SCR: Training Graph Neural Networks with Consistency Regularization

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Abstract

We present the SCR framework for enhancing the training of graph neural networks (GNNs) with consistency regularization. Regularization is a set of strategies used in Machine Learning to reduce overfitting and improve the generalization ability. However, it is unclear how to best design the generalization strategies in GNNs, as it works in a semi-supervised setting for graph data. The major challenge lies in how to efficiently balance the trade-off between the error from the labeled data and that from the unlabeled data. SCR is a simple yet general framework in which we introduce two strategies of consistency regularization to address the challenge above. One is to minimize the disagreements among the perturbed predictions by different versions of a GNN model. The other is to leverage the Mean Teacher paradigm to estimate a consistency loss between teacher and student models instead of the disagreement of the predictions. We conducted experiments on three large-scale node classification datasets in the Open Graph Benchmark (OGB). Experimental results demonstrate that the proposed SCR framework is a general one that can enhance various GNNs to achieve better performance. Finally, SCR has been the top-1 entry on all three OGB leaderboards as of this submission.

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, graph neural networks (GNNs) have also achieved significant performance improvements in graph machine learning tasks [17, 37, 43, 15, 26]. Many of these GNN models become the top-1 performers on the leaderboard of open datasets such as Open Graph Benchmark [19].

However, training a successful GNN model requires a large amount of labeled data, which is difficult to access in realistic scenarios. Studies have shown that using unlabeled data in training can effectively enhance the model performance. The line of research on semi-supervised learning on graphs thus has been a hot topic over decades [50, 49, 27, 2]. Some work has proposed to use “pseudo labeling” to exploit unlabeled nodes in the training stage [34, 48, 23]. Among them, multi-stage self-training methods have achieved the best performance. Its basic idea is to divide the training procedure into several stages. At the beginning of each stage, the training set is 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 requires much more training time than its single-stage counterpart.

In this work, we present a simple and general consistency regularization (SCR) framework to improve the performance of graph neural networks under the semi-supervised setting. Specifically, we propose two strategies based on consistency regularization for GNNs. The first one, referred to as SCR, is to minimize the disagreement among perturbed predictions by different versions of a GNN model. The different versions could be obtained by data augmentation or randomness of the given model. For example, GRAND [13] uses random propagation to generate a graph augmentation. For each graph augmentation, we can generate a version of the predictions by the GNN model. By minimizing the disagreement among the predictions from different versions, SCR is able to improve the generalization ability of the GNN model.

The other SCR strategy is referred to as mean-teacher consistency regularization (SCR-m), which leverages the teacher-student paradigm. For SCR-m, following Mean Teacher [36], we guide the training procedure by calculating a consistency loss between the perturbed prediction from the student and the prediction from the teacher rather than minimizing the disagreement of prediction results as in SCR. 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 the teacher model will be updated by the student model.

We conducted experiments on three large datasets for the node prediction task from Open Graph Benchmark (OGB) [19], which are mostly studied recently. Specifically, we apply the proposed SCR technique to two recent GNN architectures, namely SAGN [34] and GAMLP [48]. Experiments on the three datasets clearly show that SCR can effectively improve the performance of the base GNNs, in fact outperforming all entries on the three OGB leaderboards. In addition, our study also demonstrates that SCR can improve a wide range of (advanced) GNN models, such as GraphSAGE [17], SIGN [45], ClusterGCN [9], and GraphSAINT [46], demonstrating the benefit of SCR as a general framework for enhancing GNNs.

To sum up, this work makes the following contribution:

- **Effectiveness.** Experimental results demonstrate that the proposed SCR achieves the best performance on all the three large datasets from Open Graph Benchmark (OGB).
- **Scalability.** SCR is a simple and efficient framework with scalable methods of consistency regularization for GNNs, which allows it to scale to graphs with 100 million nodes and 1 billion edges.
- **Flexibility.** SCR, as a general framework, is very flexible to all genres of graph neural networks, such as SAGN, GAMLP, GraphSAGE, SIGN, ClusterGCN, and GraphSAINT.

