Graph Random Neural Networks for Semi-Supervised Learning on Graphs

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Abstract

We study the problem of semi-supervised learning on graphs, for which graph neural networks (GNNs) have been extensively explored. However, most existing GNNs inherently suffer from the limitations of over-smoothing [7, 27, 28, 34], non-robustness [54, 51], and weak-generalization when labeled nodes are scarce. In this paper, we propose a simple yet effective framework—GRAPH RANDOM NEURAL NETWORKS (GRAND)—to address these issues. In GRAND, we first design a random propagation strategy to perform graph data augmentation. Then we leverage consistency regularization to optimize the prediction consistency of unlabeled nodes across different data augmentations. Extensive experiments on graph benchmark datasets suggest that GRAND significantly outperforms state-of-the-art GNN baselines on semi-supervised node classification. Finally, we show that GRAND mitigates the issues of over-smoothing and non-robustness, exhibiting better generalization behavior than existing GNNs. The source code of GRAND is publicly available at `https://github.com/Grand20/grand`.

1 Introduction

Graphs serve as a common language for modeling structured and relational data [26], such as social networks, knowledge graphs, and the World Wide Web. Mining and learning graphs can benefit various real-world problems and applications. The focus of this work is on the problem of semi-supervised learning on graphs [52, 24, 11], which aims to predict the categories of unlabeled nodes of a given graph with only a small proportion of labeled nodes. Among its solutions, graph neural networks (GNNs) [24, 19, 41, 1] have recently emerged as powerful approaches. The main idea of GNNs lies in a deterministic feature propagation process to learn expressive node representations.

However, recent studies show that such propagation procedure brings some inherent issues: First, most GNNs suffer from *over-smoothing* [27, 7, 28, 34]. Li et al. show that the graph convolution operation is a special form of Laplacian smoothing [27], and consequently, stacking many GNN layers tends to make nodes' features indistinguishable. In addition, a very recent work [34] suggests that the coupled non-linear transformation in the propagation procedure can further aggravate this issue. Second, GNNs are often *not robust* to graph attacks [54, 51], due to the deterministic propagation adopted in most of them. Naturally, the deterministic propagation makes each node highly dependent with its (multi-hop) neighborhoods, leaving the nodes to be easily misguided by potential data noise and susceptible to adversarial perturbations.

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34th Conference on Neural Information Processing Systems (NeurIPS 2020), Vancouver, Canada.

The third issue lies in the general setting of semi-supervised learning, wherein standard training methods (for GNNs) can easily *overfit* the scarce label information [6]. Most efforts to addressing this broad issue are focused on how to fully leverage the large amount of unlabeled data. In computer vision, recent attempts, e.g. MixMatch [3], UDA [46], have been proposed to solve this problem by designing data augmentation methods for consistency regularized training, which have achieved great success in the semi-supervised image classification task. This inspires us to apply this idea into GNNs to facilitate semi-supervised learning on graphs.

In this work, we address these issues by designing graph data augmentation and consistency regularization strategies for semi-supervised learning. Specifically, we present the GRAPH RANDOM NEURAL NETWORKS (GRAND), a simple yet powerful graph-based semi-supervised learning framework.

To effectively augment graph data, we propose random propagation in GRAND, wherein each node's features can be randomly dropped either partially (dropout) or entirely, after which the perturbed feature matrix is propagated over the graph. As a result, each node is enabled to be insensitive to specific neighborhoods, *increasing the robustness of* GRAND. Further, the design of random propagation can naturally separate feature propagation and transformation, which are commonly coupled with each other in most GNNs. This empowers GRAND to safely perform higher-order feature propagation without increasing the complexity, *reducing the risk of over-smoothing for* GRAND. More importantly, random propagation enables each node to randomly pass messages to its neighborhoods. Under the assumption of homophily of graph data [30], we are able to stochastically generate different augmented representations for each node. We then utilize consistency regularization to enforce the prediction model, e.g., a simple Multilayer Perception (MLP), to output similar predictions on different augmentations of the same unlabeled data, *improving* GRAND*'s generalization behavior under the semi-supervised setting.*

Finally, we theoretically illustrate that *random propagation* and *consistency regularization* can enforce the consistency of classification confidence between each node and its multi-hop neighborhoods. Empirically, we also show both strategies can improve the generalization of GRAND, and mitigate the issues of non-robustness and over-smoothing that are commonly faced by existing GNNs. Altogether, extensive experiments demonstrate that GRAND achieves state-of-the-art semi-supervised learning results on GNN benchmark datasets.

2 Problem and Related Work

Let $G = (V, E)$ denote a graph, where V is a set of $|V| = n$ nodes and $E \subseteq V \times V$ is a set of $|E|$ edges between nodes. $\mathbf{A} \in \{0, 1\}^{n \times n}$ denotes the adjacency matrix of G, with each element $\mathbf{A}_{ij} = 1$ indicating there exists an edge between v_i and v_j, otherwise $\mathbf{A}_{ij} = 0$.

Semi-Supervised Learning on Graphs. This work focuses on semi-supervised graph learning, in which each node v_i is associated with 1) a feature vector $\mathbf{X}_i \in \mathbf{X} \in \mathbb{R}^{n \times d}$ and 2) a label vector $\mathbf{Y}_i \in \mathbf{Y} \in \{0, 1\}^{n \times C}$ with C representing the number of classes. For semi-supervised classification, m nodes ($0 < m \ll n$) have observed their labels $\mathbf{Y}^L$ and the labels $\mathbf{Y}^U$ of the remaining $n - m$ nodes are missing. The objective is to learn a predictive function $f : G, \mathbf{X}, \mathbf{Y}^L \rightarrow \mathbf{Y}^U$ to infer the missing labels $\mathbf{Y}^U$ for unlabeled nodes. Traditional approaches to this problem are mostly based on graph Laplacian regularizations [52, 50, 31, 44, 2]. Recently, graph neural networks (GNNs) have emerged as a powerful approach for semi-supervised graph learning, which are reviewed below.

Graph Neural Networks. GNNs [17, 38, 24] generalize neural techniques into graph-structured data. The core operation in GNNs is graph propagation, in which information is propagated from each node to its neighborhoods with some deterministic propagation rules. For example, the graph convolutional network (GCN) [24] adopts the propagation rule $\mathbf{H}^{(l+1)} = \sigma(\hat{\mathbf{A}}\mathbf{H}^{(l)}\mathbf{W}^{(l)})$, where $\hat{\mathbf{A}}$ is the symmetric normalized adjacency matrix, $\sigma(.)$ denotes the ReLU function, and $\mathbf{W}^{(l)}$ and $\mathbf{H}^{(l)}$ are the weight matrix and the hidden node representation in the l^{th} layer with $\mathbf{H}^{(0)} = \mathbf{X}$.

The GCN propagation rule could be explained via the approximation of the spectral graph convolutions [5, 20, 9], neural message passing [15], and convolutions on direct neighborhoods [33, 19]. Recent attempts to advance this architecture include GAT [41], GMNN [36], MixHop [1], and GraphNAS [14], etc. In addition, sampling based techniques have also been developed for fast and scalable GNN training, such as GraphSAGE [19], FastGCN [8], AS-GCN [21], and LADIES [53]. The sampling based propagation used in those models may also be used as a graph augmentation

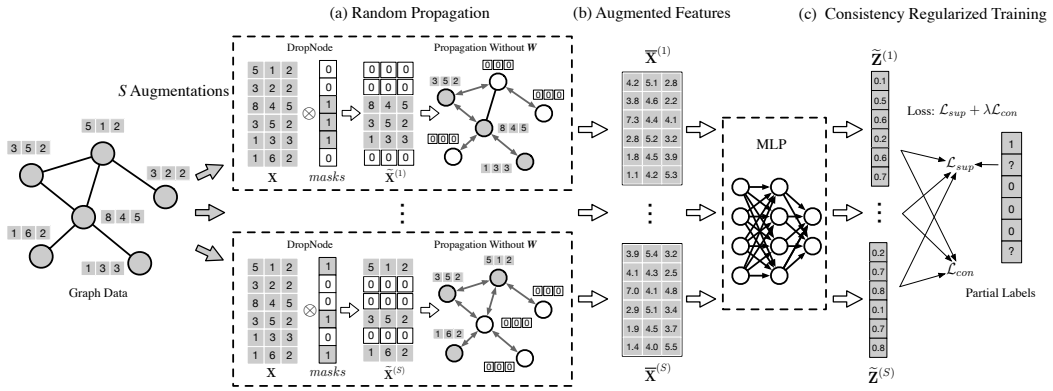


Figure 1: Illustration of GRAND with DropNode as the perturbation method. GRAND designs random propagation (a) to generate multiple graph data augmentations (b), which are further used as consistency regularization (c) for semi-supervised learning.

method. However, its potential effects under semi-supervised setting have not been well-studied, which we try to explore in future work.

