Deep Graph Neural Networks via Posteriori-Sampling-based Node-Adaptive Residual Module

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Abstract

Graph Neural Networks (GNNs), a type of neural network that can learn from graph-structured data through neighborhood information aggregation, have shown superior performance in various downstream tasks. However, as the number of layers increases, node representations become indistinguishable, which is known as over-smoothing. To address this issue, many residual methods have emerged. In this paper, we focus on the over-smoothing issue and related residual methods. Firstly, we revisit over-smoothing from the perspective of overlapping neighborhood subgraphs, and based on this, we explain how residual methods can alleviate over-smoothing by integrating multiple orders neighborhood subgraphs to avoid the indistinguishability of the single high-order neighborhood subgraphs. Additionally, we reveal the drawbacks of previous residual methods, such as the lack of node adaptability and severe loss of high-order neighborhood subgraph information, and propose a **Posterior-Sampling-based, Node-Adaptive Residual module (PSNR)**. We theoretically demonstrate that PSNR can alleviate the drawbacks of previous residual methods. Furthermore, extensive experiments verify the superiority of the PSNR module in fully observed node classification and missing feature scenarios. Our code is available at https://github.com/jingbo02/PSNR-GNN.

1 Introduction

GNNs have emerged in recent years as the most powerful model for processing graph-structured data and have demonstrated exceptional performance across various fields, such as social networks [22], recommender systems [6], and drug discovery [4]. Through the message-passing mechanism that propagates and aggregates information of neighboring nodes, GNNs provide a general framework for learning information on graph structure. Despite the remarkable success, according to previous studies [17, 32], GNNs show significant performance degradation as the number of layers increase. One of the main reasons for this situation is over-smoothing [17, 21, 32, 15]. Over-smoothing refers to the phenomenon in which node representations become increasingly similar to each other as GNNs recursively aggregate more neighborhood information. This indistinguishability will inevitably degrade the performance of deep GNNs, restricting their ability to effectively model long-range dependencies among multi-hop neighbors.

Several methods have recently been proposed to alleviate over-smoothing in deep GNNs. According to [26], these methods fall into three categories: Normalization and Regularization [34, 33], Change of GNN dynamics [5], and Residual connections [32, 16]. Among all of them, the residual-based

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38th Conference on Neural Information Processing Systems (NeurIPS 2024).

method is inspired by the success of residual neural networks (ResNets) [9] in computer vision. This type of method introduces a residual connection to the GNNs architecture. For example, JKNet [32] learns node representations by aggregating the outputs of all previous layers at the last layer. DenseGCN [16] concatenates the results of the current layer and all previous layers as the node representations of this layer. APPNP [15] uses the initial residual connection to retain the initial feature information with probability α, and utilizes information aggregated at the current layer with probability $1 - \alpha$. GCNII [3] shares a similar framework with APPNP, and it further introduces an identical mapping to avoid overfitting.

In this paper, we study the over-smoothing issue in GNNs, with a particular emphasis on residual methods. First, we revisit the over-smoothing phenomenon of GNNs from the new perspective of overlapping neighborhood subgraphs and explain the essential reason why the residual method can alleviate the over-smoothing. In essence, these methods mainly use multiple neighborhood subgraph aggregations to alleviate the indistinguishability of the single neighborhood subgraph aggregation, thereby improving the performance of the model. On this basis, we find that these residual methods often lack node adaptivity in utilizing multi-order neighborhood subgraph information, and at the same time, they still struggle to mitigate information loss when dealing with high-order neighborhood subgraphs, which hinders further improvement in the performance of deep GNNs. Although some residual methods, such as DenseGNN, can avoid these drawbacks, they tend to introduce more parameters at deeper layers. This can lead to significant memory consumption and is prone to gradient explosion, limiting the scalability of the methods.

Considering these limitations, we propose a **Posteriori-Sampling-based Node-Adaptative Residual Module (PSNR)**. More specifically, this module introduces a graph encoder to learn the posterior distribution of the required residual coefficients for each node in different layers with minor overhead. And then, we can obtain the specific fine-grained node-adaptive residual coefficients by sampling from the distribution. The contributions of this paper are as follows:

- *Perspective:* We revisit the over-smoothing issue from a novel perspective of high-order neighborhood subgraph coincidences and explain why the residual methods can alleviate it. Through this lens, we reveal several significant drawbacks of prior residual methods that limit the performance and scalability of GNNs.

- *Method:* We propose PSNR, a lightweight and model-agnostic module to mitigate the drawbacks of previous residual methods and provide theoretical justification for its advantages.

- *Experiments:* Extensive experiments verify that the PSNR module can effectively mitigate oversmoothing and further improve the performance of GNNs, especially in the case of missing feature that require deep GNNs.

2   Related Work

2.1   Notations

A connected undirected graph is represented by $\mathcal{G} = (\mathcal{V}, \mathcal{E})$, where $\mathcal{V} = \{v_1, v_2, \ldots, v_N\}$ is the set of N nodes and $\mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}$ is the edge set. The node features are represented in the matrix $\mathbf{H} \in \mathbb{R}^{N \times d}$, where d represents the length of the feature. Let $\mathbf{A} \in \{0, 1\}^{N \times N}$ denotes the adjacency matrix and $\mathbf{A}_{ij} = 1$ only if an edge exists between nodes v_i and v_j. $\mathbf{D} \in \mathbb{R}^{N \times N}$ is the diagonal degree matrix, where each element d_i represents the number of edges connected to node v_i. $\tilde{\mathbf{A}} = \mathbf{A} + \mathbf{I}, \tilde{\mathbf{D}} = \mathbf{D} + \mathbf{I}$ represent the adjacency matrix and degree matrix with self-loop, respectively.

2.2   Graph Neural Networks

A GNN layer updates the representation of each node via aggregating itself and its neighbors' representations. Specifically, a layer's output $\mathbf{H}'$ consists of new representations $\mathbf{h}'$ of each node computed as:
$$\mathbf{h}'_i = f_\theta \left(\mathbf{h}_i, \text{AGGREGATE} \left(\{\mathbf{h}_j \mid v_j \in \mathcal{V}, (v_i, v_j) \in \mathcal{E}\} \right) \right), \tag{1}$$

where $\mathbf{h}'_i$ indicates the new representation of node v_i and $f_\theta(\cdot)$ denotes the update function. The difference between different GNNs lies in the update function $\mathbf{f}_\theta(\cdot)$ and the $\text{AGGREGATE}(\cdot)$ function, which are also key to the performance of GNNs. Graph Convolutional Network (GCN) [14]

2

Table 1: Common residual connections for GNNs.

Residual Connection	Corresponding GCN	Formula
Res	ResGCN [16]	$\mathbf{H}_k = \mathbf{H}_{k-1} + \sigma\left(\tilde{\mathbf{D}}^{-\frac{1}{2}}\tilde{\mathbf{A}}\tilde{\mathbf{D}}^{-\frac{1}{2}}\mathbf{H}_{k-1}\mathbf{W}_{k-1}\right)$
InitialRes	APPNP [15]	$\mathbf{H}_k = (1-\alpha)\tilde{\mathbf{D}}^{-\frac{1}{2}}\tilde{\mathbf{A}}\tilde{\mathbf{D}}^{-\frac{1}{2}}\mathbf{H}_{k-1} + \alpha\mathbf{H}$
Dense	DenseGCN [16]	$\mathbf{H}_k = \mathrm{AGG}(\mathbf{H}, \mathbf{H}_1, \ldots, \mathbf{H}_{k-1})$
JK	JKNet [32]	$\mathbf{H}_{output} = \mathrm{AGG}(\mathbf{H}_1, \ldots, \mathbf{H}_{k-1})$

is a classical massage-passing GNNs follows layer-wise propagation rule:

$$\mathbf{H}_{k+1} = \sigma\left(\tilde{\mathbf{D}}^{-\frac{1}{2}}\tilde{\mathbf{A}}\tilde{\mathbf{D}}^{-\frac{1}{2}}\mathbf{H}_k\mathbf{W}_k\right), \tag{2}$$

where $\mathbf{H}_k$ is the feature matrix of the k-th layer, $\mathbf{W}_k$ is a layer-specific learnable weight matrix, $\sigma(\cdot)$ denotes an activation function.

2.3 Residual connection

Several works have used residual connection to alleviate the over-smoothing issue. Common residual connections for GNNs are summarized in Table 1, where $\mathbf{H}_k$ represents the output of the k-th layer, $\mathbf{W}_k$ is a learnable weight matrix for the k-th layer, α serves as a hyperparameter denoting the residual coefficient, and $\sigma(\cdot)$ denotes an activation function. Additionally, in DenseGNN, AGG represents a function with the concatenation of outputs from all previous layers as the input to the current layer, while in JKNet, AGG refers to the aggregation of all previous representations through concatenation, max-pooling, or LSTM-attention only at the final layer. Details can be found in Appendix B.

3 Why does the residual method alleviate over-smoothing?

In this section, we revisit over-smoothing from the perspective of overlapping high-order neighborhood subgraphs. Based on this, we elucidate the role of various residual methods in alleviating over-smoothing and identify their shortcomings.

3.1 Revisit over-smoothing from the perspective of neighborhood subgraphs overlapping

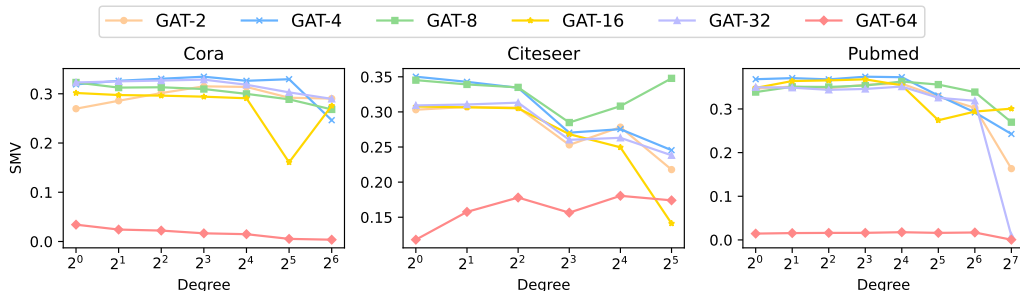



Figure 1: SMV for node groups of different degrees. More results are shown in Appendix C.

