DROPEDGE: TOWARDS DEEP GRAPH CONVOLUTIONAL NETWORKS ON NODE CLASSIFICATION

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ABSTRACT

Over-fitting and *over-smoothing* are two main obstacles of developing deep Graph Convolutional Networks (GCNs) for node classification. In particular, over-fitting weakens the generalization ability on small dataset, while over-smoothing impedes model training by isolating output representations from the input features with the increase in network depth. This paper proposes DropEdge, a novel and flexible technique to alleviate both issues. 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 retards the convergence speed of over-smoothing or relieves the information loss caused by it. More importantly, our DropEdge is a general skill that can be equipped with many other backbone models (*e.g.* GCN, ResGCN, GraphSAGE, and JKNet) for enhanced performance. Extensive experiments on several benchmarks verify that DropEdge consistently improves the performance on a variety of both shallow and deep GCNs. The effect of DropEdge on preventing over-smoothing is empirically visualized and validated as well. Codes will be made public upon the publication.

1 INTRODUCTION

Graph Convolutional Networks (GCNs), which exploit message passing or equivalently certain neighborhood aggregation function to extract high-level features from a node as well as its neighborhoods, have boosted the state-of-the-arts for a variety of tasks on graphs, such as node classification (Bhagat et al., 2011; Zhang et al., 2018), social recommendation (Freeman, 2000; Perozzi et al., 2014), and link prediction (Liben-Nowell & Kleinberg, 2007) to name some. In other words, GCNs have been becoming one of the most crucial tools for graph representation learning. Yet, when we revisit typical GCNs on node classification (Kipf & Welling, 2017), they are usually shallow (*e.g.* the number of the layers is 2[1]). Inspired from the success of deep CNNs on image classification, several attempts have been proposed to explore how to build deep GCNs towards node classification (Kipf & Welling, 2017; Li et al., 2018a; Xu et al., 2018a; Li et al., 2019); nevertheless, none of them delivers sufficiently expressive architecture. The motivation of this paper is to analyze the very factors that impede deeper GCNs to perform promisingly, and develop method to address them.

We begin by investigating two factors: *over-fitting* and *over-smoothing*. Over-fitting comes from the case when we utilize an over-parametrized model to fit a distribution with limited training data, where the model we learn fits the training data very well but generalizes poorly to the testing data. It does exist if we apply a deep GCN on small graphs (see Figure 1 for the empirical comparison between 2-layer GCN and 4-layer GCN on Cora). Over-smoothing, towards the other extreme, makes training a very deep GCN difficult. As first introduced by Li et al. (2018a) and further explained in Wu et al. (2019); Xu et al. (2018a); Klicpera et al. (2019), graph convolutions essentially push representations of adjacent nodes mixed with each other, such that, if extremely we go with an infinite number of layers, all nodes' representations will converge to a stationary point, making them unrelated to the input features and leading to vanishing gradients. We call this phenomenon as over-smoothing of node features. To illustrate its influence, we have conducted an example experiment with 8-layer GCN in Figure 1, in which the training of such a deep GCN is observed to converge poorly.

[1] When counting the number of layers (or network depth) of GCN, this paper does not involve the input layer.

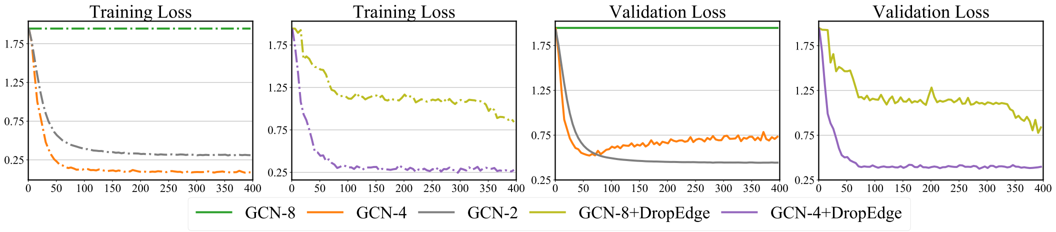


Figure 1: Training losses (in dash line) and validation losses (in bold line) of various architectures on Cora. We implement 2-layer GCN, 4-layer GCN w and w/o DropEdge, 8-layer GCN w and w/o DropEdge. GCN-4 gets stuck in the over-fitting issue attaining lower training error but higher validation error than the 2-layer one; the training of GCN-8 fails to converge satisfactorily due to over-smoothing. By applying DropEdge, both GCN-4 and GCN-8 work well for both training and validation.

Both of the above two issues can be alleviated, using the proposed method, DropEdge. The term "DropEdge" refers to randomly dropping out certain rate of edges of the input graph for each training time. There are several benefits in applying DropEdge for the GCN training (see the experimental improvements by DropEdge in Figure 1). First, DropEdge can be considered as a data augmentation technique. 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. Second, DropEdge can also 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 retards the convergence speed of over-smoothing or relieves the information loss caused by it.

We are also aware that the dense connections employed by JKNet (Xu et al., 2018a) are another kind of tools that can potentially prevent over-smoothing. In its formulation, JKNet densely connects each hidden layer to the top one, hence the feature mappings in lower layers that are hardly affected by over-smoothing are still maintained. Interestingly and promisingly, we find that the performance of JKNet can be promoted further if it is utilized along with our DropEdge. Actually, our DropEdge—as a flexible and general technique—is able to enhance the performance of various popular backbone networks on several benchmarks, including GCN (Kipf & Welling, 2017), ResGCN (Li et al., 2019), JKNet (Xu et al., 2018a), and GraphSAGE (Hamilton et al., 2017). We provide detailed evaluations in the experiments.

2 Related Work

GCNs Inspired by the huge success of CNNs in computer vision, a large number of methods come redefining the notion of convolution on graphs under the umbrella of GCNs. The first prominent research on GCNs is presented in Bruna et al. (2013), which develops graph convolution based on spectral graph theory. Later, Kipf & Welling (2017); Defferrard et al. (2016); Henaff et al. (2015); Li et al. (2018b); Levie et al. (2017) apply improvements, extensions, and approximations on spectral-based GCNs. With contending the scalability issue of spectral-based GCNs on large graphs, spatial-based GCNs have been rapidly developed (Hamilton et al., 2017; Monti et al., 2017; Niepert et al., 2016; Gao et al., 2018). These methods directly perform convolution in the graph domain by aggregating the information from neighbor nodes. By recent, several sampling-based methods have been proposed for fast graph representation learning, including the node-wise sampling methods (Hamilton et al., 2017), the layer-wise approach (Chen et al., 2018) and its layer-dependent variant (Huang et al., 2018).

