	93.8±0.0	93.7±0.0	93.1±0.0	**97.6±0.0**	**97.2±0.0**

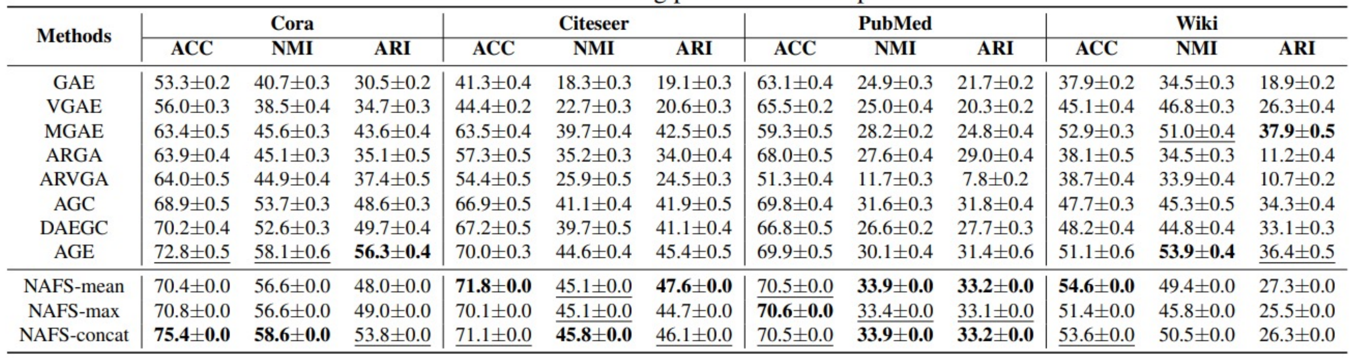


Table 2. Node clustering performance comparison.

Methods	Cora			Citeseer			PubMed			Wiki		
	ACC	NMI	ARI	ACC	NMI	ARI	ACC	NMI	ARI	ACC	NMI	ARI
GAE	53.3±0.2	40.7±0.3	30.5±0.2	41.3±0.4	18.3±0.3	19.1±0.3	63.1±0.4	24.9±0.3	21.7±0.2	37.9±0.2	34.5±0.3	18.9±0.2
VGAE	56.0±0.3	38.5±0.4	34.7±0.3	44.4±0.2	22.7±0.3	20.6±0.3	65.5±0.2	25.0±0.4	20.3±0.2	45.1±0.4	46.8±0.3	26.3±0.4
MGAE	63.4±0.5	45.6±0.3	43.6±0.4	63.5±0.4	39.7±0.4	42.5±0.5	59.3±0.5	28.2±0.2	24.8±0.4	52.9±0.3	51.0±0.4	**37.9±0.5**
ARGA	63.9±0.4	45.1±0.3	35.1±0.5	57.3±0.5	35.2±0.3	34.0±0.4	68.0±0.5	27.6±0.4	29.0±0.4	38.1±0.5	34.5±0.3	11.2±0.4
ARVGA	64.0±0.5	44.9±0.4	37.4±0.5	54.4±0.5	25.9±0.5	24.5±0.3	51.3±0.4	11.7±0.3	7.8±0.2	38.7±0.4	33.9±0.4	10.7±0.2
AGC	68.9±0.5	53.7±0.3	48.6±0.3	66.9±0.5	41.1±0.4	41.9±0.5	69.8±0.4	31.6±0.3	31.8±0.4	47.7±0.3	45.3±0.5	34.3±0.4
DAEGC	70.2±0.4	52.6±0.3	49.7±0.4	67.2±0.5	39.7±0.5	41.1±0.4	66.8±0.5	26.6±0.2	27.7±0.3	48.2±0.4	44.8±0.4	33.1±0.3
AGE	72.8±0.5	58.1±0.6	**56.3±0.4**	70.0±0.3	44.6±0.4	45.4±0.5	69.9±0.5	30.1±0.4	31.4±0.6	51.1±0.6	**53.9±0.4**	36.4±0.5
NAFS-mean	70.4±0.0	56.6±0.0	48.0±0.0	**71.8±0.0**	45.1±0.0	**47.6±0.0**	70.5±0.0	**33.9±0.0**	**33.2±0.0**	**54.6±0.0**	49.4±0.0	27.3±0.0
NAFS-max	70.8±0.0	56.6±0.0	49.0±0.0	70.1±0.0	45.1±0.0	44.7±0.0	**70.6±0.0**	33.4±0.0	33.1±0.0	51.4±0.0	45.8±0.0	25.5±0.0
NAFS-concat	**75.4±0.0**	**58.6±0.0**	53.8±0.0	71.1±0.0	**45.8±0.0**	46.1±0.0	70.5±0.0	**33.9±0.0**	**33.2±0.0**	53.6±0.0	50.5±0.0	26.3±0.0

- **Link Prediction**
  - The proposed NAFS consistently achieves the best or the second-best performance compared with all the baseline methods.
- **Node Clustering**
  - Among three ensemble strategies, NAFS-concat has the overall best performance across the three datasets, which also consistently outperforms the strongest baseline - AGE.
  - Three NAFS variants outperform training-based GAE on all the four datasets, and they outperforms the current SOTA method, AGE, in most cases.