For message-passing GNNs without the residual connection, the information domain of each node after k-layer aggregation is a corresponding k-order neighborhood subgraph. Intuitively, the size of its k-order neighborhood subgraph grows exponentially as k increases, leading to a significant increase in the overlap between the k-order neighborhood subgraphs of different nodes. As a result, the aggregation result of different nodes on their respective k-order neighborhood subgraphs becomes indistinguishable. This explanation can be partially validated from the perspective of node degrees. Considering nodes with high degrees tend to have larger neighborhood subgraph overlap, the correlation between neighborhood subgraph overlap and oversmoothiong can be validated if nodes with higher degree exhibit more pronounced over-smoothing. To verify this point, we conduct experiments on three graph datasets: Cora, Citeseer, and Pubmed. Initially, nodes are grouped based on their degrees, with nodes having degrees falling within the range of $[2^i, 2^{i+1})$ assigned to the

3

i-th group. Subsequently, we perform aggregation with different layers of GCN and GAT and then calculate the degree of smoothing of the node representations within each group separately. The metric proposed in [19] is used to measure the smoothness of the node representations within each group, namely smoothness metric value (SMV), which calculates the average distances between the nodes within the group:

$$\text{SMV}(\mathbf{X}) = \frac{1}{N(N-1)} \sum_{i \neq j} \mathcal{D}\left(\mathbf{X}_{i,:}, \mathbf{X}_{j,:}\right), \tag{3}$$

where $\mathcal{D}(\cdot, \cdot)$ denotes the normalized Euclidean distance between two vectors:

$$\mathcal{D}(\mathbf{x}, \mathbf{y}) = \frac{1}{2} \left\| \frac{\mathbf{x}}{\|\mathbf{x}\|} - \frac{\mathbf{y}}{\|\mathbf{y}\|} \right\|_2. \tag{4}$$

From the definition, a smaller value of SMV indicates a greater similarity in node representations. We show the result of GAT in Figure 1. More results can be found in Appendix C. It can be observed that the groups of nodes with higher degree tend to be more similar to each other within the group in different layers. This finding supports our claim.

3.2 The role of residual method in alleviating over-smoothing

After verifying the conclusion that neighborhood subgraph overlap leads to over-smoothing, a natural idea is to alleviate the overlap of the single neighborhood subgraph by utilizing multi-order neighborhood subgraph aggregations. In the following section, we show that the previous k-layer residual-based GNNs essentially represent different forms of utilizing neighborhood subgraph aggregations from 0 to k orders.

Table 2: Utilization of neighborhood subgraphs by various residual methods.

Model	Closed/Iterative form formulas
ResGCN	$\mathbf{H}_k = \sum_{j=0}^{k} \binom{j}{k} \mathbf{N}^j \mathbf{H}$
APPNP	$\mathbf{H}_k = (1-\alpha)^k \mathbf{N}^k \mathbf{H} + \alpha \sum_{j=0}^{k-1} \sum_{i=0}^{j} (-1)^{j-i} (1-\alpha)^i \mathbf{N}^i \mathbf{H}$
JKNet	$\mathbf{H}_k = \text{AGG}(\mathbf{N}\mathbf{H}, \dots, \mathbf{N}^{k-1}\mathbf{H})$
DenseGCN	$\mathbf{H}_k = \text{AGG}(\mathbf{H}_{k-1}, \dots, \mathbf{H}_1, \mathbf{H}_0)$

In the rest of this paper, we take GCN, a classical residual-free message-passing GNN, as an example. Assuming that $\mathbf{H}$ is non-negative, the ELU function and the weight matrix can be ignored for simplicity. Combined with the formula of GCN in Eq. 2, the k-order neighborhood subgraph aggregation can be formulated as $\mathbf{N}^k \mathbf{H}$, where $\mathbf{N} = \tilde{\mathbf{D}}^{-\frac{1}{2}} \tilde{\mathbf{A}} \tilde{\mathbf{D}}^{-\frac{1}{2}}$. To show more intuitively how different residual models utilize multi-order neighborhood subgraph aggregation $\mathbf{N}^k \mathbf{H}$, we rewrite their formula in Table 2. Details of the derivation of the closed-form formula in this part are given in Appendix D. As can be observed, the output of GCN's residual-based variants contains multi-order matrix products that represent different order neighborhood subgraph aggregations from 0 to k. There are two main ways to exploit them: **(1)** Summation, such as ResGCN and APPNP. Such methods employ linear summation over the aggregation of different order neighborhood subgraphs; **(2)** Aggregation functions, such as DenseGNN and JKNet. Such methods make direct and explicit exploitation of different order neighborhood subgraph aggregations through operations such as concatenation.

However, the utilization of multi-order neighborhood subgraph aggregations in these methods presents the following issues: Firstly, the summation methods all use a fixed coefficient to sum the neighborhood subgraph aggregations. Consequently, these methods inherently presume that the information from the neighborhood subgraph of the same order is equally important for different nodes, which lacks node adaptivity. Secondly, for ResGNN, APPNP, and JKNet, when the number of layers increases, the output of these methods still involves many high-order matrix products that are over-smoothed. This leads to severe information loss when aggregating high-order neighborhood subgraphs, which in turn degrades model performance at deeper layers. Although DenseGNN seems to alleviate the above issues to some extent, the recursive use of all previous neighborhood subgraph aggregation would introduce more parameters as the model deepens. This increases memory consumption and raises the risk of gradient explosion at deeper layers.

4

4 The Proposed Method PSNR

4.1 Methodology

To solve the above issues, we propose a node-adaptive and lightweight residual module named PSNR. The motivation is to learn the adaptive residual coefficients for each node, thereby achieving fine-grained and node-level neighborhood subgraph aggregation to improve the performance of GNNs. However, directly learning these coefficients through backpropagation presents significant challenges. The primary challenge lies in the lack of transferability of learned coefficients. Specifically, in tasks such as semi-supervised node classification, nodes in the test and validation sets often cannot propagate information to the training nodes through multiple message-passing steps. Therefore, we cannot learn effective coefficients for these nodes during the training phase.

As a remedy, we regard node-level residual coefficients as hidden parameters. Our strategy involves estimating their posterior distribution $\mathbf{P}(\eta_k|\mathbf{A}, \mathbf{H}_k, k)$. In most cases, since the training, validation, and test sets originate from the same distribution, the posterior distribution learned from the training data possesses transferability to the validation and testing nodes. We can assume the posterior distribution to be Gaussian:

$$\eta_k \sim \mathcal{N}(\mu(\mathbf{A}, \mathbf{H}_k, k), \sigma^2(\mathbf{A}, \mathbf{H}_k, k)).$$

A graph encoder can be used to model this distribution. This encoder leverages graph topology and node information as inputs. Subsequently, to enable backpropagation, we employ the reparameterization trick. This technique enables us to represent the sampling process from the aforementioned distribution as follows:

Figure 2: The framework of PSNR Module.

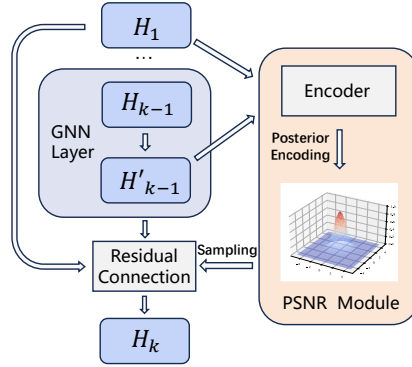
$$\eta_k = \mu(\mathbf{A}, \mathbf{H}_k, k) + \zeta \cdot \sigma(\mathbf{A}, \mathbf{H}_k, k), \ \zeta \sim \mathcal{N}(0, 1).$$

Furthermore, we parameterize $\mu(\mathbf{A}, \mathbf{H}_k, k)$ and $\sigma(\mathbf{A}, \mathbf{H}_k, k)$ as an arbitrary GNN layer. While the posterior distributions of residual coefficients vary across different layers, we do not parameterize a specific encoder for each layer. Instead, we employ the same graph encoder and use the positional embedding generated from the layer number k to differentiate the posterior distributions of residual coefficients for various layers. Consequently, the PSNR module can be formulated as follows:

$$\begin{aligned}
\mathbf{H}'_{k-1} &= \mathrm{GraphConv}\left(\mathbf{H}_{k-1}\right) \\
\mathbf{H}_k &= \mathbf{H}_1 + \phi(diag(\eta_{k-1}))\left(\mathbf{H}_1 - \mathbf{H}'_{k-1}\right), \ \eta_{k-1} \sim \mathcal{N}(\mu_{k-1}, {\sigma_{k-1}}^2) \\
\mu_k, \sigma_k &= \mathrm{GraphEncoder}_{\mu,\sigma}(\mathbf{H}_1 - \mathbf{H}'_k + \gamma\, \mathrm{LayerEmb}(k)),
\end{aligned} \tag{5}$$

where $\mathrm{GraphConv}(\cdot)$ is the k-th layer of any backbone GNN, $\mathbf{H}_k$ denotes the node representation matrix of the k-th layer, and $\mathbf{H}'_k$ represents the output matrix of the k-th layer. The first equation corresponds to the aggregation operation of the backbone GNN at the k-th layer. η_k represents the node-level residual coefficient at the k-th layer, where the element $\eta_k^{(i)}$ corresponds to the residual coefficient at the i-th node. In addition, η_k follows a high-dimensional Gaussian distribution: $\mathcal{N}(\mu_k, {\sigma_k}^2)$, and each time before each residual calculation, the distribution is first sampled to obtain the exact residual coefficients. μ_k and σ_k represent the mean and standard deviation of the distribution, respectively. $diag(\eta_k)$ represents a diagonal matrix transformed from η_k, where the i-th diagonal element is precisely the i-th element of η_k. $\phi(\cdot)$ represents the sigmoid function, which constrains the residual coefficient to $(0, 1)$. $\mathrm{GraphEncoder}_{\mu,\sigma}(\cdot)$ is a posterior encoder, which can be any graph convolution layer that is independent of the backbone GNN. $\mathrm{LayerEmb}(k)$ represents the positional embedding [29] with layer number k as input. γ is a learnable coefficient serving as the layer embedding factor. The analysis of the residual coefficients can be found in Appendix H.

Also, it is noteworthy that PSNR introduces randomness by sampling residual coefficients during both training and testing phases, thereby adding learnable random perturbations. This is different to other methods including DropEdge [24], GRAND [8] and DropMessage [7] that only incorporate randomness during the training phase and primarily introduce perturbations to node features and graph structure. We provide the theoretical analysis for this design in Section 4.2. Additionally, we clarify the difference between PSNR and other subgraph-based methods in Appendix F.

5

4.2 Theoretical justifications on the advantages of the PSNR module

In this section, we theoretically show that the PSNR module achieves finer-grained and node-adaptive neighborhood subgraph aggregations while avoiding the loss of high-order subgraph information. Firstly, combining with Equation 5, the matrix form of the iterative formula for PSNR-GCN is:

$$\mathbf{H}_k = \mathbf{H}_1 + \Lambda_{k-1} \left(\mathbf{H}_1 - \tilde{\mathbf{D}}^{-1/2} \tilde{\mathbf{A}} \tilde{\mathbf{D}}^{-1/2} \mathbf{H}_{k-1} \right).$$

For simplicity, we use Λ_k to denote $diag(\eta_k)$. Subsequently, based on this recursive form of formula, we derive the closed-form expression of PSNR-GCN as:

$$\mathbf{H}_k = \sum_{i=2}^{k-1} \prod_{j=i}^{k-1} \tilde{\mathbf{N}}_j (\mathbf{M}_i - \mathbf{M}_{i-1}) + \prod_{i=1}^{k-1} \tilde{\mathbf{N}}_i (\mathbf{H}_1 + \mathbf{M}_1) - \mathbf{M}_{k-1},$$

where $\tilde{\mathbf{N}}_i = -\Lambda_{k-1}\mathbf{N}$, and $\mathbf{M}_k = -(\Lambda_k \mathbf{N} + \mathbf{I})^{-1}(\mathbf{I} + \Lambda_k)\mathbf{H}_1$. The detailed derivation of this formula can be found in Appendix E. The first two terms consist of cumulative product terms of different orders, similar to the form of $\mathbf{N}^k \mathbf{H}$, thus approximating a new version of neighborhood subgraph aggregation. Additionally, the formula involves the aggregation of all neighborhood subgraphs from 1 to k orders. This ensures that our method, like other residual methods, can comprehensively utilize multi-order neighborhood subgraph aggregations to enhance performance. Furthermore, since Λ_k is a diagonal matrix computed by a learnable posterior encoder with graph structure, node feature and layer number as input, the neighborhood subgraph aggregation of PSNR-GCN is fine-grained and node-adaptive. This sets it apart from methods like ResGCN and APPNP.