Regularization Methods for GNNs. Another line of work has aimed to design powerful regularization methods for GNNs, such as VBAT [10], GraphVAT [12], G^{3}NN [29], GraphMix [42], and DropEdge [37]. For example, VBAT [10] and GraphVAT [12] first apply consistency regularized training into GNNs via virtual adversarial training [32], which is highly time-consuming in practice. GraphMix [42] introduces the MixUp strategy [49] for training GNNs. Different from GRAND, GraphMix augments graph data by performing linear interpolation between two samples in the hidden space, and regularizes GNNs by encouraging the model to predict the same interpolation of corresponding labels.

3 GRAPH RANDOM NEURAL NETWORKS

We present the GRAPH RANDOM NEURAL NETWORKS (GRAND) for semi-supervised learning on graphs, as illustrated in Figure 1. The idea is to design a propagation strategy (a) to stochastically generate multiple graph data augmentations (b), based on which we present a consistency regularized training (c) for improving the generalization capacity under the semi-supervised setting.

3.1 Random Propagation for Graph Data Augmentation

Given an input graph G with its adjacency matrix $\mathbf{A}$ and feature matrix $\mathbf{X}$, the random propagation module generates multiple data augmentations. For each augmentation $\overline{\mathbf{X}}$, it is then fed into the classification model, a two-layer MLP, for predicting node labels. The MLP model can also be replaced with more complex and advanced GNN models, such as GCN and GAT.

Random Propagation. There are two steps in random propagation. First, we generate a perturbed feature matrix $\widetilde{\mathbf{X}}$ by randomly dropping out elements in $\mathbf{X}$. Second, we leverage $\widetilde{\mathbf{X}}$ to perform feature propagation for generating the augmented features $\overline{\mathbf{X}}$.

In doing so, each node's features are randomly mixed with signals from its neighbors. Note that the homophily assumption suggests that adjacent nodes tend to have similar features and labels [30]. Thus, the dropped information of a node could be compensated by its neighbors, forming an approximate representation for it in the corresponding augmentation. In other words, random propagation allows us to stochastically generate multiple augmented representations for each node.

In the first step, there are different ways to perturb the input data $\mathbf{X}$. Straightforwardly, we can use the dropout strategy [40], which has been widely used for regularizing neural networks. Specifically, dropout perturbs the feature matrix by randomly setting some elements of $\mathbf{X}$ to 0 during training, i.e., $\widetilde{\mathbf{X}}_{ij} = \frac{\epsilon_{ij}}{1-\delta}\mathbf{X}_{ij}$, where ϵ_{ij} draws from $Bernoulli(1-\delta)$. In doing so, dropout makes the input feature matrix $\mathbf{X}$ noisy by randomly dropping out its elements without considering graph structures.

To account for the structural effect, we can simply remove some nodes' entire feature vectors—referred to as DropNode, instead of dropping out single feature elements. In other words, DropNode enables each node to only aggregate information from a subset of its (multi-hop) neighbors by completely ignoring some nodes' features, which reduces its dependency on particular neighbors and thus helps increase the model's robustness (Cf. Section 4.5). Empirically, it generates more stochastic data augmentations and achieves better performance than dropout (Cf. Section 4.2).

Formally, in DropNode, we first randomly sample a binary mask $\epsilon_i \sim Bernoulli(1-\delta)$ for each node v_i. Second, we obtain the perturbed feature matrix $\widetilde{\mathbf{X}}$ by multiplying each node's feature vector with its corresponding mask, i.e., $\widetilde{\mathbf{X}}_i = \epsilon_i \cdot \mathbf{X}_i$ where $\mathbf{X}_i$ denotes the i^{th} row vector of $\mathbf{X}$. Finally, we scale $\widetilde{\mathbf{X}}$ with the factor of $\frac{1}{1-\delta}$ to guarantee the perturbed feature matrix is in expectation equal to $\mathbf{X}$. Note that the sampling procedure is only performed during training. During inference, we directly set $\widetilde{\mathbf{X}}$ as the original feature matrix $\mathbf{X}$.

In the second step of random propagation, we adopt the mixed-order propagation, i.e., $\overline{\mathbf{X}} = \overline{\mathbf{A}}\widetilde{\mathbf{X}}$, where $\overline{\mathbf{A}} = \sum_{k=0}^{K} \frac{1}{K+1}\hat{\mathbf{A}}^k$ is the average of the power series of $\hat{\mathbf{A}}$ from order 0 to order K. This propagation rule enables the model to incorporate more local information, reducing the risk of over-smoothing when compared with directly using $\hat{\mathbf{A}}^K$ [1, 47]. Note that calculating the dense matrix $\overline{\mathbf{A}}$ is computationally inefficient, thus we compute $\overline{\mathbf{X}}$ by iteratively calculating and summing up the product of sparse matrix $\hat{\mathbf{A}}$ and $\hat{\mathbf{A}}^k\widetilde{\mathbf{X}}$ $(0 \leq k \leq K-1)$ in implementation.

With this propagation rule, we could observe that DropNode (dropping the i^{th} row of $\mathbf{X}$) is equivalent to dropping the i^{th} column of $\overline{\mathbf{A}}$. This is similar to DropEdge [37], which aims to address over-smoothing by randomly removing some edges. In practice, DropEdge could also be adopted as the perturbation method here. Specifically, we first generate a corrupted adjacency matrix $\tilde{\mathbf{A}}$ by dropping some elements from $\hat{\mathbf{A}}$, and then use $\tilde{\mathbf{A}}$ to perform mix-order propagation as the substitute of $\hat{\mathbf{A}}$ at each epoch. We empirically compare the effects of different perturbation methods in Section 4.2. By default, we use DropNode as the perturbation method.

Prediction. After performing random propagation for S times, we generate S augmented feature matrices $\{\overline{\mathbf{X}}^{(s)} | 1 \leq s \leq S\}$. Each of these augmented data is fed into a two-layer MLP to get the corresponding outputs:

$$\widetilde{\mathbf{Z}}^{(s)} = f_{mlp}(\overline{\mathbf{X}}^{(s)}, \Theta),$$

where $\widetilde{\mathbf{Z}}^{(s)} \in [0,1]^{n \times C}$ denotes the prediction probabilities on $\overline{\mathbf{X}}^{(s)}$ and Θ are the model parameters.

Observing the data flow from random propagation to the prediction module, it can be realized that GRAND actually separates the feature propagation step, i.e., $\overline{\mathbf{X}} = \overline{\mathbf{A}}\widetilde{\mathbf{X}}$, and transformation step, i.e., $f_{mlp}(\overline{\mathbf{X}}\mathbf{W}, \Theta)$. Note that these two steps are commonly coupled with each other in standard GNNs, that is, $\sigma(\mathbf{A}\mathbf{X}\mathbf{W})$. This separation allows us to perform the high-order feature propagation without conducting non-linear transformations, reducing the risk of over-smoothing (Cf. Section 4.6). A similar idea has been adopted by Klicpera et al. [25], with the difference that they first perform the prediction for each node and then propagate the prediction probabilities over the graph.

