Improving the Training of Graph Neural Networks with Consistency Regularization

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ABSTRACT

Graph neural networks (GNNs) have achieved notable success in the semi-supervised learning scenario. The message passing mechanism in graph neural networks helps unlabeled nodes gather supervision signals from their labeled neighbors. In this work, we investigate how consistency regularization, one of widely adopted semi-supervised learning methods, can help improve the performance of graph neural networks. We revisit two methods of consistency regularization for graph neural networks. One is simple consistency regularization (SCR), and the other is mean-teacher consistency regularization (MCR). We combine the consistency regularization methods with two state-of-the-art GNNs and conduct experiments on the ogbn-products dataset. With the consistency regularization, the performance of state-of-the-art GNNs can be improved by 0.3% on the ogbn-products dataset of Open Graph Benchmark (OGB) both with and without external data.

CCS CONCEPTS
- Theory of computation → Semi-supervised learning; • Computing methodologies → Neural networks; Regularization.

KEYWORDS

graph neural networks, consistency regularization, semi-supervised learning

1 INTRODUCTION

The graph-structured data, made up of nodes and edges, is a flexible and powerful tool to represent connected objects. With the great success of deep learning and neural networks in computer vision, natural language processing, and other fields, a series of graph neural networks (GNNs) have achieved excellent performance in graph machine learning tasks [12, 27, 31]. Some of them achieved state-of-the-art performance on the leaderboard of open datasets such as Open Graph Benchmark [14].

Training a deep learning model requires a large amount of labeled data, which is difficult to access in many realistic scenarios. Many research papers showed that using unlabeled data with small amount of labeled data in training could improve the performance of the model. Because of the characteristics of graph structure, semi-supervised learning on graphs has always been a hot research topic. For consistency regularization, there have been many in-depth studies in the field of deep learning. Some work has proposed to use "pseudo labeling" to exploit unlabeled nodes in the training stage [20, 25, 32, 34], which can be regarded as a special case of consistency regularization. Among them, multi-stage self-training methods have achieved the best performance. As the name indicated, the training procedure is divided into several stages. At the beginning of each stage, the training set are expanded by assigning pseudo labels to unlabeled nodes based on the predictions from the previous stage. This approach effectively utilizes the information of unlabeled nodes, resulting in better performance. However, the multi-stage approach is less elegant and needs more training time.

In this work, we revisit its role in the training of graph neural networks and examine the performance improvement of graph neural networks under the semi-supervised setting. We utilize two kinds of methods of consistency regularization for GNNs. One method is called simple consistency regularization (SCR) by minimizing the disagreement among perturbed predictions. The perturbed predictions can be obtained by data augmentation or the randomness of models. The other is called mean-teacher consistency regularization (MCR) by leveraging the teacher-student paradigm. For MCR, following Mean Teacher [26], we guided the training of the model by calculating a consistency loss between the student and teacher models. The parameters of the teacher model are directly derived from the Exponential Moving Average (EMA) weights of the student model without additional back propagation. In each training step,
the parameters of teacher model will be updated by the student model. Experimental results demonstrate that our methods achieve top-1 results on the ogbn-products dataset.

2 RELATED WORK

2.1 Graph Neural Networks

Due to the great success of convolutional neural networks (CNNs) in computer vision, much effort has been devoted to generalizing CNNs to graph-structured data, leading to the development of graph neural networks (GNN). GNN models are mainly divided into two categories: spectral domain based model and spatial domain based model. From a spectral perspective, Bruna et al. [4] firstly used the Fourier basis of graph in the spectral domain to develop graph convolutions. Then, Kipf et al. [17] further proposed to simplify graph convolutions with Chebyshev polynomial. In the meanwhile, spatial domain based GNNs [12, 27, 31] interpret graph convolution as us-

cing exponential moving average of model parameters. UDA [30] and ReMixMatch [18] sharpen the soft label to make the model to produce high-confidence predictions. UDA further reinforces consistency mitigates the requirement for labeled data and has attracted a lot of research work [6, 35, 36]. Consistency regularization was first proposed by [1], later referred as "TI-Model" [23]. One of the key challenges in consistency regularization is how to improve the quality of the generated labels. Temporal Ensembling [19] uses multilayer perceptrons to transform model parameters. UDA further reinforces consistency only when the highest probability of the predicted category distribution for soft labels is above a threshold.