Beyond that, we can also demonstrate that the PSNR module can reduce the information loss of high-order subgraph aggregation, thereby further improving the performance of GNNs at deeper layers. Specifically, we aim to prove that as the order k increases, the smoothing rate of the cumulative product terms in PSNR is slower than that of the matrix power terms in other methods. Since we need to analyse the smoothing rate, which involves analyzing the asymptotic behavior of cumulative product terms or matrix power terms as the order increases, we can generalize the problem setup. Therefore, we only need to prove the following proposition to support our claim.

Proposition 1 *Let $\mathcal{S} = \{\mathbf{S}_j = \Lambda_j \mathbf{N} | j \in \mathbb{N}_0\}$, where Λ_j represents a random diagonal matrix with each diagonal element $\Lambda_{j,ii}$ satisfying $0 < \Lambda_{j,ii} < 1$, and let $\mathbf{X}$ be any feature matrix. Then, as the order k increases, the product of elements in the set $\mathcal{S}$ and the matrix $\mathbf{X}$, denoted as $\mathbf{X}^{(k)} = \prod_{i=1}^k \mathbf{S}_i \mathbf{X}$, converges to a rank-one matrix with identical rows slower than $\mathbf{X}_{GCN}^{(k)} = \mathbf{N}^k \mathbf{X}$.*

Since the diagonal elements of the diagonal matrix Λ are all results of the sigmoid function, we can assume that they have a lower bound $\epsilon > 0$. Therefore, in this setting, each element $\mathbf{S}_i$ in the set $\mathcal{S}$ is a row-stochastic matrix satisfying the following property.

Property 1 *For a row-stochastic matrix $\mathbf{S}_k$, there exists an $\epsilon > 0$ satisfying the following conditions:*
1. $\epsilon \leq \mathbf{S}_{k,ij} \leq 1$, if $(i,j) \in \mathcal{E}$,
2. $\mathbf{S}_{k,ij} = 0$, if $(i,j) \notin \mathcal{E}$.

We can refer to the conclusion in [31]. [31] describes the attention matrix of GAT as a row-stochastic matrix satisfying Property 1. Leveraging mathematical tools such as joint spectral radius from the perspective of dynamical systems, this work proves that the convergence rate of GAT is bounded below by GCN. Due to all the matrix $\mathbf{S}_i$ from $\mathcal{S}$ also satisfies Property 1, this conclusion can be borrowed to prove Proposition 1, thereby demonstrating that the PSNR module can alleviate the loss of high-order neighborhood subgraph information. Furthermore, this conclusion also explains the introduction of randomness during both the training and testing phases. This random perturbation further reduces the smoothing rate, thereby enhancing the model's performance.

4.3 Complexity analysis

We take PSNR-GCN as an example to provide a complexity analysis of the PSNR module. The time complexity of a vanilla GCN layer mainly comes from the matrix multiplication of $\mathbf{N}$ and $\mathbf{H}$, hence its complexity is $O(n^2 d)$. And the main computational parts of PSNR module are the computation of mean and standard deviation, sampling of $p_k^{(i)}$, scalar multiplication and matrix

6

addition, which correspond to a complexity of $O(n^2 d)$, $O(n)$, $O(nd)$, and $O(nd)$, respectively. Thus the time complexity of the PSNR module is $O(n^2 d)$ and the time complexity of a GCN layer equipped the PSNR module is $O(n^2 d)$. As for space complexity, PSNR module needs to store the computed mean and variance for each node, i.e., $O(2n)$, which can be approximately considered as $O(n)$. Section 5.6 compares memory consumption with other residual methods on large graphs.

5   Experiment

In this section, we assess the performance of the PSNR module in comparison to other methods and answer the following research questions (**RQ**): **RQ1.** How well does the PSNR alleviate oversmoothing? **RQ2.** How does PSNR perform compared to other baseline when used with different backbone? **RQ3.** Can PSNR enable deeper networks to perform better under the missing feature scenario? **RQ4.** How scalable is the PSNR on large graph datasets?

5.1   Datasets

We conducted experiments on ten real-world datasets, including three citation network datasets, i.e., Cora, Citeseer, Pubmed [27], two web network datasets, i.e., Chameleon and Squirrel [25], co-author/co-purchase network datasets, i.e., Coauthor-CS [28], Amazon-Photo [28] and three larger datasets, i.e., Flickr [20], Coauthor-Physics [28] and Ogbn-arxiv [10]. More details of these datasets and data-splitting procedures can be found in Appendix G.

5.2   Baselines and experimental settings

We consider two fundamental GNNs, GCN [14] and GAT [30]. For GCN, we test the performance of PSNR-GCN and its residual variant models, including ResGCN [16], DenseGCN [16], GCNII [3] and JKNet [32]. For GAT, we directly equip it with the following residual module: Res-GAT, InitialRes-GAT, Dense-GAT, JK-GAT and PSNR-GAT. And we adopt the GraphSAGE layer as the GraphEncoder of the PSNR module. The impact of different graph encoders on the experiments can be found in Appendix I. In addition, we compare three recent representative methods belonging to different categories aimed at alleviating oversmoothing issues: DropMessage [7] for the drop category, DeProp [18] for the norm category, and Half-Hop [1] for graph data processing. For the missing feature setting, we also conduct comparisons with several classical oversmoothing mitigation techniques, including BatchNorm [11], PairNorm [33], DGN [34], Decorr [12], DropEdge [24]. For all baselines, the linear layers in the models are initialized with a standard normal distribution, and the convolutional layers are initialized with Xavier initialization. The Adam optimizer [13] is used for training. Experimental results are obtained from the server with four core Intel(R) Xeon(R) Platinum 8358 CPUs @ 2.60GHZ, one NVIDIA A100 GPU (80G), and models and datasets used in this paper are implemented using the Deep Graph Library (DGL) and Pytorch Geometric (PyG). Further details on the specific parameter settings can be found in Appendix G.

5.3   Effectiveness in mitigating over-smoothing (RQ1)

In this section, we aim to assess whether the PSNR module can mitigate the oversmoothing phenomenon in deep GNNs. We select representative datasets Cora, Amazon-Photo, and Chameleon. Using GCN as the backbone network, we compare our method against several residual methods: ResGCN, GCNII, JKNet, and DenseGNN. We set the number of layers to 2, 4, 8, 16, 32, 64 and test on ten random splits, with the average accuracy serving as the final result. The experimental results are depicted in Figure 3. Consistent with the analysis in the main text, most methods can alleviate over-smoothing, but at deeper layers, such as 64 layer, over-smoothing still occurs. In contrast, compared to other residual methods, PSNR maintains stable performance even at deeper layers, demonstrating remarkable effectiveness in mitigating over-smoothing in deep GNNs. This is attributed to PSNR module can effectively reduce the loss of high-order neighborhood subgraph information. It is noteworthy that among the various residual methods, another initial residual method GCNII also alleviate over-smoothing well. However, the subsequent experiment will reveal that although the performance of GCNII remains relatively stable with varying layers, it leads to a decrease in overall performance.

7

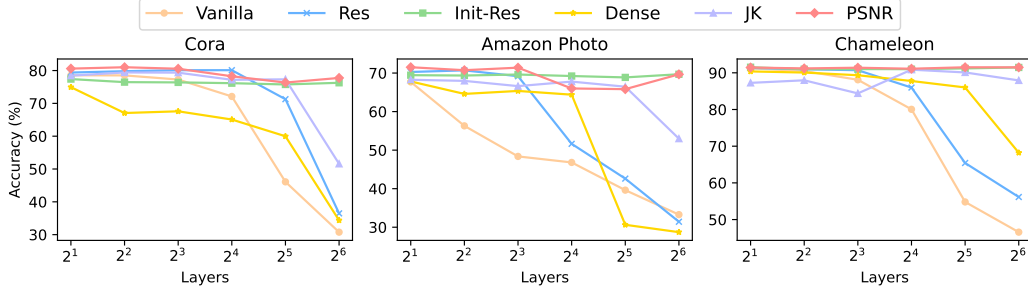



Figure 3: Different residual methods' effectiveness in mitigating over-smoothing.

Table 3: Summary of classification accuracy (%) results on real-world datasets. The best results are in bold, and the second best results are underlined.

Method	Cora	Citeseer	CS	Photo	Chameleon	Squirrel	*Avg. Rank*
GCN	78.56±1.57	66.00±2.37	90.19±0.83	91.22±0.73	67.70±0.17	47.43±1.31	6.67
ResGCN	80.11±0.98	66.40±2.29	90.86±0.99	91.31±0.85	70.70±1.54	52.43±1.72	3.67
GCNII	77.40±1.43	66.69±1.95	90.34±0.78	91.46±0.84	69.69±1.36	46.13±1.59	5.00
DenseGCN	74.94±2.46	62.54±2.56	90.28±1.06	90.38±1.02	67.82±1.27	49.57±1.58	7.17
JKNet	79.42±1.48	65.49±2.32	90.94±0.89	90.85±1.19	68.26±1.15	49.87±1.44	5.17
Half-Hop-GCN	80.74±1.80	67.76±2.19	90.30±1.83	89.32±1.17	60.07±2.34	42.78±1.01	6.33
DropMessage-GCN	80.00±2.22	67.66±1.84	90.64±2.34	91.40±0.90	65.91±2.43	45.71±1.76	4.83
DeProp-GCN	79.52±2.63	67.24±2.02	90.98±2.04	91.38±1.33	61.51±1.40	44.07±1.07	5.17
PSNR-GCN	**81.01±1.63**	**68.06±2.12**	**91.23±1.00**	**91.51±0.69**	**71.51±1.90**	**54.95±1.73**	**1.00**
GAT	79.21±1.31	67.12±1.59	89.43±1.62	89.64±0.84	68.04±1.36	47.93±1.99	6.00
Res-GAT	79.72±1.94	67.19±1.91	89.92±0.86	91.40±0.74	**72.66±0.94**	55.98±2.12	2.83
Init-Res-GAT	79.67±1.71	66.84±2.52	89.61±1.02	91.53±1.06	69.89±1.81	51.29±1.42	4.17
JK-GAT	80.04±1.61	65.83±2.21	90.10±0.94	90.82±1.24	67.98±1.71	50.43±1.45	4.50
Dense-GAT	73.39±1.52	61.23±2.53	89.72±0.86	88.92±1.66	67.36±1.95	50.25±0.88	7.00
DropMessage-GAT	80.36±1.92	67.82±2.04	**90.67±1.68**	90.98±0.90	63.23±2.23	45.23±1.35	4.33
DeProp-GAT	76.00±2.08	61.16±3.50	87.34±1.42	89.76±1.52	64.23±3.22	46.29±3.24	8.00
Half-Hop-GAT	77.24±1.69	66.74±1.98	89.66±1.45	89.92±0.77	62.86±2.04	47.84±4.36	6.83
PSNR-GAT	**80.47±1.62**	**68.01±2.14**	90.38±1.21	**91.64±0.61**	72.24±1.69	**60.85±1.61**	1.33

5.4 Fully observed feature setting (RQ2)

The PSNR module can effectively address the performance degradation of GNNs at deeper layers, but can it further enhance the overall performance of the model? In this section, we comprehensively evaluate the PSNR module across a wider range of datasets. Under the fully observed feature setting, we set the number of layers to 2, 4, 8, 16, 32, 64, and conduct experiments on ten random splits for each dataset, taking the average accuracy as the final result for each layer. The results of all layers of the model can be found in Appendix A. To evaluate the overall performance, we record the best results of each model in all layers for each dataset in Table 3.

