SkipNode: On Alleviating Over-smoothing for Deep Graph Convolutional Networks

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ABSTRACT

Over-smoothing is a challenging problem, which degrades the performance of deep graph convolutional networks (GCNs). However, existing studies for alleviating the over-smoothing problem lack either generality or effectiveness. In this paper, we analyze the underlying issues behind the over-smoothing problem, i.e., feature-diversity degeneration, gradient vanishing, and model weights over-decaying. Inspired by this, we propose a simple yet effective plug-and-play module, SkipNode, to alleviate over-smoothing. Specifically, for each middle layer of a GCN model, SkipNode randomly (or based on node degree) selects nodes to skip the convolutional operation by directly feeding their input features to the nonlinear function. Analytically, 1) skipping the convolutional operation prevents the features from losing diversity; and 2) the “skipped” nodes enable gradients to be directly passed back, thus mitigating the gradient vanishing and model weights over-decaying issues. To demonstrate the superiority of SkipNode, we conduct extensive experiments on nine popular datasets, including both homophilic and heterophilic graphs, with different graph sizes on two typical tasks: node classification and link prediction. Specifically, 1) SkipNode has strong generalizability of being applied to various GCN-based models on different datasets and tasks; and 2) SkipNode outperforms recent state-of-the-art anti-over-smoothing plug-and-play modules, i.e., DropEdge and DropNode, in different settings. Code will be made publicly available on GitHub.

KEYWORDS

Over-smoothing, deep graph neural networks, graph representation learning

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1 INTRODUCTION

Graph convolutional networks (GCNs) can capture the dependence in graphs through message passing between nodes [41, 52]. Due to the excellent ability for graph representation learning, GCNs have shown remarkable breakthroughs in numerous applications, including node classification [6, 7, 11, 18, 19, 37, 43], object detection [21, 26, 47], and visual question answering [22, 24]. However, despite the widespread success, current GCNs still suffer from a severe problem, i.e., the performance seriously degenerates with the increasing number of layers.

The performance degeneration is widely believed to be caused by the problem of over-smoothing [4, 5, 7, 29, 33, 38, 40, 44, 45, 51]. Specifically, each graph convolutional operation tends to mix the features of connected nodes through message propagation. The features between the connected nodes gradually become indistinguishable when stacking too many graph convolutional operations. This phenomenon is referred to as the over-smoothing problem. [23, 29] also investigated the asymptotic behaviors of GCNs and found that the node representations will approach an invariant space when the number of layers goes to infinity. Considering that deeper neural networks usually show a better expressive and reasoning ability [32], how to devise deeper GCNs by addressing the over-smoothing problem has received increasing attention from the community [20, 33].

To cope with the over-smoothing problem, several GCN variants were proposed recently [6–8, 11, 16, 19, 25, 39, 43, 50]. However, these methods still suffer from the following drawbacks: (1) most of these models tried to alleviate over-smoothing by sacrificing the expressiveness merit of deep learning, e.g., emphasizing low-level features when over-smoothing happens [7, 16, 43], removing nonlinearity in middle layers [19], and aggregating neighborhoods of different orders in one layer of computation [11]; (2)
We provide novel and comprehensive insight into the over-smoothing problem. We first review the phenomenon of over-smoothing and then analyze in detail the underlying issues that accompany the over-smoothing problem, i.e., feature-diversity degeneration, gradient vanishing, and model weights over-decaying. Furthermore, we explain how the above three issues hinder the deep graph learning.

We devise a novel plug-and-play module, dubbed SkipNode, for addressing over-smoothing. In each middle layer of a GCN model, SkipNode samples nodes either randomly or based on node degrees to skip the convolutional operation by directly feeding their features to the nonlinear function. For unselected nodes, they can still receive information from these selected (skipped) ones. Intuitively, 1) backtracking skipped nodes’ information reduces the degeneration of feature diversity; and 2) skipping the convolutional operation enables the gradient to be directly passed back, thus preventing the gradient from disappearing and the model weights from over-decaying.

We conduct extensive experiments to verify the generalizability and effectiveness of SkipNode. The experimental results on various datasets demonstrate good capability of our SkipNode to alleviate over-smoothing. Specifically, 1) SkipNode has a strong generalizability to improve GCN-based methods (including those designed for the over-smoothing problem) on various graphs and tasks; and 2) SkipNode consistently outperforms the commonly-used plug-and-play strategies, DropEdge and DropNode, in different settings.

2 RELATED WORK

GCNs. [3] first devised a graph convolution operation based on the graph spectral theory. However, considering the high computational cost, it is very difficult to apply spectral-based models [3, 9, 14, 18] to every node degree to skip the convolutional operation by directly feeding their features to the nonlinear function. For unselected nodes, they can still receive information from these selected (skipped) ones. Intuitively, 1) backtracking skipped nodes’ information reduces the degeneration of feature diversity; and 2) skipping the convolutional operation enables the gradient to be directly passed back, thus preventing the gradient from disappearing and the model weights from over-decaying.

We conduct extensive experiments to verify the generalizability and effectiveness of SkipNode. The experimental results on various datasets demonstrate good capability of our SkipNode to alleviate over-smoothing. Specifically, 1) SkipNode has a strong generalizability to improve GCN-based methods (including those designed for the over-smoothing problem) on various graphs and tasks; and 2) SkipNode consistently outperforms the commonly-used plug-and-play strategies, DropEdge and DropNode, in different settings.

3 PRELIMINARY

Notations. We first introduce the notations used in this paper as follows. Let $G = \{V, E\}$ denote a graph, $V = \{v_1, v_2, ..., v_N\}$ denote the node set, where $N$ is the number of all nodes. Let $E = \{e_{ij}\}, i, j \in \{1, 2, ..., N\}$ denote the edge set, where $e_{ij}$ indicates the edge between nodes $v_i$ and $v_j$. The adjacency matrix is defined as $A \in \mathbb{R}^{N \times N},$ where $A_{ij} = 1$ if $e_{ij} \in E$ otherwise $A_{ij} = 0$. Let $D$ denote the diagonal degree matrix, where $D_{ii} = \sum_{j=0}^{N} A_{ij}$. The node
feature matrix is defined as $X \in \mathbb{R}^{N \times d}$. Here, $d$ is the feature dimension of $X$. Suppose that $X_{in}^{(l)} \in \mathbb{R}^{N \times d_l}$ and $X_{out}^{(l)} \in \mathbb{R}^{N \times d_{l+1}}$ are the input and output feature matrices of the $l$-th layer, respectively, and $d_l$ is the input feature dimension for the $l$-th layer, where $l \in \{1, 2, \ldots, L\}$ and $L \geq 2$.

