Tackling Over-Smoothing for General Graph Convolutional Networks

Wenbing Huang*, Yu Rong*, Tingyang Xu, Fuchun Sun, Junzhou Huang

Abstract—Increasing the depth of Graph Convolutional Networks (GCN), which in principal can permit more expressivity, is shown to incur detriment to the performance especially on node classification. The main cause of this issue lies in over-smoothing. As its name implies, over-smoothing drives the output of GCN with the increase in network depth towards a space that contains limited distinguished information among nodes, leading to poor trainability and expressivity. Several works on refining the architecture of deep GCN have been proposed, but the improvement in performance is still marginal and it is still unknown in theory whether or not these refinements are able to relieve over-smoothing. In this paper, we first theoretically analyze the over-smoothing issue for a general family of prevailing GCNs, including generic GCN, GCN with bias, ResGCN, and APPNP. We prove that the over-smoothing of all these models is characterized by an universal process, i.e. all nodes converging to a cuboid of specific structure. Upon this universal theorem, we further propose DropEdge, a novel and flexible technique to alleviate over-smoothing. At its core, DropEdge randomly removes a certain number of edges from the input graph at each training epoch, acting like a data augmenter and also a message passing reducer. Furthermore, we theoretically demonstrate that DropEdge either reduces the convergence speed of over-smoothing for general GCNs or relieves the information loss caused by it. One group of experimental evaluations on simulated dataset has visualized the difference of over-smoothing between different GCNs as well as verifying the validity of our proposed theorems. Moreover, extensive experiments on several real benchmarks support that DropEdge consistently improves the performance on a variety of both shallow and deep GCNs.

Index Terms—Graph Convolutional Networks, Over-Smoothing, DropEdge, Node Classification.

1 INTRODUCTION

Plethora of data are in the form of graph structures, where a certain number of nodes are irregularly related via edges. Examples include social networks [1], knowledge bases [2], molecules [3], scene graphs [4], etc. Learning on graphs is crucial, not only for the analysis of the graph data themselves, but also for general data forms as graphs deliver strong inductive biases to enable relational reasoning and combinatorial generalization [5]. Recently, Graph Neural Network (GNN) [6] has become the most desired tool for the purpose of graph learning. The initial motivation of inventing GNNs is to generalize the success of traditional Neural Networks (NNs) from grid data to the graph domain.

The key spirit in GNN is that it exploits recursive neighborhood aggregation function to combine the feature vector from a node as well as its neighborhoods until a fixed number of iterations $d$ (a.k.a. network depth). Given an appropriately defined aggregation function, such message passing is proved to capture the structure around each node within its $d$-hop neighborhoods, as powerful as the Weisfeiler-Lehman (WL) graph isomorphism test [7] that is known to distinguish a broad class of graphs [8]. In this paper, we are mainly concerned with Graph Convolutional Networks (GCNs) [1], [9], [10], [11], [12], [13], [14], a central family of GNN that extends the convolution operation from images to graphs. GCNs have been employed successfully for the task of node classification which is the main focus of this paper.

As is already well-known in vision, the depth of Convolutional Neural Network (CNN) plays a crucial role in performance. For example, AlexNet [15] achieves the top-5 error as 16.4 on ImageNet [16], and this error is decreased to 3.57 by ResNet [17] where the number of layers has been increased from 8 to 152. Inspired from this, one might expect to involve more expressivity and characterize richer neighbor topology by stacking more layers for GCN. Another reason of developing deep GCN stems from that characterizing graph topology requires sufficiently deep architectures. The works by [18] and [19] have shown that GCNs are unable to learn a graph moment or estimate certain graph properties if the depth is restricted.

However, the expectation of formulating deep and expressive GCN is not easy to meet. This is because deep GCN actually suffers from the detriment of expressive power mainly caused by over-smoothing [20]. An intuitive notion of over-smoothing is that the mixture of neighborhood features by graph convolution drives the output of an infinitely-deep GCN towards a space that contains limited distinguished information between nodes. From the perspective of training, over-smoothing erases important discriminative information from the input, leading to pool trainability. We have conducted an example experiment in Figure [1] in which the training of a deep GCN is observed to converge poorly.

Although over-smoothing is well known in the community, and several attempts have been proposed to explore how to build deep GCNs [1], [12], [21], [22]. Nevertheless, none of them delivers sufficiently expressive architecture,
Deep GCNs. Despite the fruitful progress, most previous works only focus on shallow GCNs while the deeper extension is seldom discussed. The attempt for building deep GCNs is dated back to the GCN paper [1], where the residual mechanism is applied; unexpectedly, as shown in their experiments, residual GCNs still perform worse when the depth is 3 and beyond. The authors in [20] first point out the main difficulty in constructing deep networks lying in the limitations of traditional graph convolution filters into account, and proved GCN converges to a subspace formulated with the bases of node degrees, but this result is limited to generic GCN [1] without discussion of other architectures.

Hence, it remains open to answer, why and when, in theory, does over-smoothing happen for a general family of GCNs? and can we, to what degree, derive a general mechanism to address over-smoothing and recover the expressive capability of deep GCNs?

To this end, we first revisit the concept of over-smoothing in a general way. Besides generic GCN [1], we explore GCN with bias [18] that is usually implemented in practice, ResGCN [1] and APPNP [12] that refine GCN by involving attention connections. We mathematically prove, if we go with an infinite number of layers, that all these models will converge to a cuboid that expands the subspace proposed by [23] up to a certain radius \( r \). Such theoretical finding is interesting and refreshes current results by [20], [23] in several aspects. First, converging to a cuboid does not necessarily lead to information loss as the cuboid (even it could be small) preserves the full dimensionality of the input space. Second, unlike existing methods [20], [23] that focus on GCN without bias, our conclusion here shows that adding the bias leads to non-zero radius, which, interestingly, will somehow impede over-smoothing. Finally, our theorem suggests that ResGCN slows down over-smoothing and APPNP always maintains certain input information, both of which are consistent with our instinctive understanding on these two models, which, yet, has not been rigorously explored before.

Over-smoothing towards a cuboid rather than a subspace, albeit not that bad, still restricts expressive power and requires to be alleviated. In doing so, we propose DropEdge. The term “DropEdge” refers to randomly dropping out certain rate of edges of the input graph for each training time. In its particular form, each edge is independently dropped with a fixed probability \( p \), with \( p \) being a hyper-parameter and determined by validation. There are several benefits in applying DropEdge for the GCN training (see the experimental improvements by DropEdge in Fig. 1). First, DropEdge can be treated as a message passing reducer. In GCNs, the message passing between adjacent nodes is conducted along edge paths. Removing certain edges is making node connections more sparse, and hence avoiding over-smoothing to some extent when GCN goes very deep. Indeed, as we will draw theoretically in this paper, DropEdge either slows down the degeneration speed of over-smoothing, or reduces information loss caused by dimension collapse.

Anther merit of DropEdge is that it can be considered as a data augmentation technique as well. By DropEdge, we are actually generating different random deformed copies of the original graph; as such, we augment the randomness and the diversity of the input data, thus better capable of preventing over-fitting. It is analogous to performing random rotation, cropping, or flapping for robust CNN training in the context of images.

We provide a complete set of experiments to verify our conclusions related to our rethinking on over-smoothing and the efficacy of DropEdge on four benchmarks of node classification. In particular, our DropEdge—as a flexible and general technique—is able to enhance the performance of various popular backbone networks, including GCN [1], ResGCN [22], JKNet [21], and APPNP [12]. It demonstrates that DropEdge consistently improves the performance on a variety of both shallow and deep GCNs. Complete details are provided in § 5.