2.2 Semi-Supervised Learning

Semi-supervised learning provides an effective way to use unlabeled data to improve model performance. Semi-supervised learning mitigates the requirement for labeled data and has attracted a lot of research work [6, 35, 36]. Consistency regularization was first proposed by [1], later referred as "TI-Model" [23]. One of the key challenges in consistency regularization is how to improve the quality of the generated labels. Temporal Ensembling [19] uses multilayer perceptrons to transform model parameters. UDA further reinforces consistency only when the highest probability of the predicted category distribution for soft labels is above a threshold.

2.3 Self-training Methods on Graphs

Using "pseudo-label" to improve GNN performance is a common practice for semi-supervised learning tasks [20, 32]. In SAGN [25] and GAMLP [34], they proposed a multi-stage self-training approach, which divides the training process into stages. In the first stage only the training set are used. Starting from the second stage, they leverage the training results of the previous stage with pseudo labeling and knowledge distillation, respectively. Though multistage training can bring extra performance gains compared to one-stage training scheme, it suffers from long training time.

3 METHOD

In general, we use bold uppercase letters (e.g., \( \mathbf{A} \)) for matrices, and bold lowercase letters (e.g., \( \mathbf{x} \)) for vectors. The transpose of a matrix \( \mathbf{A} \) (resp. a vector \( \mathbf{x} \)) is denoted by \( \mathbf{A}^\top \) (resp. \( \mathbf{x}^\top \)). For any matrix \( \mathbf{A} \), we use \( \mathbf{A}[i, j], \mathbf{A}[i, :] \), and \( \mathbf{A}[:, j] \) to represent its \((i, j)\)-th entry, \( i\)-th row and \( j\)-th column, respectively. Likewise, we use \( \mathbf{x}[i] \) to denote the \( i\)-th entry of \( \mathbf{x} \). We denote a graph with \( N \) nodes by \( G = (\mathcal{V}, \mathcal{E}, \mathcal{X}) \), where \( \mathcal{V} = \{1, 2, \ldots, N\} \) is its node set, \( \mathcal{E} \subseteq \mathcal{V} \times \mathcal{V} \) is its edge set, \( \mathcal{X} \in \mathbb{R}^{N \times d} \) is the matrix with its \( i\)-th row being the features associated with node \( i \), and \( d \) is the number of features. The adjacency matrix of \( G \), denoted by \( \mathbf{A}_G \), is an \( N \times N \) matrix encoding the structure specified by \( G \). Its \((i, j)\)-th entry \( \mathbf{A}_G[i, j] \) is defined according the connectivity between node \( i \) and \( j \), i.e.,

\[
\mathbf{A}_G[i, j] = \begin{cases} 
1, & \text{if } (i, j) \in \mathcal{E}; \\
0, & \text{otherwise}.
\end{cases}
\]

We will drop the subscript \( G \) for simplicity when no ambiguity arises.

3.1 Graph Neural Networks

In this work, we experiment on two newly developed GNN architectures, namely SAGN [25] and GAMLP [34]. Both models enrich the node features by multiplying \( \mathcal{X} \) by a series of aggregation matrices and adopt the attention mechanism to build the final node representations. Here, an aggregation matrix \( \hat{\mathbf{A}} \) is defined as a matrix of size \( N \times N \) whose \((i, j)\)-th entry \( \hat{\mathbf{A}}[i, j] \) satisfies

\[
\hat{\mathbf{A}}[i, j] = \begin{cases} 
\geq 0, & \text{if } i = j \text{ or } (i, j) \in \mathcal{E}; \\
0, & \text{otherwise}.
\end{cases}
\]

It is therefore straightforward to see that the \( i\)-th row of the multiplication \( \hat{\mathbf{A}}\mathcal{X} \) is the aggregation of the original features of node \( i \) and its immediate neighbors \( \{j : (i, j) \in \mathcal{E}\} \).