Efficiency & Scalability

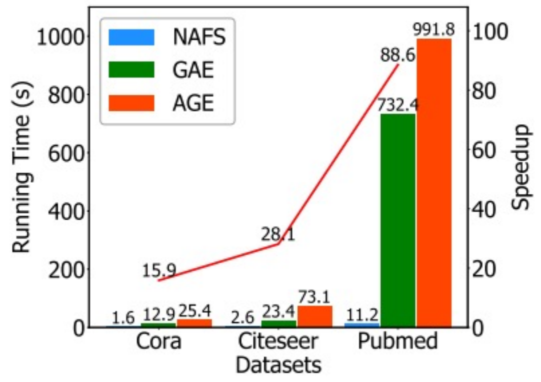


Figure 5. Efficiency comparison on the three citation networks.

Table 3. Scalablity comparison with different sample sizes on the ogbn-products dataset.

Methods	10,000	20,000	30,000	50,000	100,000
GAE	10.2s	36.3s	OOM	OOM	OOM
AGE	68.5s	256.2s	727.7s	2315.7s	OOM
NAFS-mean	2.8s	6.5s	10.8s	13.8s	23.7s

- **Efficiency Analysis**
  - NAFS is significantly faster than the considered baseline methods on the three datasets

- **Scalability Analysis**
  - NAFS can support the larger graphs (i.e., larger than 30,000 nodes) than the compared baselines. Besides, it is significantly faster than the compared baselines, especially for large graph datasets.

Interpretability

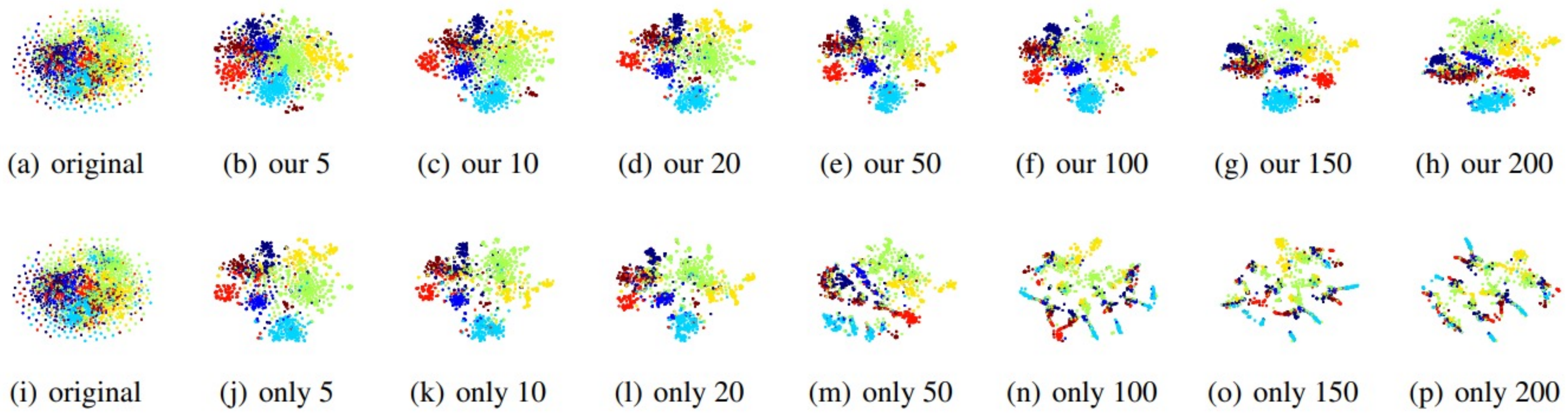


Figure 6. T-SNE visualization of node embedding on the Cora dataset.

- **Visualization**
  - At hop 10, the node embedding produced by NAFS and SGC are both distinguishable.
  - As the value of maximal smoothing step becomes larger, the node embedding of SGC falls into total disorder, like the situation showed by Figure. 6(n), 6(o) and 6(p).
  - NAFS can support large hops while maintain the distinguishable results.

Outline

Conclusion

Conclusion

1. To the best of our knowledge, we are the first to explore the possibility that simple feature smoothing without any trainable parameters could even outperform state-of-the-art GNNs; this incredible finding opens up a new direction towards efficient and scalable graph representation learning.