2 Related Work

GCNs. The first prominent research on GCNs is presented in [9], which develops graph convolution based on both the spectral and spatial views. Later, [1], [24], [25], [26], [27] apply improvements, extensions, and approximations on spectral-based GCNs. To address the scalability issue of spectral-based GCNs on large graphs, spatial-based GCNs have been rapidly developed [11], [28], [29], [30]. These methods directly perform convolution in the graph domain by aggregating the information from neighbor nodes. Recently, several sampling-based methods have been proposed for fast graph representation learning, including the node-wise sampling methods [11], the layer-wise approaches [10], [13], and the graph-wise methods [31], [32]. Specifically, GAT [33] has discussed applying dropout on edge attentions. While it actually is a post-conducted version of DropEdge before attention computation, the relation to over-smoothing is never explored in [33]. In our paper, however, we have formally presented the formulation of DropEdge and provided rigorous theoretical justification of its benefit in alleviating over-smoothing. We also carried out extensive experiments by imposing DropEdge on several popular backbones.
over-smoothing, but unfortunately, they never propose any method to address it. The follow-up study [12] solves over-smoothing by using personalized PageRank that additionally involves the rooted node into the message passing loop. JKNet [21] employs dense connections for multi-hop message passing which is compatible with DropEdge for formulating deep GCNs. The authors in [23] theoretically prove that the node features of deep GCNs will converge to a subspace and incur information loss. It generalizes the conclusion in [20] by considering the ReLu function and convolution filters.

In this paper, we investigate the over-smoothing behaviors of a broader class of GCNs, and show that general GCNs will converge to a cuboid other than a subspace. Chen et al. [34] develop a measurement of over-smoothing based on the conclusion of [20] and propose to relieve over-smoothing by using a supervised optimization-based method, while our DropEdge is proved to alleviate general GCNs by just random edge sampling, which is simple yet effective. Other recent studies to prevent over-smoothing resort to activation normalization [35] and doubly residual connections [36], which are complementary with our DropEdge. A recent method [22] has incorporated residual layers, dense connections and dilated convolutions into GCNs to facilitate the development of deep architectures. Nevertheless, this model is targeted on graph-level classification (i.e. point cloud segmentation), where over-smoothing is not discussed.

3 Preliminaries

3.1 Graph denotations and the spectral analysis.

Let \( \mathcal{G} = (\mathcal{V}, \mathcal{E}) \) represent the input graph of size \( N \) with nodes \( v_i \in \mathcal{V} \) and edges \((v_i, v_j) \in \mathcal{E} \). We denote by \( X = \{x_1, \cdots, x_N\} \in \mathbb{R}^{N \times C} \) the node features, and by \( A \in \mathbb{R}^{N \times N} \) the adjacency matrix where the element \( A(i,j) \) returns the weight of each edge \((v_i, v_j)\). The node degrees are given by \( d = \{d_1, \cdots, d_N\} \) where \( d_i \) computes the sum of edge weights connected to node \( i \). We define \( D \) as the degree matrix whose diagonal elements are obtained from \( d \).

As we will introduce later, GCN [1] applies the normalized augmented adjacency by adding self-loops followed by augmented degree normalization, which results in \( \hat{A} = D^{-1/2}(A + I)D^{-1/2} \), where \( D = D + I \). We define the augmented normalized Laplacian \([23]\) as \( \hat{L} = I - \hat{A} \). By setting up the relation with the spectral theory of generic Laplacian [37], Oono & Suzuki [23] derive the spectral for the augmented normalized Laplacian and its adjacency thereby. We summarize the result as follows.

**Theorem 1 (Augmented Spectral Property [23]).** Since \( \hat{A} \) is symmetric, let \( \lambda_1 \leq \cdots \leq \lambda_N \) be the real eigenvalues of \( A \), sorted in an ascending order. Suppose the multiplicity of the largest eigenvalue \( \lambda_N \) is \( M \), i.e., \( \lambda_{N-M} < \lambda_{N-M+1} = \cdots = \lambda_N \). Then we have:

- \(-1 < \lambda_1, \lambda_{N-M} < 1;\)
- \(\lambda_{N-M+1} = \cdots = \lambda_N = 1;\)
- \(M \) is given by the number of connected components in \( G \), and \( e_m \coloneqq D^{1/2}u_m \) is the eigenvector associated with eigenvalue \( \lambda_{N-M+m} \) where \( u_m \in \mathbb{R}^N \) is the indicator of the \( m \)-th connected component, i.e., \( u_m(i) = 1 \) if node \( i \) belongs to the \( m \)-th component and \( u_m(i) = 0 \) otherwise.

3.2 Variants of GCN

Here, we introduce several typical variants of GCN.

**Generic GCN.** As originally developed by [1], the feed forward propagation in GCN is recursively conducted as

\[
H_{l+1} = \sigma \left( \hat{A}H_lW_l \right),
\]

where \( H_l = \{h_{1,l}, \cdots, h_{N,l}\} \) are the hidden vectors of the \( l \)-th layer with \( h_{i,l} \) being the hidden feature for node \( i \); \( \sigma(\cdot) \) is a nonlinear function (it is implemented as ReLu throughout this paper); and \( W_l \in \mathbb{R}^{C_l \times C_{l+1}} \) is the filter matrix in the \( l \)-th layer. For the analyses in §4 we set the dimensions of all layers to be the same \( C_l = C \) for simplicity.

**GCN with bias (GCN-b).** In most literature, GCN is introduced in the form of Eq. (1) without the explicit involvement of the bias term that, however, is necessary in practical implementation. If adding the bias, Eq. (1) is renewed as

\[
H_{l+1} = \sigma \left( \hat{A}H_lW_l + b_l \right),
\]

where the bias is defined by \( b_l \in \mathbb{R} \times C \).

**ResGCN.** By borrowing the concept from ResNet [17], Kipf & Welling [1] utilize residual connections between hidden layers to facilitate training of deeper models by carrying over information from the previous layer’s input:

\[
H_{l+1} = \sigma \left( \hat{A}H_lW_l + \alpha H_l \right),
\]
where we have further added the weight $0 \leq \alpha \leq 1$ for more flexibility to balance between the GCN propagation and residual information.

**APPNP.** Since deep GCNs will isolate the output from the input due to over-smoothing, Klicpera et al.\cite{22} suggest to explicitly conduct skip connections from the input layer to each hidden layer to preserve input information:

$$H_{l+1} = (1 - \beta) \hat{A}H_l + \beta H_0,$$

where $0 \leq \beta \leq 1$ is the trade-off weight. Note that the original version by \cite{22} does not involve the non-linearity and weight matrix in each hidden layer. The work by \cite{36} seeks for more capacity by adding the ReLu function and trainable weights to the propagation. Here we adopt the original version and find it works promisingly.

Apart from the models introduced above, JKNet \cite{21}, GAT \cite{33}, GraphSAGE \cite{11}, FastGCN \cite{10}, and AS-GCN \cite{13} are also well studied. All these models either augment the output with every hidden layer \cite{21} or refine the adjacency by self-attention \cite{33} or node sampling \cite{10, 11, 13}, which does not change the dynamic behavior of generic GCN in essence. Hence, this paper sheds more light on the models from Eq. 1 to Eq. 4 without loss of generality.

