Effective Semi-Supervised Node Classification on Few-Labeled Graph Data

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ABSTRACT

Graph neural networks (GNNs) are designed for semi-supervised node classification on graphs where only a small subset of nodes have class labels. However, under extreme cases when very few labels are available (e.g., 1 labeled node per class), GNNs suffer from severe result quality degradation. Several existing studies make an initial effort to ease this situation, but are still far from satisfactory.

In this paper, on few-labeled graph data, we propose an effective framework ABN that is readily applicable to both shallow and deep GNN architectures and significantly boosts classification accuracy. In particular, on a benchmark dataset Cora with only 1 labeled node per class, while the classic graph convolutional network (GCN) only has 44.6% accuracy, an immediate instantiation of ABN over GCN achieves 62.5% accuracy; when applied to a deep architecture Dagnn, ABN improves accuracy from 59.8% to 66.4%, which is state of the art.

ABN obtains superior performance through three main algorithmic designs. First, it selects high-quality unlabeled nodes via an adaptive pseudo labeling technique, so as to adaptively enhance the training process of GNNs. Second, ABN balances the labels of the selected nodes on real-world skewed graph data by pseudo label balancing. Finally, a negative sampling regularizer is designed for ABN to further utilize the unlabeled nodes. The effectiveness of the three techniques in ABN is well-validated by both theoretical and empirical analysis. Extensive experiments, comparing 12 existing approaches on 4 benchmark datasets, demonstrate that ABN achieves state-of-the-art performance.

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1 INTRODUCTION

Graph is an expressive data model, representing objects and the relationships between objects as nodes and edges respectively. Graph data are ubiquitous with a wide range of real-world applications, e.g., social network analysis [28, 37], traffic network prediction [16, 29], protein interface prediction [12], recommendation systems [10, 47]. Among these applications, an important task is to classify the nodes in a graph into various classes. However, one tough situation commonly existing is the lack of labeled data, which are also expensive to collect.

To ease the situation, semi-supervised node classification on graphs has attracted much attention from both industry [28, 37] and academia [8, 17, 25, 30, 31, 42]. It aims to leverage a small amount of labeled nodes and additionally a large amount of unlabeled nodes in a graph to train an accurate classifier. Semi-supervised node classification can be framed under the graph-based semi-supervised learning paradigm. Graph convolution networks (GCNs) [24] and their variants [17, 25, 31, 32, 42] are representative solutions under this paradigm. GCNs rely on a message passing scheme called graph convolution that aggregates the neighborhood information of a node, including node features and graph topology, to learn node representations, which can then be used in downstream classification tasks.

Despite the great success of GCNs, under the extreme cases when very few labels are given (e.g., only one labeled node per class), the shallow GCN architecture, typically with two layers [24], cannot effectively propagate the training labels over the input graph, leading to inferior performance. In particular, as shown in our experiments, on a benchmark dataset Cora with 1 labeled node per class, GCN is even less accurate than unsupervised methods, such as DGI [43] and G2G [1]. Recently, several latest studies try to improve accuracy by designing deeper GNNs, e.g., DGGNN and APPNP [25, 31], which also address the over-smoothing issue identified in [5, 30, 46]. However, these deep GNNs are still not directly designed to tackle the scarcity of labeled data, especially when only very few labels are available.

On the other hand, there exist initial efforts to handle insufficient labeled data. Pseudo Labeling [26] assigns a pseudo label to each unlabeled node based on the node’s highest probability to belong to a certain class (i.e., confidence) during the training process of GCNs [24]. Self-Training enlarges training set by adding top-$K$
high-confidence unlabeled nodes [30]. Although these methods can improve the performance, we conduct a thorough analysis with empirical insights in Section 3, revealing that Pseudo Labeling and Self-Training are not adaptive and inflexible to the dynamic changes of confidence scores at different training iterations, and are not able to handle imbalanced labels on real-world skewed graph data.

Facing the challenges of semi-supervised node classification on few-labeled graph data, we propose ABN, an effective framework that is readily applicable to both shallow and deep GNNs, e.g., GCN and DAGNN, and significantly boosts classification accuracy. Figure 1 shows a brief result of ABN applied over GCN and DAGNN, dubbed as ABN$_G$ and ABN$_D$, respectively, when varying the number of labeled nodes per class in $\{1, 3, 5, 10, 20\}$ on Cora dataset. Observe that ABN$_G$ and ABN$_D$ are much more accurate than their respective base GNN models, demonstrating the effectiveness of ABN framework. Specifically, with only 1 labeled node per class, ABN$_G$ achieves 62.5% accuracy while that of GCN is only 44.6%, and compared to DAGNN (59.8%), ABN$_D$ improves accuracy to 66.4%.

ABN achieves superior performance through three main techniques: adaptive pseudo labeling, pseudo label balancing, and negative sampling regularization. Adaptive pseudo labeling selects high-confidence unlabeled nodes according to a confidence distribution per training epoch, so as to adapt to the dynamic training process, and then ABN balances the importance of the selected nodes in gradient descent. Finally, in order to further utilize the unlabeled data, a negative sampling regularization technique is designed to enhance the training process. Extensive experiments, using 4 real datasets and comparing against 12 existing solutions, demonstrate that ABN consistently obtains high classification accuracy for semi-supervised node classification on few-labeled graphs.

Summing up, our contributions in this paper are as follows:

- We conduct both empirical and theoretical analysis of semi-supervised node classification problem on graphs with few-labeled nodes, discover important insights, and uncover deficiencies of existing solutions.
- We propose an effective framework ABN with three techniques, namely adaptive pseudo labeling, pseudo label balancing, and negative sampling regularization.
- We apply ABN over both shallow and deep GNN architectures, and achieve state-of-the-art performance.
- We conduct extensive experiments on 4 benchmark datasets and compare ABN with 12 existing solutions, to evaluate the superior performance of ABN.