In SAGN, we first get a set of aggregated node features by

\[
\mathcal{X}^{(k)} = \hat{\mathbf{A}}^{k} \mathcal{X}, \forall k = 0, 1, \ldots, K
\]

where \( \hat{\mathbf{A}}^k \) is the \( k\)-th power of \( \hat{\mathbf{A}} \), the superscript \( \cdot^{(k)} \) indexes the hop count and \( K \) is the maximum hop count that is predefined. \( \mathcal{X}^{(k)} \in \mathbb{R}^{N \times d} \) is the matrix of the \( k\)-th aggregated features and its \( i\)-th row \( \mathcal{X}^{(k)}[i, :] \) gathers the information of node \( i \)'s \( k\)-hop neighbors. Then, we adopt \( (K + 1) \) multilayer perceptrons to transform these aggregated node features separately:

\[
\mathcal{Z}^{(k)} = \text{MLP}^{(k)}(\mathcal{X}^{(k)}),
\]

where \( \text{MLP} \) denotes a multilayer perceptron and \( \mathcal{Z}^{(k)} \) is the latent node representations at hop \( k \) that is solely determined by \( \mathcal{X}^{(k)} \). Now, each node \( i \) has \((K + 1)\) representations, i.e., \( \{\mathcal{Z}^{(k)}[i, :]\}_{k=0}^{K} \). To get an integrated representation for node \( i \) that exploits all these representations, the attention mechanism [2] is subsequently utilized:

\[
\mathcal{Z}_{attn}[i, :] = \sum_{k=0}^{K} \theta^{(k)}[i] \mathcal{Z}^{(k)}[i, :],
\]

where \( \theta^{(k)} \in \mathbb{R}^{N} \) is the vector with its \( i\)-th entry being the importance of the \( k\)-th latent representation to node \( i \). The above
3.2 Semi-Supervised Node Classification

Semi-supervised learning provides an efficient way to improve the performance of deep neural networks with abundant unlabeled data. In this work, we focus on the problem of semi-supervised node classification where only a small subset of nodes is labeled. Let $\mathcal{V}_L$ and $\mathcal{V}_U$ denote the set of labeled nodes and unlabeled nodes such that $\mathcal{V}_L \cup \mathcal{V}_U = \mathcal{V}$ and $\mathcal{V}_L \cap \mathcal{V}_U = \emptyset$. Each labeled node $i \in \mathcal{V}_L$ is associated with a label $y_i \in \{1, \ldots, C\}$ where $C$ is the number of classes. By leveraging both labeled nodes and unlabeled nodes, the objective of semi-supervised node classification is to minimize the following loss function:

$$L = \frac{1}{|\mathcal{V}_L|} \sum_{i \in \mathcal{V}_L} L_s(i, y_i) + \lambda \cdot \frac{1}{|\mathcal{V}_U|} \sum_{i \in \mathcal{V}_U} L_u(i),$$

where $|\cdot|$ denotes the size of a set, $L_s$ is the supervised loss that only applies on labeled data, $L_u$ is the unsupervised loss that exploits unlabeled data to regularize the model, and $\lambda$ is a weighting factor that controls the strength of the unsupervised loss.

**Supervised loss.** We are interested in learning a neural network $p_\theta : \mathcal{V} \rightarrow \mathbb{R}^C$ that maps each node to a class distribution where $\theta$ is the set of parameters to be estimated. The neural network consists of a GNN that encodes graph nodes into vectors following the process described in 3.1 and a classifier that converts node representations to class distributions. Let $p_{Y|i,\theta}$ denote the class distribution predicted by $p_\theta$ on node $i$ and $p_{Y|i,\theta}(c) = \Pr(Y = c | i, \theta)$ denote the predicted probability of node $i$ having label $c$. For classification problems, we adopt the cross entropy as the supervised loss, i.e.,

$$L_s(i, y_i) = -\log p_{Y|i,\theta}(y_i).$$

**Unsupervised loss.** There have been several strategies to design the unsupervised loss in the literature. Pseudo labeling, e.g., SLE [25], assigns artificial labels for unlabeled nodes by treating the predictions of the model, especially those with high confidence, as the ground truth. **Consistency regularization,** e.g., GRAND [9], favors models that produce consistent outputs across different views of the same input. GraphMix [28] proposed an interpolation-based regularization that puts a linear constraint on the model, i.e., a linear interpolation of two data points should result in a linear interpolation of their corresponding labels.