3.2 Consistency Regularized Training

In graph based semi-supervised learning, the objective is usually to smooth the label information over the graph with regularizations [52, 44, 24], i.e., its loss function is a combination of the supervised loss on the labeled nodes and the graph regularization loss. Given the S data augmentations generated in random propagation, we can naturally design a consistency regularized loss for GRAND's semi-supervised learning.

Supervised Loss. With m labeled nodes among n nodes, the supervised objective of the graph node classification task in each epoch is defined as the average cross-entropy loss over S augmentations:

$$\mathcal{L}_{sup} = -\frac{1}{S}\sum_{s=1}^{S}\sum_{i=0}^{m-1} \mathbf{Y}_i^\top \log \widetilde{\mathbf{Z}}_i^{(s)}. \tag{1}$$

Consistency Regularization Loss. In the semi-supervised setting, we propose to optimize the prediction consistency among S augmentations for unlabeled data. Considering a simple case of $S =$

Algorithm 1 GRAND

Input:

Adjacency matrix $\hat{\mathbf{A}}$, feature matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$, times of augmentations in each epoch S, DropNode/dropout probability δ, learning rate η, an MLP model: $f_{mlp}(\mathbf{X}, \Theta)$.

Output:

Prediction $\mathbf{Z}$.

while not convergence **do**
  for $s = 1 : S$ **do**
    Pertube the input: $\widetilde{\mathbf{X}}^{(s)} \sim \text{DropNode}(\mathbf{X}, \delta)$.
    Perform propagation: $\overline{\mathbf{X}}^{(s)} = \frac{1}{K+1} \sum_{k=0}^{K} \hat{\mathbf{A}}^k \widetilde{\mathbf{X}}^{(s)}$.
    Predict class distribution using MLP: $\widetilde{\mathbf{Z}}^{(s)} = f_{mlp}(\overline{\mathbf{X}}^{(s)}, \Theta)$
  end for
  Compute supervised classification loss $\mathcal{L}_{sup}$ via Eq. 1 and consistency regularization loss via Eq. 3.
  Update the parameters Θ by gradients descending: $\Theta = \Theta - \eta \nabla_{\Theta}(\mathcal{L}_{sup} + \lambda \mathcal{L}_{con})$
end while
Output prediction $\mathbf{Z}$ via: $\mathbf{Z} = f_{mlp}(\frac{1}{K+1} \sum_{k=0}^{K} \hat{\mathbf{A}}^k \mathbf{X}, \Theta)$.

2, we can minimize the squared L_2 distance between the two outputs, i.e., $\min \sum_{i=0}^{n-1} \|\widetilde{\mathbf{Z}}_i^{(1)} - \widetilde{\mathbf{Z}}_i^{(2)}\|_2^2$. To extend this idea into the multiple-augmentation situation, we first calculate the label distribution center by taking the average of all distributions, i.e., $\overline{\mathbf{Z}}_i = \frac{1}{S} \sum_{s=1}^{S} \widetilde{\mathbf{Z}}_i^{(s)}$. Then we utilize the *sharpening* [3] trick to "guess" the labels based on the average distributions. Specifically, the i^{th} node's guessed probability on the j^{th} class is calculated by:

$$\overline{\mathbf{Z}}_{ij}^{'} = \overline{\mathbf{Z}}_{ij}^{\frac{1}{T}} \Big/ \sum_{c=0}^{C-1} \overline{\mathbf{Z}}_{ic}^{\frac{1}{T}}, (0 \leq j \leq C-1), \tag{2}$$

where $0 < T \leq 1$ acts as the "temperature" that controls the sharpness of the categorical distribution. As $T \to 0$, the sharpened label distribution will approach a one-hot distribution. We minimize the distance between $\widetilde{\mathbf{Z}}_i$ and $\overline{\mathbf{Z}}_i^{'}$ in GRAND:

$$\mathcal{L}_{con} = \frac{1}{S} \sum_{s=1}^{S} \sum_{i=0}^{n-1} \|\overline{\mathbf{Z}}_i^{'} - \widetilde{\mathbf{Z}}_i^{(s)}\|_2^2. \tag{3}$$

Therefore, by setting T as a small value, we can enforce the model to output low-entropy predictions. This can be viewed as adding an extra entropy minimization regularization into the model, which assumes that the classifier's decision boundary should not pass through high-density regions of the marginal data distribution [18].

Training and Inference. In each epoch, we employ both the supervised classification loss in Eq. 1 and the consistency regularization loss in Eq. 3 on S augmentations. The final loss of GRAND is:

$$\mathcal{L} = \mathcal{L}_{sup} + \lambda \mathcal{L}_{con}, \tag{4}$$

where λ is a hyper-parameter that controls the balance between the two losses. Algorithm 1 outlines GRAND's training process. During inference, as mentioned in Section 3.1, we directly use the original feature $\mathbf{X}$ for propagation. This is justified because we scale the perturbed feature matrix $\widetilde{\mathbf{X}}$ during training to guarantee its expectation to match $\mathbf{X}$. Hence the inference formula is $\mathbf{Z} = f_{mlp}(\overline{\mathbf{A}}\mathbf{X}, \Theta)$.

Complexity. The complexity of random propagation is $\mathcal{O}(Kd(n + |E|))$, where K denotes propagation step, d is the dimension of node feature, n is the number of nodes and $|E|$ denotes edge count. The complexity of its prediction module (two-layer MLP) is $\mathcal{O}(nd_h(d + C))$, where d_h denotes its hidden size and C is the number of classes. By applying consistency regularized training, the total computational complexity of GRAND is $\mathcal{O}(S(Kd(n + |E|) + nd_h(d + C)))$, which is linear with the sum of node and edge counts.

Limitations. GRAND is based on the homophily assumption [30], i.e., "birds of a feather flock together", a basic assumption in the literature of graph-based semi-supervised learning [52]. Due to that, however, GRAND may not succeed on graphs with less homophily.

3.3 Theoretical Analysis

We theoretically discuss the regularization effects brought by *random propagation* and *consistency regularization* in GRAND. For analytical simplicity, we assume that the MLP used in GRAND has one single output layer, and the task is binary classification. Thus we have $\widetilde{\mathbf{Z}} = \text{sigmoid}(\overline{\mathbf{A}}\widetilde{\mathbf{X}} \cdot \mathbf{W})$, where $\mathbf{W} \in \mathbb{R}^d$ is the learnable parameter vector. For the i^{th} node, the corresponding conditional distribution is $\tilde{z}_i^{y_i}(1-\tilde{z}_i)^{1-y_i}$, in which $\tilde{z}_i \in \widetilde{\mathbf{Z}}$ and $y_i \in \{0,1\}$ denotes the corresponding label.

As for the consistency regularization loss, we consider the simple case of generating $S = 2$ augmentations. Then the loss $\mathcal{L}_{con} = \frac{1}{2}\sum_{i=0}^{n-1}\left(\tilde{z}_i^{(1)} - \tilde{z}_i^{(2)}\right)^2$, where $\tilde{z}_i^{(1)}$ and $\tilde{z}_i^{(2)}$ represent the model's two outputs on node i corresponding to the two augmentations, respectively.

With these assumptions, we have the following theorem with proofs in Appendix B.1.

Theorem 1. *In expectation, optimizing the unsupervised consistency loss $\mathcal{L}_{con}$ is approximate to optimize a regularization term:* $\mathbb{E}_\epsilon\left(\mathcal{L}_{con}\right) \approx \mathcal{R}^c(\mathbf{W}) = \sum_{i=0}^{n-1} z_i^2(1-z_i)^2 \text{Var}_\epsilon\left(\overline{\mathbf{A}}_i\widetilde{\mathbf{X}} \cdot \mathbf{W}\right)$.