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 (Kipf & Welling, 2017), 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 Li et al. (2018a) first point out the main difficulty on constructing deep networks lying in over-smoothing, but unfortunately, they never propose any method to address it. The follow-up study (Klicpera et al., 2019) solves over-smoothing by using personalized PageRank that additionally involves the rooted node into the message passing loop; however, the accuracy is still observed to decrease when the depth increases from 2. JKNet (Xu et al., 2018a) employs dense connections for multi-hop message passing which is compatible with DropEdge for formulating deep GCNs. Oono & Suzuki (2019) theoretically prove that the node features of deep GCNs will converge to a subspace and incur information loss, which is a generation of the conclusion in Li et al. (2018a) by further considering the ReLu function and convolution filters. Our interpretations on why DropEdge can impede over-smoothing is based on the concepts proposed by Oono & Suzuki (2019). A recent method (Li et al., 2019) 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 the data points are graphs and naturally disconnected between each other. In our task for node classification, the samples are nodes and they all couple with each other, thus the over-smoothing issue is more demanded to be addressed. By leveraging DropEdge, we are able to relieve over-smoothing, and derive more enhanced deep GCNs on node classification.

3 Notations and Preliminaries

Notations. Let $\mathcal{G} = (\mathbb{V}, E)$ represent the input graph of size N with nodes $v_i \in \mathbb{V}$ and edges $(v_i, v_j) \in E$. The node features are denoted as $\boldsymbol{X} = \{\boldsymbol{x}_1, \cdots, \boldsymbol{x}_n\} \in \mathbb{R}^{N \times C}$, and the adjacent matrix is defined as $\boldsymbol{A} \in \mathbb{R}^{N \times N}$ which associates each edge (v_i, v_j) with its element A_{ij}. The node degrees are given by $\boldsymbol{d} = \{d_1, \cdots, d_N\}$ where d_i computes the sum of edge weights connected to node i. We define $\boldsymbol{D}$ as the degree matrix whose diagonal elements are obtained from $\boldsymbol{d}$.

GCN is originally developed by Kipf & Welling (2017). The feed forward propagation in GCN is recursively conducted as

$$\boldsymbol{H}^{(l+1)} = \sigma\left(\hat{\boldsymbol{A}}\boldsymbol{H}^{(l)}\boldsymbol{W}^{(l)}\right), \tag{1}$$

where $\boldsymbol{H}^{(l+1)} = \{\boldsymbol{h}_1^{(l+1)}, \cdots, \boldsymbol{h}_n^{(l+1)}\}$ are the hidden vectors of the l-th layer with $\boldsymbol{h}_i^{(l)}$ as the hidden feature for node i; $\hat{\boldsymbol{A}} = \hat{\boldsymbol{D}}^{-1/2}(\boldsymbol{A} + \boldsymbol{I})\hat{\boldsymbol{D}}^{-1/2}$ is the re-normalization of the adjacency matrix, and $\hat{\boldsymbol{D}}$ is the corresponding degree matrix of $\boldsymbol{A} + \boldsymbol{I}$; $\sigma(\cdot)$ is a nonlinear function, *i.e.* the relu function; and $\boldsymbol{W}^{(l)} \in \mathbb{R}^{C_l \times C_{l-1}}$ is the filter matrix in the l-th layer. We denote one-layer GCN computed by Equation 1 as Graph Convolutional Layer (**GCL**) in what follows.

4 Our Method: DropEdge

This section first introduces the methodology of the DropEdge technique as well as its layer-independent variant where the adjacent matrix for each GCN layer is perturbed individually. We also explain how the proposed DropEdge can prevent over-fitting and over-smoothing in generic GCNs. Particularly for over-smoothing, we provide its mathematical definition and theoretical derivations on showing the benefits of DropEdge.

4.1 Methodology

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 adjacent matrix $\mathbf{A}$ to be zeros, where V is the total number of edges and p is the dropping rate. If we denote the resulting adjacent matrix as $\boldsymbol{A}_{\text{drop}}$, then its relation with $\boldsymbol{A}$ becomes

$$\boldsymbol{A}_{\text{drop}} = \boldsymbol{A} - \boldsymbol{A}', \tag{2}$$

where $\boldsymbol{A}'$ is a sparse matrix expanded by a random subset of size Vp from original edges E. Following the idea of Kipf & Welling (2017), we also perform the re-normalization trick on $\boldsymbol{A}_{\text{drop}}$, leading to $\hat{\boldsymbol{A}}_{\text{drop}}$. We replace $\hat{\boldsymbol{A}}$ with $\hat{\boldsymbol{A}}_{\text{drop}}$ in Equation 1 for propagation and training. When validation and testing, DropEdge is not utilized.

Preventing over-fitting. DropEdge produces varying perturbations of the graph connections. As a result, it generates different random deformations of the input data and can be regarded as a data augmentation skill for graphs. DropEdge is hence expected to alleviate the over-fitting issue in training GCNs, similar to typical image augmentation skills (*e.g.* rotation, cropping and flapping) that are capable of hindering over-fitting in training CNNs. We will provide experimental validations in § 5.1.

Layer-independent DropEdge. The above formulation of DropEdge is one-shot with all layers sharing the same perturbed adjacent matrix. Indeed, we can perform DropEdge for each individual layer. Specifically, we obtain $\hat{\boldsymbol{A}}^{(l)}_{\text{drop}}$ by independently computing Equation 2 for each l-th layer. Different layer could have different adjacent matrix $\hat{\boldsymbol{A}}^{(l)}_{\text{drop}}$. Such layer-independent version brings in more randomness and deformations of the original data, and we will experimentally compare its performance with the original DropEdge in § 5.2.

Over-smoothing is another obstacle of training deep GCNs, and we will detail how DropEdge can address it to some extent in the next section. For simplicity, the following derivations assume all GCLs share the same perturbed adjacent matrix, and we will leave the discussion on layer-independent DropEdge for future exploration.