As can be observed from the Table 3, PSNR outperforms all baselines in most cases. For example, compared to the vanilla model, PSNR improves the test accuracy on the Squirrel dataset by 7.52% and 12.92%, respectively. Compared with the vanilla GCN and GAT, the proposed PSNR can significantly improve the performance under the fully observed feature setting.

5.5 Missing feature setting (RQ3)

When do we need the deeper GNN? Real-world data often contain missing features. In that scenario, previous research [33] has shown that deep GNNs can help improve performance. For the nodes with missing features, due to the lack of information, they need a deeper network to gather more neighborhood information, thereby achieving better node representations. However, deep GNNs face the issue of performance degradation. In this section, we examine if PSNR module can improve the performance of GNNs in the context of missing feature.

Consistent with [33, 18, 12], we evaluate the performance of GNNs on three datasets, Cora, Citeseer, and Pubmed, and remove their node features from validation and test sets. Under this setting, the test nodes need more propagation layers to reach the training nodes. We reuse the metrics that already reported in [12] for None, BatchNorm [11], PairNorm [33], DGN [34], DeCorr [12], and DropEdge [24]. For all residual-based models, the results are obtained by varying the number of layers in

8

Table 4: Test accuracy (%) on missing feature setting. The best results are in bold and the second best results are underlined.

	GCN						GAT					
	Cora		Citeseer		Pubmed		Cora		Citeseer		Pubmed	
Module	Acc	#K	Acc	#K	Acc	#K	Acc	#K	Acc	#K	Acc	#K
None	57.3	3	44.0	6	36.4	4	50.1	2	40.8	4	38.5	4
BatchNorm	71.8	20	45.1	25	70.4	30	72.7	5	48.7	5	60.7	4
PairNorm	65.6	20	43.6	25	63.1	30	68.8	8	50.3	6	63.2	20
DGN	76.3	20	50.2	30	72.0	30	75.8	8	54.5	5	72.3	20
DeCorr	73.8	20	49.1	30	73.3	15	72.8	15	46.5	6	72.4	15
DropEdge	67.0	6	44.2	8	69.3	6	67.2	6	48.2	6	67.2	6
Res	_76.8_	_8_	60.4	10	76.6	6	76.5	8	60.5	6	_76.9_	_8_
Init-Res	65.1	6	50.7	15	70.4	10	_77.1_	_8_	60.6	8	76.8	6
Dense	66.2	4	51.5	2	74.1	8	68.5	10	52.7	2	75.1	10
JK	75.5	30	60.4	8	_76.9_	_6_	77.0	10	60.3	4	76.8	6
DropMessage	75.5	10	_61.0_	_6_	74.6	6	76.5	6	_61.1_	_8_	76.6	6
DeProp	71.4	6	59.4	2	76.1	4	68.04	2	48.3	2	75.8	4
Half-Hop	73.7	8	59.48	6	76.5	6	76.0	20	59.6	4	_76.9_	_6_
PSNR	**77.3**	**20**	**61.1**	**15**	**77.0**	**30**	**77.9**	**8**	**61.9**	**15**	**77.3**	**10**

$\{2, 4, 6, 8, 10, 15, 20, 30\}$ and running five times for each number of layers. We select the layer #K that achieves the best performance and report its average accuracy. The results are reported in Table 4. By examining the results in Table 4, under the missing feature setting, the optimal number of layers to achieve the best performance is significantly higher than in the fully observed feature setting, demonstrating the importance of deep GNNs. And PSNR outperform other baselines in all cases through alleviating over-smoothing more effectively. Specially, on the Pubmed dataset, PSNR boost the accuracy of GCN and GAT by 40.6% and 38.8%, respectively.

5.6 Performance on large graphs (RQ4)

To validate the scalability of PSNR, we conducted additional experiments on three larger graph datasets i.e., Coauthor-Physics, Flickr and Ogbn-arxiv, to further validate the effectiveness and scalability of our method. Specifically, we selected the GCN backbone for our experiment. We report the performance of GCN and various residual methods on three datasets and the memory consumption on the largest dataset, Ogbn-arxiv. The experimental results are presented in Table 5, from which we observe that PSNR-GCN scales well and achieves the best results across all three large datasets. Meanwhile, in terms of memory consumption, PSNR is slightly higher than GCN and ResGCN, comparable to GCNII with the same initial residuals, and significantly lower than JKNet and DenseGCN. Regarding training time, PSNR is roughly at the same level as JKNet, and its time is shorter than that of DenseNet.

Table 5: Comparison of different methods across various datasets and memory consumption (MB) and training time (ms / epoch) on Ogbn-arxiv. The best performance for each dataset is in bold, while the second best is underlined.

Method	Phy	Flickr	Ogbn-arxiv	Memory	Time
GCN	95.32 ± 0.11	51.40 ± 0.33	64.37 ± 0.41	2421	30.10
ResGCN	95.61 ± 0.18	51.90 ± 0.16	$\underline{66.32 \pm 0.59}$	2463	36.06
GCNII	$\underline{95.90 \pm 0.14}$	46.18 ± 0.21	61.43 ± 1.63	2525	33.33
JKNet	95.88 ± 0.15	51.65 ± 0.31	60.46 ± 1.21	2921	40.05
DenseGCN	95.50 ± 0.12	$\underline{52.18 \pm 0.25}$	62.46 ± 1.58	3131	52.24
PSNR-GCN	$\mathbf{95.92 \pm 0.17}$	$\mathbf{52.47 \pm 0.16}$	$\mathbf{67.81 \pm 0.57}$	2539	42.93

6 Conclusion and Future Work

In this paper, we addressed the oversmoothing in Graph Neural Networks (GNNs) with a focus on residual methods. We revisit the oversmoothing from the perspective of overlapping neighborhood subgraphs, explaining why residual methods can alleviate it. Our analysis revealed that current residual methods often lack node adaptivity and struggle with information loss in high-order neighborhoods subgraphs. To overcome these limitations, we introduce the Posteriori-Sampling-based Node-Adaptive Residual Module (PSNR). This innovative module uses a graph encoder to learn the posterior distribution of residual coefficients for each node at different layers, enabling fine-grained,

9

node-adaptive neighborhood subgraph aggregation with minimal overhead. Extensive experiments confirmed that the PSNR module can effectively mitigate oversmoothing and improve performance, particularly in scenarios requiring deep networks. Despite the significant progress made by PSNR, training a deeper GNN remains challenging, prompting the need for further research in the future.

7 Acknowledgements

This work was supported by National Science and Technology Major Project (No. 2022ZD0115101), National Natural Science Foundation of China Project (No. 623B2086, No. U21A20427), Project (No. WU2022A009) from the Center of Synthetic Biology and Integrated Bioengineering of Westlake University and Integrated Bioengineering of Westlake University and Project (No. WU2023C019) from the Westlake University Industries of the Future Research Funding. Carl Yang was not supported by any funds from China.

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10

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11

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12

A   Fully Observed Node Classification

Table 6: Node classification accuracy (%) on GCN backbone. The best results across different layers are highlighted.