The rest of the paper is organized as follows. In Section 2, we introduce the semi-supervised node classification problem and explain the most relevant existing solutions. We conduct empirical and theoretical analysis in Section 3, revealing the deficiencies of existing solutions. We present the ABN framework with three techniques in Section 4. Experiments are reported in Section 5. We further review other related work in Section 6. Finally, Section 7 concludes the paper. Appendix consists of proofs and details for reproducibility.

2 PRELIMINARIES

2.1 Problem Formulation

Let $G = (V, E, X)$ be a graph consisting of a node set $V$ with cardinality $n$, a set of edges $E$ of size $m$, each connecting two nodes in $V$, a feature matrix $X \in \mathbb{R}^{n \times d}$, where $d$ is the number of features in $G$. For every node $v_i \in V$, it has a feature vector $X_i \in \mathbb{R}^d$, where $X_i$ is the $i$-th row of $X$. Let $c$ be the number of classes in $G$. We use $L$ to denote the set of labeled nodes, and obviously $L \subseteq V$. Let $U$ be the set of unlabeled nodes and $U' = V \setminus L$. Each labeled node $v_i \in L$ has a one-hot vector $Y_i \in \{0, 1\}^c$, indicating the class label of $v_i$. A high-level definition of the semi-supervised node classification problem is as follows.

DEFINITION 1. Given a graph $G = (V, E, X)$, a set of labeled nodes $L \subseteq V$, and a class label $Y_i \in \{0, 1\}^c$ per node $v_i \in L$, assuming that each node belongs to exactly one class, Semi-Supervised Node Classification predicts the labels of the unlabeled nodes.

In particular, the aim is to leverage the graph $G$ with the labeled nodes in $L$, and to train a forward predicting classification model/function $f(G, \theta)$ that takes as input the graph $G$ and a set of trainable parameters $\theta$. The output of $f$ is a matrix $F \in \mathbb{R}^{n \times c}$, with each $i$-th row $F_i \in [0, 1]^c$ representing the output probability vector of node $v_i \in V$ (the 1-norm of $F_i$ is normalized to 1). Supposing that $j = \arg \max_{j'} F_{i,j'}$, we say that, with confidence $F_{i,j}$, node $v_i$ has class label $C_j$: i.e., the largest element $F_{i,j}$ in vector $F_i$ is called the confidence of node $v_i$.

We adopt the widely used cross-entropy loss as objective function. For a node $v_i$, its loss of $F_i$ with respect to its class label $Y_i$, $L(Y_i, F_i)$, is defined as follows.

$$L(Y_i, F_i) = -\sum_{j=1}^{c} Y_{i,j} \log(F_{i,j})$$

where $Y_{i,j}$ is the $j$-th value in $Y_i$ and $F_{i,j}$ is the $j$-th value in $F_i$.

2.2 Related Work

Observe that, in practice, the labeled nodes are few, i.e., $|L| \ll |U|$. In literature, there are two directions to address the scarcity of labeled data for semi-supervised node classification: (i) explore multi-hop graph topological features to propagate the labels in $L$ over the input graph, e.g., GCN [24] and DAGNN [31]; (ii) enhance labeled set $L$ by Pseudo Labeling [26] or Self-Training [30] over unlabeled set $U$. Note that these two directions are not mutually

![Figure 1: Node classification performance on Cora.](image-url)
where we review the existing studies that are most relevant to this paper.

GCN. GCN [24] is a graph neural network model for semi-supervised classification. GCN learns the representation of each node by iteratively aggregating the representations of its neighbors. Specifically, GCN consists of $k > 0$ layers, each with the same propagation rule defined as follows. At the $t$-th layer, the hidden representations $H^{(t)}$ of previous layer are aggregated to get $H^{(t)}$.

$$
H^{(t)} = \sigma(\hat{A}(H^{(t-1)}W^{(t)}), t = 1, 2, \ldots, k.
$$

$\hat{A} = \hat{D}^{-\frac{1}{2}} \hat{A} \hat{D}^{-\frac{1}{2}}$ is the graph laplacian, where $\hat{A} = A + I$ is the adjacency matrix of $G$ after adding self-loops (I is the identity matrix) and $\hat{D}$ is a diagonal matrix with $D_{ii} = \sum_j \hat{A}_{ij}$. $W^{(t)}$ is a trainable weight matrix of the $t$-th layer, and $\sigma$ is a nonlinear activation function. Initially, $H^{(0)} = X$. $H^{(k)}$ is the output $F$. Note that GCN usually achieves superior performance with 1-layer or 2-layer models [24]. When applying multiple layers to leverage large receptive fields, the performance degrades severely, due to the over-smoothing issue identified in [5, 30, 46].

DAGNN. A recent deep GNN architecture, DAGNN, tackles the over-smoothing issue and achieves state-of-the-art results by decoupling representation transformation and propagation in GNNs [31]. Then it utilizes an adaptive adjustment mechanism to balance the information from local and global neighborhoods of each node. Specifically, the mathematical expression of DAGNN is as follows. DAGNN uses a learnable parameter $s \in \mathbb{R}^{c \times 1}$ to adjust the weight of embeddings at different propagation level (from 1 to $k$).

$$
Z = \text{MLP}(X) \in \mathbb{R}^{nc}
$$

$$
H_{f} = \hat{A}^{f} \cdot Z \in \mathbb{R}^{nc}, f = 1, 2, \ldots, k
$$

$$
S_{f} = H_{f} \cdot s \in \mathbb{R}^{nc}, f = 1, 2, \ldots, k
$$

$$
\hat{S}_{f} = [\hat{S}_{f}, \hat{S}_{f}, \ldots, \hat{S}_{f}] \in \mathbb{R}^{nc}, f = 1, 2, \ldots, k
$$

$$
X_{\text{out}} = \text{softmax}(I_{f=1}^{k} H_{f} \odot \hat{S}_{f}),
$$

where $\hat{A}^{f}$ is the $f$-th power of matrix $\hat{A}$, $\odot$ is the Hadamard product, $\cdot$ is dot product, MLP is the Multilayer Perceptron and softmax operation is on the second dimension.