4.2 Towards preventing over-smoothing

By its original definition in Li et al. (2018a), the over-smoothing phenomenon implies that the node features will converge to a fixed point as the network depth increases. This unwanted convergence restricts the output of deep GCNs to be only relevant to the graph topology but independent to the input node features, which as a matter of course incurs detriment of the expressive power of GCNs. Oono & Suzuki (2019) has generalized the idea in Li et al. (2018a) 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 subspace rather than convergence to a fixed point. This paper will use the concept of subspace by Oono & Suzuki (2019) for more generality.

We first provide several relevant definitions that facilitate our later presentations.

Definition 1 (subspace)**.** *Let $\mathcal{M} := \{\boldsymbol{EC} | \boldsymbol{C} \in \mathbb{R}^{M \times C}\}$ be an M-dimensional subspace in $\mathbb{R}^{N \times C}$, where $\boldsymbol{E} \in \mathbb{R}^{N \times M}$ is orthogonal,* i.e. *$\boldsymbol{E}^{\mathrm{T}}\boldsymbol{E} = \boldsymbol{I}_M$, and $M \leq N$.*

Definition 2 (ϵ-smoothing)**.** *We call the ϵ-smoothing of node features happens for a GCN, if all its hidden vectors $\boldsymbol{H}^{(l)}$ beyond a certain layer L have a distance no larger than ϵ ($\epsilon > 0$) with respect to a subspace $\mathcal{M}$ that is independent to the input features, namely,*

$$d_{\mathcal{M}}(\boldsymbol{H}^{(l)}) < \epsilon, \forall l \geq L, \tag{3}$$

where $d_{\mathcal{M}}(\cdot)$ computes the distance between the input matrix and the subspace $\mathcal{M}$.[2]

Definition 3 (the ϵ-smoothing layer)**.** *Given the subspace $\mathcal{M}$ and ϵ, we call the minimal value of the layers that satisfy Equation 3 as the ϵ-smoothing layer, that is, $l^*(\mathcal{M}, \epsilon) := \min_l \{d_{\mathcal{M}}(\boldsymbol{H}^{(l)}) < \epsilon\}$.*

According to the conclusions by the authors in Oono & Suzuki (2019), a sufficiently deep GCN will certainly suffer from the ϵ-smoothing issue for any small value of ϵ under some mild conditions (the details are included in the supplementary material). Note that they only prove the existence of ϵ-smoothing in deep GCN without developing any method to address it.

Here, we will demonstrate that adopting DropEdge alleviates the ϵ-smoothing issue in two aspects: **1.** By reducing node connections, DropEdge is proved to slow down the convergence of over-smoothing; in other words, the value of the ϵ-smoothing layer will only increase if using DropEdge. **2.** The gap between the dimensions of the original space and the converging subspace, *i.e.* $N - M$ measures the amount of information loss; larger gap means severer information loss. As shown by our derivations, DropEdge is able to increase the dimension of the converging subspace, thus capable of reducing information loss.

We summarize our conclusions as follows.

[2] The definition of $d_{\mathcal{M}}(\cdot)$ is provided in the supplementary material.

Theorem 1. *We denote the original graph as $\mathcal{G}$ and the one after dropping one edge out as $\mathcal{G}'$. Given a small value of ϵ, we assume $\mathcal{G}$ and $\mathcal{G}'$ will encounter the ϵ-smoothing issue with regard to subspaces $\mathcal{M}$ and $\mathcal{M}'$, respectively. Then, either of the following inequalities holds.*

- *The smoothing layer only increases: $l^*(\mathcal{M}, \epsilon) \leq l^*(\mathcal{M}', \epsilon)$;*
- *The information loss is decreased: $N - dim(\mathcal{M}) > N - dim(\mathcal{M}')$.*

The proof of Theorem 1 is based on the derivations in Oono & Suzuki (2019) as well as the concept of *mixing time* that has been studied in the random walk theory (Lovász et al., 1993). We provide the full details in the supplementary material. Theorem 1 tells that DropEdge either retards the convergence speed of over-smoothing or relieves the information loss caused by it. In this way, DropEdge enables us to train deep GCNs more effectively.

4.3 DISCUSSIONS

This sections contrasts the difference between DropEdge and other related concepts including Dropout, DropNode, and Graph Sparsification.

DropEdge vs. Dropout The Dropout trick (Hinton et al., 2012) is trying to perturb the feature matrix by randomly setting feature dimensions to be zeros, which may reduce the effect of over-fitting but has no help to preventing over-smoothing since it has no touch to 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 (Hamilton et al., 2017), FastGCN (Chen et al., 2018), and AS-GCN (Huang et al., 2018). 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 (Eppstein et al., 1997) is an old research topic in the graph domain. Its optimization goal is removing unnecessary edges for graph compressing while keeping almost all information of the input graph. This is clearly district to 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.

5 EXPERIMENTS

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 (Sen et al., 2008); (2) predicting which community different posts belong to in the Reddit social network (Hamilton et al., 2017). 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 Huang et al. (2018) and Chen et al. (2018) on all datasets in our experiments. The statics of all datasets are listed in the supplemental materials.

Table 1: Testing accuracy (%) comparisons on different backbones w and w/o DropEdge.

		2 layers		8 layers		32 layers	
Dataset	Backbone	Orignal	DropEdge	Orignal	DropEdge	Orignal	DropEdge
Cora	GCN	86.10	**86.50**	78.70	**85.80**	71.60	**74.60**
	ResGCN	-	-	85.40	**86.90**	85.10	**86.80**
	JKNet	-	-	86.70	**87.80**	87.10	**87.60**
	IncepGCN	-	-	86.70	**88.20**	87.40	**87.70**
	GraphSAGE	87.80	**88.10**	84.30	**87.10**	31.90	**32.20**
Citeseer	GCN	75.90	**78.70**	74.60	**77.20**	59.20	**61.40**
	ResGCN	-	-	77.80	**78.80**	74.40	**77.90**
	JKNet	-	-	79.20	**80.20**	71.70	**80.00**
	IncepGCN	-	-	79.60	**80.50**	72.60	**80.30**
	GraphSAGE	78.40	**80.00**	74.10	**77.10**	37.00	**53.60**
Pubmed	GCN	90.20	**91.20**	90.10	**90.90**	84.60	**86.20**
	ResGCN	-	-	89.60	**90.50**	90.20	**91.10**
	JKNet	-	-	90.60	**91.20**	89.20	**91.30**
	IncepGCN	-	-	90.20	**91.50**	OOM	**90.50**
	GraphSAGE	90.10	**90.70**	90.20	**91.70**	41.30	**47.90**
Reddit	GCN	96.11	**96.13**	96.17	**96.48**	45.55	**50.51**
	ResGCN	-	-	96.37	**96.46**	93.93	**94.27**
	JKNet	-	-	96.82	**97.02**	OOM	OOM
	IncepGCN	-	-	96.43	**96.87**	OOM	OOM
	GraphSAGE	96.22	**96.28**	96.38	**96.42**	96.43	**96.47**

5.1 Can DropEdge generally improve the performance of deep GCNs?

In this section, we are interested in if applying DropEdge can promote the performance of current popular GCNs (especially their deep architectures) on node classification.