Vanilla GCN. The vanilla GCN is introduced in [18] which defines the graph convolution operation as $g_{\theta}(x) \approx \theta(1 + D^{-\frac{1}{2}} AD^{-\frac{1}{2}} x)$, where $x \in \mathbb{R}^N$ indicates the graph signal, $\star$ is convolutional operation, and $\theta$ is a learnable parameter. To avoid exploding filter coefficients, [18] further adopted re-normalization trick. The final GCN formulation can thus be defined as follows:

$$X_{out}^{(l)} = \text{ReLU}(\tilde{A}X_{in}^{(l)} W^{(l)}),$$

where $\tilde{A} = (D + I)^{-\frac{1}{2}} (A + I)(D + I)^{-\frac{1}{2}}$ is a normalized adjacency, $W^{(l)}$ indicates the $l$-th learnable weight matrix. The symmetrical augmented graph Laplacian is defined as $\tilde{L} = I - \tilde{A}$.

4 A CLOSER LOOK AT OVER-SMOOTHING

We first review the definition of over-smoothing. Over-smoothing is a problem where node representations lose their diversities, which hinders the learning of graph neural networks. We explain over-smoothing as the decreasing distance between input and a lower-information subspace $M$ after multiple convolutions, following [29]. The definition of $M$ can be found in Appendix B.2.1. Then, the convergence can be written as:

$$d_M(X_{out}^{(l)}) \leq s_l - \lambda d_M(X_{out}^{(l-1)}) \cdots \leq \sum_{i=0}^{L-1} (s_l \lambda)^i d_M(X^{(0)}),$$

where $\lambda$ is the smallest nonzero eigenvalue of $\tilde{L}$, $s_l$ is the maximum singular value of $W^{(l)}$, and $d_M(X)$ is the minimum distance between $X$ and $M$. In addition, the Proposition 3 from [29] also noted that $X_{out}^{(l)}$ will exponentially approach 0 as $l \rightarrow \infty$ if $s_l \lambda < 1$.

4.1 Underlying Problems Behind Over-smoothing

Numerous works [4, 7, 23, 29, 43] have explained the over-smoothing phenomenon. However, few methods have comprehensively analyzed the problems that follow over-smoothing. In this subsection, we would like to discuss three problems that rise as over-smoothing happens and explain how these problems hinder the training process.

4.1.1 Feature diversity degeneration. GCNs can be regarded as low-pass filters retaining low frequency in graph signal processing. Regardless of the weight matrix, the output features of nodes become linearly dependent after multiple propagations. It can be explained by $\lim_{k \rightarrow \infty} \tilde{A}^k X^{(0)} = \pi \pi^T X^{(0)}$, where $\pi_i = \frac{\sqrt{D_i}}{\sum_{i=1}^{N} \sqrt{D_i}}$ and $i \in \{1, \ldots, N\}$, since the range of $\tilde{A}$’s eigenvalue $\lambda$ lies in $(-1, 1]$, i.e., $-1 < \lambda \leq 1$.

4.1.2 Gradient vanishing. Though many recent works [6, 18, 33, 45] have mentioned the gradient vanishing when it comes to over-smoothing, there are very limited methods analyzing their relationships in detail. Here, we prove that the over-smoothing problem would trigger the gradient vanishing issue.

**Lemma 4.1.** Let $L$ denote the cross-entropy loss function and $Z \in \mathbb{R}^{N \times C}$ be the output of the last layer, where $C$ is the number of class. When the over-smoothing problem occurs, the gradient of the last layer $\sum_{l \in V_{train}} \sum_{j=1}^{C} \frac{\partial}{\partial z_{ij}}$ approaches 0.

**Proof.** See proof in Appendix B.1.

where $\sum_{j=1}^{C} Y_{ij} = 1$. As a result, model weights can not be optimized by classification objective. What is worse, it would cause the model weights to decrease to zero if weight regularization is used. The final representations $X_{out}^{(L)}$ in the last layer would approximately equal zero as the over-smoothing problem raises.

4.1.3 Model weights over-decaying. Note that model weights over-decaying only occurs when weight regularization, such as L2 loss, is considered during training as over-smoothing issue emerges. Assume the final loss contains classification loss and regularization loss. As Lemma 4.1.2 notes, the over-smoothing issue incurs gradient vanishes which disables classification objective. Therefore, the regularization objective dominates the training. The regularization objective of reducing the norm of the weight matrix without control aggravates the over-smoothing problem. As a result, the propagating features approach zero.

**Remark 4.1.** The above three problems seriously hinder the efficient learning of deep GCNs. Intuitively, addressing any one of the above problems could alleviate the over-smoothing. We further provide three visualizations of the three problems using GCNs with 9 layers on Cora in Figure 1. We can observe that 1) GCN with or without DropNode suffers from all the three problems; 2) DropEdge can only ease diversity degeneration; 3) SkipNode is capable of alleviating all the problems.

5 METHOD

In this section, we present the methodological details of SkipNode and explain how SkipNode alleviates the over-smoothing problem.

5.1 SkipNode

Suppose a deep GCN contains $L$ layers. Then, for each middle layer, the SkipNode generates a mask matrix $P^{(l)} \in \mathbb{R}^{N \times N}$, which is a diagonal matrix whose diagonal consists of $\rho \times N 0$’s and $(1 - \rho) \times N 1$’s, where $\rho$ is the sampling rate. $P_{ii} = 0$ indicates that node $i$ is the sampled node; otherwise, it is not. Then, SkipNode can be defined as follows:

$$X_{out}^{(l)} = \sigma(P^{(l)} \tilde{A}X_{in}^{(l)} W^{(l)} + (I - P^{(l)}) X_{in}^{(l)})$$

where $\sigma$ is a nonlinear function, i.e., ReLU function. The mask matrix $P^{(l)}$ is determined by the sampling strategies and sampling rate $\rho$. Here, we propose two sampling strategies: **Uniform Sampling** selects $\rho \times N$ nodes with the same probability $\frac{1}{N}$ for each node. **Biased Sampling** samples “skipped nodes” according to $\lambda$’s degree and the sampling weight of $v_i$ is $\frac{D_i}{\sum_{i=1}^{N} D_i}$. Biased sampling is adopted because [6] noted that nodes with higher degrees are more likely to suffer from over-smoothing in the deep GCNs. We employ SkipNode at training stage to GCN for each middle layer, except for the first and last one. Figure 2 describes the training procedure of SkipNode.
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5.2 Toward Alleviating Over-smoothing

SkipNode helps nodes to maintain their diversities and enables gradient to be directly passed to previous layer. Naturally, as shown in Figure 1, SkipNode alleviates all three problems of over-smoothing.