Pseudo Labeling. Pseudo Labeling assigns to each node in $\mathcal{U}$ a pseudo label based on the confidence of node $v_i$ over $F_i$ [26]. In particular, the pseudo label $\hat{Y}_i$ of node $v_i$ in $\mathcal{U}$ is as follows. If $F_{i,j}$ is the largest element in vector $F_i$, $\hat{Y}_{i,j}$ is 1, otherwise, 0.

$$
\hat{Y}_{i,j} = \begin{cases} 1 & \text{if } j = \arg \max_{j^{'}} F_{i,j^{'}}, \\ 0 & \text{otherwise}. \end{cases}
$$

Then Pseudo Labeling considers a pseudo loss $L_{ps}$ that consists of the loss of labeled nodes in $\mathcal{L}$ and the loss of all nodes in $\mathcal{U}$ with their pseudo labels as follows.

$$
L_{ps} = \frac{1}{|\mathcal{L}|} \sum_{v_i \in \mathcal{L}} L(Y_i, F_i) + \frac{\lambda}{|\mathcal{U}|} \sum_{v_i \in \mathcal{U}} L(Y_i, F_i),
$$

where $\lambda \in \mathbb{R}$ is a hyper-parameter controlling the weight of pseudo labels in the loss function.

Self-Training. Self-Training picks the top-$K$ nodes with the highest confidence in $\mathcal{U}$ and adds them with their predicted labels into labeled set $\mathcal{L}$ to extend $\mathcal{L}$ [19, 22, 34, 38, 49]. Then in the following iterations, the classifier will be trained from the extended labeled set. In literature, there are several studies on Self-Training, such as Co-Training which co-trains a GCN with a random walk model [7, 30], M3S [40] which utilizes DeepCluster technique to refine the selected pseudo labels.

3 ANALYSIS

We first conduct an empirical analysis to identify the issues of existing techniques, specifically Pseudo Labeling and Self-Training. Then we theoretically analyze these issues from the perspective of transductive learning and gradient descent. The analysis motivates the design of our ABN framework in Section 4.

3.1 Empirical Analysis

In the following, we show that (i) Pseudo Labeling and Self-Training are not adaptive to the distributions of confidence scores at various training iterations, and (ii) they are not able to handle imbalanced pseudo labels on real-world graphs that are often skewed [27]. These issues may degrade the performance of the learned classifier.

In Figures 2a, 2b, and 2c, we illustrate the distributions of the confidence scores of all nodes in unlabeled set $\mathcal{U}$ on Cora with only 1 label per class, at early (20-th), middle (100-th), and late (500-th) epochs, respectively. Observe that the number of high-confidence nodes increases gradually at middle and late epochs as in Figures 2b and 2c. At the early epoch in Figure 2a, 95.4% of the unlabeled nodes are with very low confidence (< 0.2).
where $U \lesiota (V)$ is the uniform distribution over node set $V$.

First, recall that Pseudo Labeling assigns a label to every node $v_i$ in $UU$, no matter whether the confidence of $v_i$ is actually low or high. This may lead to low-quality training process, at the early epochs when most of the confidence scores are small, which is exactly the case in Figure 2a, where 95.4% of the nodes have confidence below 0.2. Low-quality pseudo labels at early epochs will severely influence the training of later epochs, resulting to unexpected performance degradation. Self-Training, which picks the top-$K$ high-confidence nodes in $UU$ to extend labeled set $L$, suffers from the same issue at early epochs. In particular, for a fixed $K$ parameter, at early epochs in Figure 2a, there exist rarely any high-confidence nodes, but Self-Training still has to select top-$K$ nodes even with low confidence. Even worse, in Self-Training, such low-confidence nodes added at early epochs are never moved out from $L$ [40]. Further, at the 500-th epoch in Figure 2c, when there are 28.6% nodes with 0.9 or even higher confidence, Self-Training with top-$K$ selection may not be able to add all such high-confidence nodes for training.

Second, Figure 3b shows the distribution of the pseudo labels of the nodes in $UU$ at the 20-th epoch on Cora dataset with 7 classes. Obviously the distribution of pseudo labels is highly imbalanced, i.e., 92.4% of the nodes are with class 1 and 6.6% with class 4. The imbalanced classes (i.e., class 1 in Figure 3b) will heavily affect the direction of gradient descent during the training process. If too many low-confidence nodes are wrongly assigned to a single class at early epochs, Pseudo Labeling and Self-Training will suffer from such imbalanced distribution and result to inferior performance.

### 3.2 Theoretical Analysis

The semi-supervised node classification problem studied in this paper naturally fits the transductive learning setting, since all labeled and unlabeled data in the input graph $G$ are known and no more new data will be added [9, 24]. In the following, we analyze the problem from the perspective of gradient descent, to theoretically explain the issues discovered in Section 3.1.

Under the ideal case where we have the labels of all nodes in $VV$ (the population), given a classifier $f(G, \theta)$ with output probability vectors $F_i$ for all nodes $v_i \in V$, the population loss $L_{pop}$ is computed as follows. Ideally, the objective is to minimize $L_{pop}$ by evaluating population gradient $\nabla \theta L_{pop}$, and find optimal parameters $\theta^*$. However, in practice, due to the scarcity of labeled data (i.e., $|L| \ll |V|$), it is impossible to directly evaluate $\nabla \theta L_{pop}$. Therefore, as introduced in Eq. (3), Pseudo Labeling approximates population loss $L_{pop}$ by pseudo loss $L_{pse}$ with the consideration of both labeled nodes and unlabeled nodes (pseudo labels). In other words, it uses pseudo gradient $\nabla \theta L_{pse}$ to approximate $\nabla \theta L_{pop}$, so as to minimize the loss, which is a common technique in literature [14, 33].