DropNode Regularization. With DropNode as the perturbation method, we can easily check that $\text{Var}_\epsilon(\overline{\mathbf{A}}_i\widetilde{\mathbf{X}} \cdot \mathbf{W}) = \frac{\delta}{1-\delta}\sum_{j=0}^{n-1}(\mathbf{X}_j \cdot \mathbf{W})^2(\overline{\mathbf{A}}_{ij})^2$, where δ is drop rate. Then the corresponding regularization term $\mathcal{R}_{DN}^c$ can be expressed as:

$$\mathcal{R}_{DN}^c(\mathbf{W}) = \frac{\delta}{1-\delta}\sum_{j=0}^{n-1}\left[(\mathbf{X}_j \cdot \mathbf{W})^2 \sum_{i=0}^{n-1}(\overline{\mathbf{A}}_{ij})^2 z_i^2(1-z_i)^2\right]. \tag{5}$$

Note that $z_i(1-z_i)$ (or its square) is an indicator of the classification uncertainty for the i^{th} node, as $z_i(1-z_i)$ (or its square) reaches its maximum at $z_i = 0.5$ and minimum at $z_i = 0$ or 1. Thus $\sum_{i=0}^{m-1}(\overline{\mathbf{A}}_{ij})^2 z_i^2(1-z_i)^2$ can be viewed as the weighted average classification uncertainty over the j^{th} node's multi-hop neighborhoods with the weights as the square values of $\overline{\mathbf{A}}$'s elements, which is related to graph structure. On the other hand, $(\mathbf{X}_j \cdot \mathbf{W})^2$—as the square of the input of sigmoid—indicates the classification confidence for the j^{th} node. In optimization, in order for a node to earn a higher classification confidence $(\mathbf{X}_j \cdot \mathbf{W})^2$, it is required that the node's neighborhoods have lower classification uncertainty scores. Hence, *the random propagation with the consistency regularization loss can enforce the consistency of the classification confidence between each node and its multi-hop neighborhoods*.

Dropout Regularization. With $\mathbf{X}$ perturbed by dropout, the variance term $\text{Var}_\epsilon(\overline{\mathbf{A}}_i\widetilde{\mathbf{X}} \cdot \mathbf{W}) = \frac{\delta}{1-\delta}\sum_{j=0}^{n-1}\sum_{k=0}^{d-1}\mathbf{X}_{jk}^2\mathbf{W}_k^2(\overline{\mathbf{A}}_{ij})^2$. The corresponding regularization term $\mathcal{R}_{Do}^c$ is

$$\mathcal{R}_{Do}^c(\mathbf{W}) = \frac{\delta}{1-\delta}\sum_{h=0}^{d-1}\mathbf{W}_h^2\sum_{j=0}^{n-1}\left[\mathbf{X}_{jh}^2\sum_{i=0}^{n-1}z_i^2(1-z_i)^2(\overline{\mathbf{A}}_{ij})^2\right]. \tag{6}$$

Similar to DropNode, this extra regularization term also includes the classification uncertainty $z_i(1-z_i)$ of neighborhoods. However, *we can observe that different from the DropNode regularization, dropout is actually an adaptive L_2 regularization for $\mathbf{W}$, where the regularization coefficient is associated with unlabeled data, classification uncertainty, and the graph structure*.

Previous work [43] has also drawn similar conclusions for the case of applying dropout in generalized linear models.

By applying the Cauchy-Schwarz Inequality, we have $\mathcal{R}_{Do}^c \geq \mathcal{R}_{DN}^c$. That is to say, dropout's regularization term is the upper bound of DropNode's. By minimizing this term, dropout can be regarded as an approximation of DropNode.

Random propagation w.r.t supervised classification loss. We also discuss the regularization effect of random propagation with respect to the supervised classification loss.

With the previous assumptions, the supervised classification loss is: $\mathcal{L}_{sup} = \sum_{i=0}^{m-1} -y_i\log(\tilde{z}_i) - (1-y_i)\log(1-\tilde{z}_i)$. Note that $\mathcal{L}_{sup}$ refers to the perturbed classification loss with DropNode on the node features. By contrast, the original (non-perturbed) classification loss is defined as: $\mathcal{L}_{org} = \sum_{i=0}^{m-1} -y_i\log(z_i) - (1-y_i)\log(1-z_i)$, where $z_i = \text{sigmoid}(\overline{\mathbf{A}}_i\mathbf{X} \cdot \mathbf{W})$ is the output with the original feature matrix $\mathbf{X}$. Then we have the following theorem with proof in Appendix B.2.

Theorem 2. *In expectation, optimizing the perturbed classification loss $\mathcal{L}_{sup}$ is equivalent to optimize the original loss $\mathcal{L}_{org}$ with an extra regularization term $\mathcal{R}(\mathbf{W})$, which has a quadratic approximation form $\mathcal{R}(\mathbf{W}) \approx \mathcal{R}^q(\mathbf{W}) = \frac{1}{2}\sum_{i=0}^{m-1} z_i(1-z_i)\text{Var}_\epsilon\left(\overline{\mathbf{A}}_i\widetilde{\mathbf{X}}\cdot\mathbf{W}\right)$.*

This theorem suggests that DropNode brings an extra regularization loss to the optimization objective. Expanding the variance term, this extra quadratic regularization loss can be expressed as:

$$\mathcal{R}^q_{DN}(\mathbf{W}) = \frac{1}{2}\frac{\delta}{1-\delta}\sum_{j=0}^{n-1}\left[(\mathbf{X}_j\cdot\mathbf{W})^2\sum_{i=0}^{m-1}(\overline{\mathbf{A}}_{ij})^2\, z_i(1-z_i)\right]. \tag{7}$$

Different from $\mathcal{R}^c_{DN}$ in Eq. 5, the inside summation term in Eq. 7 only incorporates the first m nodes, i.e, the labeled nodes.

4 Experiments

4.1 Experimental Setup

We follow exactly the same experimental procedure—such as features and data splits—as the standard GNN settings on semi-supervised graph learning [48, 24, 41]. The setup and reproducibility details are covered in Appendix A.

Datasets. We conduct experiments on three benchmark graphs [48, 24, 41]—Cora, Citeseer, and Pubmed—and also report results on six publicly available and large datasets in Appendix C.1.

Baselines. By default, we use DropNode as the perturbation method in GRAND and compare it with 14 GNN baselines representative of three different categories, as well as its variants:

- Eight graph convolutions: GCN [24], GAT [41], APPNP [25], Graph U-Net [13], SGC [45], MixHop [1], GMNN [36] and GrpahNAS [14].
- Two sampling based GNNs: GraphSAGE [19] and FastGCN [8].
- Four regularization based GNNs: VBAT [10], G^{3}NN [29], GraphMix [42] and Dropedge [37]. We report the results of these methods with GCN as the backbone model.
- Four GRAND variants: GRAND_dropout, GRAND_DropEdge, GRAND_GCN and GRAND_GAT. In GRAND_dropout and GRAND_DropEdge, we use dropout and DropEdge as the perturbation method respectively, instead of DropNode. In GRAND_GCN and GRAND_GAT, we replace MLP with more complex models, i.e., GCN and GAT, respectively.

4.2 Overall Results

Table 1 summarizes the prediction accuracies of node classification. Following the community convention [24, 41, 36], the results of baselines are taken from the original works [24, 41, 13, 1, 14, 10, 29, 42, 37, 25]. The results of GRAND are averaged over **100** runs with random weight initializations.

From the top part of Table 1, we can observe that GRAND consistently achieves large-margin outperformance over all baselines across all datasets. Note that the improvements of GRAND over other baselines are all statistically significant (p-value $\ll 0.01$ by a t-test). Specifically, GRAND improves upon GCN by a margin of 3.9%, 5.1%, and 3.7% (absolute differences) on Cora, Citeseer, and Pubmed, while the margins improved by GAT upon GCN were 1.5%, 2.2%, and 0%, respectively. When compared to the very recent regularization based model—DropEdge, the proposed model achieves 2.6%, 3.1%, and 3.1% improvements, while DropEdge's improvements over GCN were only 1.3%, 2.0%, and 0.6%, respectively. To better examine the effectiveness of GRAND in semi-supervised setting, we further evaluate GRAND under different label rates in Appendix C.6.