5.2.1 Reducing the degeneration of feature diversity. We prove that SkipNode reduces the degeneration of feature diversity by increasing the distance between output features and the information-less subspace $\mathcal{M}$.

**Theorem 5.1.** Let $W \in \mathbb{R}^{N \times C}$ be the weight matrix, $X \in \mathbb{R}^{N \times C}$ be the input features, $P \in \mathbb{R}^{N \times N}$ be the diagonal matrix which contains 0 and 1 in its diagonal. We denote the aggregated features of GCN layer as $X_1 = AX$ and the aggregated features of GCN layer with SkipNode as $X_2 \in \mathbb{R}^{N \times C}$, where $X_2 = \bar{P}AX + (I - P)X$. We have $d_M(X_2) \geq d_M(X_1)$.

**Proof.** See proof in Appendix B.2.2.

Hence, we can conclude that SkipNode can alleviate over-smoothing problem by increasing the upper bound of distance between the output and $\mathcal{M}$.

5.2.2 Preventing gradients from vanishing. We first introduce vanishing gradient phenomena briefly and explain why SkipNode can prevent them. Assume that the graph signal $x$ is transformed by $\theta_l$ where $l \in \{1, \cdots, L\}$ to obtain the output $x^{(l)}$ and we have $x^{(l)} = \theta_l(x^{(l-1)})$. Therefore, the gradient from loss function $f(x^{(l)})$ to $x^{(0)}$ is

$$\frac{\partial f(x^{(l)})}{\partial x^{(0)}} = \frac{\partial f(x^{(l)})}{\partial x^{(l)}} \frac{\partial x^{(l)}}{\partial x^{(l-1)}} \cdots \frac{\partial x^{(1)}}{\partial x^{(0)}}$$

$$= (\prod_{l=1}^{L} \theta_l) \frac{\partial f(x^{(l)})}{\partial x^{(l)}}.$$  (4)

Figure 1: Three problems following over-smoothing on Cora. GCN (SN-U)/GCN (SN-B) stands for GCN with our SkipNode using uniform/biased sampling strategy. In (a), the features get more indistinguishable as the MAD [5] value becomes smaller. In (b), only SkipNode alleviates the gradient vanishing problem. (c) shows the sum of the L2 norm of all the model weights. Note that some curves coincide in (b) and (c).

Figure 2: The SkipNode training procedure. $X^{(l)} = \bar{A}X^{(l-1)}$. For simplicity, we omit the nonlinear function in this figure.

Figure 3: The sketch of Vanilla GCN and GCN with DropEdge/DropNode/Skip Connection/SkipNode. Vanilla GCN enables each connected node to propagate information. DropEdge randomly deletes edges to make the graph sparser. DropNode removes the node by downsampling technique. Skip Connection adds the input on the output. SkipNode maintains the selected node’s information and updates unselected nodes’.
Table 1: Full-supervised Classification Accuracy (%) Comparison. The layer number is also included. Wisconsin is not a supported dataset in the code of GPRGNN and APPNP.