### 4 Our Analysis and Method

In this section, we first derive the universal theorem \textbf{Theorem 2} to explain why and how over-smoothing will happen for all the four models introduced in §3.2. We then introduce DropEdge that is proved to relieve over-smoothing for all models. We also contend that our DropEdge is able to prevent over-fitting, and involve the discussions and extensions of DropEdge with other related notions.

#### 4.1 Rethinking Over-smoothing

By its original definition in \cite{20}, the over-smoothing phenomenon implies that the node activations will converge to a linear combination of the component indicators $u_n$ (i.e., one-dimensional line) as the network depth increases. \cite{23} has generalized the idea in \cite{20} by taking both the non-linearity (i.e., the ReLu function) and the convolution filters into account; they explain over-smoothing as convergence to a multi-dimensional subspace rather than convergence to an one-dimensional line. Here, we further develop the concept of over-smoothing upon \cite{23} and demonstrate that the output of general GCNs will converge to a cuboid that is an ambient space of the subspace within a certain radius.

We first provide the definition of the subspace.

**Definition 1 (Subspace).** We define $\mathcal{M} := \{ EC \subseteq \mathbb{R}^{M \times C}\}$ as an $M$-dimensional ($M \leq N$) subspace in $\mathbb{R}^{N \times C}$, where $E = \{e_1, \ldots, e_M\} \subseteq \mathbb{R}^{N \times M}$ collects the bases of the largest eigenvalue of $\hat{A}$ in \textbf{Theorem 1}.

The hidden layer of GCNs falling into the subspace $\mathcal{M}$ will cause information loss which has two-fold understandings: 1. For the nodes within the same connected component in $G$, they are only distinguishable by their degrees (see the form of $\hat{E}$ in \textbf{Theorem 1}), neither by node features nor local topology of each node; 2. Such information loss will become more serious if $M \ll N$, e.g., $M = 1$ when the graph is fully connected and all nodes are in a single component. Overall, over-smoothing restricts the output of deep GCNs to be only relevant to limited topology information but independent to the input features, which, as a matter of course, incurs detriment to the expressive power of GCNs.

Hence, the distance between each GCN layer and $\mathcal{M}$ measures how serious the over-smoothing is. We define the distance between matrix $H \in \mathbb{R}^{N \times M}$ and $\mathcal{M}$ as $d_M(H) := \inf_{y \in \mathcal{M}} ||H - Y||_F$, where $\cdot \ | \cdot$ computes the Frobenius norm. With this metric, we define the cuboid below.

**Definition 2 (Cuboid).** We define $O(M, r)$ as the cuboid that expands $\mathcal{M}$ up to a radius $r \geq 0$, namely, $O(M, r) := \{d_M(H) \leq r | H \in \mathbb{R}^{N \times C}\}$.

We now devise the general theorem on over-smoothing.

**Theorem 2 (Universal Over-Smoothing Theorem).** For the GCN models defined in Eq. 1 to Eq. 4 we universally have

$$d_M(H_{l+1}) - r \leq v(d_M(H_l) - r),$$

where $v \geq 0$ and $r$ describe the convergence factor and radius, respectively, depending on what the specific model is. In particular,

- For generic GCN (Eq. 1), $v = s\lambda, r = 0$;
- For GCN-b (Eq. 2), $v = s\lambda, r = \frac{d_M(b)}{s\lambda}$;
- For ResGCN (Eq. 3), $v = s\lambda + \alpha, r = 0$;
- For APPNP (Eq. 4), $v = (1 - \beta)s\lambda, r = \frac{s\lambda d_M(b)}{1 - v}$,

where, $s > 0$ is the supremum of all singular values of all $W_l$, and $\lambda := \max_{n=1}^{M-1} |\lambda_n| < 1$ is the second largest eigenvalue of $\hat{A}$. The equality in Eq. 5 is achievable under certain specification.

The proof is provided in §A. By Eq. 5 we recursively derive $d_M(H_1) - r \leq v(d_M(H_0) - r) \leq \cdots \leq v^l(d_M(H_0) - r)$. We assume $v < 1$ for any $v \in \{s\lambda, s\lambda + \alpha, (1 - \beta)s\lambda\}$ in \textbf{Theorem 2} This is reasonable since $s \leq 1$ is usually the case due to the Gaussian initialization and the $\ell_2$ penalty during training, and $\alpha$ is set to be small enough. Otherwise, if $v > 1$, it will potentially cause gradient explosion and thus unstable training for deep GCNs, which is not the focus of this paper.

**Remark 1.** For generic GCN without bias, the radius becomes $r = 0$, and we have $\lim_{l \to \infty} d_M(H_{l+1}) \leq \lim_{l \to \infty} v^l d_M(H_0) = 0$, indicating that $H_{l+1}$ exponentially converges to $\mathcal{M}$ and thus results in over-smoothing, as already studied by \cite{23}.

**Remark 2.** For GCN-b, the radius is not zero: $r > 0$, and we have $\lim_{l \to \infty} d_M(H_{l+1}) \leq \lim_{l \to \infty} r + v^l d_M(H_0) - r$, i.e., $H_{l+1}$ exponentially converges to the cuboid $O(M, r)$. Unlike $\mathcal{M}$, $O(M, r)$ shares the same dimensionality with $\mathbb{R}^{N \times C}$ and probably contains useful information (other than node degree) for node representation. It does not necessary lead to over-smoothing if the magnitude of $r$ is considerable.

**Remark 3.** For ResGCN, $v = s\lambda + \alpha \geq s\lambda$ (recall $v = s\lambda$ in generic GCN), it exhibits slower convergence speed to $\mathcal{M}$ compared to generic GCN, which is consistent with our intuitive understanding of residual connections.

**Remark 4.** In terms of APPNP, $r > 0$ similar to GCN-b, this will explain why adding the input layer to each hidden layer in APPNP impedes over-smoothing. Notice that increasing $\beta$ will
enlarge $v$ but decrease $r$ at the same time, thus leading to faster convergence to the cuboid.

The conclusion by **Theorem 2** is crucial, not only for it unifies the dynamic behavior of a general family of GCNs when the depth varies, but also for it states the difference of how over-smoothing acts in different models. Besides, the discussions above in Remarks 1–4 show that the value of $v$ plays an important role in influencing over-smoothing for different models, larger $v$ implying less over-smoothing. In the next subsection, we will introduce that our proposed method DropEdge is capable of increasing $v$ and preventing over-smoothing thereby.

### 4.2 DropEdge to Alleviate Over-Smoothing

At each training epoch, the DropEdge technique drops out a certain rate of edges of the input graph by random. Formally, it randomly enforces $Vp$ non-zero elements of the adjacency matrix $A$ to be zeros, where $V$ is the total number of edges and $p$ is the dropping rate. If we denote the resulting adjacency matrix as $A'$, then its relation with $A$ becomes

$$A' = \text{Unif}(A, 1 - p),$$

(6)

where $\text{Unif}(A, 1 - p)$ uniformly samples each edge in $A$ with property $1 - p$, namely, $A'(i,j) = \begin{cases} A(i,j) + \text{Bernoulli}(1 - p) \end{cases}$.

In our implementation, to avoid redundant sampling edge, we create $A'$ by drawing a subset of edges of size $V(1 - p)$ from $A$ in a non-replacement manner. Following the idea of [1], we also perform the re-normalization trick on $A'$, to attain $\hat{A}'$. We replace $A$ with $\hat{A}'$ in Eq. 1 for propagation and training. When validation and testing, DropEdge is not utilized.