### 3.3 Consistency Regularization

Consistency regularization techniques are developed under the assumption that a small perturbation on the input should not change the output of the model. A simple definition of this idea can be summarized as follows: (1) given a data sample, compute a set of perturbed predictions based on the sample; (2) minimize the disagreement among those predictions. The perturbed prediction can be obtained by manipulating the input (e.g., data augmentation), or injecting noise to the model (e.g., dropout). This definition is used in MixMatch [3] and GRAND [9], and we call it the simple consistency regularization (SCR). Given a graph $G = (\mathcal{V}, \mathcal{E}, X)$, a set of $S$ augmented versions of $G$, denoted by $\{G_s = (\mathcal{V}, \mathcal{E}_s, X_s)\}_{s=1}^S$, is constructed by graph augmentation approaches such as DropNode [9] and DropEdge [24]. Notice that the node set is unchanged during the augmentation process. As mentioned in Section 3.2, a neural network $p_\theta$ is used to map each node to a class distribution. We apply the neural network on those augmented graphs independently, resulting in $S$ class distributions for each node $i$. We use $p_{Y|i,\theta,G_s}$ to denote the predictions of node $i$ on the $s$-th augmented graph. The unsupervised loss is designed to minimize
The disagreement between those prediction:

$$q_{Y|i}(c) = \sum_{s=1}^{S} p_{Y|i, \hat{\gamma}, \theta}(c), \forall c \in \{1, \ldots, C\},$$

$$L_u(i) = \frac{1}{S} \sum_{s=1}^{S} D(q_{Y|i}; p_{Y|i, \hat{\gamma}, \theta}),$$

where $q_{Y|i}$ is a smoothed prediction that is likely to be a better guess for node $i$'s label, $D$ is a function that measures the disagreement between two distributions such as the mean squared error and the cross entropy.

The mean-teacher consistency regularization (MCR) is developed based on the teacher-student framework. There are two neural networks in the teacher-student framework, namely the teacher and the student. Both can be characterized as a function maps each node in $\mathcal{V}$ to a class distribution as described before. In this work, the teacher and the student share the same architecture, and we use $p_{\theta_t}: \mathcal{V} \rightarrow \mathbb{R}^C$ and $p_{\theta_s}: \mathcal{V} \rightarrow \mathbb{R}^C$ to denote the teacher and the student where $\theta_t$ and $\theta_s$ are the sets of parameters of the teacher and the student. For each node $i \in \mathcal{V}$, we can obtain two class distributions $p_{Y|i, \theta_t}$ and $p_{Y|i, \theta_s}$. The former is predicted from the teacher and the latter is predicted from the student. The unsupervised loss is constructed to penalize the disagreement between them:

$$L_u(i) = D(p_{Y|i, \theta_s}; p_{Y|i, \theta_t}).$$

Training stage. We follow the training strategy proposed in [26] to estimate the parameters in the student and the teacher. At each training step, we randomly select a batch of nodes which is a mixture of labeled and unlabeled nodes. We use $\mathcal{V}_{Bu} \subseteq \mathcal{V}_L$ and $\mathcal{V}_{Bu} \subseteq \mathcal{V}_U$ to denote the sets of labeled nodes and unlabeled nodes in the batch. The labeled nodes are processed by the student to build the supervised loss, while the unlabeled nodes are processed by both the teacher network and the student to build the unsupervised loss. The loss function of the batch can be expressed as:

$$L = \frac{1}{|\mathcal{V}_{Bu}|} \sum_{i \in \mathcal{V}_{Bu}} L_s(i, y_i) + \lambda \cdot \frac{1}{|\mathcal{V}_{Bu}|} \sum_{i \in \mathcal{V}_{Bu}} L_u(i)$$

$$= -\frac{1}{|\mathcal{V}_{Bu}|} \sum_{i \in \mathcal{V}_{Bu}} \log p_{Y|i, \theta_s}(y_i)$$

$$+ \lambda \cdot \frac{1}{|\mathcal{V}_{Bu}|} \sum_{i \in \mathcal{V}_{Bu}} D(p_{Y|i, \theta_t}; p_{Y|i, \theta_s}).$$

The parameters of the student are updated with the gradient descent algorithm:

$$\theta_s = \theta_s - \gamma \frac{\partial L}{\partial \theta_s},$$

where $\gamma$ is the learning rate. After updating $\theta_s$, the parameters of the teacher are updated form the counterparts of the student by exponential moving average (EMA):

$$\theta_t = \alpha \theta_t + (1 - \alpha) \theta_s,$$

where $\alpha \in [0, 1]$ is a predefined decay rate.