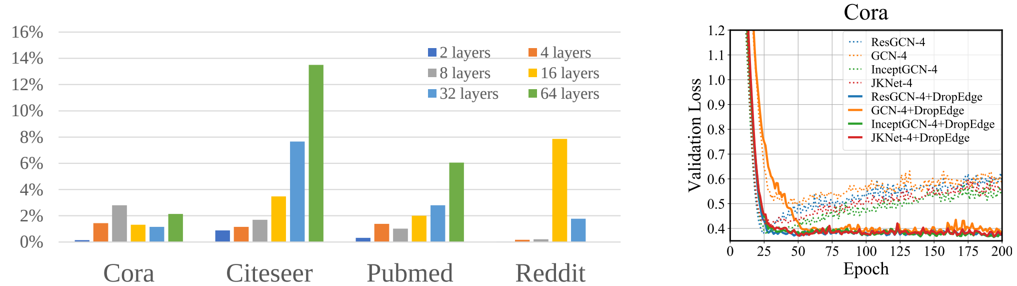
Implementations We consider five backbones: GCN (Kipf & Welling, 2017), ResGCN (He et al., 2016; Li et al., 2019), JKNet (Xu et al., 2018a), IncepGCN[3] and GraphSAGE (Hamilton et al., 2017) with varying depth from 2 to 64.[4] Since different structure exhibits different training dynamics on different dataset, to enable more robust comparisons, we perform random hyper-parameter search for each model, and report the case giving the best accuracy on validation set of each benchmark. The searching space of hyper-parameters and more details are provided in Table 4 in the supplementary material. Regarding the same architecture w or w/o DropEdge, we apply the same set of hyper-parameters except the drop rate p for fair evaluation.

Overall Results Table 1 summaries the results on all datasets. We only report the performance of the model with 2/8/32 layers here due to the space limit, and provide the accuracy under other different depths in the supplementary material. It's observed that DropEdge consistently improves the testing accuracy for all cases. The improvement is more clearly depicted in Figure 2a, where we have computed the average absolute improvement over all backbones by DropEdge on each dataset under different numbers of layers. On Citeseer, for example, DropEdge yields further improvement for deeper architecture; it gains 0.9% average improvement for the model with 2 layers while achieving a remarkable 13.5% increase for the model with 64 layers. In addition, the validation losses of all 4-layer models on Cora are shown in Figure 2b. The curves along the training epoch are dramatically pulled down after applying DropEdge, which also explains the effect of DropEdge on alleviating over-fitting. Another valuable observation in Table 1 is that the 32-layer IncepGCN without DropEdge incurs the Out-Of-Memory (OOM) issue while the model with DropEdge survives, showing the advantage of DropEdge to save memory consuming by making the adjacency matrix sparse.

Comparison with SoAs We select the best performance for each backbone with DropEdge, and contrast them with existing State of the Arts (SoA), including GCN, FastGCN, AS-GCN and GraphSAGE in Table 2; for the SoA methods, we reuse the results reported in Huang et al. (2018). We have these findings: (1) Clearly, our DropEdge obtains significant enhancement against SoAs; particularly on Reddit, the best accuracy by our method is 97.02%, and it is better than the previous best by AS-GCN (96.27%), which is regarded as a remarkable boost considering the challenge on this benchmark. (2) For most models with DropEdge, the best accuracy is obtained under the depth beyond 2, 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.

[3] The formulation is given in the appendix.

[4] For Reddit, the maximum depth is 32 considering the memory bottleneck.



(a) The average absolute improvement by DropEdge.

(b) The validation loss on different backbones w and w/o DropEdge.

Figure 2

Albeit in not exactly fair comparison, the DropEdge based approaches outperform the DropNode based variants as shown in Table 2, which somehow confirms the effectiveness of DropEdge. Actually, employing DropEdge upon the DropNode methods further delivers promising enhancement, which can be checked by revisiting the increase by DropEdge for GraphSAGE in Table 1

Table 2: Accuracy (%) comparisons with SoAs. The number in parenthesis denotes the network depth for the models with DropEdge.

	Transductive			Inductive
	Cora	Citeseer	Pubmed	Reddit
GCN	86.64	79.34	90.22	95.68
FastGCN	85.00	77.60	88.00	93.70
ASGCN	87.44	79.66	90.60	96.27
GraphSAGE	82.20	71.40	87.10	94.32
GCN+DropEdge	87.60(4)	79.20(4)	91.30(4)	96.71(4)
ResGCN+DropEdge	87.00(4)	79.40(16)	91.10(32)	96.48(16)
JKNet+DropEdge	88.00(16)	80.20(8)	91.60(64)	**97.02(8)**
IncepGCN+DropEdge	**88.20(8)**	**80.50(8)**	91.60(4)	96.87(8)
GraphSAGE+DropEdge	88.10(4)	80.00(2)	**91.70(8)**	96.54(4)

5.2 How does DropEdge help?

This section continues a more in-depth analysis on DropEdge and attempts to figure out why it works. Due to the space limit, we only provide the results on Cora, and defer the evaluations on other datasets to the supplementary material.

Note that this section mainly focuses on analyzing DropEdge and its variants, without the concern with pushing state-of-the-art results. So, we do not perform delicate hyper-parameter selection. We employ GCN as the backbone in this section. Here, GCN-n denotes GCN of depth n. 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 “withbn” operation (see their definitions in Table 4 in the appendix).