**Theorem 2** demonstrates the degenerated expressivity of deep GCNs is closely related to the values of $v$ and $r$. Here, we will demonstrate that adopting DropEdge alleviates over-smoothing in two aspects.

**Theorem 3 (DropEdge).** We denote the original graph as $G$ and the one after dropping certain edges out as $G'$. Regarding the GCN models in Eq. 1 to Eq. 4, we assume by $v$, $M$ the convergence factor and subspace in Eq. 5 on $G$, and by $v'$, $M'$ on $G'$. Then, either of the following inequalities holds after sufficient edges removed.

- The convergence factor and radius only increase: $v \leq v'$;
- The information loss is decreased: $N - \text{dim}(M) > N - \text{dim}(M')$.

The proof of **Theorem 3** is based on **Theorem 2** as well as the concept of effective resistance that has been studied in the random walk theory [38]. We provide the full details in §5.3. **Theorem 3** tells that: 1. By reducing node connections, DropEdge is proved to increase $v$ that will slow down the degeneration speed. 2. The gap between the dimensions of the original space and the convergence subspace, i.e., $N - M$ measures the amount of information loss; larger gap means more severe information loss. As shown by our derivations, DropEdge is able to increase the dimension of the convergence subspace, thus capable of reducing information loss caused by dimension collapse.

**Theorem 3** does suggest that DropEdge is able to alleviate over-smoothing, but it does not mean preventing over-smoothing by DropEdge will always deliver enhanced classification performance. For example, dropping all edges will address over-smoothing completely, which yet will weaken the model expressive power as well since the GCN model has degenerated to an MLP without considering topology modeling. In general, how to balance between preventing over-smoothing and expressing graph topology is critical, and one should take care of choosing an appropriate edge dropping rate $p$ to reflect this. In our experiments, we select the value of $p$ by using validation data, and find it works well in a general way.

**Preventing over-fitting.** Another hallmark of DropEdge is that it is unbiased if we look at the neighborhood aggregation in each layer of GCN. To explain why this is valid, we provide an intuitive understanding here. The neighborhood aggregation can be understood as a weighted sum of the neighbor features (the weights are associated with the edges). As for DropEdge, it enables a random subset aggregation instead of the full aggregation during training. This random aggregation, statistically, only changes the expectation of the neighbor aggregation up to a multiplier $1 - p$ that will be actually removed after adjacency re-normalization. Therefore, DropEdge is unbiased and can be regarded as a data augmentation skill for training GCN by generating different random deformations of the input data. In this way, DropEdge is able to prevent over-fitting, similar to typical image augmentation skills (e.g., rotation, cropping and flipping) to hinder over-fitting in training CNNs. We will provide experimental validations in §5.2.

**Layer-Wise DropEdge.** The above formulation of DropEdge is one-shot with all layers sharing the same perturbed adjacency matrix. Indeed, we can perform DropEdge for each individual layer. Specifically, we obtain $A'_l$ by independently computing Equation 6 for each $l$-th layer. Different layer could have different adjacency matrix $A'_l$. Such layer-wise version brings in more randomness and deformations of the original data, and we will experimentally compare its performance with the original DropEdge in §5.3.

### 4.3 Discussions

This section contrasts the difference between DropEdge and other related concepts including Dropout, DropNode, and Graph Sparsification. We also discuss the difference of over-smoothing between node classification and graph classification.

**DropEdge vs. Dropout.** The Dropout trick [39] is trying to perturb the feature matrix by randomly setting feature dimensions to be zeros, which may reduce the effect of over-fitting but is of no help to preventing over-smoothing since it does not make any change of the adjacency matrix. As a reference, DropEdge can be regarded as a generation of Dropout from dropping feature dimensions to dropping edges, which mitigates both over-fitting and over-smoothing. In fact, the impacts of Dropout and DropEdge are complementary to each other, and their compatibility will be shown in the experiments.

**DropEdge vs. DropNode.** Another related vein belongs to the kind of node sampling based methods, including GraphSAGE [11], FastGCN [10], and AS-GCN [13]. We name this category of approaches as DropNode. For its original motivation, DropNode samples sub-graphs for mini-batch
training, and it can also be treated as a specific form of dropping edges since the edges connected to the dropping nodes are also removed. However, the effect of DropNode on dropping edges is node-oriented and indirect. By contrast, DropEdge is edge-oriented, and it is possible to preserve all node features for the training (if they can be fitted into the memory at once), exhibiting more flexibility. Further, to maintain desired performance, the sampling strategies in current DropNode methods are usually inefficient, for example, GraphSAGE suffering from the exponentially-growing layer size, and AS-GCN requiring the sampling to be conducted recursively layer by layer. Our DropEdge, however, neither increases the layer size as the depth grows nor demands the recursive progress because the sampling of all edges are parallel.

DropEdge vs. Graph-Sparsification. Graph-Sparsification [40] is an old research topic in the graph domain. Its goal is removing unnecessary edges for graph compressing while keeping almost all information of the input graph. This is clearly distinct from the purpose of DropEdge where no optimization objective is needed. Specifically, DropEdge will remove the edges of the input graph by random at each training time, whereas Graph-Sparsification resorts to a tedious optimization method to determine which edges to be deleted, and once those edges are discarded the output graph keeps unchanged.

Node Classification vs. Graph Classification. The main focus of our paper is on node classification, where all nodes are in an identical graph. In graph classification, the nodes are distributed across different graphs; in this scenario, Theorem 2 is still applicable per graph, and node activations of an infinitely-deep GCN in the same graph instance are only distinguishable by node degrees. Yet, this is not true for those nodes in different graphs, since they will converge to different positions in $\mathcal{M}$ (i.e. $C$ in Definition 1). To illustrate this, we suppose all graph instances are fully connected graphs and share the same form of $\hat{A} = \{ \frac{1}{N} \}_{N \times N}$, the node features $X_i$ ($i \geq 0$) within graph $i$ are the same but different from those in different graphs, and the weight matrix is fixed as $W = I$ in Eq. 1. Then, any layer of generic GCN keeps outputting $X_i$ for graph $i$, which indicates no information confusion happens across different graphs. Note that for graph classification over-smoothing per graph still hinders the expressive capability of GCN, as it will cause dimension collapse of the input data.

5 Experiments

Our experimental evaluations are conducted with the goal to answer the following questions:

- Is our proposed universal over-smoothing theorem in line with the experimental observation?
- How does our DropEdge help in relieving over-smoothing of different GCNs?

To address the first question, we display on a simulated dataset how the node activations will behave when the depth grows. We also calculate the distance between the node activations and the subspace to show the convergence dynamics. As for the second question, we contrast the classification performance of varying models of different depths with and without DropEdge on several real node classification benchmarks. The comparisons with state-of-the-art methods are involved as well.

Node classification datasets. Joining the previous works’ practice, we focus on four benchmark datasets varying in graph size and feature type: (1) classifying the research topic of papers in three citation datasets: Cora, Citeseer and Pubmed [41]; (2) predicting which community different posts belong to in the Reddit social network [11]. Note that the tasks in Cora, Citeseer and Pubmed are transductive underlying all node features are accessible during training, while the task in Reddit is inductive meaning the testing nodes are unseen for training. We apply the full-supervised training fashion used in [13] and [10] on all datasets in our experiments. The statistics of all datasets are listed in Tab. 1.