We rewrite pseudo loss in Eq. (3) as in Eq. (4), and write its gradient $\nabla \theta L_{pse}$ in Eq. (5).

$$L_{pse} = E_{UU \cap L}(L(Y_i, F_i)) + \lambda \cdot E_{U \cap U}(L(\hat{Y}_i, F_i)),$$  

$$\nabla \theta L_{pse} = E_{UU \cap L}(\nabla \theta L(Y_i, F_i)) + \lambda \cdot E_{U \cap U}(\nabla \theta L(\hat{Y}_i, F_i)).$$

where $U(L)$ and $U(U)$ are the uniform distributions over labeled node set $L$ and unlabeled node set $U$, respectively.

In a similar way, the population gradient $\nabla \theta L_{pop}$ is as follows. Note that we break $V$ into $L$ and $U$.

$$\nabla \theta L_{pop} = E_{UU \cap L}(\nabla \theta L(Y_i, F_i)) = \frac{|L|}{|V|} E_{UU \cap L}(\nabla \theta L(Y_i, F_i)) + \frac{|U|}{|V|} E_{U \cap U}(\nabla \theta L(\hat{Y}_i, F_i)).$$

Then, we derive a bound of the difference between $\nabla \theta L_{pop}$ and $\nabla \theta L_{pse}$ in Eq. (6). Specifically, let $\lambda = \frac{|U|}{|L|}$, and assume that any gradient satisfies a bounded norm (i.e., $\|\nabla \theta L\| \leq \Theta$, for any loss $L$), which is a common assumption in the analysis of gradient descent [51]. Then the difference between $\nabla \theta L_{pop}$ and $\nabla \theta L_{pse}$ is bounded as follows. The proof of Eq. (6) is in Appendix A.1.

$$\left\| \nabla \theta L_{pop} - \frac{|V|}{|L|} \nabla \theta L_{pse} \right\| \leq \frac{|U|}{|L|} \cdot E_{U \cap U}(\nabla \theta L(\hat{Y}_i, F_i) - \nabla \theta L(Y_i, F_i)) \leq |U| \cdot P_{\hat{U} \cap U}(\hat{Y}_i \neq Y_i) \cdot E_{U \cap U}(\left\| \nabla \theta L(\hat{Y}_i, F_i) - \nabla \theta L(Y_i, F_i) \right\|) \leq 2\Theta|U| \cdot P_{\hat{U} \cap U}(\hat{Y}_i \neq Y_i).$$

where $P_{\hat{U} \cap U}(\hat{Y}_i \neq Y_i)$ is the probability that a randomly sampled node $v_i \in U$ has a wrongly predicted label.

Obviously, $P_{\hat{U} \cap U}(\hat{Y}_i \neq Y_i)$ is exactly the classification error on unlabeled set $U$. Observe that the bound at the last line in Eq. (6) mainly relies on the quality of pseudo labels $Y_i$ of nodes $v_i \in U$. In other words, if we have low-quality pseudo labels from $U$, then $P_{\hat{U} \cap U}(\hat{Y}_i \neq Y_i)$ tends to be large, leading to a large difference between $\nabla \theta L_{pop}$ and $\nabla \theta L_{pse}$ and consequently resulting to suboptimal performance. This situation is likely to happen at the early epochs when most nodes have low confidence, but are still assigned with pseudo labels by Pseudo Labeling or chosen by Self-Training, as we have analyzed in Section 3.1. Moreover, at the early epochs when most nodes are with low confidence, the imbalance of pseudo labels may make $P_{\hat{U} \cap U}(\hat{Y}_i \neq Y_i)$ even larger, further hampering the training process.
4 THE ABN FRAMEWORK

In this section, we present ABN that addresses the issues identified in Section 3. In a nutshell, ABN develops new gradient formula to be used in the training process and consists of three techniques, namely, adaptive pseudo labeling in Section 4.1, pseudo label balancing in Section 4.2, and negative sampling regularization in Section 4.3. We present the overall ABN framework in Section 4.4.

4.1 Adaptive Pseudo Labeling

First, intuitively, nodes with higher confidence tend to be predicted more accurately, meaning that if a framework selects more nodes with high confidence into the training process, it tends to be more accurate. We verify this assumption in Figure 3a, which shows the positive correlation between confidence and accuracy per confidence interval. For each confidence interval (x-axis), we report the percentage of nodes with pseudo labels same as ground-truth labels (y-axis). Second, a new pseudo labeling technique should be adaptive to the evolving of confidence distribution per epoch as shown in Figure 2.

To achieve the above goals, we propose adaptive pseudo labeling that only assigns labels to high-confidence unlabeled nodes per epoch, so as to reduce the effect of pseudo-labeling with low-confidence nodes in the training process. Specifically, at current epoch, only unlabeled nodes with confidence larger than a threshold  \( \beta \) are assigned with an adaptive pseudo label  \( \hat{Y}_i \) as in Eq. (7). Note that  \( \hat{Y}_i \) in Eq. (7) and  \( \hat{Y}_i \) in Eq. (2) have a similar but vital difference: for any node  \( v_i \in \mathcal{U} \),  \( \hat{Y}_i \) can be a zero vector, meaning that  \( v_i \) has too low confidence (\(< \beta\)) to earn a label at current epoch, while  \( \hat{Y}_i \) always has a 1-element regardless of its confidence. From now on, we refer to  \( \hat{Y}_i \) as the adaptive pseudo label of  \( v_i \), and  \( \hat{Y}_i \) as the pseudo label of  \( v_i \).

\[
\hat{Y}_{l,j} = \begin{cases} 
1 & \text{if } j = \arg \max_{j'} F_{i,j'} \text{ and } F_{i,j} \geq \beta, \\
0 & \text{otherwise},
\end{cases} 
\]  

(7)

where  \( \beta \in (0, 1) \) is a confidence threshold.