5.2.1 On preventing over-smoothing

As discussed in § 4.2, the over-smoothing issue exists when the top-layer outputs of GCN converge to a subspace and become unrelated to the input features with the increase in depth. Since we are unable to derive the converging subspace explicitly, we measure the degree of over-smoothing by instead computing the difference between the output of the current layer and that of the previous one. We adopt the Euclidean distance for the difference computation. Lower distance means more serious over-smoothing. Experiments are conducted on GCN-8.

Figure 3 (a) shows the distances of different intermediate layers (from 2 to 6) under different edge dropping rates (0 and 0.8). Clearly, over-smoothing becomes more serious in GCN as the layer grows, which is consistent with our conjecture. Conversely, the model with DropEdge ($p = 0.8$) reveals higher distance and slower convergent speed than that without DropEdge ($p = 0$), implying

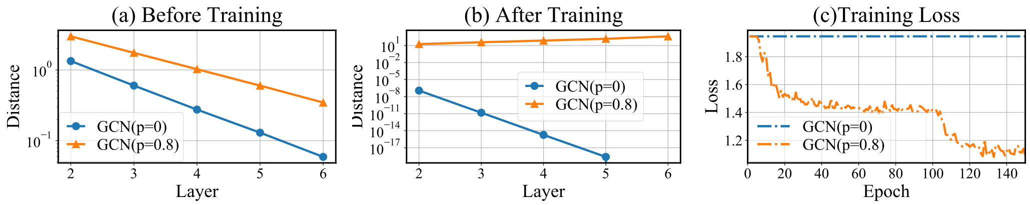
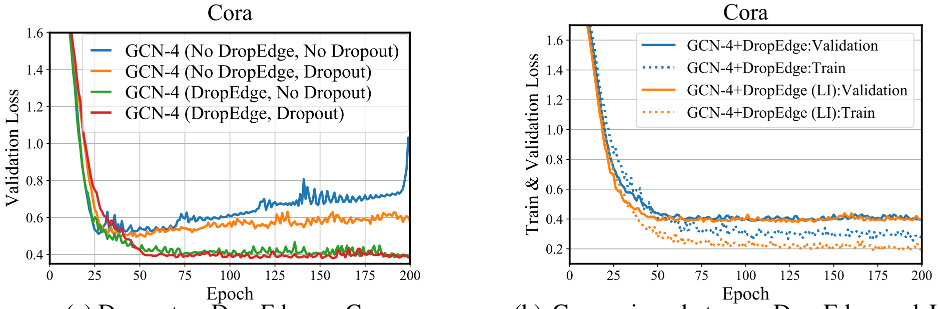


Figure 3: Analysis on over-smoothing. Smaller distance means more serious over-smoothing.



(a) Dropout vs DropEdge on Cora.

(b) Comparison between DropEdge and Layer-Independent (LI) DropEdge.

Figure 4

the importance of DropEdge to alleviating over-smoothing. We are also interested in how the over-smoothing will act after training. For this purpose, we display the results after 150-epoch training in Figure 3 (b). For GCN without DropEdge, the difference between outputs of the 5-th and 6-th layers is equal to 0, indicating that the hidden features have converged to a certain stationary point. On the contrary, GCN with DropEdge performs promisingly, as the distance does not vanish to zero when the number of layers grows; it probably has successfully learned meaningful node representations after training, which could also be validated by the training loss in Figure 3 (c).

5.2.2 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 4a. 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.

5.2.3 On layer-independent DropEdge

§ 4.1 has descried the Layer-Independent (LI) extension of DropEdge. Here, we provide the experimental evaluation on assessing its effect. As observed from Figure 4b, the LI DropEdge achieves lower training loss than the original version, whereas the validation value between two models is comparable. It implies that LI DropEdge can facilitate the training further than original DropEdge. However, we prefer to use DropEdge other than the LI variant so as to not only avoid the risk of over-fitting but also reduces computational complexity since LI DropEdge demands to sample each layer and spends more time.

6 Conclusion

We have presented DropEdge, a novel and efficient technique to facilitate the development of deep Graph Convolutional Networks (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, Pubmed and Reddit have verified that DropEdge can generally and consistently promote the performance of current popular GCNs, such as GCN, ResGCN, JKNet, IncepGCN, and GraphSAGE. 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.

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A Appendix: Proof of Theorem 1

To prove theorem 1, we need following definitions and corollaries from Oono & Suzuki (2019). First, we denote the maximum singular value of $\boldsymbol{W}_l$ by s_l and set $s := \sup_{l \in \mathbb{N}_+} s_l$. We assume that $\boldsymbol{W}_l$ of all layers are initialized so that $s \leq 1$. Second, we denote the distance that induced as the Frobenius norm from $\boldsymbol{X}$ to $\mathcal{M}$ by $d_{\mathcal{M}}(\boldsymbol{X}) := \{\inf ||\boldsymbol{X} - \boldsymbol{Y}||_{\mathrm{F}} | \boldsymbol{Y} \in \mathcal{M}\}$. Then, we recall Corollary 3 in Oono & Suzuki (2019).

Corollary 1. *Let $\lambda_1 \leq \cdots \leq \lambda_N$ be the eigenvalues of $\boldsymbol{A}$, sorted in ascending order. Suppose the multiplicity of the largest eigenvalue λ_N is $M (\leq N)$, i.e., $\lambda_{N-M} < \lambda_{N-M+1} = \cdots = \lambda_N$. Then the second largest eigenvalue is defined as*

$$\lambda := \max_{n=1}^{N-M} |\lambda_n| < |\lambda_N|.$$

Let $\boldsymbol{E}$ to be the eigenspace associated with $\lambda_{N-M+1}, \cdots, \lambda_N$ and it has an orthonormal basis that consists of non-negative vectors. Then we have

$$d_{\mathcal{M}}(\boldsymbol{H}^{(l)}) \leq s_l \lambda d_{\mathcal{M}}(\boldsymbol{H}^{(l-1)}), \tag{4}$$

where $\mathcal{M} := \{\boldsymbol{EC} | \boldsymbol{C} \in \mathbb{R}^{M \times C}\}$.