Simulated dataset. We have constructed a small dataset from Cora. In detail, we sample two connected components from the training graph of Cora, with the numbers of nodes being 654 and 26, respectively. The original feature dimension of nodes is 1433 which is not suitable for visualization on a 2-dimension plane. Hence, we apply truncated SVD for dimensionality reduction with output dimension as 2. The left sub-figure in Fig. 3 displays the distribution of the node features. We call this simulated dataset as Small-Cora.

5.1 Visualizing over-smoothing on Small-Cora

Theorem 2 has derived the universality of over-smoothing for the four models: GCN, GCN-b, ResGCN, and APPNP. Here, to check if it is consistent with empirical observations, we visualize the dynamics of the node activations on Small-Cora.

Implementations. To better focus on how the different structure of different GCN influences over-smoothing, the experiments in this section fix the hidden dimension of all GCNs to be 2, randomly initialize an orthogonal weight matrix $W$ for each layer and keep them untrained, which leads to $s = 1$ in Eq. 5. We also remove ReLu function, as we find that, with ReLu, the node activations will degenerate to zeros given the rotation caused by $W$ when the layer number grows, which will hinder the visualization. Regarding GCN-b, the bias of each layer is set as 0.05. We fix $\alpha = 0.2$ and $\beta = 0.5$ for ResGCN and APPNP, respectively. Fig. 3 demonstrates the outputs of all models with varying depth in [10, 100, 400]. Since the total number of nodes is small (i.e. 680), we are able to exactly devise the bases of the subspace,

| Datasets  | Nodes | Edges | Classes | Features | Training/Validation/Testing | Type     |
|----------|-------|-------|---------|----------|-----------------------------|----------|
| Cora     | 2,708 | 5,429 | 7       | 1,433    | 1,208/500/1,000             | Transductive |
| Citeseer | 3,327 | 4,732 | 6       | 3,703    | 1,812/500/1,000             | Transductive |
| Pubmed   | 19,717| 44,338| 3       | 500      | 18,217/500/1,000            | Transductive |
| Reddit   | 2,329,65 | 11,606,919 | 41      | 602      | 152,410/23,699/55,334       | Inductive  |

TABLE 1: Dataset Statistics
Fig. 3: Output dynamics of GCN. From left to right, the sub-figures display the node activations (the axes corresponded to the feature dimensions) of the depth \(d\) as 0, 10, 100, and 400. The size of each node reflects the value of its degree, and \(d_M\) computes the distance between the node activations and the subspace (below figures are the same).

Fig. 4: Output dynamics of GCN-b. The left sub-figure plots the value of \(d_M\) for GCN and GCN-b under varying depth. Other sub-figures depict the node activations of the depth as 10, 100, and 400.

Fig. 5: Output dynamics of ResGCN. The left sub-figure plots the value of \(d_M\) for GCN and ResGCN under varying depth. Other sub-figures depict the node activations of the depth as 10, 100, and 400.

Fig. 6: Output dynamics of APPNP. The left sub-figure plots the value of \(d_M\) for GCN and APPNP under varying depth. Other sub-figures depict the node activations of the depth as 10, 100, and 400.

Fig. 7: Output dynamics of GCN with DropEdge. The left sub-figure plots the value of \(d_M\) for GCN and GCN with DropEdge (the dropping rate \(p = 0.5, 0.7\)) under varying depth. Other sub-figures depict the node activations of the depth as 10, 100, and 400 (\(p = 0.5\)).
When we perform DropEdge on GCN with the dropping which confirms the conclusion by Remark 4. In APPNP, as within different components are colinear onto different lines, d when Theorem 3, where the convergence to the subspace becomes slower and the number of connected components is larger, and the bigger (of larger degree) the node is, the farther it is from the zero point. Such observation is consistent with Remark \[1\] as different lines indeed represent different bases of the subspace.

Results in Fig. 4. The output dynamics of GCN-b is distinct from GCN. It turns out the nodes within the same component keep non-collinear when \(d = 400\). For better visualization, we plot the exact values of \(d_M\) for both GCN and GCN-b with respect to \(d\) in the left sub-figure; in contrast to GCN, the curve of GCN-b fluctuates within a certain bounded area. This result coincides with Remark \[2\] and supports that adding the bias term enables the node activations to converge to a cuboid surrounding the subspace under a certain radium.

Results in Fig. 5. Akin to GCN, the output of ResGCN approaches the subspace in the end, but its convergence dynamics as shown in the left sub-figure is a bit different. The curve shakes up and down for several rounds before it eventually degenerates. This could because the skip connection in ResGCN helps prevent over-smoothing or even reverse the convergence direction during the early period. When \(d\) is sufficiently large, each node will exponentially fall into the subspace at the rate of \(\lambda + \alpha\) as proven in Remark \[3\]. Note that the average speed of ResGCN is smaller than that of GCN (recalling \(\lambda + \alpha > \lambda\)).

Results in Fig. 6. The behavior of APPNP is completely different. It quickly becomes stationary and this stationary point is beyond the subspace up to a fixed distance \(r > 0\), which confirms the conclusion by Remark \[4\] in APPNP, as the rate \(v = \lambda \beta\) is smaller than that of GCN, its convergence speed is faster.

Results in Fig. 7. Clearly, the results in Fig. 2 verify Theorem \[5\], where the convergence to the subspace becomes slower and the number of connected components is larger when we perform DropEdge on GCN with the dropping rate \(p = 0.5\). If we further increase \(p\) to 0.7, the convergence speed will be further decreased.

Comparison with SOTAs. We select the best performance for each backbone with DropEdge, and contrast them with existing State of the Arts (SOTA), including KLED [42], DCNN [43], FastGCN [10], AS-GCN [13], and GraphSAGE [44] in Tab. 2. For the SOTA methods, we reuse the results reported in [13]. Besides GCN, ResGCN, and APPNP. We have these findings in Tab. 2: (1) Clearly, our DropEdge obtains significant enhancement against SOTAs; particularly on Cora and Citeseer, the best accuracies by APPNP+DropEdge are 89.10% and 81.30%, which are clearly better than the previous best (87.44% and 79.7%), and obtain around 1% improvement compared to the no-drop APPNP. Such improvement is regarded as a remarkable boost considering the challenge on these benchmarks. (2) For most models with DropEdge, the best accuracy is obtained under the depth beyond 4, which again verifies the impact of DropEdge on formulating deep networks. (3) As mentioned in §4.3, FastGCN, AS-GCN and GraphSAGE are considered as the DropNode extensions of GCNs. The DropEdge based approaches outperform the DropNode based variants as shown in Tab. 2 which somehow confirms the effectiveness of DropEdge.
Fig. 8: Test-Accuracy vs. Depth comparison of GCN with and without DropEdge. From left to right: the results under different numbers of layers on Cora, Citeseer, Pubmed, and Reddit (Below figures are the same).

Fig. 9: Test-Accuracy vs. Depth comparison of GCN-b with and without DropEdge.

Fig. 10: Test-Accuracy vs. Depth comparison of ResGCN with and without DropEdge.

Fig. 11: Test-Accuracy vs. Depth comparison of APPNP with and without DropEdge.

Fig. 12: Test-Accuracy vs. Depth comparison of JKNet with and without DropEdge (16-layer JKNet meets OOM on Reddit).
This section continues two other ablation studies: 1. assessing the compatibility of DropEdge with Dropout; 2. justifying the performance of layer-wise DropEdge. We employ GCN as the backbone in this section. The hidden dimension, learning rate and weight decay are fixed to 256, 0.005 and 0.0005, receptively. The random seed is fixed. We train all models with 200 epochs. Unless otherwise mentioned, we do not utilize the “withloop” and “within” operation (see their definitions in Tab. 5 in Appendix).