At each epoch, we generate a new adaptive pseudo-labeled set with nonzero  \( \hat{Y}_i \),  \( \mathcal{U}' \subseteq \mathcal{U} \), based on the confidence distribution of current epoch and Eq. (7), to facilitate the computation of pseudo gradient at current epoch. A node that had confidence larger than  \( \beta \) in previous epochs is not guaranteed to be in the  \( \mathcal{U}' \) of current epoch if its confidence is changed below  \( \beta \). Note that there is a trade-off: if  \( \beta \) is too large, though the selected nodes are with high confidence, but the number of nodes that contribute to the training process is small; if  \( \beta \) is too small, too many low-confidence nodes will be selected into the training process. We experimentally evaluate the choice of  \( \beta \) in Section 5.5.

Discussion. Compared with Pseudo Labeling that assigns a pseudo label  \( Y_i \) to every node  \( v_i \) in  \( \mathcal{U} \) regardless of confidence level, we only assign adaptive pseudo labels  \( \hat{Y}_i \) to nodes with high confidence and generate a new adaptive pseudo-labeled set  \( \mathcal{U}' \) per epoch.  \( \mathcal{U}' \) changes in a way adaptive to the confidence distribution per epoch. Each unlabeled node earns its adaptive pseudo label  \( \hat{Y}_i \) per epoch by its current confidence. But Self-Training has a fixed top-\( K \) parameter to add unlabeled nodes into training and never move such nodes out even if they are with low confidence later.

4.2 Pseudo Label Balancing

Figure 3b illustrates pseudo label imbalance at early epochs. Initially, while the confidence of all unlabeled nodes is low (shown in Figure 2a), if too many unlabeled nodes are rashly assigned to a class, this will severely influence the search direction of gradient descent.

Inspired by classic class-reweight techniques [18, 21], we design a pseudo label balancing technique to ease the situation. In a nutshell, at each epoch, after pseudo-labeling by Eq. (2), if a pseudo-labeled node  \( v_i \) belongs to a class with  \( N_i \) pseudo-labeled nodes, we reduce the importance of  \( v_i \) in gradient descent by a factor of  \( \frac{1}{N_i} \). Specifically, the pseudo gradient update formula by considering adaptive pseudo labeling and pseudo label balancing is in Eq. (8).

\[
\nabla_{\theta} L_{\text{pse}} = \frac{1}{|L|} \sum_{v_i \in L} \nabla_{\theta} L(Y_i, F_i) + \lambda \cdot \frac{1}{n_i} \sum_{v_i \in U'} \nabla_{\theta} L(\hat{Y}_i, F_i),
\]

(8)

4.3 Negative Sampling Regularization

Under extreme cases with very few labeled nodes (e.g., 1 labeled node per class), we further design a negative sampling regularization technique to utilize the input graph for training. Negative sampling is widely used in unsupervised learning, such as network embedding [48]. Intuitively, the embedding of a node  \( v \) should be distant to the embedding of another node  \( u \) if these two nodes are faraway on the input graph  \( G \) [43, 48].

For semi-supervised node classification, we apply negative sampling over labels instead of embeddings. Specifically, a positive sample is a node  \( v_i \) in  \( L \) or  \( U' \). We sample a set  \( \mathcal{I} \) of positive samples from  \( L \cup U' \) uniformly at random. The negative samples of a positive sample  \( v_i \) are the nodes that are not directly connected to  \( v_i \) in graph  \( G \). For each positive sample  \( v_i \) in  \( I \), we sample a fixed-size set  \( J_i \) of negative samples uniformly at random.

For a positive-negative pair  \( (v_i, v_j) \), compared with the  \( Y_i \) (or  \( \hat{Y}_i \)) of  \( v_i \in \mathcal{L} \cup \mathcal{U}' \), the intention is to let the output vector  \( F_j \) of  \( v_j \) to be as different as possible. Here, without ambiguity, we abuse the symbol  \( \hat{Y}_i \) and use it to represent the adaptive pseudo label or ground-truth label of node  \( v_i \). Denote  \( I \) as the all-one vector in  \( \mathbb{R}^t \). Then we have the following loss of all positive-negative pairs.

\[
L_{\text{neg}} = \frac{1}{|I| - |J_i|} \sum_{v_i \in I} \sum_{v_j \in J_i} L(\hat{Y}_i, 1 - F_j)
\]

(9)

4.4 Put Things Together

In summary, by Eq. (8) and Eq. (9), we compute the following pseudo gradient per epoch and use it to optimize the training process.

\[
\nabla_{\theta} L_{\text{pse}} = \frac{1}{|L|} \sum_{v_i \in L} \nabla_{\theta} L(Y_i, F_i) + \lambda \cdot \frac{1}{n_i} \sum_{v_i \in U'} \nabla_{\theta} L(\hat{Y}_i, F_i)
+ \frac{\lambda_1}{|I| - |J_i|} \sum_{v_i \in I} \sum_{v_j \in J_i} \nabla_{\theta} L(\hat{Y}_i, 1 - F_j),
\]

(10)
We experimentally evaluate ABN on GNNs against 12 competitors \( \theta \), \( \lambda \) where \( \theta \) is a factor controlling the weight of negative sampling.

Algorithm 1 summarizes the pseudo-code of ABN over GNNs, and it takes as input a graph \( G \) with labeled nodes \( L \) and unlabeled nodes \( U \). Note that ABN can be instantiated over either a shallow or a deep GNN, e.g., GCN and DAGNN introduced in Section 2.2. The output of Algorithm 1 is the learned classification model \( f \) with trainable parameters \( \theta \). At Line 3, ABN initializes the trainable parameters \( \theta \) by Xavier [13]. Then from Lines 4 to 14, ABN trains the classification model per epoch \( t \) iteratively, until convergence or the max number \( T \) of iterations is reached. Specifically, at Line 5, ABN first use a GNN to observe the forward prediction output \( F \). Then (Line 6) ABN detects the adaptive pseudo-labeled set \( U' \) and assigns pseudo labels to these nodes by Eq. (7). Next (Line 7), we obtain the pseudo label balancing factor \( \frac{1}{N} \) per node \( v_i \in U' \), after which, at Line 8 we perform negative sampling to obtain \( I \) and \( J \). At Line 9, ABN computes the gradient \( \nabla_{\theta} L_{pse} \) of current epoch according to Eq. (10). And at Line 10, ABN updates model parameters \( \theta \) for next epoch by Adam optimizer [23] over \( \nabla_{\theta} L_{pse} \).