2 Related Work

**Graph Neural Networks.** Due to the great success of deep learning in various areas, much effort has been devoted to generalizing neural networks to graph-structured data, resulting in the development of graph neural networks (GNNs). As a pioneer work, Kipf and Welling [22] proposed graph convolution network (GCN) which adopted Chebyshev polynomials to approximate the graph spectral filter. After that, spatial domain based GNNs [17, 37, 43] are proposed by generalizing the graph convolution to various neighborhood aggregation functions, making GNNs become the mainstream for graph modeling. Based on the formulation of spatial GNNs, there have been several sampling strategies proposed to scale up GNNs on large graphs, e.g., FastGCN [8], AS-GCN [21], and GraphSAINT [46].

**Regularization Methods for GNNs.** In the meanwhile of developing GNN architectures, several works also focus on improving the training of GNNs with the consistency regularization technique. Consistency regularization was first proposed by [11], which employs a consistency loss to enforce the model to give similar predictions among different augmentations of unlabeled data. To extend this idea onto graphs, the main efforts concentrates on designing data augmentation strategies for For example, VBAT [11] and GraphVAT [12] utilized virtual adversarial training to generate graph data augmentations. GraphMix [38] borrowed the idea from MixMatch [3] by adopting MixUp [47] to facilitate GNN training. GRAND [13] and NodeAug [40] further explored more
complex augmentation strategies for graph data and achieved significant performance gains on small graphs. However, these data augmentation methods are usually time-consuming especially on large-scale graphs because it needs to be executed in each training step.

A similar technique to consistency regularization is self-training, which employs the “pseudo-labels” of unlabeled nodes to facilitate model training. Li et al. [23] was an early-stage work to explore co-training and self-training of GCNs, which significantly boosted the performance of GCNs when using very few labels in training. Sun et al. [35] proposed a Multi-Stage Self-Supervised (M3S) training algorithm, which used clustering approach to construct pseudo-labels.

3 Preliminaries

We denote a graph with \( N \) nodes by \( G = (V, E) \) where \( V \) is its node set, and \( E \subseteq V \times V \) is a set of edges. The adjacency matrix of \( G \) is denoted by \( A \in \mathbb{R}^{N \times N} \) with its \((i, j)\)-th entry \( A[i, j] = \mathbb{I}(\langle i, j \rangle \in E) \) indicating whether there is an edge from node \( i \) to node \( j \). We also assume that each node \( i \in V \) is associated with a feature vector \( x_i \in \mathbb{R}^d \).

We illustrate our approach in the context of node classification, though it can be easily generalized to other tasks such as link prediction and subgraph classification. In the setting of node classification, we are given a graph \( G = (V, E) \) and a set of labeled nodes, denoted by \( V_L \subset V \). Each labeled node \( i \in V_L \) is associated with a one-hot vector \( y_i \in \{0, 1\}^C \) which encodes its ground-truth class. \( C \) is the number of predefined classes. Our goal is to learn a function \( f_\theta(i | G) \) parameterized by \( \theta \) which can predict the correct class for a given unlabeled node \( i \).

Decoupled GNNs. Conventional GNN architectures alternate between the feature transformation and feature aggregation operators. E.g., in the GCN model [22]. A feature transformation operation and a feature aggregation operator are coupled together to form a graph convolution layer. However, recent studies also suggest that this coupling paradigm is practically unnecessary and develop a series of decoupled GNNs [30, 42]. Such GNNs first propagate the input feature \( X \) on graph for \( K \) steps by iteratively calculating:

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

where \( X^{(0)} = X \) and \( \hat{A} \in \mathbb{R}^{N \times N} \) is an aggregation matrices. The generated feature matrices \( \{X^{(0)}, X^{(1)}, \ldots, X^{(K)}\} \) are then fed into a neural network \( f_\theta \) to make predictions:

\[
\hat{Y} = f_\theta(\{X^{(0)}, X^{(1)}, \ldots, X^{(K)}\}),
\]

where \( \hat{Y} \in [0, 1]^{N \times C} \) denotes the generated prediction probability matrix. And the model is usually trained with the cross entropy loss on labeled nodes:

\[
\mathcal{L}_{sup} = \frac{1}{|V_L|} \sum_{i \in V_L} \text{CrossEntropy}(y_i, \hat{y}_i).
\]

In practice, the labeled nodes can be scarce while there are abundant unlabeled nodes in the graph. In this paper, we will investigate how much performance can be gained when training GNNs with both labeled and unlabeled nodes. To this end, we adopt two advanced decoupled GNN architectures—SAGN [34] and GAMLP [48] as backbone models due to their SOTA performances on quite a few open datasets.