### 5.3.1 On Compatibility with Dropout

§ 4.3 has discussed the difference between DropEdge and Dropout. Hence, we conduct an ablation study on GCN-4, and the validation losses are demonstrated in Figure 14. It reads that while both Dropout and DropEdge are able to facilitate the training of GCN, the improvement by DropEdge is more significant, and if we adopt them concurrently, the loss is decreased further, indicating the compatibility of DropEdge with Dropout.

### 5.3.2 On layer-wise DropEdge

§ 4.2 has descried the Layer-Wise (LW) extension of DropEdge. Here, we provide the experimental evaluation on assessing its effect. As observed from Figure 15, the LW DropEdge achieves lower training loss than the original version, whereas the validation value between two models is comparable. It implies that LW DropEdge can facilitate the training further than original DropEdge. However, we prefer to use DropEdge other than the LW variant so as to not only avoid the risk of over-fitting but also reduces computational complexity since LW DropEdge demands to sample each layer and spends more time.

### 6 Conclusion

We have analyzed the universal process of over-smoothing for 4 popular GCN models, including generic GCN, GCN with bias, ResGCN, and APPNP. Upon our analyses, we propose DropEdge, a novel and efficient technique to facilitate the development of general GCNs. By dropping out a certain rate of edges by random, DropEdge includes more diversity into the input data to prevent over-fitting, and reduces message passing in graph convolution to alleviate over-smoothing. Considerable experiments on Cora, Citeseer,
We first provide the following lemma.

We also define the orthogonal complement of \(\hat{E}\). We additionally discuss Ineq. 10, and prove all the four popular GCNs. It is expected that our research will open up a new venue on a more in-depth exploration of deep GCNs for broader potential applications.

\section*{Appendix A}
\subsection*{Proof of Theorem 2}
We first provide the following lemma.

\textbf{Lemma 4.} For any \(H, B \in \mathbb{R}^{N \times C}\) and \(\alpha_1, \alpha_2 \geq 0\), we have:

\[
\begin{align*}
\hat{d}_M(\hat{A}H) &\leq \lambda d_M(H), \\
\hat{d}_M(\hat{E}^T H) &\leq \|F\|_F d_M(H), \\
\hat{d}_M(\sigma(H)) &\leq d_M(H), \\
\hat{d}_M(\alpha_1 H + \alpha_2 B) &\leq \alpha_1 \hat{d}_M(H) + \alpha_2 \hat{d}_M(B),
\end{align*}
\]

where \(\sigma\) is ReLu function.

Proof. \cite{Oono & Suzuki} has proved the first three inequalities. Their proof is based on eigen-decomposition with Kronecker product, which is sort of tedious. Here, we additionally discuss Ineq. 10 and prove all the four inequalities in a new and concise way.

Our proof is mainly based on the notion of projection \cite{45} that returns the projected vector/matrix onto a subspace from any given vector/matrix. In terms of the subspace \(M\), the projection matrix is given by \(\hat{E}^T \hat{E}\), where \(\hat{E}\) is the normalized bases of the subspace \(M\) defined in Theorem 1. We also define the orthogonal complement of \(\hat{E}\) as \(\hat{F}\). Then, the distance \(\hat{d}_M(H)\) of arbitrary \(H\) is derived as

\[
\hat{d}_M(H) = \| (I - \hat{E}^T \hat{E}) H \|_F
\]

With Eq. 11 at hand, we justify Ineq. 7, 8 and 10 by

\[
\hat{d}_M(\hat{A}H) = \| F^T (\hat{A}H) \|_F
\]

\[
\leq \| F^T \hat{E}^T + \hat{F} \hat{A} \|_F
\]

\[
\leq \| \hat{A} \|_F \| \hat{F}^T H \|_F
\]

\[
\leq \lambda \hat{d}_M(H),
\]

where we have applied the fact \(\hat{A} = \hat{E}^T \hat{E} + \hat{F} \hat{A} \hat{F}^T\).

\[
\hat{d}_M(\hat{E}^T H) = \| F^T (\hat{E}^T H) \|_F
\]

\[
\leq \| F^T \|_F \| \hat{E}^T H \|_F
\]

\[
\leq \| \hat{E}^T H \|_F \| \hat{W} \|_F
\]

\[
\leq \hat{d}_M(H),
\]

\[
\hat{d}_M(\alpha_1 H + \alpha_2 B) = \| F^T (\alpha_1 H + \alpha_2 B) \|_F
\]

\[
\leq \| \alpha_1 F^T H \|_F + \| \alpha_2 F^T B \|_F
\]

\[
= \alpha_1 \hat{d}_M(H) + \alpha_2 \hat{d}_M(B).
\]

Notice that the above inequation can be extended for the vector \(b \in \mathbb{R}^{1 \times C}\) (such as the bias in GCN-b), and we define \(\hat{d}_M(b) = \hat{d}_M(B)\) where \(B \in \mathbb{R}^{N \times C}\) is broadcasted from \(b\) in the first dimension.

We now prove Eq. 9. As \(\hat{E}\) is defined by the node indicator of connected components in Theorem 1, all elements in \(\hat{E}\) are non-negative. Moreover, since each node can only belong to one connected component, the non-zero entries in different column \(e_i\) of \(\hat{E}\) are located in a non-overlap way. It means, Eq. 11 can be further decomposed as

\[
\hat{d}_M(H) = \sum_{i=1}^M \| (I - e_i e_i^T) H \|_F,
\]

where the \(j\)-th row of \(H \in \mathbb{R}^{N \times C}\) is copied from \(H\) if \(j\) belongs to component \(i\) and is zero otherwise. Then,

\[
\hat{d}_M^2(H) = \sum_{i=1}^M \| (I - e_i e_i^T) H \|_F^2
\]

\[
= \sum_{i=1}^M \| (I - e_i e_i^T) H \|_F^2
\]

\[
= \sum_{i=1}^M \| H_i^T (I - e_i e_i^T) H_i \|
\]

\[
= \sum_{i=1}^M \sum_{c} h_{ic}^2 h_{ic} - \| (h_{ic})^T e_i \|^2.
\]

Then, we minus Eq. 18 with Eq. 17

\[
\hat{d}_M^2(H) - \hat{d}_M^2(\sigma(H)) = \sum_{i=1}^M \sum_{c} h_{ic}^2 h_{ic} - \| (h_{ic})^T e_i \|^2.
\]

Based on Lemma 4, we can immediately justify Theorem 2 as follows.

For GCN in Eq. 2 we apply Ineq. 7, 8 and 9

\[
\hat{d}_M(H_{i+1}) \leq \hat{d}_M(\hat{A}H_{i}) \leq \lambda \| \hat{W} \|_F \hat{d}_M(H_i) \leq s \hat{d}_M(H_i).
\]

For GCN-b in Eq. 2 we apply Ineq. 7, 10

\[
\hat{d}_M(H_{i+1}) \leq s \lambda \hat{d}_M(H_i) + \hat{d}_M(b_i)
\]

\[
\Rightarrow \hat{d}_M(H_{i+1}) \leq \frac{\hat{d}_M(b_i)}{1 - s \lambda}.
\]
For ResGCN in Eq. 3 we apply Ineq. [7] [10]

\[ d_M(H_{l+1}) \leq s \lambda d_M(H_l) + \alpha d_M(H_l) \]

(22)

For APPNP in Eq. 4 we apply Ineq. [7] [10]

\[ d_M(H_{l+1}) \leq (1 - \beta) \lambda d_M(H_l) + \beta d_M(H_0) \]

\[ \Rightarrow d_M(H_{l+1}) - \frac{\beta d_M(H_0)}{1 - (1 - \beta) \lambda} \leq (1 - \beta) \lambda \left( d_M(H_l) - \frac{\beta d_M(H_0)}{1 - (1 - \beta) \lambda} \right). \]

(23)

Clearly, Ineq. [20] [23] imply the general form in Theorem 2.