5 EXPERIMENTS

We experimentally evaluate ABN on GNNs against 12 competitors for semi-supervised node classification on 4 real-world benchmark graph datasets. All experiments are conducted on a machine powered by an Intel(R) Xeon(R) E5-2603 v4 @ 1.70GHz CPU, 131GB RAM, 16.04.1-Ubuntu, and 4 Nvidia Geforce 1080ti Cards with Cuda version 10.2. Source codes of all competitors are obtained from the respective authors. Our ABN framework is implemented in Python, using libraries including PyTorch [35] and PyTorch Geometric [11]. An anonymous link of our source code is provided in Appendix B. Apart from the descriptions in this section, we explain more details on reproducibility in Appendix B.

5.1 Datasets and Competitors

Datasets. Table 2 shows the statistics of the 4 real-world graphs used in our experiments. We list the number of nodes, edges, features and classes in each graph dataset respectively. Specifically, the 4 datasets are Cora [39], Citeseer [39], Pubmed [39], and Corefull [1], all of which are widely used for benchmarking node classification performance in existing studies [30, 31, 40]. Notice that every node in these graphs has a ground-truth class label.

Competitors. We compare with 12 existing solutions, including LP (Label Propagation) [45], DeepWalk [36], LINE [41], G2G [1], DGI [43], GCN [24], GAT [42], MoNet [32], APPNP [25], DAGNN [31], STs (Self-Training and its variants) [30], and PL (Pseudo Labeling [26] on GCN). In particular, GCN, GAT, MoNet, APPNP, and DAGNN are GNNs with either shallow or deep architectures. DeepWalk, DGI, LINE, and G2G are unsupervised network embedding methods. STs represents the four variants over GCN in [30], including Self-Training, Co-Training, Union, and Intersection; we summarize the best results among these four variants as the results of STs. Remark that there are other existing solutions, such as M3S [40], but their codes are not available yet when this paper is submitted, and thus these solutions are not compared.

5.2 Experimental Settings

We evaluate our framework and the competitors on semi-supervised node classification tasks with various settings. In particular, for each graph dataset, we repeat experiments on 100 random data splits as suggested in [30, 31] and report the average performance. For each graph dataset, we vary the number of labeled nodes per class in \{1, 3, 5, 10, 20\}. Now we explain what a random data split is. For example, when the number of labeled nodes per class on Cora is 3 (denoted as Cora-3), since Cora has 7 classes, we randomly pick 3 nodes per class, combining together as a training set of size 21 (i.e., the labeled node set \( L \)), and then, among the remaining nodes, we randomly select 500 nodes as a validation set, and 1000 nodes as a test set, following convention in existing work [31]. Each data split consists of a training set, a validation set, and a test set as mentioned above. Table 1 summarizes the size of training, validation, test sets and corresponding label rate of all datasets.

We use the classification accuracy on test set as evaluation metric. Specifically, accuracy is defined as the fraction of the testing nodes whose class labels are correctly predicted by the learned classifier.

5.3 Implementation Details

Competitors. We use the parameters suggested in the original papers of the competitors to tune their models under various classification task settings explained in Section 5.2, and report the best results of the competitors. Notice that for unsupervised network embedding methods, including DeepWalk, DGI, LINE, and G2G, after obtaining the embedding results, we use logistic regression to train a node classifier over the embedding results [1, 43].

ABN over GCN and DAGNN. We instantiate ABN framework over the classic GCN model with 2 layers and a recent deep GNN architecture DAGNN to demonstrate the effectiveness and applicability of ABN. The instantiation of ABN over GCN and DAGNN are dubbed as ABNG and ABN_D respectively for brevity. ABNG and
ABN₃ has parameters (i) inherited from GCN and DAGNN and (ii) developed in ABN. Hence, we first tune the best parameters of the base models under each classification task setting on each dataset. After obtaining the best parameters of the base models, we then tune ABN₂ and ABN₃ for adaptive pseudo labeling parameter β in range [0, 1], and its weight λ in [0, 1], pseudo label balancing enable in {True, False}, negative sampling regularization weight λ₁ in [0, 0.1, 0.3, 1, 3], and the number of positive samples and the number of negative samples per positive sample in {(1, 10), (2, 5), (5, 2), (10, 1)}. The best parameters of each task setting are in Appendix B as well as in the submitted source code.

### 5.4 Overall Results

Table 3 reports the classification accuracy (in percentage) of all methods on CiteSeer and Cora, when varying the number of labeled nodes per class in [1,3,5,10,20]. For each classification task, the best (i.e., highest) accuracy is in bold, and the second and third best accuracy are underlined.

An overall observation is that ABN₃ and ABN₄ consistently outperform their respective base GNN models, i.e., GCN and DAGNN respectively, by a significant margin under all settings on both CiteSeer and Cora, and they achieve state-of-the-art performance. This demonstrates the power of the proposed ABN framework to boost classification performance. In particular, on the left side of Table 3 (CiteSeer), ABN₂ consistently achieves the highest accuracy under all settings, compared with all competitors. For instance, on CiteSeer-1 with only 1 labeled node per class, ABN₂ has 56.2% accuracy, while the best competitor DAGNN only achieves 46.5% accuracy. Further, ABN₃ outperforms GCN that has 40.4% on CiteSeer-1 by 15.8%. Moreover, ABN₃ is always the second best performer among all methods on CiteSeer dataset. Similarly, on the right side of Table 3 (Cora), ABN₃ achieves the best accuracy under all classification task settings. For instance, on Cora-1, ABN₃ improves GCN from 44.6% to 62.5% (i.e., 17.9% improvement), and ABN₄ has 66.4% accuracy, outperforming DAGNN that has 59.8% accuracy by a significant margin.