Datasets	Model	Layer 2	Layer 4	Layer 8	Layer 16	Layer 32	Layer 64
Cora	GCN	78.56±1.57	78.52±2.02	77.27±2.29	72.11±6.30	46.09±12.12	30.76±1.30
	ResGCN	79.39±1.12	79.80±1.53	80.10±1.46	80.11±0.98	71.27±3.65	36.48±7.53
	GCNII	77.40±1.43	76.47±1.96	76.39±1.88	76.15±1.70	75.76±1.83	76.27±1.46
	DenseGCN	74.94±2.46	67.06±2.02	67.58±2.66	65.08±3.71	59.98±2.30	34.37±5.69
	JKNet	78.44±2.10	79.42±1.48	79.36±2.23	77.18±2.17	77.33±2.88	51.58±7.29
	DropMessage-GCN	80.00±2.22	79.88±1.81	78.14±1.65	76.40±1.22	52.18±1.06	30.34±0.63
	DeProp-GCN	79.52±2.63	78.44±2.39	33.02±5.64	31.28±3.24	30.20±0.01	30.20±0.01
	Half-Hop-GCN	78.92±2.08	80.74±1.80	80.24±1.61	46.66±13.37	43.68±7.14	31.03±7.39
	PSNR-GCN	80.59±1.57	81.01±1.63	80.55±1.57	78.26±1.36	76.34±2.18	77.75±2.27
Citeseer	GCN	66.00±2.37	64.13±2.31	64.13±2.10	58.52±3.31	27.21±3.98	27.52±5.04
	Res-GCN	66.11±1.65	66.40±2.29	65.97±1.93	65.46±2.02	48.70±3.77	33.74±4.79
	GCNII	66.69±1.95	66.18±1.74	66.50±1.77	66.31±2.08	66.27±1.92	66.50±2.59
	Dense-GCN	62.54±2.56	58.99±3.74	54.35±5.42	50.10±5.24	49.09±4.03	31.43±5.54
	JKNet	65.49±2.32	64.40±2.28	64.18±3.07	63.77±1.87	60.88±3.53	29.66±7.51
	DropMessage-GCN	67.66±1.84	67.04±2.20	63.84±2.66	59.82±2.75	22.68±3.77	21.38±1.72
	Half-Hop-GCN	67.76±2.19	67.46±1.99	67.02±2.53	54.48±3.93	38.40±8.33	24.14±3.48
	DeProp-GCN	67.24±2.02	64.86±2.93	29.08±10.03	21.72±0.91	21.94±1.18	20.98±1.13
	PSNR-GCN	68.06±2.12	66.03±1.93	65.46±1.59	65.81±2.39	65.52±1.76	65.85±2.30
CS	GCN	90.19±0.83	88.81±0.62	86.93±0.83	84.47±0.95	71.40±4.93	36.74±4.57
	Res-GCN	90.86±0.99	90.63±0.96	89.97±0.90	88.40±0.90	85.01±1.53	64.39±3.86
	GCNII	90.34±0.78	90.02±0.81	90.07±0.77	90.09±0.94	90.17±0.52	89.93±0.70
	Dense-GCN	89.01±1.09	89.99±1.27	90.28±1.06	89.33±1.73	88.92±1.08	88.40±1.37
	JKNet	90.81±1.35	90.94±0.89	90.53±1.41	89.52±1.11	88.81±1.14	88.44±1.44
	DropMessage-GCN	90.64±2.34	89.18±1.76	89.38±1.52	85.62±7.01	87.94±6.18	84.44±1.13
	Half-Hop-GCN	90.30±1.83	89.30±2.23	88.98±1.81	82.98±1.88	54.60±4.55	25.36±10.27
	DeProp-GCN	90.98±2.04	89.10±2.23	71.24±4.18	72.34±2.26	52.60±0.03	22.60±0.01
	PSNR-GCN	91.23±1.00	90.70±1.49	90.26±1.17	90.26±0.98	90.52±1.02	90.30±0.88
Photo	GCN	91.22±0.73	90.49±0.76	88.10±1.02	80.05±4.25	54.80±8.00	46.57±9.64
	Res-GCN	91.31±0.85	90.97±0.78	90.71±0.78	85.98±2.36	65.42±6.75	56.15±10.43
	GCNII	91.02±0.93	90.98±0.92	91.02±0.70	90.99±0.76	91.20±0.81	91.46±0.84
	Dense-GCN	90.38±1.02	90.07±1.76	89.34±1.40	87.77±2.00	86.01±1.91	68.22±17.58
	JKNet	87.26±1.77	87.96±1.91	84.39±2.76	90.85±1.19	90.10±1.20	87.93±2.66
	DropMessage-GCN	91.40±0.90	90.22±1.19	87.57±2.74	87.82±1.21	86.12±1.05	80.40±1.07
	Half-Hop-GCN	52.00±17.28	67.48±24.16	89.32±1.17	83.66±3.02	64.40±4.30	39.00±9.42
	DeProp-GCN	91.38±1.33	89.50±5.31	78.12±3.66	81.86±9.36	87.74±4.19	84.43±2.31
	PSNR-GCN	91.44±0.82	91.20±1.03	91.39±0.76	91.11±0.68	91.51±0.69	91.49±0.88
Chameleon	GCN	67.70±0.17	56.30±2.28	48.37±1.56	46.81±2.06	39.62±2.13	33.27±1.86
	Res-GCN	70.28±1.14	70.70±1.54	69.18±0.78	51.64±2.11	42.61±3.60	31.42±2.73
	GCNII	69.45±1.63	69.36±1.13	69.62±1.61	69.23±1.21	68.87±2.16	69.69±1.36
	Dense-GCN	67.82±1.27	64.59±1.29	65.36±1.50	64.39±1.37	30.63±3.98	28.72±4.66
	JKNet	68.26±1.15	67.97±1.59	66.61±1.76	67.78±1.60	66.46±2.25	52.98±2.79
	DropMessage-GCN	65.91±2.43	60.50±2.84	47.29±2.00	42.66±1.60	34.56±1.61	31.74±1.56
	Half-Hop-GCN	60.07±2.34	55.72±3.12	52.64±1.99	43.19±2.55	36.26±2.12	29.34±2.20
	DeProp-GCN	61.51±1.40	58.25±2.22	46.46±2.18	31.88±2.52	30.81±2.07	33.36±0.96
	PSNR-GCN	71.51±1.90	70.74±2.24	71.40±1.83	66.00±1.97	65.82±2.02	69.67±4.59
Squirrel	GCN	47.43±1.31	41.68±1.80	37.43±1.35	33.17±1.22	31.99±1.14	29.83±1.98
	Res-GCN	51.72±1.63	52.43±1.72	50.38±1.90	38.35±1.56	26.30±2.06	22.66±1.01
	GCNII	46.13±1.59	45.28±1.59	45.71±2.08	45.37±1.72	45.06±1.50	45.32±1.85
	Dense-GCN	49.57±1.58	49.01±0.98	49.51±1.30	49.08±1.36	49.29±1.25	49.04±1.30
	JKNet	49.87±1.44	49.11±2.27	46.62±1.44	24.79±3.88	45.73±1.80	41.75±1.96
	DropMessage-GCN	45.71±1.76	38.68±2.02	26.67±3.06	25.71±1.15	23.77±1.18	20.06±0.23
	Half-Hop-GCN	42.78±1.01	41.87±1.36	37.84±1.68	31.60±2.12	26.36±1.66	21.07±1.53
	DeProp-GCN	44.07±1.07	40.98±1.29	33.38±1.70	28.33±0.96	28.42±0.54	29.98±2.78
	PSNR-GCN	54.95±1.73	54.13±1.41	50.68±1.45	50.22±6.32	50.06±0.97	50.24±1.58

13

Table 7: Node classification accuracy (%) on GAT backbone. The best results across different layers are highlighted.

Datasets	Model	Layer 2	Layer 4	Layer 8	Layer 16	Layer 32	Layer 64
Cora	GAT	79.21±1.31	78.83±1.78	41.48±2.84	30.20±0.00	30.20±0.00	30.20±0.00
	Res-GAT	79.42±1.46	79.72±1.94	78.88±1.69	78.71±2.13	77.80±2.25	30.22±0.12
	InitRes-GAT	79.32±1.65	79.39±1.45	79.00±1.97	79.16±1.68	79.67±1.71	79.42±1.97
	Dense-GAT	73.39±1.52	69.07±2.76	58.85±3.02	60.34±2.12	59.44±3.03	55.80±3.12
	JK-GAT	79.32±1.06	80.04±1.61	77.28±1.62	77.58±1.51	77.53±1.29	77.58±2.91
	DropMessage-GAT	80.06±2.50	80.36±1.92	79.20±0.22	76.54±2.49	52.54±1.02	30.17±0.06
	DeProp-GAT	76.00±2.08	69.06±3.94	30.22±0.06	31.20±0.02	30.20±0.01	30.20±0.01
	Half-Hop-GAT	77.20±1.86	76.98±1.42	77.24±1.69	75.84±1.68	70.50±4.69	30.20±0.10
	PSNR-GAT	80.47±1.62	80.22±0.98	79.96±1.69	80.02±1.64	79.43±1.78	79.69±1.29
Citeseer	GAT	67.12±1.59	65.14±3.02	21.90±2.40	21.10±0.00	21.10±0.00	21.10±0.00
	Res-GAT	67.19±1.91	65.65±2.21	63.26±2.31	63.47±1.18	62.82±2.92	22.66±1.31
	InitRes-GAT	66.84±2.52	64.15±2.44	65.80±1.89	64.89±2.65	64.69±2.49	65.11±2.65
	Dense-GAT	61.63±2.53	54.84±2.34	50.69±3.79	49.21±3.48	47.24±3.08	46.34±3.62
	JK-GAT	65.83±2.21	64.79±2.46	63.44±2.51	65.00±1.43	63.57±2.27	62.08±2.26
	DropMessage-GAT	67.82±2.04	66.64±2.51	65.10±3.32	58.20±2.55	21.90±1.64	20.90±2.04
	DeProp-GAT	61.16±3.50	51.52±11.25	23.20±2.77	21.12±1.76	21.00±1.67	20.50±0.92
	Half-Hop-GAT	66.74±1.98	66.70±2.58	63.12±3.49	60.00±3.30	45.98±4.63	24.32±4.46
	PSNR-GAT	68.01±2.14	65.61±2.05	66.46±2.14	65.48±2.59	66.36±2.25	65.50±2.35
CS	GAT	89.43±1.62	77.23±10.14	72.63±5.30	38.81±6.52	22.60±0.00	22.60±0.00
	Res-GAT	89.48±1.25	83.48±3.39	89.92±0.86	64.30±19.93	23.10±1.45	22.46±2.22
	InitRes-GAT	89.61±1.02	77.82±5.90	89.43±1.23	88.50±1.17	88.20±1.22	86.90±2.30
	Dense-GAT	89.72±0.86	88.81±0.89	88.28±0.72	87.01±1.52	86.47±1.13	87.23±1.78
	JK-GAT	89.77±1.02	90.10±0.94	90.03±1.26	89.68±1.41	89.66±1.04	89.86±1.12
	DropMessage-GAT	90.67±1.68	89.20±1.58	87.58±1.46	85.68±1.29	84.58±1.40	81.43±1.13
	DeProp-GAT	87.34±1.42	84.18±1.99	72.26±2.77	72.36±2.34	52.60±0.02	22.60±0.01
	Half-Hop-GAT	89.66±1.45	89.30±1.84	84.12±2.27	84.75±2.96	56.20±5.96	29.61±9.70
	PSNR-GAT	90.38±1.12	86.31±2.68	84.48±1.24	83.84±1.38	81.85±3.55	79.85±5.24
Photo	GAT	89.64±0.84	42.4±18.86	51.13±10.00	27.97±7.71	25.40±0.00	25.40±0.00
	Res-GAT	89.03±1.33	89.30±4.68	91.40±0.74	88.60±1.79	25.61±4.23	26.16±1.88
	InitRes-GAT	88.92±2.22	31.74±3.12	91.23±1.22	90.72±1.40	91.53±1.06	91.11±1.21
	Dense-GAT	88.92±1.66	88.10±1.50	87.03±2.22	86.79±1.97	86.24±2.65	85.63±2.15
	JK-GAT	87.55±1.39	90.82±1.24	90.35±1.61	90.30±1.37	90.29±1.49	90.07±1.48
	DropMessage-GAT	90.98±0.90	90.29±0.97	82.15±2.82	84.96±1.56	85.10±0.90	82.15±1.32
	DeProp-GAT	89.76±1.52	87.98±1.05	82.54±1.01	81.25±2.88	82.26±2.17	80.00±2.11
	Half-Hop-GAT	89.92±0.77	85.48±1.89	85.16±2.77	72.12±1.54	67.84±1.08	45.51±0.65
	PSNR-GAT	90.93±1.42	91.48±0.94	91.33±1.05	91.05±0.95	91.64±0.61	91.37±0.96
Chameleon	GAT	68.04±1.36	48.37±3.71	26.86±6.17	22.86±0.00	22.86±0.00	22.86±0.00
	Res-GAT	70.90±1.34	67.87±3.43	72.66±0.94	66.68±1.13	27.54±3.63	27.27±3.44
	InitRes-GAT	69.87±1.65	61.63±5.02	69.89±1.81	69.34±1.34	68.62±1.32	68.53±1.23
	Dense-GAT	67.36±1.95	66.87±2.07	66.21±2.03	61.95±2.14	62.32±2.10	61.71±1.69
	JK-GAT	67.98±1.71	65.71±1.40	66.75±1.88	66.99±2.23	66.24±1.42	66.31±1.56
	DropMessage-GAT	63.23±2.23	56.98±2.54	48.53±2.95	47.00±1.93	40.19±1.82	33.75±2.23
	DeProp-GAT	64.23±3.22	53.31±4.19	42.29±2.77	41.19±2.17	32.29±2.77	32.26±0.85
	Half-Hop-GAT	62.86±2.04	60.34±2.01	50.58±7.19	43.05±1.74	33.75±2.37	32.27±1.42
	PSNR-GAT	71.29±1.64	72.04±1.82	71.58±1.99	71.78±1.51	71.47±2.54	72.24±1.69
Squirrel	GAT	47.93±1.99	32.96±1.85	20.57±1.02	20.00±0.00	20.00±0.00	20.00±0.00
	Res-GAT	52.87±1.68	49.87±4.74	55.98±2.12	50.31±1.68	23.07±1.98	22.01±1.26
	InitRes-GAT	51.29±1.42	43.92±5.77	49.83±1.55	50.34±1.17	50.30±1.81	50.46±1.75
	Dense-GAT	50.25±0.88	49.57±1.80	46.71±1.69	47.83±1.70	47.54±1.58	46.87±1.65
	JK-GAT	50.43±1.45	44.41±2.33	49.08±0.79	49.31±1.99	48.87±1.74	49.56±1.31
	DropMessage-GAT	45.23±1.35	40.31±1.25	30.69±1.84	29.44±1.34	28.35±2.50	25.47±1.33
	DeProp-GAT	45.76±1.32	46.29±3.24	29.99±0.28	28.97±0.56	28.91±0.23	20.00±0.04
	Half-Hop-GAT	43.46±1.57	47.84±4.36	42.53±1.53	29.19±1.50	24.37±1.54	23.79±0.65
	PSNR-GAT	57.81±2.08	60.85±1.61	59.58±2.09	60.43±2.20	60.00±2.20	60.20±1.53

14

B   Residual Connection Defination

Common residual connection for GNNs and their corresponding GNNs are described below.