APPENDIX B
PROOF OF THEOREM 3

We need to adopt some concepts from [38] in proving Theorem 3. Consider the graph \( G \) as an electrical network, where each edge represents an unit resistance. Then the effective resistance, \( R_{st} \) from node \( s \) to node \( t \) is defined as the total resistance between node \( s \) and \( t \). According to Corollary 3.3 and Theorem 4.1 (i) in [38], we can build the connection between \( \lambda \) and \( R_{st} \) for each connected component via commute time as the following inequality:

\[ \lambda \geq 1 - \frac{1}{R_{st}} \left( \frac{1}{d_s} + \frac{1}{d_t} \right). \]

(24)

Now, we prove Theorem 3.

Proof. Our proof relies basically on the connection between \( \lambda \) and \( R_{st} \) in Equation (24). We recall Corollary 4.3 in [38] that removing any edge from \( G \) can only increase any \( R_{st} \), then according to [24], the lower bound of \( \lambda \) only increases if the removing edge is not connected to either \( s \) or \( t \) (i.e. the degree \( d_s \) and \( d_t \) keep unchanged). Since there must exist a node pair satisfying \( R_{st} = \infty \) after sufficient edges (except self-loops) are removed from one connected component of \( G \), we have the infinite case \( \lambda = 1 \) given in Equation (24) that both \( 1/d_s \) and \( 1/d_t \) are consistently bounded by a finite number. i.e. 1. It implies \( \lambda \) does increase before it reaches \( \lambda = 1 \) as \( \nu \rightarrow 1 \) and we have proved the first part of Theorem 3, i.e., \( \nu \leq \nu' \) after removing sufficient edges.

When there happens \( R_{st} = \infty \), the connected component is disconnected into two parts, which leads to the increment of the dimension of \( M \) by 1 and proves the second part of Theorem 3, i.e., the information loss is decreased: \( N - \text{dim}(M) > N - \text{dim}(M') \).

\[ \square \]

APPENDIX C
MODELS AND BACKBONES

Backbones We employ one input GCL and one output GCL on ResGCN, APPNP, and JKNet. Therefore, the layers in ResGCN, APPNP and JKNet are at least 3 layers. All backbones are implemented in Pytorch [46].

Self Feature Modeling We also implement a variant of graph convolution layer with self feature modeling [47]:

\[ H_{l+1} = \sigma \left( A \tilde{H} W_L + H_{l, \text{self}} \right), \]

(25)

where \( W_{self_i} \in \mathbb{R}^{C_l \times C_l - 1} \).

| Hyper-parameter | Description             |
|-----------------|-------------------------|
| learning rate   | weight-decay            |
| L2 regulation weight | edge preserving percent (1 - p) |
| dropout rate    | the propagation models |
| normalization   | using self feature modeling |
| withinloop      | using batch normalization |

TABLE 3: Hyper-parameter Description

ACKNOWLEDGMENTS

The authors would like to thank...

REFERENCES

[1] T. N. Kipf and M. Welling, “Semi-supervised classification with graph convolutional networks,” in Proceedings of the International Conference on Learning Representations, 2017.
[2] H. Ren, W. Hu, and J. Leskovec, “Query2box: Reasoning over knowledge graphs in vector space using box embeddings,” in International Conference on Learning Representations, 2019.
[3] D. K. Duvenaud, D. Maclaurin, J. Iparraguirre, R. Bombarell, T. Hirzel, A. Aspuru-Guzik, and R. P. Adams, “Convolutional networks on graphs for learning molecular fingerprints,” in Advances in neural information processing systems, 2015, pp. 2224–2232.
[4] D. Xu, Y. Zhu, C. B. Choy, and L. Fei-Fei, “Scene graph generation by iterative message passing,” in Proceedings of the IEEE conference on computer vision and pattern recognition, 2017, pp. 5410–5419.
[5] P. W. Battaglia, J. B. Hamrick, V. Bapst, A. Sanchez-Gonzalez, V. Zambaldi, M. Malinowski, A. Tacchetti, D. Raposo, A. Santoro, R. Faulkner et al., “Relational inductive biases, deep learning, and graph networks,” arXiv preprint arXiv:1806.01261, 2018.
[6] Z. Wu, S. Pan, F. Chen, G. Long, C. Zhang, and P. S. Yu, “A comprehensive survey on graph neural networks,” arXiv preprint arXiv:1901.00596, 2019.
[7] B. Weisfeiler and A. A. Lehman, “A reduction of a graph to its chromatic class,” Nauchno-Technicheskaya Informatsia, vol. 2, no. 9, pp. 12–16, 1968.
[8] K. Xu, W. Hu, J. Leskovec, and S. Jegelka, “How powerful are graph neural networks?” arXiv preprint arXiv:1810.00826, 2018.
[9] J. Bruna, W. Zaremba, A. Szlam, and Y. LeCun, “Spectral networks and locally connected networks on graphs,” in Proceedings of International Conference on Learning Representations, 2013.
[10] J. Chen, T. Ma, and C. Xiao, “Fastgcn: Fast learning with graph convolutional networks via importance sampling,” in Proceedings of the 6th International Conference on Learning Representations, 2018.
[11] W. Hamilton, Z. Ying, and J. Leskovec, “Inductive representation learning on large graphs,” in Advances in Neural Information Processing Systems, 2017, pp. 1025–1035.
[12] J. Klicpera, A. Bojchevski, and S. Günnemann, “Predict then propagate: Graph neural networks meet personalized pagerank,” in Proceedings of the 7th International Conference on Learning Representations, 2019.
[13] W. Huang, T. Zhang, Y. Rong, and J. Huang, “Adaptive sampling towards fast graph representation learning,” in Advances in Neural Information Processing Systems, 2018, pp. 4558–4567.
[14] K. Xu, C. Li, Y. Tian, T. Sonobe, K.-i. Kawarabayashi, and S. Jegelka, “Representation learning on graphs with jumping knowledge networks,” arXiv preprint arXiv:1806.03536, 2018.
[15] A. Krizhevsky, I. Sutskever, and G. E. Hinton, “Imagenet classification with deep convolutional neural networks,” in Advances in neural information processing systems, 2012, pp. 1097–1105.
TABLE 4: The normalization / propagation models

| Description                                      | Notation                  | $A'$                                      |
|--------------------------------------------------|---------------------------|-------------------------------------------|
| First-order GCN                                  | FirstOrderGCN             | $I + D^{-1/2} AD^{-1/2}$                   |
| Augmented Normalized Adjacency                   | AugNormAdj                | $(I + D)^{-1/2}(A + I)(D + I)^{-1/2}$      |
| Augmented Normalized Adjacency with Self-loop    | AugGeNormAdj              | $I + (D + I)^{-1/2}(A + I)(D + I)^{-1/2}$  |
| Augmented Random Walk                            | AugRWalk                  | $(D + I)^{-1}(A + I)$                      |

[16] J. Deng, W. Dong, R. Socher, L.-J. Li, K. Li, and L. Fei-Fei, “Imagenet: A large-scale hierarchical image database,” in 2009 IEEE conference on computer vision and pattern recognition. Ieee, 2009, pp. 248–255.

