Structure-Aware Label Smoothing for Graph Neural Networks

Yiwei Wang¹, Yujun Cai², Yuxuan Liang¹, Wei Wang¹, Henghui Ding², Muhao Chen³, Jing Tang³ and Bryan Hooi¹

¹National University of Singapore
²Nanyang Technological University
³Department of Computer Science, USC
⁴The Hong Kong University of Science and Technology

wangyw_seu@foxmail.com, {yujun001, ding0093}@e.ntu.edu.sg, yuxliang@outlook.com, wangwei.cs@gmail.com, muhaochen@ucla.edu, jingtang@ust.hk, bhooi@comp.nus.edu.sg

Abstract

Representing a label distribution as a one-hot vector is a common practice in training node classification models. However, the one-hot representation may not adequately reflect the semantic characteristics of a node in different classes, as some nodes may be semantically close to their neighbors in other classes. It would cause over-confidence since the models are encouraged to assign full probabilities when classifying every node. While training models with label smoothing can ease this problem to some degree, it still fails to capture the nodes’ semantic characteristics implied by the graph structures. In this work, we propose a novel SALS (Structure-Aware Label Smoothing) method as an enhancement component to popular node classification models. SALS leverages the graph structures to capture the semantic correlations between the connected nodes and generate the structure-aware label distribution to replace the original one-hot label vectors, thus improving the node classification performance without inference costs. Extensive experiments on seven node classification benchmark datasets reveal the effectiveness of our SALS on improving both transductive and inductive node classification. Empirical results show that SALS is superior to the label smoothing method and enhances the node classification models to outperform the baseline methods.

1 Introduction

Node classification is a fundamental machine learning task on graphs [Wu et al., 2019]. It supports numerous practical applications, such as learning molecular fingerprints [Kearnes et al., 2016] and predicting entity properties [Schlichtkrull et al., 2018]. Since the introduction of the Graph Convolutional Network [Kipf and Welling, 2016], graph neural networks (GNNs) have become the modern tools of choice for node classification.

GNNs devise the ‘message passing’ mechanism, which aggregates the features for every node from its neighbors in the feed-forward process [Kipf and Welling, 2016]. ‘Message passing’ offers the inductive bias of reducing the semantic distances between connected nodes [Rong et al., 2019; Wang and Leskovec, 2020]. This inductive bias matches the prior knowledge that the edges naturally imply the connectivity or relatedness between the connected nodes [Hartuv and Shamir, 2000], which is the basis of GNNs’ superior performance [Wang and Leskovec, 2020].

On the other hand, how to utilize the graph structural information to generate effective supervision signals remains under-explored. As far as we know, most of the existing work trains GNNs with the label distribution of one-hot vectors, namely the hard targets [Wu et al., 2019]. However, recent research has found that using the hard targets to train neural networks tends to cause over-fitting and over-confidence [Szegedy et al., 2016; Müller et al., 2019]. To combat these problems, [Szegedy et al., 2016] have proposed the label smoothing (LS) technique that applies the uniform noise to the label distribution. Although LS can prevent the learned models from being over-confident, it cannot describe the characteristics of a node in different classes implied by the graph structures. For example, if node i in class yᵢ has a neighbor j in class yⱼ, node i should be more semantically close to yⱼ than other classes due to the connectivity between nodes i and j. Equally treating all the classes for every node overlooks the graph structures and could limit the GNNs’ performance.

The central idea of this paper is to enrich the supervision of GNNs by incorporating the graph structural information into the label distribution. We encapsulate this idea in a simple yet effective method, called SALS (Structure Aware Label Smoothing), to generate more ‘faithful’ soft targets on node classification. SALS takes the neighborhood labels as the prior distribution for the label smoothing of every node. It reflects the semantic characteristics of a target node in different classes implied by the graph structures. In the semantic space, our SALS reduces the optimum distances from a target node to its neighbors so as to guide the target node’s representation toward an appropriate position. This suits the inductive bias of GNNs and calibrates them by adaptively offering the structure-aware training targets for every node.

SALS is a general method for node classification that offers improvements by regularizing GNN models without ex-
tra inference costs. We evaluate SALS on both transductive and inductive node classification tasks using the Citeseer, Cora, Pubmed [London and Getoor, 2014], CoraFull [Bojchevski and Günnemann, 2018], Coauthor-Physics [Shchur et al., 2018], Flickr [McAuley and Leskovec, 2012], and Reddit [Hamilton et al., 2017] datasets. Qualitatively, SALS learns more discriminative node representations (see Fig. 6). We also observe consistent quantitative improvements measured by test accuracy. Overall, SALS improves the popular GCN [Kipf and Welling, 2016], ResGCN [Li et al., 2019], GraphSAGE [Hamilton et al., 2017], GraphSAINT [Zeng et al., 2019], and SIGN [Frasca et al., 2020] models by a significant margin, and enhances them to outperform the baseline methods.