Remark 1. *Let $\{\mathcal{G}_1, \ldots, \mathcal{G}_M\}$ be M connected graphs in $\mathcal{G}$. Since $\lambda_N = 1$ for $\hat{\boldsymbol{A}}$ in GCN, $\hat{\boldsymbol{A}}$ contains M multiplicity of the largest eigenvalue λ_N that $\lambda_{N-M+1} = \cdots = \lambda_N = 1$ and $\lambda < 1$. Therefore, we have $s_l \lambda < 1$.*

We also need to adopt some concepts of the conductance of a graph from Lovász et al. (1993) in proving Theorem 1. Consider the graph $\mathcal{G}$ as electrical networks, where each edge represents a unit resistance. Then the effective resistance, $R_{eff}^{(s,t)}$ from node s to node t is defined as the total resistance between node s and t. Moreover, the conductance of the graph is defined as the following.

Definition 4. *Let $\mathcal{G}$ as a graph and $\mathbb{S} \subset \mathbb{V}, \neq \emptyset$. The conductance of the $\mathrm{cut}(\mathbb{S}, \bar{\mathbb{S}})$ is defined as:*

$$\Phi(\mathbb{S}) = \frac{|\{e_{v_i, v_j} | v_i \in \mathbb{S}, v_j \in \bar{\mathbb{S}}\}|}{\min(|\mathbb{S}|, |\bar{\mathbb{S}}|)}.$$

and the conductance of the graph is defined as

$$\psi = \min_{\mathbb{S}} \Phi(\mathbb{S})$$

By the graph theory in Lovász et al. (1993), the conductance of the graph is bounded by λ as:

$$\frac{\psi^2}{8} \leq 1 - \lambda. \tag{5}$$

Let $l^* = l^*(\mathcal{M}, \epsilon)$ be the ϵ-smoothing layer. According to above theorems and definitions, we have the lower bound of l^*.

Lemma 2. *Let ψ be the conductance of the graph. Then the ϵ-smoothing happens whenever*

$$l^* > \frac{\log \frac{\epsilon}{d_{\mathcal{M}}(\boldsymbol{X})}}{\log s \left(1 - \frac{\psi^2}{8}\right)}.$$

Proof. We start our proof from Inequality 4 first. By substituting Inequality 5, we have

$$\begin{aligned} d_{\mathcal{M}}(\boldsymbol{H}^{(l)}) &\leq s_l \lambda d_{\mathcal{M}}(\boldsymbol{H}^{(l-1)}) \\ &\leq s_l \left(1 - \frac{\psi^2}{8}\right) d_{\mathcal{M}}(\boldsymbol{H}^{(l-1)}) \\ &\leq \prod_l s_l \left(1 - \frac{\psi^2}{8}\right)^l d_{\mathcal{M}}(\boldsymbol{X}) \\ &\leq s^l \left(1 - \frac{\psi^2}{8}\right)^l d_{\mathcal{M}}(\boldsymbol{X}) \end{aligned}$$

It is obvious that as l becomes larger, $s^l\left(1-\frac{\psi^2}{8}\right)^l$ is closing to 0 since $s<1$ and $\left(1-\frac{\psi^2}{8}\right)\leq\lambda<1$. When it reaches ϵ-smoothing, the following inequality should be satisfied as

$$\begin{aligned} d_{\mathcal{M}}(\boldsymbol{H}^{(l^*)}) \leq s^{l^*}\left(1-\frac{\psi^2}{8}\right)^{l^*} d_{\mathcal{M}}(\boldsymbol{X}) < \epsilon, \\ l^* \log s\left(1-\frac{\psi^2}{8}\right) < \log\frac{\epsilon}{d_{\mathcal{M}}(\boldsymbol{X})}. \end{aligned} \tag{6}$$

Since $0\leq 1-\frac{\psi^2}{4}\leq 1$, then $\log\left(1-\frac{\psi^2}{8}\right)\leq 0$. Therefore, the Inequality 6 becomes

$$l^* > \frac{\log\frac{\epsilon}{d_{\mathcal{M}}(\boldsymbol{X})}}{\log s\left(1-\frac{\psi^2}{8}\right)}.$$

□

Corollary 2. *By decreasing the conductance of a graph, the lower bound of the mixing layer is increasing.*

Then, we prove the first part of Theorem 1, i.e.

the smoothing layer only increases: $l^*(\mathcal{M},\epsilon)\leq l^*(\mathcal{M}',\epsilon)$,

when the dropped edge does not split any $\mathcal{G}_m$ into two connected graphs.

Proof. According to Lemma 2, the graph with smaller conductance needs larger ϵ-smoothing layer since $\log\frac{\epsilon}{d_{\mathcal{M}}(\boldsymbol{X})}<0$. To reduce the conductance of a graph, we recall the graph theory in Lovász et al. (1993) which implies that the conductance of the graph is bounded by the effective resistance as

$$\frac{\psi^2}{8}\leq\frac{1}{R_{eff}^{(s,t)}}\left(\frac{1}{d_s}+\frac{1}{d_t}\right).$$

Therefore,

$$\psi^2\leq\frac{8}{R_{eff}^{(s,t)}}\left(\frac{1}{d_s}+\frac{1}{d_t}\right) \tag{7}$$

By the properties of effective resistance, the effective resistance can only increase if one edge that not connected to either s or t is removed from the circuit Ghosh et al. (2008). It means that according to Inequality 7, the conductance of the graph can only decrease if one edge is removed from the graph $\mathcal{G}$. Consequently, it enlarges l^* after DropEdge by Inequality 5 which proves the first part of Theorem 1. □

The proof of the second part of Theorem 1 is straight forward. We sketch the proof here. According to the graph theory, the multiplicity of the largest eigenvalue is equal to the number of connected graph in $\mathcal{G}$. Therefore, when one connected graph $\mathcal{G}_m$ in $\mathcal{G}$ is dis-connected into two parts as $\mathcal{G}_m\to\{\mathcal{G}_m,\mathcal{G}_{M+1}\}$ by deleting one edge, M is increased to $M+1$ (Remark 1), which leads the increment of the dimension of $\mathcal{M}$ and proves the second part of Theorem 1. i.e.

The information loss is decreased: $N-\mathit{dim}(\mathcal{M})>N-\mathit{dim}(\mathcal{M}')$.

B Appendix: More Details in Experiments

B.1 Datasets Statistics

Datasets The statistics of all datasets are summarized in Table 3.