| Model        | Datasets | Cora | Citeseer | Pubmed | Chameleon | Cornell | Texas | Wisconsin |
|--------------|----------|------|----------|--------|-----------|---------|-------|-----------|
| GCN          |          | 86.1 (2) | 79.1 (2) | 86.2 (2) | 42.1 (2) | 70.2 (2) | 67.5 (2) | 60.7 (2) |
| GCN (DropEdge) |         | 88.9 (3) | 79.2 (3) | 86.9 (3) | 42.3 (3) | 73.9 (3) | 70.2 (5) | 62.7 (4) |
| GCN (SN-U)   |          | 89.7 (3) | **79.4 (3)** | 87.0 (3) | **43.2 (3)** | 75.6 (3) | 72.9 (3) | 62.7 (4) |
| GCN (SN-B)   |          | 89.7 (3) | 79.2 (3) | **87.3 (3)** | **43.2 (3)** | **78.3 (5)** | 70.2 (6) | **68.6 (3)** |
| JKNet        |          | 88.4 (8) | 77.1 (4) | 87.2 (8) | 40.5 (8) | 70.2 (8) | 72.4 (8) | 62.7 (8) |
| JKNet (DropEdge) |        | 88.4 (8) | 78.3 (16) | 87.9 (8) | 41.2 (8) | 71.3 (8) | 72.9 (8) | 64.7 (8) |
| JKNet (SN-U) |          | 89.3 (6) | **79.4 (4)** | **87.0 (3)** | 43.2 (3) | 75.6 (3) | 75.6 (12) | 66.6 (4) |
| JKNet (SN-B) |          | 89.7 (4) | 79.0 (4) | **87.3 (4)** | 43.2 (3) | 75.6 (8) | 75.6 (8) | 66.6 (4) |
| Incep        |          | 88.0 (12) | 76.6 (8) | 87.9 (8) | 41.6 (8) | 75.6 (16) | 70.2 (32) | 60.7 (16) |
| Incep (DropEdge) |        | 88.3 (8) | 77.1 (8) | 87.5 (8) | 42.0 (8) | 78.3 (8) | 70.2 (8) | 62.7 (8) |
| Incep (SN-U) |          | 87.5 (16) | 77.3 (16) | 87.2 (4) | 42.1 (8) | 78.0 (8) | 72.4 (8) | 64.7 (8) |
| Incep (SN-B) |          | 87.5 (8) | 77.3 (16) | 87.6 (4) | 40.5 (8) | 78.3 (8) | 72.9 (4) | 64.7 (16) |
| GCNII        |          | 88.4 (64) | 77.0 (64) | 89.5 (64) | 60.2 (8) | 74.8 (16) | 76.8 (32) | 74.1 (16) |
| GCNII (DropEdge) |       | 88.0 (64) | 76.8 (64) | 87.8 (64) | 59.6 (8) | 75.0 (16) | 72.9 (32) | 73.3 (16) |
| GCNII (SN-U) |          | 88.6 (64) | 77.3 (64) | **89.7 (64)** | **60.9 (8)** | **75.4 (16)** | **77.6 (32)** | **73.7 (16)** |
| GCNII (SN-B) |          | 88.4 (64) | 76.8 (64) | 88.8 (64) | 60.2 (8) | 75.4 (16) | 70.5 (32) | 73.1 (16) |
| GRAND        |          | 87.4 (6) | 76.2 (3) | 86.2 (3) | 42.3 (3) | 58.9 (9) | 58.9 (9) | 56.4 (3) |
| GRAND (DropEdge) |       | 87.5 (6) | 76.2 (3) | 86.1 (3) | **44.2 (3)** | 58.9 (9) | 57.5 (9) | 56.8 (3) |
| GRAND (SN-U) |          | 88.4 (10) | 76.1 (4) | 86.1 (5) | 43.2 (3) | 58.9 (8) | 58.9 (9) | 56.0 (3) |
| GRAND (SN-B) |          | 88.1 (10) | **76.6 (9)** | **86.3 (5)** | **44.2 (5)** | **60.0 (10)** | **59.4 (10)** | **57.2 (4)** |
| GPRGNN       |          | 88.0 (10) | 78.9 (10) | 86.9 (10) | 54.7 (10) | 69.0 (10) | 57.2 (10) | - |
| GPRGNN (DropEdge) |       | 88.1 (10) | 78.6 (10) | 86.6 (10) | 54.4 (10) | 69.1 (10) | 57.3 (10) | - |
| GPRGNN (SN-U) |          | 88.6 (10) | **79.6 (10)** | **87.5 (10)** | **55.0 (10)** | **69.8 (10)** | **57.0 (10)** | - |
| GPRGNN (SN-B) |          | 88.4 (10) | 79.1 (10) | 87.0 (10) | 54.6 (10) | 69.3 (10) | **64.5 (10)** | - |
| APPNP        |          | 86.4 (10) | 78.4 (10) | 84.3 (10) | 50.0 (10) | 55.4 (10) | 56.0 (10) | - |
| APPNP (DropEdge) |       | 87.1 (10) | 79.6 (10) | 83.6 (10) | **51.2 (10)** | **55.7 (10)** | **57.4 (10)** | - |
| APPNP (SN-U) |          | **87.8 (10)** | **80.6 (10)** | 84.5 (10) | **51.2 (10)** | **56.5 (10)** | **58.3 (10)** | - |
| APPNP (SN-B) |          | 87.5 (10) | 80.2 (10) | **84.8 (10)** | 51.1 (10) | 56.4 (10) | 56.7 (10) | - |

where $|\theta| < 1$. The successive multiplication of $\theta$ possibly converges to zero, which indicates the gradient vanishing. Our SkipNode lets some nodes skip several transformations to slow down the convergence speed since $n$ decreases.

5.2.3 Preventing model weights from over-decaying. As we have analyzed in Sec 4.1, the model weights over-decaying issue is mainly triggered by gradient vanishing and regularization. Since we alleviated the vanishing gradient, the model weights can be updated by the gradients from last layer. Therefore, SkipNode maintains the norm of model weights at a relatively high value to prevent over-smoothing.

5.3 Discussion

In this section, we discuss the difference between our SkipNode and three widely used strategies, i.e., DropEdge, DropNode, and Skip Connection. In addition, we visualize their differences in Figure 3.

5.3.1 SkipNode vs. DropEdge. DropEdge [33] randomly deletes a part of edges during training to alleviate over-smoothing since more sparsity of the graph results in less over-smoothing. To some extent, SkipNode also masks the edges of sampled nodes and improves the graph sparsity. However, the graph sparsity is only one of the factors that induces over-smoothing. As we discussed previously, SkipNode can also solve the problem of vanishing gradient and model weights over-decaying, which are ignored by DropEdge. Besides, DropEdge requires re-normalizing the adjacency matrix at each epoch and it is time-consuming when dealing with large graphs.

5.3.2 SkipNode vs. DropNode. There are two works [10, 11] which proposed DropNode technique. In [11], DropNode is used as a data augmentation method to randomly masks nodes’ features before propagation. In addition, it requires extra regularization on the outputs from different augmentations to maintain the robustness of the model. Therefore, it’s not a plugin for alleviating over-smoothing and we don’t regard [11] as a comparing strategy.
DropNode scheme used in [10] down-samples the graph between layers and then has to normalize the new adjacency matrix since the selected nodes are dropped. Furthermore, the above-mentioned two DropNode schemes only ease the feature diversity degeneration and cannot directly be used on different models. Our SkipNode differs from them by its simplicity to be easily applied to various models, and the theoretically guaranteed effectiveness to alleviate all the three issues.

5.3.3 SkipNode vs. Skip Connection. Residual (or Skip) connection has been widely used to prevent gradient vanishing. However, [29, 38] proved that adding skip connections to GCNs acts similar to a lazy random walk in a graph that eventually converges to a stationary distribution. In contrast, our SkipNode directly replaces the aggregated features of the sampled nodes by their input features, to alleviate the over-smoothing. And the node-wise "skip" operation also prevent deep GCNs from gradient vanishing.

6 EXPERIMENTS

6.1 Tasks, Datasets, and Baselines

We evaluate our SkipNode on various graphs by different tasks as follows: 1) For semi-supervised node classification task, we use three widely-used graphs, including Cora [35], Citeseer [35], and Pubmed [35]. All the models are evaluated on public splits [46]. 2) For full-supervised node classification task, we use Cora, Citeseer, Pubmed, Chameleon [34], Cornell [31], Texas [31], and Wisconsin [31] under ten different splits (60%, 20% and 20% for training, validation, and testing). 3) For node classification task on a large-scale graph, we choose a challenging dataset, ogbn-arxiv [15]. 4) For link prediction task, ogbl-ppa [15] is considered and the evaluation metric is the ratio of predicted positive edges that are ranked at K-th place or above (Hits@K).