2 Related Work

Graph Neural Networks (GNNs) for node classification have seen a long history of studies, we thus refer readers to [Wu et al., 2019] and [Zhou et al., 2018] for a comprehensive review. The first work that proposes the convolution operation on graph data is [Bruna et al., 2013]. More recently, [Kipf and Welling, 2016] made breakthrough advancements in the task of node classification. After [Kipf and Welling, 2016], numerous GNN methods have been proposed for better performance on node classification. There are two main lines of research in this field. The first one is to propose new GNN architectures to improve the model capacity [Veličković et al., 2017; Zhang et al., 2018; Haonan et al., 2019; Zhuang and Ma, 2018; Qu et al., 2019]. Another one is to propose new mini-batch training techniques for GNNs to enhance their scalability without the loss of effectiveness [Hamilton et al., 2017; Chiang et al., 2019; Zeng et al., 2019]. A common design among these GNN models is the ‘message passing’ mechanism, which matches the characteristics of graph data that the edges imply the connectivity or relatedness between nodes.

Our work is orthogonal to the above two lines in the sense that it does not alter the GCN architecture, or introduce any new mini-batch technique. Instead, we propose a new label smoothing method that enriches the supervision of GNNs without introducing extra inference costs. SALS incorporates the rich graph structures into the supervision of GNNs. We find that the favorable characteristics of SALS lead to more accurate predictions.

Label smoothing (LS) is first proposed in image classification tasks as a regularization technique [Szegedy et al., 2016], and has been used in many state-of-the-art models, including computer vision [Zoph et al., 2018; Zhang et al., 2021], and natural language processing [Chorowski and Jaitly, 2016; Vaswani et al., 2017]. However, the soft targets produced by the LS cannot describe the structural characteristics of nodes implied by the connectivity. In contrast, we use the graph structural information to guide the label smoothing so as to supervise GNNs with the structure-aware label distribution. As far as we know, our work is the first to devise the label smoothing method for the graph data.

3 Methodology

In this section, we introduce the technical details of our proposed structure-aware label smoothing (SALS). Our SALS incorporates the idea of modeling deterministic data, namely observed class labels, in terms of a set of probability distributions instead of a hard target. SALS utilizes the rich graph structure information for supervising graph neural networks on node classification, so as to produce more ‘faithful’ training targets reflecting the connectivity or relatedness between the connected nodes. Consequently, SALS yields the soft target for every node to be adaptive to its neighborhood, which is shown to be crucial to learning effective node embeddings.

3.1 Preliminaries

We hereby introduce the preliminaries by introducing the node classification problem, graph neural networks, and the original label smoothing technique.

Node Classification Consider a graph $G = (V, E)$, where $V$ is the set of nodes and $E = \{(i, j) \mid i, j \in V\}$ is the set of edges. The goal of node classification is to learn a mapping $M: V \rightarrow \mathbb{P}(Y)$, where $Y$ is a set of class labels, and $\mathbb{P}(Y)$ is the space of probability distributions over $Y$.

Node classification has been mainly addressed by Graph Neural Network (GNN) based methods in recent literature. The edges in a graph imply the connectivity or relatedness between the connected nodes [Hartuv and Shamir, 2000]. Based on this prior knowledge, GNNs utilize the connectivity of nodes in graph structures to learn the nodes’ representations. GNNs are a kind of multi-layer neural networks that propagates the nodes’ representations across edges between different nodes, which is also known as the ‘message passing’ mechanism. GNNs stack multiple trainable layers to achieve message passing over edges, where every GNN layer updates a target node $i$’s representations by aggregating the last layer’s representations from the target node’s neighbors (in the training set) denoted as $N(i)$.

Existing work finds that ‘message passing’ reduces the distance in the embedding space between the connected nodes [Rong et al., 2019; Wang and Leskovec, 2020]. This property matches the characteristics of the graph data that every node
is correlated to its neighbors. It acts as a useful inductive bias that supports GNNs’ state-of-the-art performance.

**Label Smoothing**  The classical training is based on the deterministic label, which is (explicitly or implicitly) treated as a one-hot vector, namely the hard targets. The recent study [Müller et al., 2019] finds that the hard targets are too extreme to express the normally realistic assumption of a non-deterministic dependency between the features and labels. Some instances are semantically close to other instances in the classes different from themselves [Zhang et al., 2021]. Instead of using hard labels for training, label smoothing (LS) replaces the surrogate distribution $q$ with a less extreme surrogate

$$q^{LS} = (1 - \epsilon)q + \epsilon u_c$$

as a soft target for the learner, where $u_c \in \mathbb{P}(Y)$ is a uniform distribution among all the classes in $Y$ and $\epsilon \in (0, 1]$ is a smoothing factor. LS can be seen as an attempt at presenting the training information in a more ‘faithful’ way: a smoothed target probability $q^{LS}$ is arguably more realistic than a degenerated hard distribution $q$ assigning the full probability mass to a single class label.