[17] K. He, X. Zhang, S. Ren, and J. Sun, “Deep residual learning for image recognition,” in Proceedings of the IEEE conference on computer vision and pattern recognition, 2016, pp. 770–778.

[18] N. Dehghani, A.-L. Barabási, and R. Yu, “Understanding the representation power of graph neural networks in learning graph topology,” in Advances in Neural Information Processing Systems, 2019, pp. 1413–1423.

[19] A. Loukas, “What graph neural networks cannot learn: depth vs width,” in International Conference on Learning Representations, 2019.

[20] Q. Li, Z. Han, and X.-M. Wu, “Deeper insights into graph convolutional networks for semi-supervised learning,” in Thirty-Second AAAI Conference on Artificial Intelligence, 2018.

[21] K. Xu, C. Li, Y. Tian, T. Sonobe, K.-i. Kawarabayashi, and S. Jegelka, “Representation learning on graphs with jumping knowledge networks,” in Proceedings of the 35th International Conference on Machine Learning, 2018.

[22] G. Li, M. Müller, A. Thabet, and B. Ghanem, “Deepgcn: Can gcns go as deep as cnns?” in International Conference on Computer Vision, 2019.

[23] K. Oono and T. Suzuki, “Graph neural networks exponentially lose expressive power for node classification,” in International Conference on Learning Representations, 2020.

[24] M. Defferrard, X. Bresson, and P. Vandergheynst, “Convolutional neural networks on graphs with fast localized spectral filtering,” in Advances in Neural Information Processing Systems, 2016, pp. 3844–3852.

[25] M. Henaff, J. Bruna, and Y. LeCun, “Deep convolutional networks on graph-structured data,” arXiv preprint arXiv:1506.05163, 2015.

[26] R. Li, S. Wang, F. Zhu, and J. Huang, “Adaptive graph convolutional neural networks,” in Thirty-Second AAAI Conference on Artificial Intelligence, 2018.

[27] R. Levie, F. Monti, X. Bresson, and M. M. Bronstein, “Cayleynets: Graph convolutional neural networks with complex rational spectral filters,” IEEE Transactions on Signal Processing, vol. 67, no. 1, pp. 97–109, 2017.

[28] F. Monti, D. Boscaini, J. Masci, E. Rodola, J. Svoboda, and M. M. Bronstein, “Geometric deep learning on graphs and manifolds using mixture model cnns,” in Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition, 2017, pp. 5115–5124.

[29] M. Niepert, M. Ahmed, and K. Kutzkov, “Learning convolutional neural networks for graphs,” in International conference on machine learning, 2016, pp. 2014–2023.

[30] H. Gao, Z. Wang, and S. Ji, “Large-scale learnable graph convolutional networks,” in Proceedings of the 24th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining, ACM, 2018, pp. 1416–1424.

[31] W.-L. Chiang, X. Liu, S. Si, Y. Li, S. Bengio, and C.-J. Hsieh, “Cluster-gcn: An efficient algorithm for training deep and large graph convolutional networks,” in KDD, 2019, pp. 257–266.

[32] Z. Lin, A. Desmaison, L. Antiga, and A. Lerer, “Automatic differentiation in PyTorch,” in NIPS Autodiff Workshop, 2017.

[33] A. Fout, J. Byrd, B. Shariat, and A. Ben-Hur, “Protein interface prediction using graph convolutional networks,” in Advances in Neural Information Processing Systems, 2017, pp. 6530–6539.
TABLE 5: The hyper-parameters of best accuracy for each backbone on all datasets.

| Dataset | Backbone | nlayers | Acc. | Hyper-parameters |
|---------|----------|---------|------|------------------|
| Cora    | GCN      | 2       | 0.880| lr:0.008, weight-decay:1e-5, sampling-percent:0.4, dropout:0.8, normalization:AugRWalk |
|         | GCN-b    | 2       | 0.880| lr:0.008, weight-decay:1e-5, sampling-percent:0.6, dropout:0.8, normalization:AugRWalk |
|         | ResGCN   | 4       | 0.870| lr:0.001, weight-decay:1e-5, sampling-percent:0.1, dropout:0.5, normalization:FirstOrderGCN |
|         | JKNet    | 16      | 0.880| lr:0.008, weight-decay:5e-4, sampling-percent:0.2, dropout:0.8, normalization:AugNormAdj |
|         | APPNP    | 64      | 0.891| lr:0.006, weight-decay:5e-5, sampling-percent:0.4, dropout:0.1, normalization:AugRWalk, alpha:0.2 |
| Citeseer| GCN      | 2       | 0.800| lr:0.003, weight-decay:1e-4, sampling-percent:0.6, dropout:0.3, normalization:AugNormAdj, withloop |
|         | GCN-b    | 2       | 0.796| lr:0.003, weight-decay:1e-4, sampling-percent:0.6, dropout:0.3, normalization:AugNormAdj, withloop |
|         | ResGCN   | 16      | 0.794| lr:0.001, weight-decay:5e-3, sampling-percent:0.5, dropout:0.3, normalization:BingGeNormAdj, withloop |
|         | JKNet    | 8       | 0.802| lr:0.004, weight-decay:5e-3, sampling-percent:0.5, dropout:0.3, normalization:BingGeNormAdj, withloop |
|         | APPNP    | 64      | 0.813| lr:0.010, weight-decay:1e-5, sampling-percent:0.8, dropout:0.8, normalization:AugNormAdj, alpha:0.4 |
| Pubmed  | GCN      | 2       | 0.913| lr:0.009, weight-decay:5e-5, sampling-percent:0.4, dropout:0.8, normalization:BingGeNormAdj, withloop, withbn |
|         | GCN-b    | 2       | 0.911| lr:0.009, weight-decay:5e-5, sampling-percent:0.4, dropout:0.8, normalization:BingGeNormAdj, withloop, withbn |
|         | ResGCN   | 32      | 0.911| lr:0.003, weight-decay:5e-5, sampling-percent:0.7, dropout:0.8, normalization:BingGeNormAdj, withloop, withbn |
|         | JKNet    | 64      | 0.916| lr:0.005, weight-decay:1e-4, sampling-percent:0.5, dropout:0.8, normalization:BingGeNormAdj, withloop, withbn |
|         | APPNP    | 4       | 0.907| lr:0.008, weight-decay:1e-4, sampling-percent:0.8, dropout:0.1, normalization:FirstOrderGCN, alpha:0.4 |
| Reddit  | GCN      | 8       | 0.9673| lr:0.005, weight-decay:5e-5, sampling-percent:0.6, dropout:0.5, normalization:BingGeNormAdj, withloop, withbn |
|         | GCN-b    | 4       | 0.9684| lr:0.001, weight-decay:5e-5, sampling-percent:0.4, dropout:0.5, normalization:BingRWalk, withloop |
|         | ResGCN   | 16      | 0.9648| lr:0.009, weight-decay:1e-5, sampling-percent:0.2, dropout:0.5, normalization:BingGeNormAdj, withloop, withbn |
|         | JKNet    | 8       | 0.9702| lr:0.010, weight-decay:5e-5, sampling-percent:0.6, dropout:0.5, normalization:BingGeNormAdj, withloop, withbn |
|         | APPNP    | 8       | 0.9585| lr:0.004, weight-decay:1e-5, sampling-percent:0.5, dropout:0.1, normalization:BingRWalk, alpha:0.1 |