We consider eight typical GCNs-based baselines for experiments, namely, GCN [18], JKNet [43], InceptGCN [16], ResGCN [18], GCNII [6], GPRGNN [7], APPNP [19], and GRAND [11]. In addition, DropEdge [33] and DropNode [10] are used as comparing strategies. It is worth noting that we only compare SkipNode with DropNode [10] in Table 3 and 6 since DropNode can not scale to all the selected baselines except for GCN and InceptGCN.

The statistics of all the graphs are described in Table 7 in Appendix A.2.

6.2 Implementation Details.

For a fair comparison, we first perform grid hyper-parameter searching for each baseline and obtain all hyperparameters based on the best accuracy of the validation set of each benchmark. Then, we adopt SkipNode and other comparing strategies by only tuning the new strategy-related hyperparameter and dropout rate while fixing the other hyperparameters. SN-U and SN-B in the experiments indicate uniform sampling and biased sampling SkipNode, respectively.
6.3 Performance Studies

6.3.1 Generalizability. To demonstrate generalizability of SkipNode, we evaluate it by two common tasks, i.e., node classification and link prediction, on various graphs with different homophily and scales. Table 1 summarized the accuracy and the corresponding depth of full-supervised node classification on seven graphs. We can observe that SkipNode obtains better performance in the most cases. What’s more, we use GCN with SkipNode on ogbn-arxiv which is a large-scale graph and the results are recorded in Table 5. Besides, we conduct experiment of GCN with SkipNode on ogbl-ppa since link prediction also depends on the quality of node representations. Results in Table 4 demonstrates that SkipNode is also useful to protect GCN from degenerating in link prediction task.

6.3.2 Effectiveness. We then verify the effectiveness of SkipNode for deep GCNs with different layers. We first evaluate our SkipNode method by semi-supervised node classification task on three popular graphs, i.e., Cora, Citeseer, and Pubmed. Specifically, deep GCNs with various depth $L \in \{4, 8, 16, 32, 64\}$ are considered. Table 2 provides the results. The best performance of each baseline is highlighted by boldface. We can observe that SkipNode effectively enhances most methods with different depth. We also compare SkipNode with two anti-over-smoothing strategies, i.e., DropEdge [33] and DropNode [10] in Table 3. The great improvement demonstrates that SkipNode are more effective than the comparing strategies.

Table 3: Accuracy (%) Comparison with DropEdge and DropNode on Semi-supervised Classification on Cora.

| Methods      | 3 layers | 5 layers | 7 layers | 9 layers |
|--------------|----------|----------|----------|----------|
| GCN          | 82.3     | 80.6     | 79.1     | 78.4     |
| GCN (DropEdge) | 81.3     | 79.9     | 77.3     | 78.7     |
| GCN (DropNode) | 82.5     | 81.7     | 82.1     | 81.2     |
| GCN (SN-U)   | 82.9     | 81.7     | 82.1     | 81.2     |
| GCN (SN-B)   | 82.8     | 82.3     | 81.4     | 80.2     |
| Incep        | 82.0     | 82.3     | 80.4     | 82.2     |
| Incep (DropEdge) | 81.7     | 82.0     | 79.5     | 81.9     |
| Incep (DropNode) | 81.5     | 81.7     | 78.2     | 80.5     |
| Incep (SN-U) | 82.4     | 82.7     | 81.0     | 82.5     |
| Incep (SN-B) | 82.5     | 82.5     | 80.8     | 82.7     |

6.4 Ablation Studies

The sampling rate $\rho$ is the only one parameter of our technique. Thus, we would investigate the influence of sampling rate $\rho$ on SkipNode. Specifically, we fix the number of the layer in the model, hidden dimension, learning rate, and weight decay at 32, 64, 0.01 and 0.0005 respectively. The range of $\rho$ is $\{0.1, 0.2, \cdots, 0.9\}$, and each trail is conducted with 500 epochs. We use the best performance of GCN as the baseline and apply SkipNode by tuning different $\rho$. We can observe that SkipNode achieves better performance with a large sampling rate since the over-smoothing issue is much serious in such deep GCN. The results are illustrated in Figure 4(a).

6.5 Efficiency Studies

Besides, we further explore the smoothness of node features in the last layer by MAD metric [5], which is the mean of the average cosine distance from nodes to their connected nodes. We use the MAD value of output representations after 500 epochs training as the resulting smoothness, which is depicted in Figure 4(b). The smoothness of output representations that GCN obtains from the 32-th layer in each dataset is always zero, which indicates little diversity. SkipNode successfully maintains information diversities in feature propagating.

Table 4: Link Prediction Results of GCN on Ogbn-ppa.

| Metric | Methods      | 4 layers | 6 layers | 8 layers |
|--------|--------------|----------|----------|----------|
| GCN    | 3.19         | 5.29     | 3.68     |
| GCN (SN-U) | 3.11       | 5.86     | 7.25     |
| GCN (SN-B) | 3.48       | 5.72     | 5.86     |
| GCN    | 11.92        | 13.61    | 12.83    |
| GCN (SN-U) | 12.01       | 14.95    | 14.39    |
| GCN (SN-B) | 13.31       | 14.17    | 14.95    |
| GCN    | 17.11        | 18.54    | 16.50    |
| GCN (SN-U) | 17.57       | 18.92    | 19.08    |
| GCN (SN-B) | 17.54       | 18.74    | 18.92    |

Table 5: Node Classification Accuracy (%) for Ogbn-arxiv.

| Methods      | 10 layers | 12 layers | 14 layers | 16 layers |
|--------------|-----------|-----------|-----------|-----------|
| GCN          | 66.5      | 62.3      | 58.7      | 53.2      |
| GCN (DropEdge) | 66.7      | 62.8      | 60.3      | 55.1      |
| GCN (SN-U)   | 67.3      | 65.6      | 62.9      | 56.3      |
| GCN (SN-B)   | 67.0      | 65.4      | 62.1      | 58.5      |

Besides, we further explore the smoothness of node features in the last layer by MAD metric [5], which is the mean of the average cosine distance from nodes to their connected nodes. We use the MAD value of output representations after 500 epochs training as the resulting smoothness, which is depicted in Figure 4(b). The smoothness of output representations that GCN obtains from the 32-th layer in each dataset is always zero, which indicates little diversity. SkipNode successfully maintains information diversities in feature propagating.