LS obviously leads to less extreme predictions than the hard targets. However, the adjusted distribution $q^{LS}$ assigns the uniform noise to all the classes, which may not reflect the intrinsic characteristics of an instance to be classified.

### 3.2 Structure-Aware Label Smoothing

For training GNNs, most of existing work minimizes the expected value of the cross-entropy loss between the true targets $q(c|i)$ and the network’s prediction $p(c|i)$ in

$$H(q, p) = -\sum_{c=1}^{C} q(c|i) \log p(c|i).$$

Minimizing this loss is equivalent to maximizing the expected log-likelihood of the label that is selected according to the distribution $q(c|i)$, of which the gradient is bounded between $-1$ and $1$ [Szegedy et al., 2016].

Consider the case of the hard target, where $q(y_i|i) = 1$ and $q(c|i) = 0$ for $c \neq y_i$, training GNNs with hard targets has several limitations. First, it overlooks the correlations between connected nodes. The edges in a graph naturally imply the connectivity or relatedness between connected nodes [Hartuv and Shamir, 2000]. Second, using hard targets to supervise GNNs does not match their inductive bias of reducing the semantic distances between connected nodes [Wang and Leskovec, 2020]. To classify node $i$, the ‘message passing’ mechanism of GNNs aggregates the features from $i$’s neighbors, while its neighbor $j \in \mathcal{N}(i)$ can belong to any other classes than $y_i$. Enforcing GNNs to assign full probabilities as prediction for connected nodes in different classes ignores their structural relationship, and is hard to generalize to the unseen nodes.

To address the above issues, intuitively, we aim to find a label distribution that reveals the semantic characteristics of a node in each class implied by the graph structures. Consider an example in Fig. 1. In a social network of athletes where the edges represent the ‘teammate’ relations, the node ‘Michael Jordan’ is a famous professional basketball athlete, and he is meanwhile an expert in baseball, which is implied by his neighbors of professional baseball athletes [Mathur et al., 1997]. Here, ‘basketball’ and ‘baseball’ should be assigned a higher probability mass than the other sports, e.g., ‘soccer’, at which the node ‘Michael Jordan’ is not a professional. It would be beneficial to consider these genuine ‘preferences’ of a node on different classes implied by the graph structures for label smoothing.

We propose a method called **SALS** (Structure-aware Label Smoothing) to mine the intrinsic semantic characteristics of every node from rich graph structures for node classification, and produce structure-aware soft targets for training GNNs. Specifically, we use the labels of a node’s neighbors to mine its characteristics beyond its own hard target, and use the structural information to produce the soft targets that are adaptive to the graph structures. SALS regularizes GNNs for better generalization and makes node representation more adaptable by leveraging the rich graph structural knowledge for supervision. For node $i$ with ground-truth labels $y_i$, consider the distributions of its neighbors’ labels $\{y_j, j \in \mathcal{N}(i)\}$. First, we analyze the ratio of neighbors (in the training set) of nodes $i$ in different classes. In particular, let the ratio of node $i$’s neighbors in class $y$ be

$$r_c(i) := \frac{1}{|\mathcal{N}(i)|} \sum_{j \in \mathcal{N}(i)} 1[y_j = c].$$

We define the neighborhood label of node $i$, which is the average label of $i$’s neighbors in the training set, to be

$$\eta(i) := \frac{1}{|\mathcal{N}(i)|} \sum_{j \in \mathcal{N}(i)} \delta_{c,y_j} = \sum_{y \in Y} r_y(i) \delta_{c,y},$$

where $\delta_{c,y}$ is Dirac delta, which equals 1 for $c = y_j$ and 0 otherwise. We replace the label distribution of $q(c|i) = \delta_{c,y_i}$ with

$$q^{SALS}(c|i) = (1 - \epsilon)\delta_{c,y_i} + \epsilon \left(\gamma \eta(i) + (1 - \gamma)u_c\right),$$

which is a mixture of the original hard target $q(c|i)$ and its neighbors’ label distributions, with weights $1 - \epsilon$ and $\epsilon$, respectively. $\epsilon$ is a hyper-parameter for weighting the label
the supervision of node classification. An interpretation of

In this section, we analyze how our SALS method influences
vision signals with graph structural knowledge, which regular-
rizes GNNs to adapt to complex graph topology.