We observe GRAND_dropout and GRAND_DropEdge also outperform most of baselines, though still lower than GRAND. This indicates DropNode is the best way to generate graph data augmentations in random propagation. Detailed experiments to compare DropNode and dropout under different propagation steps K are shown in Appendix C.4.

We interpret the performance of GRAND_GAT, GRAND_GCN from two perspectives. First, both GRAND_GAT and GRAND_GCN outperform the original GCN and GAT models, demonstrating the positive effects of the proposed random propagation and consistency regularized training methods. Second, both of them are inferior to GRAND with the simple MLP model, suggesting GCN and GAT are relatively easier to over-smooth than MLP. More analyses can be found in Appendix C.5.

Method	Cora	Citeseer	Pubmed
GCN [24]	81.5	70.3	79.0
GAT [41]	83.0±0.7	72.5±0.7	79.0±0.3
APPNP [25]	83.8±0.3	71.6± 0.5	79.7 ± 0.3
Graph U-Net [13]	84.4±0.6	73.2±0.5	79.6±0.2
SGC [45]	81.0 ±0.0	71.9 ± 0.1	78.9 ± 0.0
MixHop [1]	81.9± 0.4	71.4±0.8	80.8±0.6
GMNN [36]	83.7	72.9	81.8
GraphNAS [14]	84.2±1.0	73.1±0.9	79.6±0.4
GraphSAGE [19]	78.9±0.8	67.4±0.7	77.8±0.6
FastGCN [8]	81.4±0.5	68.8±0.9	77.6±0.5
VBAT [10]	83.6±0.5	74.0±0.6	79.9±0.4
G^3NN [29]	82.5±0.2	74.4±0.3	77.9 ±0.4
GraphMix [42]	83.9±0.6	74.5±0.6	81.0±0.6
DropEdge [37]	82.8	72.3	79.6
GRAND_dropout	84.9±0.4	75.0±0.3	81.7±1.0
GRAND_DropEdge	84.5±0.3	74.4±0.4	80.9±0.9
GRAND_GCN	84.5±0.3	74.2±0.3	80.0±0.3
GRAND_GAT	84.3±0.4	73.2± 0.4	79.2±0.6
GRAND	**85.4±0.4**	**75.4±0.4**	**82.7±0.6**
w/o CR	84.4±0.5	73.1±0.6	80.9±0.8
w/o mDN	84.7±0.4	74.8±0.4	81.0±1.1
w/o sharpening	84.6±0.4	72.2±0.6	81.6±0.8
w/o CR & DN	83.2±0.5	70.3±0.6	78.5±1.4

Table 1: Overall classification accuracy (%).

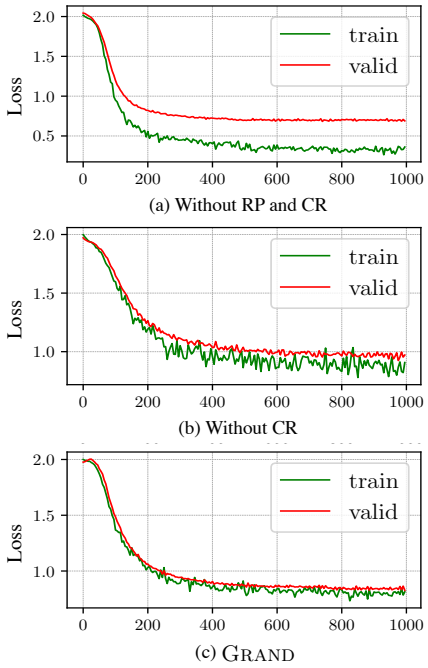


Figure 2: Generalization on Cora (x: epoch).

4.3 Ablation Study

We conduct an ablation study to examine the contributions of different components in GRAND.

- **Without consistency regularization (CR):** We only use the supervised classification loss, i.e., $\lambda = 0$.
- **Without multiple DropNode (mDN):** Do DropNode once at each epoch, i.e., $S = 1$, meaning that CR only enforces the model to give low-entropy predictions for unlabeled nodes.
- **Without sharpening:** The sharpening trick in Eq. 2 is not used in getting the distribution center, i.e., $T = 1$.
- **Without CR and DropNode (CR & DN):** Remove DropNode (as a result, the CR loss is also removed), i.e., $\delta = 0, \lambda = 0$. In this way, GRAND becomes the combination of deterministic propagation and MLP.

In Table 1, the bottom part summarizes the results of the ablation study, from which we have two observations. First, all GRAND variants with some components removed witness clear performance drops when comparing to the full model, suggesting that each of the designed components contributes to the success of GRAND. Second, GRAND without consistency regularization outperforms almost all eight non-regularization based GCNs and DropEdge in all three datasets, demonstrating the significance of the proposed random propagation technique for semi-supervised graph learning.

4.4 Generalization Analysis

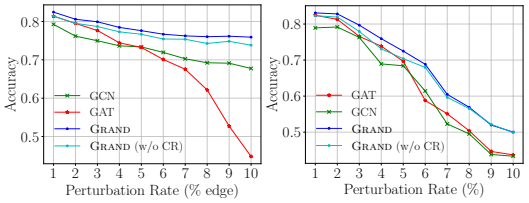
We examine how the proposed techniques—random propagation and consistency regularization—improve the model's generalization capacity. To achieve this, we analyze the model's cross-entropy losses on both training and validation sets on Cora. A small gap between the two losses indicates a model with good generalization. Figure 2 reports the results for GRAND and its two variants. We can observe the significant gap between the validation and training losses when without both consistency regularization (CR) and random propagation (RP), indicating an obvious overfitting issue. When applying only the random propagation (without CR), the gap becomes much smaller. Finally, when

further adding the CR loss to make it the full GRAND model, the validation loss becomes much closer to the training loss and both of them are also more stable. This observation demonstrates both the random propagation and consistency regularization can significantly improve GRAND's generalization capability.

4.5 Robustness Analysis

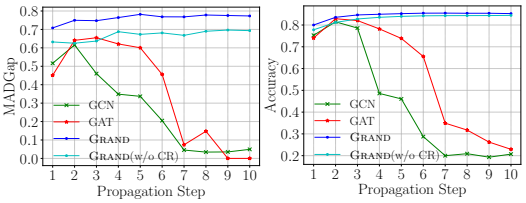
We study the robustness of GRAND by generating perturbed graphs with two adversarial attack methods: Random Attack perturbs the graph structure by randomly adding fake edges, and Metattack [55] attacks the graph by removing or adding edges based on meta learning.

Figure 3 presents the classification accuracies of different methods with respect to different perturbation rates on the Cora dataset. We observe that GRAND consistently outperforms GCN and GAT across all perturbation rates on both attacks. When adding 10% new random edges into Cora, we observe only a 7% drop in classification accuracy for GRAND, while 12% for GCN and 37% for GAT. Under Metattack, the gap between GRAND and GCN/GAT also enlarges with the increase of the perturbation rate. This study suggests the robustness advantage of the GRAND model (with or without) consistency regularization over GCN and GAT.



(a) Random Attack (b) Metattack

Figure 3: Robustness Analysis on Cora.



(a) MADGap (b) Classification Result

Figure 4: Over-Smoothing on Cora

4.6 Over-Smoothing Analysis

Many GNNs face the over-smoothing issue—nodes with different labels become indistinguishable—when enlarging the feature propagation steps [27, 7]. We study how vulnerable GRAND is to this issue by using MADGap [7], a measure of the over-smoothness of node representations. A smaller MADGap value indicates the more indistinguishable node representations and thus a more severe over-smoothing issue.