Table 2: Datasets

|            | Cora | CiteSeer | Pubmed | Cora-full |
|------------|------|----------|--------|-----------|
| # of Nodes | 2708 | 3327     | 19717  | 19793     |
| # of Edges | 5429 | 4732     | 44338  | 65311     |
| # of Features | 1433 | 3703     | 500    | 8710      |
| # of Classes | 7    | 6        | 3      | 6         |

Table 3: Accuracy results (in percentage) on CiteSeer and Cora respectively, averaged over 100 random data splits. (The best accuracy is in bold, second and third are underlined.)

| # of Labels per class | CiteSeer | Cora |
|-----------------------|----------|------|
| 1                     | 3        | 5    |
| 10                    | 20       |      |

|            | LP       | DeepWalk | LINE | G2G     | DGI     | STs     | PL      | GAT     | MoNet   | APPNP   | DAGNN   | GCN     | ABN₃    | ABN₄    |
|------------|----------|----------|------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|
| 1          | 30.1     | 34.7     | 38.0 | 45.1    | 46.1    | 57.2    | 15.3    | 32.8    | 38.8    | 34.6    | 46.5    | 40.4    | 56.2    | 48.5    |
| 3          | 37.0     | 41.8     | 43.1 | 60.3    | 64.1    | 51.8    | 17.3    | 48.6    | 59.7    | 52.2    | 68.6    | 53.5    | 66.4    | 65.9    |
| 5          | 39.3     | 42.0     | 43.8 | 63.1    | 67.6    | 60.7    | 18.7    | 54.9    | 64.6    | 59.4    | 70.7    | 58.4    | 70.9    | 62.5    |
| 10         | 41.9     | 45.6     | 48.5 | 63.1    | 68.7    | 70.4    | 22.8    | 60.8    | 66.9    | 66.3    | 71.2    | 65.8    | 70.9    | 64.2    |
| 20         | 44.8     | 45.6     | 48.5 | 63.1    | 68.7    | 70.4    | 22.8    | 60.8    | 66.9    | 66.3    | 71.2    | 65.8    | 70.9    | 64.2    |

From the superior performance of our ABN framework, in Table 3, we can observe three interesting findings. First, under extremely-few-labels settings (e.g., CiteSeer-3), unsupervised methods G2G (56.4%) and DGI (59.2%) achieve better performance than GNNs, e.g., GCN (53.5%) and DAGNN (58.8%). One reason is that the unsupervised methods are good at cases when no labeled data are available, while GNNs still require a sufficient amount of labeled data. This finding demonstrates the intuition of the negative sampling regularization technique in Section 4.3, and also sheds light on possible future research directions to use unsupervised techniques further enhance the performance of semi-supervised learning. Second, PL (Pseudo Labeling in Section 2.2) has low accuracy as reported in Table 3, validating our analysis of its potential issues in Section 3. Third, the performance gap between our methods and competitors enlarges as the number of labels per class decreases, which further illustrates the effectiveness of the proposed ABN framework under extreme settings on graphs with very few-labeled nodes per class.

Table 4 presents the classification accuracy of all methods under all settings in [1,3,5,10,20] on PubMed and Cora-full datasets. We exclude from this table, the inaccurate competitors (e.g., DeepWalk and LINE) that are obviously outperformed by other competitors. Observe that on PubMed and Cora-full, ABN₄ and ABN₃ achieve either the highest accuracy in bold or top-3 accuracy underlined.
Table 4: Accuracy results (in percentage) on PubMed and Cora-full respectively, averaged over 100 random data splits. (The best accuracy is in bold, second and third are underlined.)

| # of Labels per class | PubMed                  | Cora-full               |
|-----------------------|-------------------------|-------------------------|
|                       | 1 3 5 10 20            | 1 3 5 10 20            |
| LP                    | 55.7 61.9 63.5 65.2 66.4 | 26.3 32.4 35.1 38.0 41.0 |
| G2G                   | 55.2 64.5 67.4 72.0 74.3 | 25.8 36.4 43.3 49.3 54.3 |
| DGI                   | 55.1 63.4 65.3 71.8 73.9 | 26.2 37.9 46.5 55.3 59.8 |
| STs                   | 55.1 65.4 69.7 74.0 78.5 | 29.2 43.6 48.9 53.4 60.8 |
| PL                    | 34.9 35.1 49.2 49.9 77.5 | 23.5 19.1 24.2 31.3 57.9 |
| APPNP                 | 54.8 66.9 70.8 76.0 79.4 | 24.3 41.5 48.5 55.3 60.1 |
| DAGNN                 | 59.4 69.5 72.0 76.8 80.1 | 27.3 43.2 49.8 55.8 60.4 |
| GCN                   | 55.5 66.0 70.4 74.6 78.7 | 24.5 41.4 48.1 55.8 60.2 |
| ABNG                  | 60.8 67.8 71.6 76.1 79.4 | 30.8 44.9 49.4 56.6 60.9 |
| ABND                  | 61.0 72.1 74.9 78.2 80.6 | 27.6 44.4 51.1 56.8 61.2 |

Also, ABNG and ABND are consistently better than their base GNN models GCN and DAGNN respectively. For instance, on PubMed-1, ABNG achieves 60.8% accuracy; 5.3% better than GCN; ABND has 61.0% accuracy while that of DAGNN is 59.4%.

In summary, the experimental results presented in Tables 3 and 4 validate the effectiveness of the proposed ABN framework to boost classification performance under the graph-based semi-supervised learning paradigm.