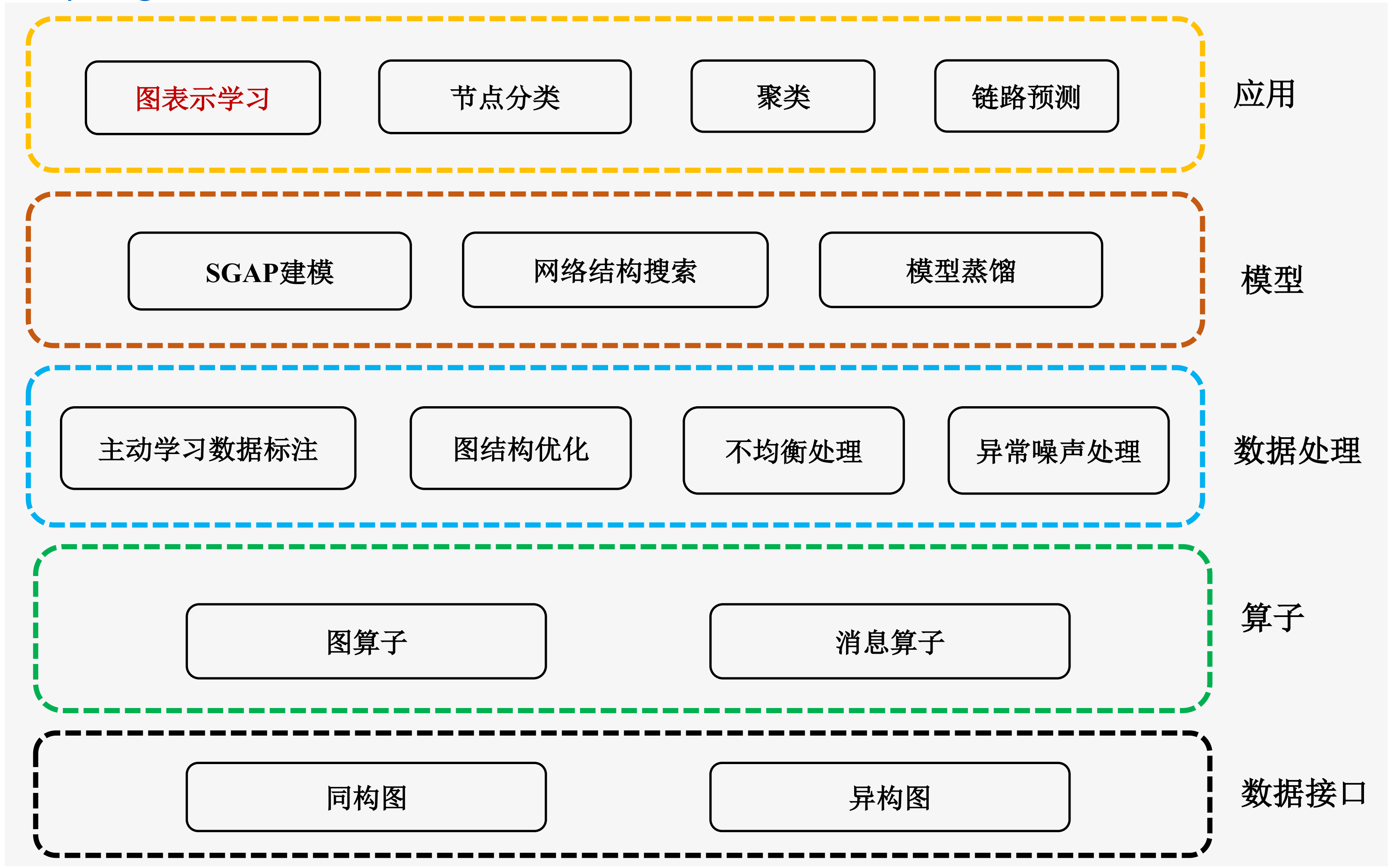
2. We propose NAFS, a node-adaptive feature smoothing approach along with various feature ensemble strategies, to fully exploit knowledge from both the graph structure and node features.

3. Empirical results demonstrate that NAFS performs comparably with or even outperforms the state-of-the-art GNNs, and achieves up to two orders of magnitude speedup.

SGL系统

https://github.com/PKU-DAIR/SGL/blob/main/sgl/models/homo/nafs.py

https://github.com/PKU-DAIR/SGL/



SGL系统设计目标

1.高可扩展性:
基于**SGAP建模范式**, SGL 能处理超大规模图数据

2.自动化**:**
根据指定的多个目标自动化搜索网络结构

3.易用性:
针对多个任务定制的用户友好的接口

4. 针对数据的优化
多种数据处理操作

5. Bag of Tricks
内置多种有效的提点方法

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Thanks