4 The SCR Framework

In this section, we introduce the proposed SCR framework to improve the training of graph neural networks. SCR is based on the concept of consistency regularization [30, 42]. Briefly, consistency regularization encourages the learned model to be in line with the low-density separation assumption [7], i.e., the learned decision boundary should lie in the low-density region. In other words, a small perturbation on the input data should not change the prediction significantly.

Figure 1 illustrates the process of training a graph neural network under the SCR framework. Given an input graph with 1 labeled node and 4 unlabeled nodes on the left, it is fed into an encoder \( S \) times
Figure 1: Illustration of the proposed SCR framework. The total training loss is divided into the supervised loss and unsupervised consistency loss. The difference between SCR and SCR-m mainly lies on how to estimate pseudo labels. In SCR, the pseudo label is the average of the outputs over multiple runs, while in SCR-m, the pseudo label is predicted by an EMA teacher. Confidence-based masking is used to get rid of pseudo labels with high uncertainty.

(e.g., $S = 3$ in the figure) to get $S$ noisy predictions (Cf. § 4.1). These predictions are different due to the stochastic property of the encoder, e.g., a neural network with dropout. Then, we assign a pseudo label, e.g., the average of these noisy predictions, to every unlabeled node (Cf. § 4.2). Next, a confidence mask is computed according to the pseudo labels, which filters out unlabeled nodes that the model cannot predict well. The loss function consists of two components. The first one is the standard cross entropy loss between ground-truth labels and predictions from labeled nodes. The second component is evaluated based on the confident unlabeled nodes, and used to penalize a distance metric between predictions and pseudo labels (Cf. § 4.3).

The SCR framework is a general consistency regularization technique for improving graph learning models. For example, the encoder can be a simple MLP or any graph neural networks, e.g., GCN [22], GraphSAGE [17], and GAMLP [48].

4.1 Noisy Prediction Generation

Injecting noise to the model in the training stage is a simple yet efficient technique to regularize deep neural networks. The noise can be added into the input, e.g., data augmentation [42], or directly added into the model, e.g., dropout [33]. For example, there are many semantic-preserving transformations, such as flipping, rotation and color jitter, to augment image data. However, these cannot be directly applied to the graph data. Furthermore, existing data augmentation approaches for graphs, such as DropNode [13] and DropEdge [29], are operated on the entire graph. This means that we need to load the entire graph into the memory at each training step, which is time-consuming and memory inefficient for large graphs.

In SCR, we only use the simple dropout strategy to generate noisy predictions. For each node $i \in \mathcal{V}$, we can obtain a total of $S$ noisy predictions $\{\hat{y}_i^{(s)}\}_{s=1}^{S}$ by evaluating the model $f_\theta(i \mid G)$ for $S$ times under different dropout conditions. During the training stage, the dropout regularization randomly disables a predefined proportion of hidden units of the model to avoid co-adapting and overfitting, and the output is a random variable. Therefore, multiple evaluations of the same input will yield different results. According to the low-density separation assumption [7], this difference should be small, given that the input data is the same. Thus, minimizing the output difference caused by the dropout regularization is reasonable. Moreover, by using dropout, the SCR framework is in nature a lightweight and scalable method that can regulate models on large-scale graphs.

4.2 Pseudo Labeling

In order to extract information from the unlabeled data, we need to construct learning tasks on them. Pseudo labelling is a popular method which produces pseudo labels for unlabeled data using the model itself and trains the model against them. Denoting the pseudo label of node $i$ as $\bar{y}_i$, the regularization term used in SCR framework is defined as:

$$L_{SCR} = \frac{1}{S \cdot |\mathcal{V}_U|} \sum_{i \in \mathcal{V}_U} \sum_{s=1}^{S} \text{dist} \left( \bar{y}_i, \hat{y}_i^{(s)} \right).$$

(3)
We use \( B \) to denote the sets of labeled nodes and unlabeled nodes in the batch.