Res. Res is composed of multiple residual blocks containing few stacked layers. Taking the initial input of the n-th residual block as $\mathbf{X}_n$, and the stacked nonlinear layers within the residual block as $\mathbf{F}(\mathbf{X})$:

$$\mathbf{X}_{n+1} = \mathbf{F}(\mathbf{X}_n) + \mathbf{X}_n,$$

where residual mapping and identity mapping refer to $\mathbf{F}(\mathbf{X})$ and $\mathbf{X}$ on the right side of the above equation, respectively. Inspired by Res, Guohao Li & Matthias Müller(2019) proposed a residual connection learning framework for GCN and called this model ResGCN which can be simply described as follows:

$$\mathbf{H}_k = \sigma \left(\tilde{\mathbf{D}}^{-\frac{1}{2}} \tilde{\mathbf{A}} \tilde{\mathbf{D}}^{-\frac{1}{2}} \mathbf{H}_{k-1} \mathbf{W}_{k-1} \right) + \mathbf{H}_{k-1}.$$

InitialRes. InitialRes is proposed for the first time in APPNP, unlike Res that carries information from the previous layers, it constructs a connection to the initial representation $\mathbf{X}_0$ at each layer:

$$\mathbf{X}_{n+1} = (1 - \alpha)\mathbf{H}(\mathbf{X}_n) + \alpha\mathbf{X}_0,$$

where $\mathbf{H}(\mathbf{X})$ denotes the aggregation operation within one layer. InitialRes ensures that each node's representation retains at least an α-sized portion of the initial feature information. Correspondingly, APPNP can be formulated as:

$$\mathbf{H}_k = (1 - \alpha) \tilde{\mathbf{D}}^{-\frac{1}{2}} \tilde{\mathbf{A}} \tilde{\mathbf{D}}^{-\frac{1}{2}} \mathbf{H}_{k-1} + \alpha\mathbf{H}.$$

Based on APPNP, GCNII introduces identity mapping from Res to make up for the deficiency in APPNP.

Dense. Dense proposes a more efficient way to reuse features between layers. The input is the outputs of all previous layers of the network and at each layer Dense concats them together:

$$\mathbf{X}_{n+1} = \mathbf{H}([\mathbf{X}_0, \mathbf{X}_1, \dots, \mathbf{X}_n]),$$

where $[\cdot]$ denotes the concatenation of the feature map for the output of layers 0 to n. Inspired by Dense, DenseGCN applies a similar idea to GCN, i.e., let the output of the k-th layer contains transformations from all previous GCN layers to exploit the information from different GCN layers:

$$\mathbf{H}_k = \mathbf{AGG}_{dense}(\mathbf{H}, \mathbf{H}_1, \dots, \mathbf{H}_{k-1}).$$

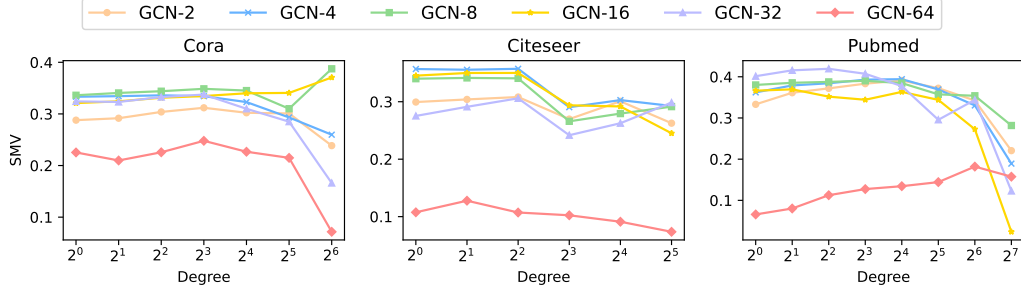
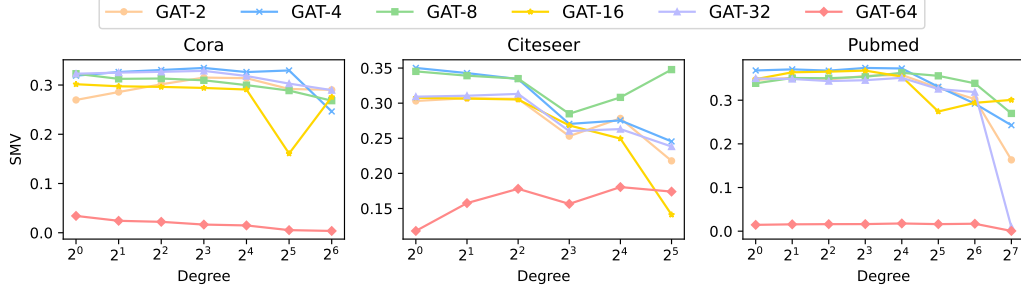
JK. At the last layer, JK sifts from all previous representations $[\mathbf{X}_1, \dots, \mathbf{X}_N]$ and combines them:

$$\mathbf{X}_{output} = \mathbf{AGG}(\mathbf{X}_1, \dots, \mathbf{X}_N).$$

The $\mathcal{AGG}$ operation includes concatenation, Maxpooling and LSTM-attention. When it is introduced to GNN, i.e., JKNet, can be formulated as:

$$\mathbf{H}_{output} = \mathbf{AGG}_{jk}(\mathbf{H}_1, \dots, \mathbf{H}_{k-1}).$$

15

C   SMV for Node Groups of Different Degrees

Result of GCN.

Result of GAT.

D   Derivation of the closed-form formulas in the table

ResGCN: We can write the recursive formula for ResGCN in the following form:

$$\mathbf{H}_k = (\mathbf{I} + \mathbf{N})\mathbf{H}_{k-1}. \tag{6}$$

In turn, the following form can be obtained by recursion:

$$\mathbf{H}_k = (\mathbf{I} + \mathbf{N})^k \mathbf{H}. \tag{7}$$

Using the binomial theorem, we can obtain the closed-form formula for ResGCN as follows:

$$\mathbf{H}_k = \sum_{j=0}^{k} \mathbf{C}_k^j \mathbf{N}^j \mathbf{H}. \tag{8}$$

APPNP: According to the recurrence formula of APPNP:

$$\mathbf{H}_k = \alpha \mathbf{H} + (1 - \alpha) \mathbf{N} \mathbf{H}_{k-1}. \tag{9}$$

To obtain the closed-form formula, we can add a term $\mathbf{T}$ to both sides of the equation:

$$\mathbf{H}_k + \mathbf{T} = (1 - \alpha)\, \mathbf{N} \mathbf{H}_{k-1} + \alpha \mathbf{H} + \mathbf{T}. \tag{10}$$

We aim to transform the equation into the following form:

$$\mathbf{H}_k + \mathbf{T} = (1 - \alpha)\, \mathbf{N} \left(\mathbf{H}_{k-1} + \mathbf{T}\right). \tag{11}$$

Then we need to make sure that there exists a very $\mathbf{T}$ that satisfies the following equation:

$$(1 - \alpha)\, \mathbf{N}\mathbf{T} = \alpha \mathbf{H} + \mathbf{T}, \tag{12}$$

which can be transformed into the following form:

$$((1 - \alpha)\, \mathbf{N} - \mathbf{I})\, \mathbf{T} = \alpha \mathbf{H}. \tag{13}$$

We can proof the following lemma:

16

Lemma 1 *Given that $\alpha \in (0,1)$, $(1-\alpha)\mathbf{N} - \mathbf{I}$ is invertible.*

Proof 1 *Proving that $(1-\alpha)\mathbf{N} - \mathbf{I}$ is invertible is equivalent to demonstrating that it does not possess an eigenvalue of 0. Consider the Rayleigh quotient of $(1-\alpha)\mathbf{N} - \mathbf{I}$:*

$$\frac{\mathbf{X}^T\left((1-\alpha)\mathbf{N} - \mathbf{I}\right)\mathbf{X}}{\mathbf{X}^T\mathbf{X}} = (1-\alpha)\frac{\mathbf{X}^T\left(\tilde{\mathbf{D}}^{-\frac{1}{2}}\tilde{\mathbf{A}}\tilde{\mathbf{D}}^{-\frac{1}{2}}\right)\mathbf{X}}{\mathbf{X}^T\mathbf{X}} - 1. \tag{14}$$

From spectral graph theory, we can know the following equation holds:

$$\mathbf{X}^T\left(\tilde{\mathbf{D}}^{-\frac{1}{2}}\mathbf{L}\tilde{\mathbf{D}}^{-\frac{1}{2}}\right)\mathbf{X} = \sum_{(v_i,v_j)\in\mathcal{E}}\left(\frac{\mathbf{X}_i}{\sqrt{d_i+1}} - \frac{\mathbf{X}_j}{\sqrt{d_j+1}}\right)^2 > 0. \tag{15}$$

We can decompose $\mathbf{L}$ into $\tilde{\mathbf{D}} - \tilde{\mathbf{A}}$, then we have:

$$\frac{\mathbf{X}^T\left(\tilde{\mathbf{D}}^{-\frac{1}{2}}\tilde{\mathbf{D}}\tilde{\mathbf{D}}^{-\frac{1}{2}}\right)\mathbf{X}}{\mathbf{X}^T\mathbf{X}} - \frac{\mathbf{X}^T\left(\tilde{\mathbf{D}}^{-\frac{1}{2}}\tilde{\mathbf{A}}\tilde{\mathbf{D}}^{-\frac{1}{2}}\right)\mathbf{X}}{\mathbf{X}^T\mathbf{X}} > 0, \tag{16}$$

which is equivalent to:

$$\frac{\mathbf{X}^T\left(\tilde{\mathbf{D}}^{-\frac{1}{2}}\tilde{\mathbf{A}}\tilde{\mathbf{D}}^{-\frac{1}{2}}\right)\mathbf{X}}{\mathbf{X}^T\mathbf{X}} < \frac{\mathbf{X}^T\mathbf{I}\mathbf{X}}{\mathbf{X}^T\mathbf{X}} = 1. \tag{17}$$

Combining Eq. 14 and Ineq. 17, we can obtain:

$$\frac{\mathbf{X}^T\left((1-\alpha)\mathbf{N} - \mathbf{I}\right)\mathbf{X}}{\mathbf{X}^T\mathbf{X}} < (1-\alpha) - 1 = -\alpha < 0. \tag{18}$$

Hence, 0 can't be the eigenvalue of $(1-\alpha)\mathbf{N} - \mathbf{I}$. Therefore, $(1-\alpha)\mathbf{N} - \mathbf{I}$ is invertible.