Figure 4 shows both the MADGap values of the last layer's representations and classification results w.r.t. different propagation steps. In GRAND, the propagation step is controlled by the hyperparameter K, while for GCN and GAT, it is adjusted by stacking different hidden layers. The plots suggest that as the propagation step increases, both metrics of GCN and GAT decrease dramatically—MADGap drops from $\sim$0.5 to 0 and accuracy drops from 0.75 to 0.2—due to the over-smoothing issue. However, GRAND behaves completely different, i.e., both the performance and MADGap benefit from more propagation steps. This indicates that GRAND is much more powerful to relieve over-smoothing, when existing representative GNNs are very vulnerable to it.

5 Conclusions

In this work, we study the problem of semi-supervised learning on graphs and present the GRAPH RANDOM NEURAL NETWORKS (GRAND). In GRAND, we propose the random propagation strategy to stochastically generate multiple graph data augmentations, based on which we utilize consistency regularization to improve the model's generalization on unlabeled data. We demonstrate its consistent performance superiority over fourteen state-of-the-art GNN baselines on benchmark datasets. In addition, we theoretically illustrate its properties and empirically demonstrate its advantages over conventional GNNs in terms of robustness and resistance to over-smoothing. To conclude, the simple and effective ideas presented in GRAND may generate a different perspective in GNN design, in particular for semi-supervised graph learning. In future work, we aim to further improve the scalability of GRAND with some sampling methods.

Broader Impact

Over the past years, GNNs have been extensively studied and widely used for semi-supervised graph learning, with the majority of efforts devoted to designing advanced and complex GNN architectures. Instead of heading towards that direction, our work focuses on an alternative perspective by examining whether and how simple and traditional machine learning (ML) techniques can help overcome the common issues that most GNNs faced, including over-smoothing, non-robustness, and weak generalization.

Instead of the nonlinear feature transformations and advanced neural techniques (e.g., attention), the presented GRAND model is built upon dropout (and its simple variant), linear feature propagation, and consistency regularization—the common ML techniques. Its consistent and significant outperformance over 14 state-of-the-art GNN baselines demonstrates the effectiveness of our alternative direction. In addition, our results also echo the recent discovery in SGC [45] to better understand the source of GCNs' expressive power. More importantly, these simple ML techniques in GRAND empower it to be more robust, better avoid over-smoothing, and offer stronger generalization than GNNs.

In light of these advantages, we argue that the ideas in GRAND offer a different perspective in understanding and advancing GNN based semi-supervised learning. For future research in GNNs, in addition to designing complex architectures, we could also invest in simple and traditional graph techniques under the regularization framework which has been widely used in (traditional) semi-supervised learning.

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Appendix—Graph Random Neural Network for Semi-Supervised Learning on Graphs

A Reproducibility

A.1 Datasets Details

Table 2 summarizes the statistics of the three benchmark datasets — Cora, Citeseer and Pubmed. Our preprocessing scripts for Cora, Citeseer and Pubmed is implemented with reference to the codes of Planetoid [48]. We use exactly the same experimental settings—such as features and data splits—on the three benchmark datasets as literature on semi-supervised graph mining [48, 24, 41] and run 100 trials with 100 random seeds for all results on Cora, Citeseer and Pubmed reported in Section 4. We also evaluate our method on six publicly available and large datasets, the statistics and results are summarized in Appendix C.1.

Table 2: Benchmark Dataset statistics.

Dataset	Nodes	Edges	Train/Valid/Test Nodes	Classes	Features
Cora	2,708	5,429	140/500/1,000	7	1,433
Citeseer	3,327	4,732	120/500/1,000	6	3,703
Pubmed	19,717	44,338	60/500/1,000	3	500

A.2 Implementation Details

We make use of PyTorch to implement GRAND and its variants. The random propagation procedure is efficiently implemented with sparse-dense matrix multiplication. The codes of GCN and GRAND_GCN are implemented referring to the PyTorch version of GCN [1]. As for GRAND_GAT and GAT, we adopt the implementation of GAT layer from the PyTorch-Geometric library [2] in our experiments. The weight matrices of classifier are initialized with Glorot normal initializer [16]. We employ Adam [23] to optimize parameters of the proposed methods and adopt early stopping to control the training epochs based on validation loss. Apart from DropNode (or dropout [40]) used in random propagation, we also apply dropout on the input layer and hidden layer of the prediction module used in GRAND as a common practice of preventing overfitting in optimizing neural network. For the experiments on Pubmed, we also use batch normalization [22] to stabilize the training procedure. All the experiments in this paper are conducted on a single NVIDIA GeForce RTX 2080 Ti with 11 GB memory size. Server operating system is Unbuntu 18.04. As for software versions, we use Python 3.7.3, PyTorch 1.2.0, NumPy 1.16.4, SciPy 1.3.0, CUDA 10.0.

A.3 Hyperparameter Details

Overall Results in Section 4.2. GRAND introduces five additional hyperparameters, that is the DropNode probability δ in random propagation, propagation step K, data augmentation times S at each training epoch, sharpening temperature T when calculating consistency regularization loss and the coefficient of consistency regularization loss λ trading-off the balance between $\mathcal{L}_{sup}$ and $\mathcal{L}_{con}$. In practice, δ is always set to 0.5 across all experiments. As for other hyperparameters, we perform hyperparameter search for each dataset. Specifically, we first search K from { 2,4,5,6,8}. With the best selection of K, we then search S from {2,3,4}. Finally, we fix K and S to the best values and take a grid search for T and λ from {0.1, 0.2, 0.3,0.5} and {0.5, 0.7, 1.0} respectively. For each search of hyperparameter configuration, we run the experiments with 20 random seeds and select the best configuration of hyperparameters based on average accuracy on validation set. Other hyperparameters used in our experiments includes learning rate of Adam, early stopping patience, L2 weight decay rate, hidden layer size, dropout rates of input layer and hidden layer. We didn't spend much effort to tune these hyperparameters in practice, as we observe that GRAND is not very

[1] `https://github.com/tkipf/pygcn`

[2] `https://pytorch-geometric.readthedocs.io`

sensitive with those. Table 3 reports the best hyperparameters of GRAND we used for the results reported in Table 1.

Table 3: Hyperparameters of GRAND for results in Table 1

Hyperparameter	Cora	Citeseer	Pubmed
DropNode probability δ	0.5	0.5	0.5
Propagation step K	8	2	5
Data augmentation times S	4	2	4
CR loss coefficient λ	1.0	0.7	1.0
Sharpening temperature T	0.5	0.3	0.2
Learning rate	0.01	0.01	0.2
Early stopping patience	200	200	100
Hidden layer size	32	32	32
L2 weight decay rate	5e-4	5e-4	5e-4
Dropout rate in input layer	0.5	0.0	0.6
Dropout rate in hidden layer	0.5	0.2	0.8

Robustness Analysis in Section 4.5. For random attack, we implement the attack method with Python and NumPy library. The propagation step K of GRAND (with or without CR) is set to 5. And the other hyperparameters are set to the values in Table 3. As for Metattack [55], we use the publicly available implementation[3] published by the authors with the same hyperparameters used in the original paper. We observe GRAND (with or without CR) is sensitive to the propagation step K under different perturbation rates. Thus we search K from {5,6,7,8} for each perturbation rate. The other hyperparameters are fixed to the values reported in Table 3.

Other Experiments. For the other results reported in Section 4.2 — 4.6, the hyperparameters used in GRAND are set to the values reported in Table 3 with one or two changed for the corresponding analysis.

Baseline Methods. For the results of GCN or GAT reported in Section 4.5 — 4.6, the learning rate is set to 0.01, early stopping patience is 100, L2 weight decay rate is 5e-4, dropout rate is 0.5. The hidden layer size of GCN is 32. For GAT, the hidden layer consists 8 attention heads and each head consists 8 hidden units.