Table 3: Dataset Statistics

Datasets	Nodes	Edges	Classes	Features	Traing/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	232,965	11,606,919	41	602	152,410/23,699/55,334	Inductive

B.2 Models and Backbones

Backbones Other than multi-layer GCN, we replace the CNN layer with graph convolution layer to implement three popular backbones recasted from image classification. They are residual network (ResGCN)(He et al., 2016; Li et al., 2019), inception network (IncepGCN)(Szegedy et al., 2016) and dense network (JKNet) (Huang et al., 2017; Xu et al., 2018b). Figure 5 shows the detailed architectures of four backbones. Furthermore, we employ one input GCL and one output GCL on these four backbones. Therefore, the layers in ResGCN, JKNet and InceptGCN are at least 3 layers. All backbones are implemented in Pytorch (Paszke et al., 2017). For GraphSAGE, we utilize the Pytorch version implemented by DGL(Wang et al., 2019).

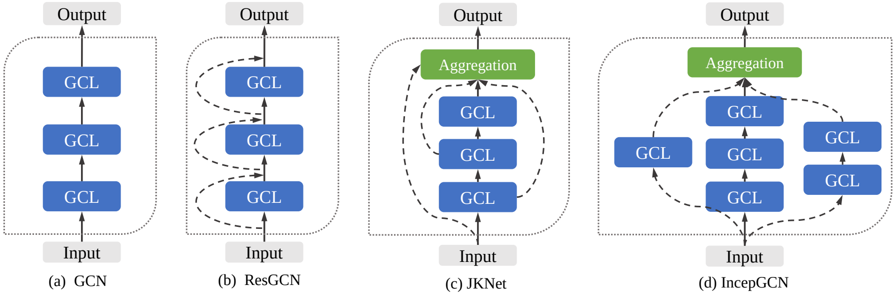


Figure 5: The illustration of four backbones. GCL indicates graph convolutional layer.

Self Feature Modeling We also implement a variant of graph convolution layer with self feature modeling (Fout et al., 2017):

$$\mathbf{H}^{(l+1)} = \sigma\left(\hat{\mathbf{A}}\mathbf{H}^{(l)}\mathbf{W}^{(l)} + \mathbf{H}^{(l)}\mathbf{W}^{(l)}_{\text{self}}\right), \tag{8}$$

where $\mathbf{W}^{(l)}_{\text{self}} \in \mathbb{R}^{m_l \times m_{l-1}}$.

Hyper-parameter Optimization We adopt the Adam optimizer for model training. To ensure the re-productivity of the results, the seeds of the random numbers of all experiments are set to the same. We fix the number of training epoch to 400 for all datasets. All experiments are conducted on a NVIDIA Tesla P40 GPU with 24GB memory.

Given a model with $n \in \{2, 4, 8, 16, 32, 64\}$ layers, the hidden dimension is 128 and we conduct a random search strategy to optimize the other hyper-parameter for each backbone in § 5.1. The decryptions of hyper-parameters are summarized in Table 4. Table 5 depicts the types of the normalized adjacency matrix that are selectable in the "normalization" hyper-parameter. For GraphSAGE, the aggregation type like GCN, max, mean, or LSTM is a hyper-parameter as well.

For each model, we try 200 different hyper-parameter combinations via random search and select the best test accuracy as the result. Table 6 summaries the hyper-parameters of each backbone with the best accuracy on different datasets and their best accuracy are reported in Table 2.

B.3 The Validation Loss on Different Backbones w and w/o DropEdge.

Figure 6 depicts the additional results of validation loss on different backbones w and w/o DropEdge.

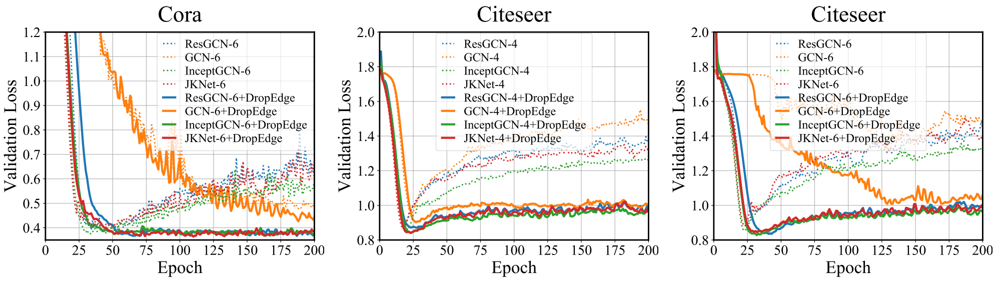
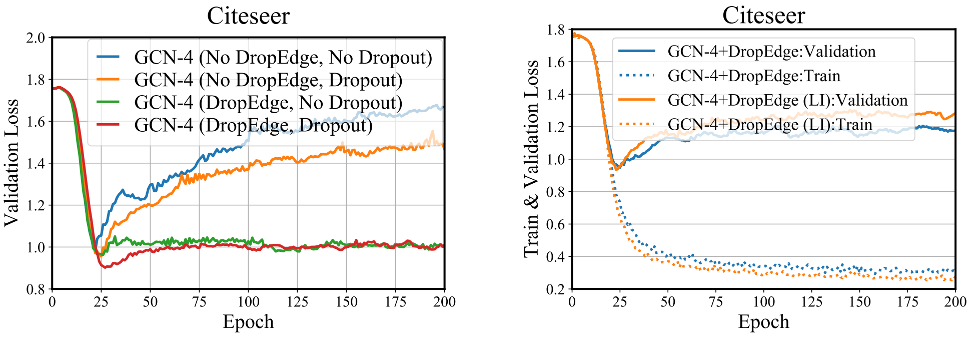


Figure 6: The validation loss on different backbones w and w/o DropEdge. GCN-n denotes PlainGCN of depth n; similar denotation follows for other backbones.

B.4 The Ablation Study on Citeseer

Figure 7a shows the ablation study of Dropout vs. DropEdge and Figure 4b depicts a comparison between the proposed DropEdge and the layer-independent DropEdge on Citeseer.



(a) Ablation study of Dropout vs. DropEdge on Citeseer.

(b) Performance comparison of layer-independent DropEdge.

Figure 7

Table 4: Hyper-parameter Description

Hyper-parameter	Description
lr	learning rate
weight-decay	L2 regulation weight
sampling-percent	edge preserving percent $(1 - p)$
dropout	dropout rate
normalization	the propagation models (Kipf & Welling, 2017)
withloop	using self feature modeling
withbn	using batch normalization

Table 5: The normalization / propagation models

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

Table 6: The hyper-parameters of best accuracy for each backbone on all datasets.