3.3 Discussion

SALS can be obtained by considering the cross entropy:

\[
H \left( q^{\text{SALS}}(c|i), p(c|i) \right) = 1 - \epsilon + (1 - \gamma) \sum_{j \in N(i)} H(q(c|j), p(c|i)) + (1 - \gamma) H(u,p)
\]

Thus, SALS is to add a group of losses \(\{H(q(c|j), p(c|i)), j \in N(i)\}\), which penalizes the deviation of predicted label distribution \(p(c|i)\) from the label distributions of neighbors. Note that this deviation could be equivalently captured by the KL divergence, which is a measure of how dissimilar the predicted distribution \(p(c|v)\) is to its neighbors’ label distributions. This is in accordance with the characteristics of the graph data. In a graph, edges represent the natural connectivity or relatedness between nodes [Hartuv and Shamir, 2000]. Motivated by this, we use the loss in Eq. (7) to encourage the nodes to have the final-layer representations that are closer to the class templates of their neighbors.

To intuitively understand the role of our SALS, we draw an analogy with a physical equilibrium model as shown in Fig. 3. Each node is seen as a particle, while the supervised classification signals act as the implicit force pulling the nodes away from the decision boundary. Without edges (Fig. 1(a)), nodes are loosely placed in the embedding space. In contrast, with message passing, edges act as the rubber bands and expose explicit constraints on the representations of connected nodes. In an ideal case where edges only connect nodes with the same label, the message passing will pull nodes within the same class together, which greatly benefits classification (Fig. 1(b)).

The connected nodes may have different class labels from each other. These edges pull the nodes of low \(r_y\), (see Eq. (3)) towards the decision boundaries (see Fig. 1(c)). If training with the hard targets, the nodes of lower \(r_y\) have larger losses and gradient magnitudes on the final layer, since these nodes are closer to the decision boundary than the nodes of higher \(r_y\). These gradients of higher magnitudes influence the updating of GNNs’ learnable weights more heavily during training. Enforcing the nodes of low \(r_y\)(i) to be far away from the decision boundary can lead to the over-confidence problem, and is hard to generalize to unseen nodes. This is meanwhile conflicted with the graphs’ characteristics that the

Figure 3: The message passing of GNNs reduce the embedding distances between the connected nodes. We compare the node embeddings retrieved by GNNs to a physical equilibrium mode, where edges connecting nodes serve as the rubber bands that expose explicit constraints to pull the connected nodes together.

Figure 4: Our SALS produces the soft targets for every node adaptable to graph structures. The structure-aware soft targets produced by SALS match the inductive bias of GNNs’ message passing that reduces the semantic distances between the connected nodes.
connected nodes are semantically close to each other. On the other hand, since the gradients on the nodes of lower $r_y(i)$ dominate the gradients for updating GNNs, the optimizer takes relatively lower efforts to form the discriminative representations for the nodes of higher $r_y(i)$. In contrast, with our SALS, the soft targets (see Eq. (5)) reflect the influence of neighbors in different classes. As a result, the gradient magnitudes of lower $r_y(i)$ are balanced with the nodes of higher $r_y(i)$. Moreover, if the number of nodes in class $c$ increases, the influence from the class $c$ improves, and our SALS’s soft can reflect this change with higher target probability on class $c$. These structure-aware soft targets align well with the prior knowledge of the graph structures. SALS matches the inductive bias of graph neural networks and can generalize to the unseen nodes in a better calibrated manner with more appropriate confidence targets (see Fig. 7). Overall, our soft targets correspond to the appropriate positions in the embedding space, which are adaptive to graph structures, and meanwhile maintain the correctness of classification.

4 Experiments

In this section, we evaluate the effectiveness of our SALS by applying it to various GNN architectures. We report the experimental results under both the transductive and inductive settings. In the transductive setting, the training phase has access to the features of all nodes but only the labels of nodes in the training set. In the inductive setting, neither the features nor labels of nodes in the validation/testing set are available during training. In addition, we visualize the learned representations of GNNs with SALS compared with those from the original GNNs without SALS. Last but not least, we conduct ablation studies to show the influence of SALS, as well as the sensitivity with respect to the hyper-parameters.

We use seven benchmark datasets: Cora, Citeseer, Pubmed [London and Getoor, 2014], CoraFull [Bojchevski and Günnemann, 2018], Coauthor-Physics (short as Coauthor-Phy) [Shchur et al., 2018], Flickr [McAuley and Leskovec, 2012], and Reddit [Zeng et al., 2019] for evaluation. The former three are citation networks, where each node is a document and each edge is a citation record. CoraFull is the larger version of the well-known citation network Cora dataset, where nodes represent publications and edges represent their citations, and the nodes are labeled based on the research topics. In Flickr, each node represents one image. An edge is built between two images if they share some common properties (e.g., same geographic location, same gallery, etc.). Reddit is collected from an online discussion forum where users comment on different topical communities. Two posts (nodes) are connected if some users comment on both posts. Each of them contains an unweighted adjacency matrix and bag-of-words features. The statistics of these datasets are summarized in Table 1.