We describe two strategies to generate the pseudo labels — SCR and SCR-m. In SCR, the pseudo label for node \( i \) is defined as the average of its noisy predictions, i.e.,

\[
\hat{y}_i = \frac{1}{S} \sum_{s=1}^{S} y_i^{(s)}.
\]  

(4)

In SCR-m, we use a teacher network to generate pseudo labels:

\[
\hat{y}_i = f_{\theta'}(i \mid G),
\]  

(5)

where \( f_{\theta'}(i \mid G) \) is the teacher network. Motivated by the Mean-Teacher paradigm described in [36], the teacher network shares the same network architecture with the student model \( f_{\theta}(i \mid G) \), and its parameters at training step \( t \), expressed by \( \theta'_t = \alpha \theta'_{t-1} + (1 - \alpha) \theta_t \), are an exponential moving average of the parameters of the student where \( \alpha \in (0, 1) \) is a decay rate.

**Pseudo label sharpening.** After obtaining the pseudo label via Equation [4] or [5] we further apply a sharpening function to reduce the entropy of the pseudo label.

\[
\hat{y}_i^{(\text{sharp})} = \text{sharpen}(\hat{y}_i) = \frac{(\hat{y}_i[c])^{1/T}}{\sum_{c'=1}^{C}(\hat{y}_i[c'])^{1/T}}
\]

where \( T \in (0, 1) \) is a temperature hyperparameter controlling the sharpness of the pseudo label. This operation is motivated by the idea of entropy minimization [16] which encourages the model to produce low-entropy (high-confident) predictions, and is widely used in other consistency regularization methods [42,3,12].

### 4.3 Loss Function

As aforementioned, the loss function of the SCR framework consists of two parts. The first part is evaluated on the labeled nodes while the second part is evaluated on the unlabeled nodes. At each training step, we randomly select a batch of nodes which is a mixture of labeled and unlabeled nodes. We use \( B_L \subseteq \mathcal{V}_L \) and \( B_U \subseteq \mathcal{V}_U \) to denote the sets of labeled nodes and unlabeled nodes in the batch.

The loss function of the batch can be expressed as:

\[
\mathcal{L} = \frac{1}{S \cdot N_L} \sum_{i \in B_L} \sum_{s=1}^{S} \text{CrossEntropy}(y_i, \hat{y}_i^{(s)}) + \frac{\lambda}{S \cdot N_U} \sum_{i \in B_U} \sum_{s=1}^{S} \text{dist}(\hat{y}_i^{(\text{sharp})}, \hat{y}_i^{(s)})
\]

(6)

where \( N_L \) and \( N_B \) denote the size of \( B_L \) and \( B_U \), respectively. \( \lambda \) is a hyperparameter that controls the strength of the regularizer. Following [36,42,3], we do not propagate gradients through pseudo labels.
Table 1: Statistics of three OGB datasets.

| Datasets          | #Nodes      | #Feat. | #Edges     | #Classes |
|-------------------|-------------|--------|------------|----------|
| ogbn-products     | 2,449,029   | 100    | 61,859,140 | 47       |
| ogbn-mag          | 1,939,743   | 128    | 21,111,007 | 349      |
| ogbn-papers100m   | 111,059,956 | 128    | 1,615,685,872 | 172     |

4.4 Training Algorithm

Algorithm 1 summaries the training process of the SCR framework. In this section, we present several useful techniques that help improve the training effectiveness. These techniques can be easily extended to other consistency regularization frameworks.

**Confidence-based masking.** Minimizing the regularization term via Equation 3 is to pull the predictions of the model towards the generated pseudo labels. It is desirable when the pseudo labels are of high confidence. However, the pseudo labels are not always reliable, especially at the beginning of the training process. Poor pseudo labels could even hinder the model from fitting to the labeled data. To solve this, we filter out low-quality predictions with the confidence-based masking strategy [42]. Specifically, we maintain a confident node set $V_C = \{ i : i \in V_U \cap \max_{c \in \{1, \ldots, C\}} \bar{y}[c] \geq \eta \}$ in the training stage whose elements are unlabeled node with highly skewed predictions. Here, $\eta \in [0, 1]$ is a threshold that controls the size of the confident set. This is based on the assumption that the skewed predictions are more likely to be a confident one as they are far away from the decision boundary. At each training step, the unlabeled nodes in the minibatch are selected from this confident node set $V_C$, instead of the entire 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 process in some situations, which allows more nodes to contribute to the consistency regularization as the training proceeds.