Dataset	Backbone	nlayers	Acc.	Hyper-parameters
Cora	GCN	4	0.876	lr:0.010, weight-decay:5e-3, sampling-percent:0.7, dropout:0.8, normalization:FirstOrderGCN
	ResGCN	4	0.87	lr:0.001, weight-decay:1e-5, sampling-percent:0.1, dropout:0.5, normalization:FirstOrderGCN
	JKNet	16	0.88	lr:0.008, weight-decay:5e-4, sampling-percent:0.2, dropout:0.8, normalization:AugNormAdj
	IncepGCN	8	0.882	lr:0.010, weight-decay:1e-3, sampling-percent:0.05, dropout:0.5, normalization:AugNormAdj
	GraphSage	4	0.881	lr:0.010, weight-decay:5e-4, sampling-percent:0.4, dropout:0.5, aggregator:mean
Citeseer	GCN	4	0.792	lr:0.009, weight-decay:1e-3, sampling-percent:0.05, dropout:0.8, normalization:BingGeNormAdj, withloop, withbn
	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-5, sampling-percent:0.6, dropout:0.3, normalization:AugNormAdj, withloop
	IncepGCN	8	0.805	lr:0.002, weight-decay:5e-3, sampling-percent:0.2, dropout:0.5, normalization:BingGeNormAdj, withloop
	GraphSage	2	0.8	lr:0.001, weight-decay:1e-4, sampling-percent:0.1, dropout:0.5, aggregator:mean
Pubmed	GCN	4	0.913	lr:0.010, weight-decay:1e-3, sampling-percent:0.3, dropout:0.5, normalization:BingGeNormAdj, withloop, withbn
	ResGCN	32	0.911	lr:0.003, weight-decay:5e-5, sampling-percent:0.7, dropout:0.8, normalization:AugNormAdj, withloop, withbn
	JKNet	64	0.916	lr:0.005, weight-decay:1e-4, sampling-percent:0.5, dropout:0.8, normalization:AugNormAdj, withloop,withbn
	IncepGCN	4	0.916	lr:0.002, weight-decay:1e-5, sampling-percent:0.5, dropout:0.8, normalization:BingGeNormAdj, withloop, withbn
	GraphSage	8	0.917	lr:0.007, weight-decay:1e-4, sampling-percent:0.8, dropout:0.3, aggregator:mean
Reddit	GCN	4	0.9671	lr:0.005, weight-decay:1e-4, sampling-percent:0.6, dropout:0.5, normalization:AugRWalk, withloop
	ResGCN	16	0.9648	lr:0.009, weight-decay:1e-5, sampling-percent:0.2, dropout:0.5, normalization:BingGeNormAdj, withbn
	JKNet	8	0.9702	lr:0.010, weight-decay:5e-5, sampling-percent:0.6, dropout:0.5, normalization:BingGeNormAdj, withloop,withbn
	IncepGCN	8	0.9687	lr:0.008, weight-decay:1e-4, sampling-percent:0.4, dropout:0.5, normalization:FirstOrderGCN, withbn
	GraphSAGE	4	0.9654	lr:0.005, weight-decay:5e-5, sampling-percent:0.2, dropout:0.3, aggregator:mean

Table 7: Accuracy (%) comparisons on different backbones with and without DropEdge

		2		4		8		16		32		64	
Dataset	Backbone	Orignal	DropEdge	Orignal	DropEdge	Orignal	DropEdge	Orignal	DropEdge	Orignal	DropEdge	Orignal	DropEdge
Cora	GCN	86.10	86.50	85.50	87.60	78.70	85.80	82.10	84.30	71.60	74.60	52.00	53.20
	ResGCN	-	-	86.00	87.00	85.40	86.90	85.30	86.90	85.10	86.80	79.80	84.80
	JKNet	-	-	86.90	87.70	86.70	87.80	86.20	88.00	87.10	87.60	86.30	87.90
	IncepGCN	-	-	85.60	87.90	86.70	88.20	87.10	87.70	87.40	87.70	85.30	88.20
	GraphSAGE	87.80	88.10	87.10	88.10	84.30	87.10	84.10	84.50	31.90	32.20	31.90	31.90
Citeseer	GCN	75.90	78.70	76.70	79.20	74.60	77.20	65.20	76.80	59.20	61.40	44.60	45.60
	ResGCN	-	-	78.90	78.80	77.80	78.80	78.20	79.40	74.40	77.90	21.20	75.30
	JKNet	-	-	79.10	80.20	79.20	80.20	78.80	80.10	71.70	80.00	76.70	80.00
	IncepGCN	-	-	79.50	79.90	79.60	80.50	78.50	80.20	72.60	80.30	79.00	79.90
	GraphSAGE	78.40	80.00	77.30	79.20	74.10	77.10	72.90	74.50	37.00	53.60	16.90	25.10
Pubmed	GCN	90.20	91.20	88.70	91.30	90.10	90.90	88.10	90.30	84.60	86.20	79.70	79.00
	ResGCN	-	-	90.70	90.70	89.60	90.50	89.60	91.00	90.20	91.10	87.90	90.20
	JKNet	-	-	90.50	91.30	90.60	91.20	89.90	91.50	89.20	91.30	90.60	91.60
	IncepGCN	-	-	89.90	91.60	90.20	91.50	90.80	91.30	OOM	90.50	OOM	90.00
	GraphSAGE	90.10	90.70	89.40	91.20	90.20	91.70	83.50	87.80	41.30	47.90	40.70	62.30
Reddit	GCN	96.11	96.13	96.62	96.71	96.17	96.48	67.11	90.54	45.55	50.51	-	-
	ResGCN	-	-	96.13	96.33	96.37	96.46	96.34	96.48	93.93	94.27	-	-
	JKNet	-	-	96.54	96.75	96.82	97.02	OOM	96.78	OOM	OOM	-	-
	IncepGCN	-	-	96.48	96.77	96.43	96.87	OOM	OOM	OOM	OOM	-	-
	GraphSAGE	96.22	96.28	96.45	96.54	96.38	96.42	96.15	96.18	96.43	96.47	-	-