![Table 1: Statistics of the datasets for node classification.]

| Dataset          | #Nodes | #Edges | #Classes |
|------------------|--------|--------|----------|
| Cora             | 2,708  | 5,429  | 7        |
| Citeseer         | 3,327  | 4,732  | 6        |
| Pubmed           | 19,717 | 44,338 | 3        |
| CoraFull         | 19,793 | 65,311 | 70       |
| Coauthor-Phy     | 34,493 | 247,962| 5        |
| Flickr           | 89,250 | 899,756| 7        |
| Reddit           | 232,965| 11,606,919| 41      |

4.1 Transductive Node Classification

In the transductive setting, we take the popular GNN models of GCN [Kipf and Welling, 2016], GAT [Veličković et al., 2017], JKNet [Xu et al., 2018], LGCN [Gao et al., 2018], GMNN [Qu et al., 2019], ResGCN [Li et al., 2019], the original label smoothing (LS), and the recently proposed Online Label Smoothing (OLS) for image classification [Zhang et al., 2021] as the baselines for comparison. We follow the prior studies [Xu et al., 2018] to split nodes in each graph into 60%, 20%, 20% for training, validation, and testing for a fair comparison. We make 10 random splits and conduct the experiments for 100 trials with random weight initialization for each split.

We vary the number of layers from 1 to 10 for each model and choose the best performing number with respect to the validation set. The results are reported in Table 2. We observe that SALS improves the test accuracy of GCN by 0.9% on Citeseer, 0.7% on Cora, 1.4% on Pubmed, 2.6% on CoraFull, 0.3% on Coauthor-Phy, and improves ResGCN by 0.6% on Citeseer, 0.7% on Cora, 0.9% on Pubmed, 2.7% on CoraFull, 0.5% on Coauthor-Phy respectively. As a result, SALS regularizes GCN and ResGCN to outperform all the baseline methods.

Taking a closer look, we find that given the same GNN model, SALS consistently produces larger improvements than LS and OLS. The advantages come from our structure-aware soft targets that utilize the structural information on label smoothing, while neither LS nor OLS utilizes the connectivity characteristics of the graph data for supervising GNNs. SALS regularizes GNNs to adapt to the complex topology for every node at different positions of the graph.

4.2 Inductive Node Classification

In the inductive settings, we follow the existing work to use the datasets Flickr, Reddit with the fixed partition for evaluation [Zeng et al., 2019; Frasca et al., 2020]. These datasets can be too large to be handled well by the full-batch training. Hence, existing work devises the advanced scalable GraphSAGE [Hamilton et al., 2017] and GraphSAINT [Zeng et al., 2019], and SIGN [Frasca et al., 2020] models to deal with the large-scale graphs. We take them as the baselines for comparison. We implement SALS with GraphSAGE, GraphSAINT, and SIGN to study whether SALS can improve the performance of GNNs under the inductive setting.
Table 2: Test Accuracy (%) of transductive node classification. We conduct 100 trials with random weight initialization. The mean and standard derivations are reported.