**Warmup for SCR-m.** When training SCR-m, we found that the teacher network performs worse than the student network at the early stage of the training, and thus, may hurt the stability of the student network. This might be due to that the student network is updated via gradient descent, and fits to the labeled data very quickly, while the teacher network is updated via EMA, and lags behind the student at the early stage of training. Accordingly, we design a warmup stage for SCR-m by disabling its regularizer at the first $\tau$ training epochs, preventing the model from fitting to the predictions made by the insufficiently-trained teacher model.

5 Experiments

We evaluate the SCR (and SCR-m) on the node classification task, which is one of the most popular benchmark tasks for graph learning. We use three large datasets from Open Graph Benchmark (OGB) [19], including ogbn-products, ogbn-mag and ogbn-papers100M. Table 1 summarizes statistics of the three benchmark datasets. We follow exactly the experimental procedure suggested by OGB, such as features, data splits and evaluation protocol. More details are covered in Appendix.

Overall, the proposed SCR framework has been the top-1 entry on all the three OGB datasets as of today—the submission deadline.

5.1 Comparison with Peer Methods

**Baselines.** *ogbn-products* is a co-purchasing network of Amazon products [4], and the task is to predict the category of a product. For comparison, we include classic GNN models and several top-performing methods, including MLP, GCN [22], GraphSAGE [17], SIGN [14], SAGN [34] and GAMLIP [48] as baselines. We evaluate SCR with the two GNN models—GAMLIP [48] and SAGN [34]—We also make comparisons of C&S [20], which utilizes two post-processing steps, an
Table 2: Accuracy on ogbn-products. Results with gray are obtained by our proposed framework.

| Methods     | Arch. | C&S     | Validation | Test     |
|-------------|-------|---------|------------|----------|
| - MLP       | -     |         | 75.54±0.14 | 61.06±0.08 |
| - MLP       | ✓     |         | 91.47±0.09 | 84.18±0.07 |
| - GCN       | -     |         | 92.00±0.03 | 75.64±0.21 |
| - GraphSAGE | -     |         | 92.24±0.07 | 78.50±0.14 |
| - SIGN      | -     |         | 92.99±0.04 | 80.52±0.16 |
| - SAGN      | -     |         | 93.09±0.04 | 81.20±0.07 |
| - GAMLP     | -     |         | 93.12±0.03 | 83.54±0.09 |
| RLU GAMLP   | -     | ✓       | 93.24±0.05 | 84.59±0.10 |
| SCR GAMLP   | -     | ✓       | 93.30±0.06 | 84.07±0.06 |
| SCR-m GAMLP | -     | ✓       | 93.19±0.03 | 84.62±0.03 |
| RLU+SCR GAMLP | - | ✓ | 92.92±0.05 | 85.05±0.09 |
| RLU+SCR GAMLP | ✓ | ✓ | 93.04±0.05 | 85.20±0.08 |

using node features generated by GIANT-XRT

| SLE SAGN   | -     | ✓       | 93.63±0.03 | 86.22±0.22 |
| SCR SAGN   | -     | ✓       | 93.52±0.03 | 86.43±0.20 |
| SCR-m SAGN | -     |         | 93.64±0.03 | 86.67±0.09 |
| SCR SAGN   | ✓     |         | 93.57±0.04 | 86.80±0.07 |
| SCR-m SAGN | ✓     |         | 93.89±0.02 | 86.51±0.09 |
| SCR-m SAGN | ✓     | ✓       | 93.87±0.02 | 86.73±0.08 |

“error correlation” and a “prediction correlation”, that exploit correlation in the label structure. C&S is considered as a standard module for performance improvement especially on the ogbn-product dataset. In addition, we report the results using the GIANT-XRT features that are generated from an encoder trained on an eXtreme Multi-label Classification (XMC) formalism in the graph domain.

ogbn-mag is a heterogeneous academic graph from a subset of the MAG. The task of ogbn-mag is to predict the venue information (conference or journal) of each paper, which is consistent with practical interests of MAG. For ogbn-mag, we selected MLP, R-GCN, SIGN, NARS, NARS_SAGN, and NARS_GAMLP as baselines.

To demonstrate the scalability of our proposed framework, we conduct an experiment on an extremely large citation network, ogbn-papers100M, which has more than 100 million nodes and 1 billion edges. As the ogbn-papers100M dataset is such a giant graph, only a few scalable GNNs could handle it. Here, we report the results of MLP, SGC, SIGN, SAGN, GAMLP.