B Theorem Proofs

B.1 Proof for Theorem 1

Proof. The expectation of $\mathcal{L}_{con}$ is:

$$\frac{1}{2}\sum_{i=0}^{n-1}\mathbb{E}\left[(\tilde{z}_i^{(1)}-\tilde{z}_i^{(2)})^2\right]=\frac{1}{2}\sum_{i=0}^{n-1}\mathbb{E}\left[\left((\tilde{z}_i^{(1)}-z_i)-(\tilde{z}_i^{(2)}-z_i)\right)^2\right]. \tag{8}$$

Here $z_i=\text{sigmoid}(\overline{\mathbf{A}}_i\mathbf{X}\cdot\mathbf{W})$, $\tilde{z}_i=\text{sigmoid}(\overline{\mathbf{A}}_i\widetilde{\mathbf{X}}\cdot\mathbf{W})$. For the term of $\tilde{z}_i-z_i$, we can approximate it with its first-order Taylor expansion around $\overline{\mathbf{A}}_i\mathbf{X}\cdot\mathbf{W}$, i.e., $\tilde{z}_i-z_i\approx z_i(1-z_i)(\overline{\mathbf{A}}_i(\widetilde{\mathbf{X}}-\mathbf{X})\cdot\mathbf{W})$. Applying this rule to the above equation, we have:

$$\begin{aligned}\frac{1}{2}\sum_{i=0}^{n-1}\mathbb{E}\left[(\tilde{z}_i^{(1)}-\tilde{z}_i^{(2)})^2\right]&\approx\frac{1}{2}\sum_{i=0}^{n-1}z_i^2(1-z_i)^2\mathbb{E}\left[(\overline{\mathbf{A}}_i(\widetilde{\mathbf{X}}^{(1)}-\widetilde{\mathbf{X}}^{(2)})\cdot\mathbf{W})^2\right]\\&=\sum_{i=0}^{n-1}z_i^2(1-z_i)^2\text{Var}_\epsilon\left(\overline{\mathbf{A}}_i\widetilde{\mathbf{X}}\cdot\mathbf{W}\right).\end{aligned} \tag{9}$$

□

B.2 Proof for Theorem 2

Proof. Expanding the logistic function, $\mathcal{L}_{org}$ is rewritten as:

[3] https://github.com/danielzuegner/gnn-meta-attack

$$\mathcal{L}_{org} = \sum_{i=0}^{m-1} \left[-y_i \overline{\mathbf{A}}_i \mathbf{X} \cdot \mathbf{W} + \mathcal{A}(\overline{\mathbf{A}}_i, \mathbf{X}) \right], \tag{10}$$

where $\mathcal{A}(\overline{\mathbf{A}}_i, \mathbf{X}) = -\log\left(\frac{\exp(-\overline{\mathbf{A}}_i \mathbf{X} \cdot \mathbf{W})}{1+\exp(-\overline{\mathbf{A}}_i \mathbf{X} \cdot \mathbf{W})}\right)$. Then the expectation of perturbed classification loss can be rewritten as:

$$\mathbb{E}_\epsilon(\mathcal{L}_{sup}) = \mathcal{L}_{org} + \mathcal{R}(\mathbf{W}), \tag{11}$$

where $\mathcal{R}(\mathbf{W}) = \sum_{i=0}^{m-1} \mathbb{E}_\epsilon \left[\mathcal{A}(\overline{\mathbf{A}}_i, \widetilde{\mathbf{X}}) - \mathcal{A}(\overline{\mathbf{A}}_i, \mathbf{X}) \right]$. Here $\mathcal{R}(\mathbf{W})$ acts as a regularization term for $\mathbf{W}$. To demonstrate that, we can take a second-order Taylor expansion of $\mathcal{A}(\overline{\mathbf{A}}_i, \widetilde{\mathbf{X}})$ around $\overline{\mathbf{A}}_i \mathbf{X} \cdot \mathbf{W}$:

$$\mathbb{E}_\epsilon \left[\mathcal{A}(\overline{\mathbf{A}}_i, \widetilde{\mathbf{X}}) - \mathcal{A}(\overline{\mathbf{A}}_i, \mathbf{X}) \right] \approx \frac{1}{2} \mathcal{A}^{''}(\overline{\mathbf{A}}_i, \mathbf{X}) \mathrm{Var}_\epsilon \left(\overline{\mathbf{A}}_i \widetilde{\mathbf{X}} \cdot \mathbf{W} \right). \tag{12}$$

Note that the first-order term $\mathbb{E}_\epsilon \left[\mathcal{A}^{'}(\overline{\mathbf{A}}_i, \mathbf{X})(\widetilde{\mathbf{X}} - \mathbf{X}) \right]$ vanishes since $\mathbb{E}_\epsilon(\widetilde{\mathbf{X}}) = \mathbf{X}$. We can easily check that $\mathcal{A}^{''}(\overline{\mathbf{A}}_i, \mathbf{X}) = z_i(1 - z_i)$. Applying this quadratic approximation to $\mathcal{R}(\mathbf{W})$, we get the quadratic approximation form of $\mathcal{R}(\mathbf{W})$:

$$\mathcal{R}(\mathbf{W}) \approx \mathcal{R}^q(\mathbf{W}) = \frac{1}{2} \sum_{i=0}^{m-1} z_i(1 - z_i) \mathrm{Var}_\epsilon(\overline{\mathbf{A}}_i \widetilde{\mathbf{X}} \cdot \mathbf{W}). \tag{13}$$

□

C Additional Experiments

C.1 Results on Large Datasets

Table 4: Statistics of Large Datasets.

	Classes	Features	Nodes	Edges
Cora-Full	67	8,710	18,703	62,421
Coauthor CS	15	6,805	18,333	81,894
Coauthor Physics	5	8,415	34,493	247,962
Aminer CS	18	100	593,486	6,217,004
Amazon Computers	10	767	13,381	245,778
Amazon Photo	8	745	7,487	119,043

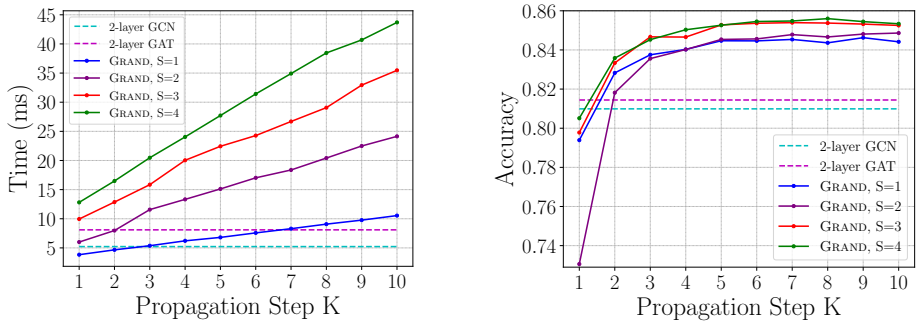
We also evaluate our methods on six relatively large datasets, i.e., Cora-Full, Coauthor CS, Coauthor Physics, Amazon Computers, Amazon Photo and Aminer CS. The statistics of these datasets are given in Table 4. Cora-Full is proposed in [4]. Coauthor CS, Coauthor Physics, Amazon Computers and Amazon Photo are proposed in [39]. We download the processed versions of the five datasets here[4]. Aminer CS is extracted from the DBLP data downloaded from `https://www.aminer.cn/citation`. In Aminer CS, each node corresponds to a paper in computer science, and edges represent citation relations between papers. These papers are manually categorized into 18 topics based on their publication venues. We use averaged GLOVE-100 [35] word vector of paper abstract as the node feature vector. Our goal is to predict the corresponding topic of each paper based on feature matrix and citation graph structure.