| Method                       | Citeseer    | Cora       | Pubmed     | CoraFull   | Coauthor-Phy |
|------------------------------|-------------|------------|------------|------------|---------------|
| GCN [Kipf and Welling, 2016] | 77.1 ± 1.4  | 88.3 ± 0.8 | 86.4 ± 1.1 | 64.5 ± 1.3 | 96.0 ± 0.5    |
| GAT [Veličković et al., 2017]| 76.3 ± 0.8  | 87.6 ± 0.5 | 85.7 ± 0.7 | 65.3 ± 0.9 | 96.2 ± 0.8    |
| JKNet [Xu et al., 2018]      | 78.1 ± 0.9  | 89.1 ± 1.2 | 86.9 ± 1.3 | 65.0 ± 1.1 | 95.1 ± 0.5    |
| LGCN [Gao et al., 2018]      | 77.5 ± 1.1  | 89.0 ± 1.2 | 86.5 ± 0.6 | 64.6 ± 1.0 | 95.4 ± 0.6    |
| GMNN [Qi et al., 2019]       | 77.4 ± 1.5  | 88.7 ± 0.8 | 86.7 ± 1.0 | 64.9 ± 1.1 | 95.6 ± 0.9    |
| ResGCN [Li et al., 2019]     | 77.9 ± 0.8  | 88.1 ± 0.6 | 87.1 ± 1.2 | 64.8 ± 1.2 | 95.3 ± 1.0    |
| GCN + LS [Szegedy et al., 2016]| 77.5 ± 1.3  | 88.5 ± 0.6 | 86.7 ± 0.6 | 64.9 ± 1.1 | 96.2 ± 0.5    |
| ResGCN + LS [Szegedy et al., 2016]| 78.1 ± 0.9  | 88.3 ± 0.7 | 87.2 ± 0.9 | 65.2 ± 1.3 | 95.6 ± 1.0    |
| GCN + OLS [Zhang et al., 2021]| 77.7 ± 1.1  | 88.6 ± 1.0 | 86.8 ± 0.7 | 65.0 ± 1.2 | 96.1 ± 0.7    |
| ResGCN + OLS [Zhang et al., 2021]| 78.2 ± 0.9  | 88.3 ± 0.6 | 87.3 ± 0.8 | 65.1 ± 1.1 | 95.4 ± 0.9    |
| GCN + SALS (Ours)            | 77.8 ± 1.0  | **88.9 ± 0.7** | 87.6 ± 0.6 | 66.2 ± 1.0 | **96.3 ± 0.4** |
| ResGCN + SALS (Ours)         | **78.4 ± 0.9** | 88.7 ± 0.7 | **87.9 ± 0.8** | **66.5 ± 1.1** | 95.8 ± 0.9 |

We vary the number of layers of each method from 1 to 10 for each model and choose the best performing model with respect to the validation set. The results are reported in Table 3. We observe that SALS improves the test accuracy of GraphSAGE by 2.0% on Flickr, 0.7% on Reddit, GraphSAINT by 1.6% on Flickr, 0.3% on Reddit, and SIGN by 1.6%, 0.3% on Reddit respectively. As a result, SALS enhances them to outperform the baseline methods.

Overall, the results above demonstrate the effectiveness of SALS to improve a wide range of GNN models in terms of both transductive and inductive node classification, and consistently outperforms LS and OLS.

### 4.3 Visualization and Ablation Study

We conduct a number of visualization and ablation studies to analyze our SALS. First, we investigate the distribution of the classification losses and the final-layer gradients on nodes of different $r_y(i)$. In Fig. 5, we sort the nodes in the training set by the ascending order of $r_y(i)$ as defined in Eq. (3), i.e., the ratio of neighbors that are in the same class as the target node. We train a 3-layer GCN with and without SALS on different datasets and record the node-wise classification losses and gradients after convergence. In Fig 5(a), we visualize the normalized accumulative classification loss (y-axis) versus the index of nodes in Citeseer in the ascending order of $r_y(i)$ (x-axis). (b) The average $\ell_2$-norm of gradients on the nodes in a bucket (y-axis) versus the index of node buckets in Pubmed in the ascending order of $r_y(i)$ (x-axis). Without our SALS, the nodes of lower $r_y(i)$ dominate the training losses and the gradients magnitudes, while our SALS balances the losses and gradients.

![Figure 5: The losses and gradient norms on nodes of different $r_y(i)$.](image)

(a) Accumulative Losses  
(b) Gradient Magnitudes
to the structure-aware soft targets. In this way, the nodes with lower $r_{y_i}(i)$ no longer dominate the weight updating of GNNs’ training, so that GNNs can be trained to form more discriminative representations for the nodes of higher $r_{y_i}(i)$.

Fig. 6 presents the learned representations obtained by a 3-layer GCN trained with hard targets and one with SALS, where we visualize the representations of the half of nodes in the Pubmed’s training set of higher $r_{y_i}(i)$. It is shown that the hidden layers supported by SALS learn more discriminative features, thanks to the regularization given by SALS. This meets our analysis in the Section 3.3 and observations from Fig. 5. The structure-aware soft targets produced by our SALS supervised GNNs to have more balanced gradient magnitudes on the nodes of different $r_{y_i}(i)$, which enables GNNs to take more efforts to learn more discriminative node representations than the original hard targets. These highly discriminative features potentially help produce better class predictions than less discriminative features.

Fig. 7 shows the 10-bin reliability diagram of a 3-layer GCN trained on Cora [Guo et al., 2017]. The grey dashed line represents perfect calibration where the output likelihood (confidence) perfectly predicts the accuracy. Without label smoothing, the model trained with hard targets is clearly over-confident, since in expectation the accuracy is always below the confidence. With our SALS, we observe that the reliability diagram slope is now much closer to a slope of 1 and the model is better calibrated than the original GCN and it with LS. This meets our analysis in Sec. 3.3, that the structure-aware soft targets correspond to suitable semantic positions that match the GNNs’ inductive bias. Our SALS smoothens the targets to make the labels of connected nodes correlated, which aligns better with the characteristics of graph data than the hard targets, LS, and OLS.