The results of these aforementioned baselines are directly taken from the OGB leaderboards.

Results. Table[2] summarizes the validation and test accuracy of baselines and our methods on ogbn-products. The prediction accuracy of test set is improved by 0.53% and 1.08% by using SCR and SCR-m on GAMLP, respectively. We can also observe that SCR-m is competitive with RLU, a multi-stage self-training methods. In addition, SCR is more compatible with RLU. Based on GAMLP, after applying SCR as a training technique, the performance could be further improved by 0.46%, which is currently the best performance on the dataset. After further applying C&S as the post-processing step, the performance can be improved by 0.15%. By using the node features provided by GIANT-XRT, our method can also bring performance gains. Applying SCR and SCR-m to the SAGN model, the performance exceeds all existing baselines. Compared with the SAGN (RLU), we improve the test accuracy by 0.45% and 0.29%. After adding C&S as post-processing, we improve the test accuracy by 0.37% and 0.30%. Overall, our proposed framework brings 0.37% and 0.46% improvements on ogbn-products with and without GIANT-XRT features, respectively.

Table[3] lists the performances of our methods and baseline methods on the ogbn-mag dataset. We used NARS_GAMLP as the base model, which shows superior performance than NARS_SAGN. Compared with NARS_GAMLP, the test accuracy could be improved by 0.36% and 0.55% when applying SCR.
and SCR-m. Meanwhile, when adding SCR to NARS_GAML (RLU), the performance can be still improved by 0.41%.

Table 4 shows the performances of all methods on the ogbn-papers100M dataset. For the basic architecture, by using SCR and SCR-m on GAML (RLU), the test accuracy could be improved by 0.43% and 0.45%. Moreover, by applying SCR to GAML (RLU), the final performance exceeds all the compared baselines.

5.2 Experiments on Different Graph Neural Networks

By design, the SCR framework is a general consistency regularization framework with the goal to improve the base graph models. As shown above, it can help both GAML and SAGN—the previous top entries on three OGB leaderboardsto improve their performance. Herein we examine whether SCR can broadly help other graph encoders as promised. Specifically, we consider the following five architectures, namely MLP, GraphSAGE [17], ClusterGCN [9], GraphSAINT [46] and SIGN [45], as the base graph encoder in SCR. Table 5 reports the results of the original models as well as those with SCR on ogbn-products. We observe consistent performance gains brought by the SCR framework for all five encoders, further demonstrating that SCR is a general consistency regularization technique that can benefit the performance of graph models.

5.3 Comparison of Training Efficiency

Multi-stage training methods, such as RLU, rely on repeated retraining to produce new pseudo labels. Our proposed SCR and SCR-m avoid this unnecessary overhead and are therefore more efficient, with a significantly reduced number of training epochs required. To verify the efficiency of our methods, we used GAML (as the base model and conducted comparative experiments with RLU on three OGB datasets. Figure 2 shows the test accuracy per epoch on the ogbn-products and ogbn-papers100M datasets. On the ogbn-products dataset, it takes 200 epochs for the SCR-m to reach the accuracy of 84% while RLU needs about 450 epochs to reach this level. On the ogbn-papers100M dataset, it takes around 200 epochs for the SCR and the SCR-m to reach the accuracy of 68% while RLU needs about 350 epochs.
Figure 2: Classification accuracy of the SCR framework and our baseline RLU when training epochs increase.

Figure 3: Effects of hyper-parameters on GAMLP + SCR and GAMLP + SCR-m.

5.4 Hyper-parameter Sensitivity

We mainly performed hyper-parameter studies on ogbn-products with GAMLP + SCR and GAMLP + SCR-m. In Figure 3a and Figure 3c, we analyzed the influence of $\lambda$ of consistency loss on training. It is an important issue to balance the proportion of supervised loss and consistency loss in the process of tuning models. From the results, we can see that too large $\lambda$ or too small $\lambda$ will affect the final performance. In Figure 3b, we explored the influence of masking threshold on experimental results. Too large threshold will reduce the number of nodes involved in calculating consistency loss, and too small threshold will make some bad predictions affect the overall training direction. In Figure 3d, we analyzed the influence of different EMA (Exponential Moving Average) decay on experimental results. Different decay can be regarded as an 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.