Inference stage. When predicting the label for a given node $i$, only the student is used to infer the class distribution. The final label of node $i$, denoted as $\hat{y}_i$, is defined as the class with the highest
probability in the distribution $p_{Y|\theta_i,c}$:
$$\hat{y}_i = \arg\max_{c \in \{1, \ldots, C\}} p_{Y|\theta_i,c}(c).$$

### 3.4 Additional Training Techniques

In this section, we present additional useful training techniques that help improve the performance of the MCR. These techniques can be easily extended to other consistency regularization techniques. **Confidence-based masking.** The effect of the MCR is to pull the class distributions of the student towards those of the teacher. It is desirable when the teacher can make creditable predictions. However, the predictions made by the teacher could be noisy, especially at the beginning of the training process, which hinders the model from fitting to the supervised loss. A solution is to filter out low-quality predictions with the confidence-based masking strategy [30]. Specifically, we maintain a confident node set $V_C \subseteq V_U$ in the training stage whose elements are unlabeled node with highly skewed predictions, i.e.,

$$V_C = \{ i : i \in V_U \cap \max_{c \in \{1, \ldots, C\}} p_{Y|\theta_i,c}(c), \eta \}$$

where $\eta \in [0, 1]$ is a threshold that controls the size of the confident set. In each training batch, the unlabeled nodes are selected from this confident node set $V_C$ instead of the original unlabeled node set $V_U$. In our experiments, the confident node set is updated every $\beta$ epochs. Furthermore, we find it helpful to gradually lower the threshold $\eta$ during the training course. This setting allows more nodes to contribute to the unsupervised loss as the training proceeds. We also disable the unsupervised loss at the first $r$ training epochs, preventing the model from fitting to the predictions made by the insufficiently-trained teacher.

### 4 EXPERIMENTS

To demonstrate the effectiveness of our methods, we present our performance on the ogbn-products dataset from OGB. We select MLP, GCN [17], GraphSAGE [12], SIGN [10], SAGN (+SLE) [25], GAMLP (+RLU) [34], MLP + C&S [15], GIANT-XRT+SAGN+SLE [8] as baselines. Our proposed methods are implemented using CogDL [5], a popular toolkit for deep learning on graphs. For baselines we use metrics from official reports and Open Graph Benchmark (OGB) leaderboard. For our methods, the experiments are conducted on a machine with Intel(R) Xeon(R) Gold 6240 CPU @ 2.60GHz, and a single GeForce RTX 3090 with 24GB GPU memory.

#### 4.1 Experimental Results

Table 1 shows the validation and test accuracy of our method and all the baseline methods without external data. On the ogbn-products dataset, the prediction accuracy of test set is improved by 1.12% and 1.08% respectively by using MCR on SAGN and GAMLP, two state-of-the-art GNN models. MCR is also very competitive with SLE and RLU, two multi-stage self-training methods. In addition, based on GAMLP+RLU, after adding SCR in each stage of training, the performance can be improved by 0.46%, which is the current state-of-the-art performance. After using C&S as post-processing, performance will be also improved by 0.15%. Table 2 shows that, by using the node features provided by GIANT-XRT [8], our method can further improve the performance of the model. Applying MCR to SAGN model, performance exceeds all existing baselines. After adding C&S as post-processing, compared with the top-1 method on the current OGB leaderboard, we improve the test accuracy by 0.3%. So far, we have achieved top-1 performance on the ogbn-products dataset both with and without external data.

#### 4.2 Hyper-parameter Sensitivity

We mainly performed sensitivity studies on ogbn-products with GAMLP+MCR. In Table 3, we analyzed the influence of $\lambda$ of consistency loss on training. How to balance the proportion of supervised
loss and consistency loss is an important issue in the process of tuning model. We can see from the results that too large $\lambda$ or too small $\lambda$ will affect the final performance. In Table 4, we analyzed the influence of different EMA decay on experimental results. Different decay can be regarded as ensemble of different numbers of past model parameters. Experimental results show that large decay can avoid the vibration of the model and bring better results.

5 CONCLUSION

This paper demonstrates how consistency regularization improves the results of state-of-the-art GNN models can be consistently improved. The training performance of graph neural networks under semi-supervised learning can avoid the vibration of the model and bring better results.

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