Last but not least, we evaluate how sensitive our SALS is to the hyper-parameters: $\epsilon$ that controls effects of label smoothing, and $\gamma$ that balances the neighborhood label and the pre-defined uniform distribution. We visualize the results in Fig. 8. The performance of GNNs with SALS is generally smooth when parameters are in different ranges. However, too small values of $\epsilon$ and $\gamma$ result in low performances, which should be avoided in practice. Moreover, increasing $\epsilon$ from 0.1 to 0.3 and $\gamma$ from 0.5 to 0.7 improves the effectiveness of SALS on all datasets, demonstrating that the label smoothing guided by graph structures plays an important role in improving the performance of GNNs.

5 Conclusion
In this work, we propose Structure-aware Label Smoothing (SALS) as an enhancement component to popular node classification models. SALS can capture the prior knowledge about the graph structures for supervising the label distributions. It produces structure-aware soft targets for every node in an adaptive manner. Experiments on seven benchmark datasets proved our SALS’s enhancement on various models for both transductive and inductive node classification. Specifically, SALS reduces the over-fitting and calibration errors of GCN models, which uses the graph structural knowledge to enrich the label distribution. An interesting future direction is to extend our methods to other modalities such as text and images, where we can construct graph topology in the semantic space and extend our SALS to learn better label distributions.

References
[Bojchevski and Günnewinn, 2018] Aleksandar Bojchevski and Stephan Günnewinn. Deep gaussian embedding of graphs: Unsupervised inductive learning via ranking, 2018.
[Bruna et al., 2013] Joan Bruna, Wojciech Zaremba, Arthur Szlam, and Yann LeCun. Spectral networks and locally connected networks on graphs. *arXiv preprint arXiv:1312.6203*, 2013.

[Chiang et al., 2019] Wei-Lin Chiang, Xuanqing Liu, Si Si, Yang Li, Samy Bengio, and Cho-Jui Hsieh. Cluster-gcn: An efficient algorithm for training deep and large graph convolutional networks. In *Proceedings of the 25th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining*, pages 257–266, 2019.

[Chorowski and Jaitly, 2016] Jan Chorowski and Navdeep Jaitly. Towards better decoding and language model integration in sequence to sequence models, 2016.

[Frasca et al., 2020] Fabrizio Frasca, Emanuele Rossi, Davide Eynard, Ben Chamberlain, Michael Bronstein, and Federico Monti. Sign: Scalable inception graph neural networks. *arXiv preprint arXiv:2004.11198*, 2020.

[Gao et al., 2018] Hongyang Gao, Zhengyang Wang, and Shuiwang Ji. Large-scale learnable graph convolutional networks. In *Proceedings of the 24th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining*, pages 1416–1424, 2018.

[Guo et al., 2017] Chuan Guo, Geoff Pleiss, Yu Sun, and Kilian Q Weinberger. On calibration of modern neural networks. In *Proceedings of the 34th International Conference on Machine Learning-Volume 70*, pages 1321–1330. JMLR. org, 2017.

[Hamilton et al., 2017] Will Hamilton, Zhitao Ying, and Jure Leskovec. Inductive representation learning on large graphs. In *Advances in neural information processing systems*, pages 1024–1034, 2017.

[Haonan et al., 2019] Lu Haonan, Seth H Huang, Tian Ye, and Guo Xiuyan. Graph star net for generalized multi-task learning. *arXiv preprint arXiv:1906.12330*, 2019.

[Hartuv and Shamir, 2000] Erez Hartuv and Ron Shamir. A clustering algorithm based on graph connectivity. *Information processing letters*, 76(4-6):175–181, 2000.

[Kearnes et al., 2016] Steven Kearnes, Kevin McCloskey, Marc Berndl, Vijay Pande, and Patrick Riley. Molecular graph convolutions: moving beyond fingerprints. *Journal of computer-aided molecular design*, 30(8):595–608, 2016.

[Kipf and Welling, 2016] Thomas N Kipf and Max Welling. Semi-supervised classification with graph convolutional networks. *arXiv preprint arXiv:1609.02907*, 2016.

[Li et al., 2019] Guohao Li, Matthias Müller, Ali Thabet, and Bernard Ghanem. Deepgcns: Can gcns go as deep as cnns? *arXiv preprint arXiv:1904.03751*, 2019.

[London and Getoor, 2014] Ben London and Lise Getoor. Collective classification of network data. *Data Classification: Algorithms and Applications*, 399, 2014.

[Mathur et al., 1997] Lynette Knowles Mathur, Ike Mathur, and Nanda Rangan. The wealth effects associated with a celebrity endorser: The michael jordan phenomenon. *Journal of Advertising research*, 37(3):67–74, 1997.