Table 6: Efficiency Evaluation on Cora: Average running time per epoch(ms) at different layers.

| Methods      | 3 layers | 5 layers | 7 layers | 9 layers |
|--------------|----------|----------|----------|----------|
| GCN          | 6.5       | 8.7      | 12.6     | 14.0     |
| GCN (DropEdge) | 23.4     | 29.5     | 36.6     | 41.2     |
| GCN (DropNode) | 13.4     | 23.6     | 34.1     | 40.6     |
| GCN (SN-U)   | 8.4       | 14.3     | 20.4     | 26.0     |
| GCN (SN-B)   | 8.3       | 14.5     | 20.7     | 24.6     |
6.6 Robustness Studies

To examine the robustness of our technique, we conducted experiments by employing SkipNode/DropEdge to GCN with different layers $L \in \{4, 8, 12, 16\}$. We fix sampling rate of SkipNode at 0.8, edge sampling rate of DropEdge at 0.5, dropout at 0, weight decay at 0.0005, and learning rate at 0.01. And the results are obtained under 10 random seeds. Figure 5 illustrates that SkipNode can improve models by obtaining higher and stable performance.

7 CONCLUSION

Our study of tackling over-smoothing problem proposes an effective and general framework to address the limitations of current deep GCNs. Also, we discuss the resulting issues caused by over-smoothing to offer a novel perspective to understand GCNs losing their expressive abilities. Our theoretical analysis and experimental results demonstrate the benefits of adopting SkipNode on deep GCNs.
Table 8: Hyperparameter Searching Space. Sampling rate is for SkipNode, DropEdge, and DropNode.

| Baseline Models | Dropout | Weight Decay | Learning Rate | Hidden Dimension |
|-----------------|---------|--------------|---------------|-----------------|
|                 | {0, 0.05, 0.1, 0.2, ..., 0.8} | {5e−4, 5e−7, 5e−9} | {0.01, 0.05, 0.1} | 64 |

**A.4 Empirical Instructions for SkipNode**

Our SkipNode has only one hyperparameter, i.e., the sampling rate. Empirically, for an unseen model, the setting of sampling rate depends on the degree of over-smoothing. In the following, we would like to provide some insights on the sampling rate of SkipNode:

- High sampling rate, e.g., (0.5, 0.9), for the models 1) suffering more from over-smoothing and 2) using small graphs.
- Small sampling rate, e.g., (0, 0.4), for the models 1) suffering less from over-smoothing and 2) using large graphs.

**A.5 Discussions on Uniform Sampling and Biased Sampling**

Uniform sampling strategy tends to randomly select nodes to skip convolution operation. As a result, we can increase the diversity of features for the model to leverage information from all the nodes. Besides, it can also be regarded as a data augmentation technique since it can generate different deformed input data for each model layer. Hence, for those models designed to solve over-smoothing, the uniform sampling is more effective in avoiding over-fitting problems because all the nodes are equally considered.

Motivated by [6], high-degree nodes suffer more from over-smoothing. Hence, we designed biased sampling, which selects nodes based on their degrees. For those models, such as GCN and ResGCN, which suffer more from over-smoothing, biased sampler tends to prevent high-degree nodes’ diversities from disappearing. In addition, the biased sampling prefers to choose a specific part of nodes with higher degree in order to keep the learning stability.

**B PROOF DETAILS**

**B.1 Proof of Lemma 4.1.2**

We first restate Lemma 4.1.2 here:

**Lemma B.1.** Let $\mathcal{L}$ denote the cross-entropy loss function and $Z \in \mathbb{R}^{N \times C}$ be the output of the last layer, where $C$ is the number of class. When the over-smoothing problem occurs, the gradient of the last layer $\sum_{i \in \mathcal{V}_{train}} \sum_{j=1}^{C} \frac{\partial \mathcal{L}}{\partial z_{ij}}$ approaches 0.

**Lemma B.2.** Let $\mathcal{L}$ denote the cross-entropy loss function and $Z \in \mathbb{R}^{N \times C}$ be the output of the last layer, where $C$ is the number of class. When the over-smoothing problem occurs, the gradient of the last layer $\sum_{i \in \mathcal{V}_{train}} \sum_{j=1}^{C} \frac{\partial \mathcal{L}}{\partial z_{ij}}$ approaches 0.

**Proof.** Let $\tilde{Y} = \text{softmax}(Z)$ denote the prediction score, $Y \in \mathbb{R}^{N \times C}$ denote the ground truth indicator, and $\mathcal{L}$ denote the cross-entropy loss function. Then, we have:

$$
\mathcal{L} = -\frac{1}{|\mathcal{V}_{train}|} \sum_{i \in \mathcal{V}_{train}} \sum_{j=1}^{C} Y_{ij} \log \tilde{Y}_{ij}
$$

Thus, we have:

$$
= -\frac{1}{|\mathcal{V}_{train}|} \sum_{i \in \mathcal{V}_{train}} \sum_{j=1}^{C} Y_{ij} \log \left( \frac{\exp(Z_{ij})}{\sum_{k=1}^{C} \exp(Z_{ik})} \right)
$$

where $\mathcal{V}_{train}$ indicates the training set and $|\mathcal{V}_{train}|$ indicates training set size.