6 Conclusion

This paper demonstrates how consistency regularization improves the training performance of graph neural networks under semi-supervised setting. We design SCR—a simple graph learning consistency regularization technique—as well as its variant SCR-m. With these methods of consistency regularization, the results of state-of-the-art GNN models can be consistently improved. At the time of writing, we achieve the top-1 performance on the three large-scale OGB datasets: ogbn-products, ogbn-mag, and ogbn-papers100M. Moreover, SCR (and SCR-m) are a general regularization framework that by design can take any graph models as the base encoder and thus improve their performance. This attempt provides inspiration for further exploration of consistency regularization on graph neural networks. In the future, we plan to design more effective consistency regularization strategies for graph-structured data.

Limitations of the work. Our work assumes that the labeled data and the unlabeled data are generated from the same distribution. However, this assumption is not always hold in real applications. If the distribution mismatch between labeled data and unlabeled data is identifiable, we would not generate reliable pseudo labels for unlabeled data with the model learned from the labeled data.
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A Appendix

A.1 Connections with Previous Work

GRAND \[13\] can be also viewed as a consistency regularization method for graph data. It utilizes random propagation, a data augmentation technique designed for graph data, to generate noisy predictions. In GRAND, every noisy prediction relies on a single run of the random propagation. To train a neural network with GRAND for \(N_t\) training steps, we need to run the random propagation \(N_t \cdot S\) times. The total complexity of the random propagation is \(O(N_tSKd(N + M))\), where \(K\), \(d\), \(N\), \(M\) are the numbers of the propagation steps, node features, nodes and edges, respectively. In practice, it is computationally infeasible to perform this operation for large graphs. In addition, the random propagation in GRAND needs to load the entire graph into memory at each training step, making its scalability constrained by the memory size. In contrast, the noisy predictions in SCR do not rely on the randomness of the propagation. Therefore, we only need to run the propagation one time and the propagated node features can be reused in the following training steps, which results in a complexity of \(O(Kd(N + M))\), which is practically much cheap. To conclude, the performance of SCR does not rely on the expensive data augmentation procedure used in GRAND, enabling it to scale to any size of networks as long as the underlying graph encoder can handle them.

R-Drop \[24\] is a regularization method to reduce the inconsistency between the training and inference stages caused by dropout. The key idea is to minimize the Kullback-Leibler divergence between two outputs generated by the same input data. The R-Drop regularization is applied in the supervised setting where each data point has a ground-truth target. Thus, the pseudo labeling is unnecessary for R-Drop. In the SCR framework, the consistency regularization is applied to the unlabeled data, and uses pseudo labels to align model outputs, making it fundamentally different from R-Drop.

SLE \[34\] & RLU \[48\] utilize unlabeled nodes by self training. When applying SLE or RLU to train a GNN model, the training phase is divided into several stages. In the first stage, only the labeled data is used to train the model. From the second stage, the model trained at the previous stage is used to label nodes that have not been labeled yet. The training data is enlarged by adding node-label pairs with high prediction confidence. A new model will be trained on the enlarged training data. As it needs to train a model to converge at each stage, the training time is much longer than SCR.
A.2 Implementation Notes

Running Environment. Our proposed framework is implemented via PyTorch [28] and CogDL [5], a toolkit for deep learning on graphs. For our methods, the experiments are conducted on a linux machine with Intel(R) Xeon(R) Gold 6240 CPU @ 2.60GHz, 377G RAM, and 10 NVIDIA GeForce RTX 3090 with 24GB GPU memory. For a fair comparison, we repeat each experiment ten times and report the mean and standard deviation except for the largest ogbn-papers100M dataset. For the ogbn-papers100M dataset, we run each method three times following the official requirements of OGB leaderboards. As for software versions, we use Python 3.8, PyTorch 1.7.1, CogDL 0.5.2, OGB 1.3.2, and CUDA 11.2.