[McAuley and Leskovec, 2012] Julian McAuley and Jure Leskovec. Image labeling on a network: using social-network metadata for image classification. In *European conference on computer vision*, pages 828–841. Springer, 2012.

[Müller et al., 2019] Rafael Müller, Simon Kornblith, and Geoffrey E Hinton. When does label smoothing help? In *Advances in Neural Information Processing Systems*, pages 4696–4705, 2019.

[Qu et al., 2019] Meng Qu, Yoshua Bengio, and Jian Tang. Gmn: Graph markov neural networks. *arXiv preprint arXiv:1905.06214*, 2019.

[Rong et al., 2019] Yu Rong, Wenbing Huang, Tingyang Xu, and Junzhou Huang. Dropedge: Towards deep graph convolutional networks on node classification. In *International Conference on Learning Representations*, 2019.

[Schlichtkrull et al., 2018] Michael Schlichtkrull, Thomas N Kipf, Peter Bloem, Rianne Van Den Berg, Ivan Titov, and Max Welling. Modeling relational data with graph convolutional networks. In *European Semantic Web Conference*, pages 593–607. Springer, 2018.

[Shchur et al., 2018] Oleksandr Shchur, Maximilian Mumme, Aleksandar Bojchevski, and Stephan Günnemann. Pitfalls of graph neural network evaluation. *arXiv preprint arXiv:1811.05868*, 2018.

[Szegedy et al., 2016] Christian Szegedy, Vincent Vanhoucke, Sergey Ioffe, Jon Shlens, and Zbigniew Wojna. Rethinking the inception architecture for computer vision. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pages 2818–2826, 2016.

[Vaswani et al., 2017] Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N. Gomez, Łukasz Kaiser, and Illia Polosukhin. Attention is all you need. In *Proceedings of the 31st International Conference on Neural Information Processing Systems*, NIPS’17, page 6000–6010, Red Hook, NY, USA, 2017. Curran Associates Inc.

[Velicković et al., 2017] Petar Velicković, Guillem Cucurull, Arantxa Casanova, Adriana Romero, Pietro Lio, and Yoshua Bengio. Graph attention networks. *arXiv preprint arXiv:1710.10903*, 2017.

[Wang and Leskovec, 2020] Hongwei Wang and Jure Leskovec. Unifying graph convolutional neural networks and label propagation. *arXiv preprint arXiv:2002.06755*, 2020.

[Wu et al., 2019] Zonghan Wu, Shirui Pan, Fengwen Chen, Guodong Long, Chengqi Zhang, and Philip S Yu. A comprehensive survey on graph neural networks. *arXiv preprint arXiv:1901.00596*, 2019.

[Xu et al., 2018] Keyulu Xu, Chengtao Li, Yonglong Tian, Tomohiro Sonobe, Ken-ichi Kawarabayashi, and Stefanie Jegelka. Representation learning on graphs with jumping knowledge networks. *arXiv preprint arXiv:1806.05356*, 2018.
[Zeng et al., 2019] Hanqing Zeng, Hongkuan Zhou, Ajitesh Srivastava, Rajgopal Kannan, and Viktor Prasanna. Graphsaint: Graph sampling based inductive learning method. *arXiv preprint arXiv:1907.04931*, 2019.

[Zhang et al., 2018] Jiani Zhang, Xingjian Shi, Junyuan Xie, Hao Ma, Irwin King, and Dit-Yan Yeung. Gaan: Gated attention networks for learning on large and spatiotemporal graphs. *arXiv preprint arXiv:1803.07294*, 2018.

[Zhang et al., 2021] Chang-Bin Zhang, Peng-Tao Jiang, Qibin Hou, Yunchao Wei, Qi Han, Zhen Li, and Ming-Ming Cheng. Delving deep into label smoothing. *IEEE Transactions on Image Processing*, 30:5984–5996, 2021.

[Zhou et al., 2018] Jie Zhou, Ganqu Cui, Zhengyan Zhang, Cheng Yang, Zhiyuan Liu, Lifeng Wang, Changcheng Li, and Maosong Sun. Graph neural networks: A review of methods and applications. *arXiv preprint arXiv:1812.08434*, 2018.

[Zhuang and Ma, 2018] Chenyi Zhuang and Qiang Ma. Dual graph convolutional networks for graph-based semi-supervised classification. In *Proceedings of the 2018 World Wide Web Conference*, pages 499–508, 2018.

[Zoph et al., 2018] Barret Zoph, Vijay Vasudevan, Jonathon Shlens, and Quoc V. Le. Learning transferable architectures for scalable image recognition. In *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition (CVPR)*, June 2018.