Following the evaluation protocol used in [39], we run each model on 100 random train/validation/test splits and 20 random initializations for each split (with **2000** runs on each dataset in total). For each trial, we choose 20 samples for training, 30 samples for validation and the remaining samples for test. We ignore 3 classes with less than 50 nodes in Cora-Full dataset as done in [39]. The results are presented in Table 5. The results of GCN and GAT on the first five datasets are taken from [39]. We can observe that GRAND *significantly outperforms GCN and GAT on all these datasets.*

[4] `https://github.com/shchur/gnn-benchmark`

Table 5: Results on large datasets.

Method	Cora Full	Coauthor CS	Coauthor Physics	Amazon Computer	Amazon Photo	Aminer CS
GCN	62.2 ± 0.6	91.1 ± 0.5	92.8 ± 1.0	82.6 ± 2.4	91.2 ± 1.2	49.9 ± 2.0
GAT	51.9 ± 1.5	90.5 ± 0.6	92.5 ± 0.9	78.0 ± 19.0	85.7 ± 20.3	49.6 ± 1.7
GRAND	**63.5 ±0.6**	**92.9 ± 0.5**	**94.6 ± 0.5**	**85.7 ± 1.8**	**92.5 ± 1.7**	**52.8 ± 1.2**



(a) Per-epoch Training Time (b) Classification Accuracy

Figure 5: Efficiency Analysis for GRAND.

C.2 Efficiency Analysis

The efficiency of GRAND is mainly influenced by two hyperparameters: the propagation step K and augmentation times S. Figure 5 reports the average per-epoch training time and classification accuracy of GRAND on Cora under different values of K and S with #training epochs fixed to 1000. It also includes the results of the two-layer GCN and two-layer GAT with the same learning rate, #training epochs and hidden layer size as GRAND.

From Figure 5, we can see that when $K = 2, S = 1$, GRAND outperforms GCN and GAT in terms of both efficiency and effectiveness. In addition, we observe that increasing K or S can significantly improve the model's classification accuracy at the cost of its training efficiency. In practice, we can adjust the values of K and S to balance the trade-off between performance and efficiency.

C.3 Parameter Sensitivity

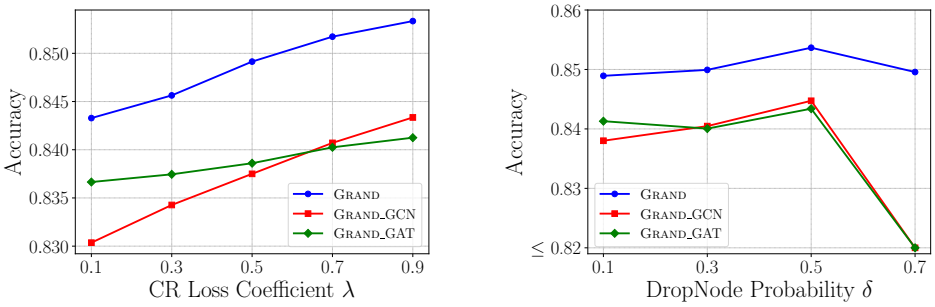
We investigate the sensitivity of consistency regularization (CR) loss coefficient λ and DropNode probability δ in GRAND and its variants on Cora. The results are shown in Figure 6. We observe that their performance increase when enlarging the value of λ. As for DropNode probability, GRAND, GRAND_GCN and GRAND_GAT reach their peak performance at $\delta = 0.5$. This is because the augmentations produced by random propagation in that case are more stochastic and thus make GRAND generalize better with the help of consistency regularization.

C.4 DropNode vs Dropout

We compare GRAND and GRAND_dropout under different values of propagation step K. The results on Cora, Citeseer and Pubmed are illustrated in Figure 7. We observe GRAND always achieve better performance than GRAND_dropout, suggesting *DropNode is much more suitable for graph data augmentation*.

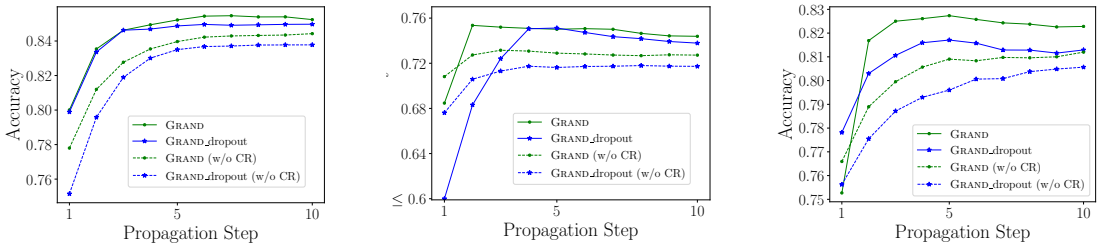
C.5 GRAND vs. GRAND_GCN & GRAND_GAT

As shown in Table 1, GRAND_GCN and GRAND_GAT get worse performances than GRAND, indicating GCN and GAT perform worse than MLP under the framework of GRAND. Here we



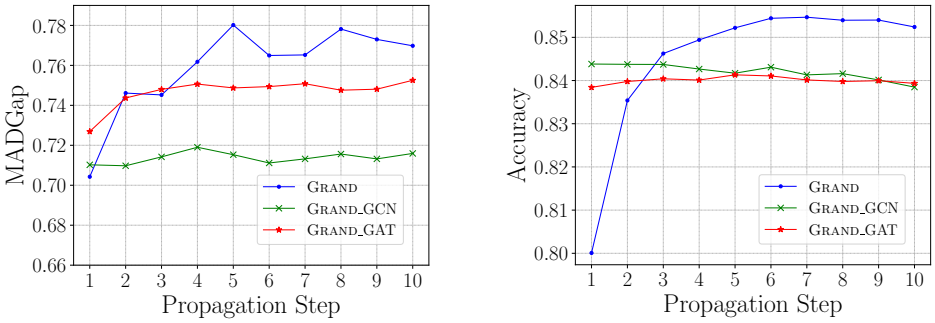
(a) CR loss coefficient λ (b) DropNode probability δ

Figure 6: Parameter sensitivity of λ and δ on Cora.



(a) Cora (b) Citeseer (c) Pubmed

Figure 7: GRAND vs. GRAND_dropout.



(a) MADGap (b) Classification Results

Figure 8: Over-smoothing: GRAND vs. GRAND_GCN & GRAND_GAT on Cora.

conduct a series of experiments to analyze the underlying reasons. Specifically, we compare the MADGap values and accuracies GRAND, GRAND_GCN and GRAND_GAT under different values of propagation step K with other parameters fixed. The results are shown in Figure 8. We find that the MADGap and classification accuracy of GRAND increase significantly when enlarging the value of K. However, both the metrics of GRAND_GCN and GRAND_GAT have little improvements or even decrease. This indicates that *GCN and GAT have higher over-smoothing risk than MLP*.

C.6 Performance of GRAND under different label rates

We have conducted experiments to evaluate GRAND under different label rates. For each label rate setting, we randomly create 10 data splits, and run 10 trials with random initialization for each split.

We compare GRAND with GCN and GAT. The results are shown in Table 6. We observe that GRAND consistently outperforms GCN and GAT across all label rates on three benchmarks.

Table 6: Classification Accuracy under different label rates (%).

Dataset	Cora			Citeseer			Pubmed		
Label Rate	1%	3%	5%	1%	3%	5%	0.1%	0.3%	0.5%
GCN	62.8±5.3	76.1±1.9	79.6±2.1	63.4±2.9	70.6±1.7	72.2±1.1	71.5±2.1	77.5±1.8	80.8±1.5
GAT	64.3±5.8	77.2±2.4	80.8±2.1	64.4±2.9	70.4±1.9	72.0±1.3	72.0±2.1	77.6±1.6	80.6±1.2
GRAND	**69.1±4.0**	**79.5±2.2**	**83.0±1.6**	**65.3±3.3**	**72.3±1.8**	**73.8±0.9**	**74.7±3.4**	**81.4±2.1**	**83.8±1.3**