Since **Lemma 1** holds, we can derive the concrete form of $\mathbf{T}$:

$$\mathbf{T} = \alpha\left((1-\alpha)\mathbf{N} - \mathbf{I}\right)^{-1}\mathbf{H}. \tag{19}$$

Thus we can keep recurring from Eq. 11 and obtain the following equation:

$$\mathbf{H}_k + \mathbf{T} = \left((1-\alpha)\mathbf{N}\right)^k\left(\mathbf{H} + \mathbf{T}\right), \tag{20}$$

which also can be written as:

$$\mathbf{H}_k = \left((1-\alpha)\mathbf{N}\right)^k\mathbf{H} + \left((1-\alpha)\mathbf{N}\right)^k\mathbf{T} - \mathbf{T}. \tag{21}$$

For the second and third terms in Eq. 21, we write $(1-\alpha)\mathbf{N}$ as $(1-\alpha)\mathbf{N} - \mathbf{I} + \mathbf{I}$. We can use the binomial theorem to write $\left((1-\alpha)\mathbf{N}\right)^k$ as $\sum_{j=0}^{k}\left((1-\alpha)\mathbf{N} - \mathbf{I}\right)^j$, then Eq. 21 can be written as :

$$\mathbf{H}_k = \left((1-\alpha)\mathbf{N}\right)^k\mathbf{H} + \sum_{j=1}^{k}\left((1-\alpha)\mathbf{N} - \mathbf{I}\right)^j\mathbf{T}. \tag{22}$$

Bring in the specific form of $\mathbf{T}$ and further derive the closed-form formula of APPNP:

$$\mathbf{H}_k = \left((1-\alpha)\mathbf{N}\right)^k\mathbf{H} + \alpha\sum_{j=0}^{k-1}\left((1-\alpha)\mathbf{N} - \mathbf{I}\right)^j\mathbf{H} \tag{23}$$

$$= (1-\alpha)^k\mathbf{N}^k\mathbf{H} + \alpha\sum_{j=0}^{k-1}\sum_{i=0}^{j}(-1)^{j-i}(1-\alpha)^i\mathbf{N}^i\mathbf{H}. \tag{24}$$

17

E Derivation of the closed-form formula of PSNR-GCN

For each diagonal element $\Lambda_{k,ii}$ of Λ_k, it is trivial to obtain:

$$0 < \Lambda_{k,ii} < 1.$$

To derive the closed-form formula of PSNR-GCN, we need proof the following lemma first.

Lemma 2 *Set all the diagonal elements of Λ to satisfy $0 < \Lambda_{ii} < 1$, then $(\Lambda\mathbf{N} + \mathbf{I})$ is invertible.*

Proof 2 *Proving that $\Lambda\mathbf{N} + \mathbf{I}$ is invertible is equivalent to demonstrating that its determinant is not equal to 0. Because all the diagonal elements of Λ satisfy $0 < \Lambda_{ii} < 1$, then Λ is invertible. And due to*

$$|\Lambda\mathbf{N} + \mathbf{I}| = |\Lambda||\mathbf{N} + \Lambda^{-1}|. \tag{25}$$

Therefore, proving that its determinant is not equal to 0 is equivalent to demonstrating that $|\mathbf{N} + \Lambda^{-1}|$ is not equal to 0, and further equivalent to demonstrating that $\mathbf{N} + \Lambda^{-1}$ does not have an eigenvalue of 0.

Consider the Rayleigh quotient of $\mathbf{N} + \Lambda^{-1}$:

$$\mathbf{R}_1 = \frac{\mathbf{X}^T \left(\mathbf{N} + \Lambda^{-1}\right) \mathbf{X}}{\mathbf{X}^T\mathbf{X}}. \tag{26}$$

Split Eq. 26, and we can derive:

$$\mathbf{R}_1 = \frac{\mathbf{X}^T\mathbf{N}\mathbf{X}}{\mathbf{X}^T\mathbf{X}} + \frac{\mathbf{X}^T\Lambda^{-1}\mathbf{X}}{\mathbf{X}^T\mathbf{X}}. \tag{27}$$

The second term of Eq. 27 can be easily written as follows:

$$\frac{\mathbf{X}^T\Lambda^{-1}\mathbf{X}}{\mathbf{X}^T\mathbf{X}} = \frac{\sum_{i=1}^N \Lambda_{ii}^{-1} x_i^2}{\sum_{i=1}^N x_i^2}.$$

Since $0 < \Lambda_{ii} < 1$, therefore $\Lambda_{ii}^{-1} > 1$, then

$$\frac{\mathbf{X}^T\Lambda^{-1}\mathbf{X}}{\mathbf{X}^T\mathbf{X}} > 1. \tag{28}$$

For the first item, we write its specific form as follows:

$$\frac{\mathbf{X}^T\mathbf{N}\mathbf{X}}{\mathbf{X}^T\mathbf{X}} = \frac{\mathbf{X}^T \left(\tilde{\mathbf{D}}^{-\frac{1}{2}}\tilde{\mathbf{A}}\tilde{\mathbf{D}}^{-\frac{1}{2}}\right) \mathbf{X}}{\mathbf{X}^T\mathbf{X}}. \tag{29}$$

From spectral graph theory, we know that the following formula holds:

$$\mathbf{X}^T \left(\tilde{\mathbf{D}}^{-\frac{1}{2}} \left(\mathbf{A} + \mathbf{D}\right) \tilde{\mathbf{D}}^{-\frac{1}{2}}\right) \mathbf{X} = \sum_{(v_i,v_j)\in\mathcal{E}} \left(\frac{\mathbf{X}_i}{\sqrt{d_i+1}} + \frac{\mathbf{X}_j}{\sqrt{d_j+1}}\right)^2 > 0. \tag{30}$$

Further mathematically transforming this formula, we can get the following form:

$$\frac{\mathbf{X}^T \left(\tilde{\mathbf{D}}^{-\frac{1}{2}} \left(\mathbf{A} + \mathbf{D}\right) \tilde{\mathbf{D}}^{-\frac{1}{2}}\right) \mathbf{X}}{\mathbf{X}^T\mathbf{X}}$$

$$= \frac{\mathbf{X}^T \left(\tilde{\mathbf{D}}^{-\frac{1}{2}} \left(\tilde{\mathbf{A}} + \tilde{\mathbf{D}} - 2\mathbf{I}\right) \tilde{\mathbf{D}}^{-\frac{1}{2}}\right) \mathbf{X}}{\mathbf{X}^T\mathbf{X}} \tag{31}$$

$$= \frac{\mathbf{X}^T \left(\tilde{\mathbf{D}}^{-\frac{1}{2}}\tilde{\mathbf{A}}\tilde{\mathbf{D}}^{-\frac{1}{2}}\right) \mathbf{X}}{\mathbf{X}^T\mathbf{X}} + \frac{\mathbf{X}^T \left(\tilde{\mathbf{D}}^{-\frac{1}{2}}\tilde{\mathbf{D}}\tilde{\mathbf{D}}^{-\frac{1}{2}}\right) \mathbf{X}}{\mathbf{X}^T\mathbf{X}} - \frac{2\mathbf{X}^T\tilde{\mathbf{D}}^{-1}\mathbf{X}}{\mathbf{X}^T\mathbf{X}} \tag{32}$$

$$= \frac{\mathbf{X}^T \left(\tilde{\mathbf{D}}^{-\frac{1}{2}}\tilde{\mathbf{A}}\tilde{\mathbf{D}}^{-\frac{1}{2}}\right) \mathbf{X}}{\mathbf{X}^T\mathbf{X}} + 1 - \frac{2\mathbf{X}^T\tilde{\mathbf{D}}^{-1}\mathbf{X}}{\mathbf{X}^T\mathbf{X}} > 0. \tag{33}$$

18

Further, we get the following result:

$$\frac{\mathbf{X}^T \left(\tilde{\mathbf{D}}^{-\frac{1}{2}} \tilde{\mathbf{A}} \tilde{\mathbf{D}}^{-\frac{1}{2}} \right) \mathbf{X}}{\mathbf{X}^T \mathbf{X}} > \frac{2 \mathbf{X}^T \tilde{\mathbf{D}}^{-1} \mathbf{X}}{\mathbf{X}^T \mathbf{X}} - 1. \tag{34}$$

It is trivial to obtain:

$$\frac{2 \mathbf{X}^T \tilde{\mathbf{D}}^{-1} \mathbf{X}}{\mathbf{X}^T \mathbf{X}} = \frac{2 \sum_{i=1}^{N} (\mathbf{d}_i + 1)^{-1} \mathbf{x}_i^2}{\sum_{i=1}^{N} x_i^2} > 0. \tag{35}$$

Combining Eq. 27, Ineq. 28, Ineq. 34 and Ineq. 35, we can get the following inequality:

$$\frac{\mathbf{X}^T \left(\tilde{\mathbf{D}}^{-\frac{1}{2}} \tilde{\mathbf{A}} \tilde{\mathbf{D}}^{-\frac{1}{2}} + \Lambda^{-1} \right) \mathbf{X}}{\mathbf{X}^T \mathbf{X}} > 0. \tag{36}$$

It can be obtained that the eigenvalue of $\tilde{\mathbf{D}}^{-\frac{1}{2}} \tilde{\mathbf{A}} \tilde{\mathbf{D}}^{-\frac{1}{2}} + \Lambda^{-1}$ is greater than 0, so 0 is not an eigenvalue of it. Further, $\Lambda \mathbf{N} + \mathbf{I}$ is invertible.