For a node $v_i$ with the $c$-th class in the training set, we have $Y_{ic} = 1$ and $Y_{ij} = 0$ for $j \neq c$. Then, for $j = c$, the gradient of $Z_{ic}$ is calculated as:

$$
\frac{\partial \mathcal{L}}{\partial z_{ic}} = -\frac{1}{|\mathcal{V}_{train}|} \sum_{i \in \mathcal{V}_{train}} \frac{1}{Y_{ic}} \left( \frac{\exp(Z_{ic}) \sum_{k=1}^{C} \exp(Z_{ik}) - \exp(Z_{ic})^2}{\sum_{k=1}^{C} \exp(Z_{ik})^2} \right)
$$

and the gradient of $Z_{ij}$ for $j \neq c$ is calculated as:

$$
\frac{\partial \mathcal{L}}{\partial z_{ij}} = \frac{1}{|\mathcal{V}_{train}|} \sum_{i \in \mathcal{V}_{train}} \frac{1}{Y_{ic}} \frac{\exp(Z_{ic}) \exp(Z_{ij})}{\left( \sum_{k=1}^{C} \exp(Z_{ik}) \right)^2}
$$

Since the study [29] has proved that when over-smoothing rises, $Z_{ij} \rightarrow 0$ as $l \rightarrow \infty$, we have $\tilde{Y}_{ij} \approx \frac{1}{c}$. Accordingly, we can further derive the gradient as follows:

$$
\sum_{i \in \mathcal{V}_{train}} \sum_{j=1}^{C} \frac{\partial \mathcal{L}}{\partial z_{ij}} = \sum_{i \in \mathcal{V}_{train}} \sum_{j=1}^{C} \frac{Y_{ij}(\tilde{Y}_{ij} - 1)}{|\mathcal{V}_{train}|} + \frac{(1 - Y_{ij}) \tilde{Y}_{ij}}{|\mathcal{V}_{train}|}
$$

$$
= \frac{1}{|\mathcal{V}_{train}|} \sum_{i \in \mathcal{V}_{train}} \sum_{j=1}^{C} \left( \frac{Y_{ij}}{c} - 1 + \frac{(1 - Y_{ij})}{c} \right)
$$

$$
= \frac{1}{|\mathcal{V}_{train}|} \sum_{i \in \mathcal{V}_{train}} \sum_{j=1}^{C} \left( \frac{1}{c} - Y_{ij} \right)
$$

$$
= \frac{1}{|\mathcal{V}_{train}|} \sum_{i \in \mathcal{V}_{train}} \left( 1 - \sum_{j=1}^{C} Y_{ij} \right) = 0,
$$

□
B.2 Proof of Theorem 5.1

B.2.1 Preparations. We first introduce the Kronecker product operation \( \otimes \) between two vectors. Given \( \mathbf{v} \in \mathbb{R}^d \) and \( \mathbf{w} \in \mathbb{R}^d \), \( \mathbf{v} \otimes \mathbf{w} \) results in a \( \mathbb{R}^{d \times d} \) matrix, and \( (\mathbf{v} \otimes \mathbf{w})_{ij} := v_i w_j \). For \( N \in \mathbb{N} \), we denote \( [N] := \{1, \cdots, N\} \). We define \( U \) as a \( M \)-dimensional \( (0 < M < N) \) subspace of \( \mathbb{R}^N \), which is the eigenspace corresponding to the \( M \) smallest eigenvalues of augmented normalized graph Laplacian \( \tilde{L} = L - \mathbf{1} \mathbf{1}^T \). Assume the eigenvalues of \( \tilde{A} \) are sorted in ascending order as: \( \lambda_1 \leq \cdots \leq \lambda_N \). Further, we have \( -1 < \lambda_1 < \cdots < \lambda_{N-M} \) and \( \lambda_{N-M+1} = \cdots = \lambda_N = 1 \). We also define \( \tilde{\mathbf{d}} \in \mathbb{R}^N \) as an indicator vector where \( \tilde{d}_i = 0 \) \( (i \in [N]) \) or 1, and define \( \mathbf{P} = \text{diag}(\tilde{\mathbf{d}}) \in \mathbb{R}^{N \times N} \) as a diagonal matrix where \( \text{diag}(\tilde{\mathbf{d}}) \) is the diagonalization of \( \tilde{\mathbf{d}} \).

Following [29], we make some assumptions and definitions as follows.

Assumption 1. \( U \) has an orthonormal basis \( \mathbf{e}_m \) \( (m \in [M]) \) that consists of non-negative vectors.

Assumption 2. \( U \) is invariant under \( \tilde{A} \), i.e., if \( \mathbf{u} \in U \), then \( \tilde{A} \mathbf{u} \in U \).

Definition 1. (subspace \( M \)) Let \( \mathcal{M} := U \otimes \mathbb{R}^d = \{\sum_{m=1}^{M} \mathbf{e}_m \otimes w_m \mid w_m \in \mathbb{R}^d\} \) be a subspace of \( \mathbb{R}^{N \times d} \), where \( \mathbf{e}_m \) is the orthonormal basis of \( U \). The distance between subspace \( M \) and input matrix \( X \) is denoted as \( d_M(X) := \inf \{ \|X - H\|_F \mid H \in M \} \), where \( \|\cdot\|_F \) is the Frobenius norm of matrix.

We introduce a lemma to benefit the proof of Theorem 5.1.

Lemma B.3. For \( \mathbf{e}_m \) \( (m \in [M]) \), \( \mathbf{w}_m \in \mathbb{R}^d \), and \( w_m \in \mathbb{R}^d \), we have \( \sum_{m=1}^{M} \tilde{A} \mathbf{e}_m \otimes \mathbf{w}_m = \sum_{m=1}^{M} \mathbf{e}_m \otimes \mathbf{w}_m \).

Proof. Since \( U \) is invariant under \( \tilde{A} \), for any \( m \in [M] \), \( \tilde{A} \mathbf{e}_m \) can be written as a linear combination of \( \mathbf{e}_k \), \( k \in [M] \). There exist \( \mathbf{e}_m \in \mathbb{R} \), we have

\[
\sum_{m=1}^{M} \tilde{A} \mathbf{e}_m \otimes \mathbf{w}_m = \sum_{m=1}^{M} \left( \sum_{k=1}^{M} \mathbf{e}_{mk} \mathbf{e}_k \right) \otimes \mathbf{w}_m
= \sum_{m=1}^{M} \left( \sum_{k=1}^{M} \mathbf{e}_{mk} \mathbf{e}_k \right) \otimes \mathbf{w}_m
= \sum_{m=1}^{M} \mathbf{e}_m \otimes \mathbf{w}_m.
\]

\[\square\]

B.2.2 Proof of Theorem 5.1. We first restate Theorem 5.1 here.