Implementation Details. We adopt the SCR framework on 7 GNN architectures. The codes are adapted from the following repositories:

- MLP: [https://github.com/snap-stanford/ogb/blob/master/examples/nodeproppred/products/mlp.py](https://github.com/snap-stanford/ogb/blob/master/examples/nodeproppred/products/mlp.py)
- GraphSAGE: [https://github.com/pyg-team/pytorch_geometric/blob/master/examples/ogbn_products_sage.py](https://github.com/pyg-team/pytorch_geometric/blob/master/examples/ogbn_products_sage.py)
- ClusterGCN: [https://github.com/snap-stanford/ogb/blob/master/examples/nodeproppred/products/cluster_gcn.py](https://github.com/snap-stanford/ogb/blob/master/examples/nodeproppred/products/cluster_gcn.py)
- GraphSAINT: [https://github.com/snap-stanford/ogb/blob/master/examples/nodeproppred/products/graph_saint.py](https://github.com/snap-stanford/ogb/blob/master/examples/nodeproppred/products/graph_saint.py)
- SIGN: [https://github.com/dmlc/dgl/blob/master/examples/pytorch/ogb/sign/sign.py](https://github.com/dmlc/dgl/blob/master/examples/pytorch/ogb/sign/sign.py)
- SAGN: [https://github.com/skepsun/SAGN_with_SLE](https://github.com/skepsun/SAGN_with_SLE)
- GAMLP: [https://github.com/PKU-DAIR/GAMLP](https://github.com/PKU-DAIR/GAMLP)

A.3 Hyperparameter Settings

For all experiments, we set the hyperparameters related to the model architecture, such as hidden size, model depth, and propagation steps, as the defaults. The hyperparameters introduced by the SCR framework are listed as follows:

- $\lambda$: the weight of the consistency regularizer
- $\text{dist}$: distance function
- $S$: the number of views
- $\eta$: threshold for confidence-based masking
- $T$: the sharpening temperature
- $\beta$: update frequency for confidence-based masking
- $\alpha$: EMA decay rate, only applied on SCR-m
- $\tau$: warmup epochs, only applied on SCR-m

We set $T$ as 0.5 and $\beta$ as 20 across all experiments, as the SCR framework is not very sensitive to them in the experiments.

Table 6 lists the hyperparameters corresponding to the results on the SCR framework reported in Table 2, 3, and 4. The confidence threshold $\eta$ in SCR-m is linearly reduced from the initial value to the minimum value.

Table 7 lists the hyperparameters used for the experiments on RLU + SCR. For these experiments, we use the mean squared error as the distance function, and set $S = 2$. The training stage is set as follows:

- On the ogbn-products dataset, we split the training process into 6 stages. The first stage has 400 epochs and the rest has 300 epochs for each.
Table 6: Detailed hyperparameter setting on SCR.

| Dataset                  | SCR | SCR-m |
|-------------------------|-----|-------|
| ogbn-products           | 0.5 | 0.2   |
| ogbn-mag                | 0.1 | 0.025 |
| ogbn-papers100M         | 0.2 | 0.03  |

| dist | MSE | MSE | MSE | KL | KL | KL |
|------|-----|-----|-----|----|----|----|
| S    | 2   | 2   | 2   | 1  | 1  | 1  |
| η    | 0.85| 0.5 | 0.9 | 0.9-0.8 | 0.5-0.4 | 0.9-0.8 |
| α    | —   | —   | —   | 0.999 | 0.99 | 0.99 |
| τ    | —   | —   | —   | 150 | 60 | 100 |

Table 7: Detailed hyperparameter setting on RLU + SCR.

| Dataset                  | λ   | η    | η   |
|-------------------------|-----|------|------|
| ogbn-products           | 0.1 | 0.995| 0.1  |
| ogbn-mag                | 0.07| 0.4  |      |
| ogbn-papers100M         | 0.1 | 0.9  |      |

- On the ogbn-products dataset, we split the training process into 6 stages. The first stage has 400 epochs and the rest has 300 epochs for each.
- On the ogbn-papers100M dataset, we split the training process into 4 stages and each has 400 epochs.

Table 8 lists the hyperparameters used for the experiments using node features generated by GIANT. For these experiments, we use the Kullback-Leibler divergence as the distance function.

Table 8: Detailed hyperparameter setting using GIANT-XRT features.

| Dataset                  | SCR | SCR-m |
|-------------------------|-----|-------|
| ogbn-products           | 0.2 | 0.02  |
| ogbn-mag                | 0.02|       |
| ogbn-papers100M         | 0.2 | 0.02  |

| S    | 2   | 2    |
| ---- | ----|------|
| η    | 0.85-0.8 | 0.85-0.75 |
| α    | —   | 0.99  |