Now, we derive the closed form of the formula. Given the following recursive formula:

$$\mathbf{H}_k = \mathbf{H}_1 + \Lambda_{k-1} \left(\mathbf{H}_1 - \tilde{\mathbf{D}}^{-1/2} \tilde{\mathbf{A}} \tilde{\mathbf{D}}^{-1/2} \mathbf{H}_{k-1} \right), \tag{37}$$

where $\mathbf{H}_1 = \tilde{\mathbf{D}}^{-1/2} \tilde{\mathbf{A}} \tilde{\mathbf{D}}^{-1/2} \mathbf{H}$, $\mathbf{\Lambda}_k = diag\{\lambda_k^{(1)}, ... \lambda_k^{(n)}\}$, $\lambda_k^{(i)} \sim Sigmoid(\mathcal{N}(\alpha_k^{(i)}, \beta_k^{(i)^2}))$. After mathematical transformation, Eq. 37 can be written as:

$$\mathbf{H}_k = (\mathbf{I} + \Lambda_{k-1}) \mathbf{H}_1 - \Lambda_{k-1} \tilde{\mathbf{D}}^{-1/2} \tilde{\mathbf{A}} \tilde{\mathbf{D}}^{-1/2} \mathbf{H}_{k-1}. \tag{38}$$

Set $\mathbf{N} = \tilde{\mathbf{D}}^{-1/2} \tilde{\mathbf{A}} \tilde{\mathbf{D}}^{-1/2}$, then Eq. 38 can be abbreviated as:

$$\mathbf{H}_k = (\mathbf{I} + \Lambda_{k-1}) \mathbf{H}_1 - \Lambda_{k-1} \mathbf{N} \mathbf{H}_{k-1}. \tag{39}$$

We try to modify Eq. 39 to the form that is more suitable for obtaining the closed form of the formula:

$$\mathbf{H}_k + \mathbf{M}_{k-1} = -\Lambda_{k-1} \mathbf{N} \left(\mathbf{H}_{k-1} + \mathbf{M}_{k-1} \right). \tag{40}$$

To verify whether there exists such $\mathbf{M}$ that satisfies the equation, we need to solve the following equation:

$$-\Lambda_{k-1} \mathbf{N} \mathbf{M}_{k-1} = (\mathbf{I} + \Lambda_{k-1}) \mathbf{H}_1 + \mathbf{M}_{k-1}, \tag{41}$$

which is equivalent to the following form:

$$-\left(\Lambda_{k-1} \mathbf{N} + \mathbf{I}\right) \mathbf{M}_{k-1} = (\mathbf{I} + \Lambda_{k-1}) \mathbf{H}_1. \tag{42}$$

Based on the definition, all the diagonal elements of Λ_k satisfy $0 < \lambda_k^{(i)} < 1$, so according to **Lemma 2**, $(\Lambda_{k-1} \mathbf{N} + \mathbf{I})$ is invertible. Then $\mathbf{M}_{k-1} = -\left(\Lambda_{k-1} \mathbf{N} + \mathbf{I}\right)^{-1} (\mathbf{I} + \Lambda_{k-1}) \mathbf{H}_1$, which means such $\mathbf{M}_{k-1}$ that we require exists.

First, we perform the following mathematical transformation on Eq. 40:

$$\mathbf{H}_k + \mathbf{M}_{k-1} = -\Lambda_{k-1} \mathbf{N} \left(\mathbf{H}_{k-1} + \mathbf{M}_{k-2} + \mathbf{M}_{k-1} - \mathbf{M}_{k-2} \right), \tag{43}$$

which can be split into the following form:

$$\mathbf{H}_k + \mathbf{M}_{k-1} = -\Lambda_{k-1} \mathbf{N} \left(\mathbf{H}_{k-1} + \mathbf{M}_{k-2} \right) + \left(-\Lambda_{k-1} \mathbf{N} \right) \left(\mathbf{M}_{k-1} - \mathbf{M}_{k-2} \right). \tag{44}$$

Let $\tilde{\mathbf{N}}_{k-1}$ denotes $-\Lambda_{k-1} \mathbf{N}$, so the formula can be simply written as:

$$\mathbf{H}_k + \mathbf{M}_{k-1} = \tilde{\mathbf{N}}_{k-1} \left(\mathbf{H}_{k-1} + \mathbf{M}_{k-2} \right) + \tilde{\mathbf{N}}_{k-1} \left(\mathbf{M}_{k-1} - \mathbf{M}_{k-2} \right). \tag{45}$$

We first use Eq. 40 to recurse once, then derive the following formula:

$$\mathbf{H}_k + \mathbf{M}_{k-1} = \tilde{\mathbf{N}}_{k-1} \tilde{\mathbf{N}}_{k-2} \left(\mathbf{H}_{k-2} + \mathbf{M}_{k-3} \right) + \tilde{\mathbf{N}}_{k-1} \left(\mathbf{M}_{k-1} - \mathbf{M}_{k-2} \right). \tag{46}$$

By analogy, continuing to split and iterate, we can get the closed form of the output of the k-th layer:

$$\mathbf{H}_k = \sum_{i=2}^{k-1} \prod_{j=i}^{k-1} \tilde{\mathbf{N}}_j \left(\mathbf{M}_i - \mathbf{M}_{i-1} \right) + \prod_{i=1}^{k-1} \tilde{\mathbf{N}}_i \left(\mathbf{H}_1 + \mathbf{M}_1 \right) - \mathbf{M}_{k-1}. \tag{47}$$

19

F Comparing with other subgraph-based methods

It is worth noting that a lot of previous work mentions "subgraph". However, our approach is fundamentally different from these approaches.

Relation with other subgraph-based methods. While there are existing works [2, 23] related to subgraphs, they primarily focus on graph classification tasks, aiming to learn representations of entire graphs. Given the limited capacity of GNNs to effectively represent the entire graphs, these subgraph-based approaches employ various strategies to leverage information from multiple subgraph structures within the overall graph to improve the representation.

In contrast, our focus is on node-level tasks, specifically, enhancing the representations of individual nodes. In our context, we naturally refer to neighborhood subgraphs as different orders of ego-networks centered on a node (which can be regarded as subgraphs of the entire graph). Our work uncovers the relationship between these subgraphs and over-smoothing, as well as how to utilize them to enhance node representations. This distinction fundamentally sets our approach apart from other subgraph methods.

G Experiment Setup

G.1 Details of Datasets

The dataset statistics are shown in Table 8, and details on dataset splits are summarized as follows:

Experiment 5.3 & 5.4. For Cora, Citeseer, Coauthor-CS, Amazon-Photo, we randomly select 20 nodes per class for training set, 500 nodes for validation and 1000 nodes for testing. For Chameleon and Squirrel, we randomly divide each class's nodes into 60%, 20%, and 20% as the train, validation, and test sets, respectively.

Experiment 5.5. We follow the widely used semi-supervised setting in [14].

Experiment 5.6. For larger datasets, We randomly divide each class's nodes into 20%, 20%, and 60% as the train, validation, and test sets, respectively.

Table 8: Dataset statistics of real-world datasets.

	Cora	Citeseer	Pubmed	Amazon-Photo	Ogbn-arxiv	Chameleon	Squirrel	Coauthor-CS	Coauthor-Phy	Flickr
#Nodes	2708	3327	19717	7650	169343	2277	5201	18333	34493	89250
#Edges	5429	4732	119081	126842	1166243	36101	217073	81894	247962	899756
#Features	1433	3703	500	745	128	2325	2089	6805	8415	500
#Classes	7	6	3	8	39	5	5	5	10	7

G.2 Parameter Settings

We summarized the hyperparameters used in different experiments in Table 9.

Table 9: Hyperparameters for experiments

Experiment	Backbone	Learning Rate	Dropout	Weight Decay	Hidden State	Attention Head	Max Epoch	Early Stopping Epoch
Experiment 5.3 & 5.4	GCN	{0.01, 0.001}	0.5	0.0005	128	-	500	100
	GAT	{0.01, 0.001}	0.5	0.0005	64	3	500	100
Experiment 5.5	GCN	{0.01, 0.001}	0.5	0.0005	128	-	1000	1000
	GAT	{0.01, 0.001}	0.5	0.0005	32	1	1000	1000
Experiment 5.6	GCN	{0.01, 0.001}	0.5	0.0005	128	-	500	100

H. The Analysis of PSNR Residual Coefficients

We conducted an empirical study using an 8-layer PSNR-GCN trained on the Cora dataset to obtain the best-performing model. We saved the mean and standard deviation of the learned residual coefficient distribution for each layer. Nodes were evenly divided into four groups based on their degree, with each group containing a similar number of nodes, and the average mean and standard

20

deviation for each group across different layers are reported in Table 10. The following observations can be obtained from the table: the mean residual coefficient increases with the number of layers, suggesting that PSNR effectively retains high-order subgraph information. In certain layers, the variance of the residual coefficients rises, indicating that added randomness helps mitigate information loss in higher-order subgraphs. In the shallow layers, the mean values show no significant differences across node degrees; however, in deeper layers, nodes with higher degrees tend to exhibit lower mean values, indicating that these nodes retain more initial information due to significant subgraph overlap. All of these observations align with our expectations, illustrating how residual coefficients adapt based on node degree and layer depth.

Table 10: Summary of means and standard deviations for different layers

Layer	Mean Group 1	Mean Group 2	Mean Group 3	Mean Group 4	Std Group 1	Std Group 2	Std Group 3	Std Group 4
Layer 0	0.0043	0.0049	0.0063	0.0099	0.0002	0.0001	0.0002	0.0001
Layer 1	0.0009	0.0017	0.0013	0.0016	0.3102	0.3120	0.3130	0.2410
Layer 2	0.0000	0.0000	0.0003	0.0008	0.0480	0.0431	0.0446	0.0170
Layer 3	0.5582	0.6017	0.5972	0.4979	0.0084	0.0118	0.0105	0.0080
Layer 4	1.4898	1.5238	1.5212	1.3478	8.3354e-05	5.4541e-05	0.0001	0.0002
Layer 5	2.4080	2.3974	2.3981	2.1414	0.0062	0.0081	0.0078	0.0059
Layer 6	5.2347	5.3148	5.2070	3.8177	0.0046	0.0089	0.0075	0.0069
Layer 7	11.0787	11.1253	10.9247	8.7238	0.1642	0.2089	0.2128	0.0677

I. Comparison of Experimental Results of Different GraphEncoders.

In practice, in addition to SAGE, encoders such as GAT and GCN can also be utilized. To provide further insight, we have included results for different encoders on the classical semi-supervised node classification task. The results are summarized in the table blow.

Table 11: Different GraphEncoder performance for SSNC task (layer 2)

Graph Encoder	Cora	Citeseer	CS	Photo	Chameleon	Squirrel
GCN	**80.98±1.60**	68.46±2.28	90.52±0.82	**91.56±0.74**	**72.02±1.60**	56.14±1.51
GAT	80.89±1.63	**68.77±1.89**	90.61±0.89	91.18±0.92	71.97±1.28	**56.24±1.11**
SAGE	80.59±1.57	68.06±2.12	**91.23±1.00**	91.44±0.82	71.51±1.90	54.95±1.73

Table 12: Different GraphEncoder performance for SSNC task (layer 4)

Graph Encoder	Cora	Citeseer	CS	Photo	Chameleon	Squirrel
GCN	81.65±1.70	**68.11±1.24**	90.66±0.70	91.14±0.90	**71.58±2.07**	56.34±1.48
GAT	**82.21±1.41**	67.96±1.20	90.57±0.89	91.17±0.81	71.29±1.75	**56.50±1.45**
SAGE	81.01±1.63	66.03±1.93	**90.70±1.49**	**91.20±1.03**	70.74±2.24	54.13±1.41

The results indicate that each encoder has its strengths and performs differently across various datasets, demonstrating superior performance compared to the baseline and emphasizing the potential of PSNR.

21

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22

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24

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27

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28