Theorem B.1. Let \( W \in \mathbb{R}^{N \times C} \) be the weight matrix, \( X \in \mathbb{R}^{N \times N} \) be the input features, and \( P \in \mathbb{R}^{N \times N} \) be the diagonal matrix which contains \( 0 \) and \( 1 \) in its diagonal. We denote the aggregated features of GCN layer as \( X_1 \in \mathbb{R}^{N \times C} \), where \( X_1 = \tilde{A} \tilde{X} \tilde{W} \) and the aggregated features of GCN layer with SkipNode as \( X_2 \in \mathbb{R}^{N \times C} \), where \( X_2 = P \tilde{A} \tilde{X} \tilde{W} + (I-P)X \). We have \( d_M(X_2) \geq d_M(X_1) \).

Proof. To make the proof more intuitive, we let \( W = I \). Then we have

\[ X_1 = \tilde{A} \tilde{X}, \]

and

\[ X_2 = P \tilde{A} \tilde{X} + (I-P)X, \]

Following the settings in the proof of Theorem 1 from [29], we let \( \mathbf{e}_m \) \( (m \in [N]) \) denote the orthonormal basis of \( \mathbb{R}^N \), and accordingly, \( X = \sum_{m=1}^{N} \mathbf{e}_m \otimes \mathbf{w}_m \) where \( \mathbf{w}_m \in \mathbb{R}^d \).

For \( X_1 \), we have:

\[
d_M(X_1) = \inf \{ \| \tilde{A} \tilde{X} - H\|_F \mid H \in M \}
= \inf \left\{ \| \tilde{A} \sum_{m=1}^{N} \mathbf{e}_m \otimes \mathbf{w}_m - \sum_{m=1}^{M} \mathbf{e}_m \otimes \mathbf{w}_m \|_F \mid \mathbf{w}_m \in \mathbb{R}^d \right\}
= \inf \left\{ \| \tilde{A} \sum_{m=1}^{M} \mathbf{e}_m \otimes \mathbf{w}_m - \sum_{m=1}^{M} \mathbf{e}_m \otimes \mathbf{w}_m \|_F \mid \mathbf{w}_m \in \mathbb{R}^d \right\}
= \inf \left\{ \| \sum_{m=1}^{M} \mathbf{e}_m \otimes \mathbf{w}_m \|_F \mid \mathbf{w}_m \in \mathbb{R}^d \right\}
= \inf \left\{ \| \sum_{m=1}^{M} \mathbf{e}_m \otimes \mathbf{w}_m \|_F \mid \mathbf{w}_m \in \mathbb{R}^d \right\}
= \inf \left\{ \| \sum_{m=1}^{M} \mathbf{e}_m \otimes (\lambda_m \mathbf{w}_m) \|_F \mid \mathbf{w}_m \in \mathbb{R}^d \right\}
= \inf \left\{ \| \sum_{m=1}^{M} \mathbf{e}_m \otimes (\lambda_m \mathbf{w}_m) \|_F \mid \mathbf{w}_m \in \mathbb{R}^d \right\}
= \| \sum_{m=M+1}^{N} \mathbf{e}_m \otimes (\lambda_m \mathbf{w}_m) \|_F.
\]
For $X_2$, we have:

$$d_M(X_2) = \inf \left\{ \| PAX + (I - P)X - H \|_F : H \in M \right\}$$

$$= \inf \left\{ \| P \sum_{m=1}^N \mathbf{A}_m \otimes \omega_m + (I - P) \sum_{m=1}^N \mathbf{e}_m \otimes \omega_m \right\}$$

$$- \| P + (I - P) \| \sum_{m=1}^M \mathbf{e}_m \otimes \omega_m \|_F \|w_m \in \mathbb{R}^d \}$$

$$= \inf \left\{ \| P \sum_{m=1}^M \mathbf{A}_m \otimes \omega_m + P \sum_{m=M+1}^N \mathbf{A}_m \otimes \omega_m \right\}$$

$$+ (I - P) \sum_{m=1}^N \mathbf{e}_m \otimes \omega_m \|_F \|w_m \in \mathbb{R}^d \}$$

$$= \inf \left\{ \| P \sum_{m=1}^M \mathbf{A}_m \otimes \omega_m + P \sum_{m=M+1}^N \mathbf{A}_m \otimes \omega_m \right\}$$

$$+ (I - P) \sum_{m=1}^N \mathbf{e}_m \otimes \omega_m \|_F \|w_m \in \mathbb{R}^d \}$$

$$= \| P \sum_{m=1}^M \mathbf{A}_m \otimes \omega_m + P \sum_{m=M+1}^N \mathbf{e}_m \otimes \omega_m \|_F \|\omega_m \in \mathbb{R}^d \}$$

$$= \| P \sum_{m=1}^M \mathbf{e}_m \otimes \lambda_m \omega_m + (I - P) \sum_{m=M+1}^N \mathbf{e}_m \otimes \omega_m \|_F.$$  \hfill (13)

Here, without loss of generality, assume $\delta_i = 1$ for $i \in \{1, \ldots, k\}$, and $\delta_i = 0$ for $i \notin \{1, \ldots, k\}$ ($0 < k \leq N$). For any vector $v \in \mathbb{R}^N$, we let $(u)_n$ denote the $n$-th element of $u$, where $n \in \mathbb{N}$. Then, the term $P \sum_{m=M+1}^N \mathbf{e}_m \otimes (\lambda_m \omega_m) + (I - P) \sum_{m=M+1}^N \mathbf{e}_m \otimes \omega_m$ can be represented as:

$$\sum_{m=M+1}^N (\mathbf{e}_m \otimes (\lambda_m \omega_m)_{1, \ldots, d}) \cdots \sum_{m=M+1}^N (\mathbf{e}_m \otimes (\lambda_m \omega_m)_{1, \ldots, d})$$

$$\cdots$$

Since $|\lambda_m| < 1$ for $m \in \mathbb{M}$, we have:

$$d_M(X_2) \geq \| P \sum_{m=1}^M \mathbf{e}_m \otimes (\lambda_m \omega_m) + (I - P) \sum_{m=M+1}^N \mathbf{e}_m \otimes (\lambda_m \omega_m) \|_F$$

$$= \| \sum_{m=M+1}^N \mathbf{e}_m \otimes (\lambda_m \omega_m) \|_F$$

$$= d_M(X_1).$$  \hfill (14)

Therefore, we prove that $d_M(X_2) \geq d_M(X_1)$, which means that SkipNode can slow down the convergence to subspace $M$ so as to relieve the over-smoothing problem. \hfill □
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