5.5 Ablation Study and Parameter Evaluation

Ablation Study. We conduct ablation study to evaluate the contributions of the three techniques of ABN presented in Section 4. Denote (i) ABN as the framework with all techniques enabled, (ii) ABN-N as ABN excluding negative sampling regularization in Section 4.3, and (iii) ABND as ABN excluding both pseudo label balancing in Section 4.2 and negative sampling regularization. In other words, ABND is the method with only adaptive pseudo labeling enabled (Section 4.1).

Figures 4a and 4b report the ablation results of ABNG and ABND respectively, on Cora when varying the number of labels per class. Observe that the accuracy indeed improves significantly when adding pseudo label balancing and negative sampling regularization one after another. Moreover, comparing ABNG-N-B in Figure 4a with the results of PL (Pseudo Labeling on GCN) on Cora in Table 3, it is easy to see that ABNG-N-B outperforms PL by a significant margin, demonstrating the effectiveness of adaptive pseudo labeling technique presented in Section 4.1. For example, on Cora-3, ABNG-N-B has 45.2% accuracy (Figure 4a) while that of PL is just 18.2% in Table 3. The ablation study on ABND in Figure 4b yields the same observations and indicates the effectiveness of the three techniques in ABN framework. In addition, one may observe that ABN-N is slightly better than ABN when the number of labels per class is 10 and 20 in Figure 4a. The reason is that, on Cora-10 and Cora-20, there are enough labels for semi-supervised training. Thus, in Eq. (10), there is a $\lambda_1$ parameter to limit the importance of negative sampling regularization when there are sufficient labels.

Parameter Evaluation. As mentioned in Section 4.1, there exists a trade-off on the choice of $\beta$. Here we report the results when varying $\beta$ from 0.1 to 0.9 with step 0.1, on Cora-1, Cora-3, and Cora-5 in Figure 5. Observe that, as $\beta$ increases, especially on Cora-1, the accuracy increases gradually to a peak and then drops, illustrating the trade-off of $\beta$ in adaptive pseudo labeling. Also when there are more labels, e.g., Cora-5, the performance is relatively stable. Nevertheless, the results in Figure 5 demonstrate that adaptive pseudo labeling is effective when $\beta$ is fine-tuned on each classification task of each dataset.

6 OTHER RELATED WORK

We review other related work here, excluding GCN [24], DAGNN [31], Pseudo Labeling [26], and Self-Training [30] that are already explained in Section 2.2.

Graph Neural Networks. Apart from GCN and DAGNN, in literature, there exist many other GNN variants, to leverage graph topology and node features for graph representation learning and downstream tasks. Initial studies apply convolution operation in the spectral domain, where the eigenvectors of the graph Laplacian are considered as the Fourier basis [3, 8, 20]. Then GAT [42] assigns different weights to nodes in the same neighborhood via attention mechanisms. MoNet [52] defines convolutions directly in the spatial domain using mixture model CNNs. The above GNNs are with shallow architecture. There are many deep GNNs proposed, e.g., DAGNN and others in [6, 25, 31]. For instance, APPNP [25] proposes a propagation rule based on personalized PageRank [2], so as to gather both local and global information on graphs. However, as evaluated in our experiments, these methods still have space for improvement since they are not directly designed to tackle the scarcity of labeled data.

Network Embedding. Network embedding aims to learn a low-dimensional embedding vector per node in an unsupervised manner. The learned embedding vectors can be then used in downstream tasks, including node classification. There exists a collection of network embedding solutions, e.g., [1, 15, 36, 41, 44]. DeepWalk uses truncated random walks to learn latent representations, with the assumption that nodes are similar if they are close by random walks [36]. LINE preserves and concatenates the first-order and second-order proximity representations between nodes [41]. G2G [1] embeds each node as a Gaussian distribution according to a novel ranking similarity based on the shortest path distances.
orthogonal to our work.

7 CONCLUSION

This paper presents ABN, an effective framework for semi-supervised node classification on few-labeled graph data. ABN achieves superior performance on graphs with extremely few labeled nodes, through three main designs: adaptive pseudo labeling that adaptively selects high-confidence unlabeled nodes, pseudo label balancing that handles label imbalance in real-world skewed graph data, and negative sampling regularization that further fully utilizes unlabeled data to train a high-quality classifier. The effectiveness of ABN is extensively evaluated on 4 real graphs, compared against 12 existing solutions. Regarding future work, we plan to enhance ABN by investigating other unsupervised techniques, and also implement ABN on top of more GNN architectures as evaluated in experiments.

Orthogonal Self-training Studies. Self-training itself is a general methodology [22] and is used in various domains in addition to graph data. It is used in word-sense disambiguation [19, 49], bootstrapping for information extraction and handling subjective nouns [38], and text classification [34]. In [50], it suggests that selecting informative unlabeled data using a guided search algorithm can significantly improve performance over standard self-training framework. Buchnik and Cohen [4] mainly consider self-training through three main designs: adaptive pseudo labeling that adapts then Propagate: Graph Neural Networks meet Personalized PageRank. In ICLR.

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A PROOF

A.1 Proof of Eq. (6)

Proof. The first inequality of Eq. (6) is from the property of conditional expectation. Specifically, for a random variable \( X = \nabla_\theta L(\tilde{Y}_i, F_i) - \nabla_\theta L(Y_i, F_i) \) and a partition of sampling space into two parts:

\[
A = \{ u_i \sim U(\mathcal{U}) \; | \; \tilde{Y}_i \neq Y_i \} \\
B = \{ u_i \sim U(\mathcal{U}) \; | \; \tilde{Y}_i = Y_i \}
\]

Then the following holds since \( \mathbb{E}[X|B] = 0 \):

\[
\mathbb{E}[X] = \mathbb{E}[X|A]P(A) + \mathbb{E}[X|B]P(B) = \mathbb{E}[X|A]P(A)
\]

Based on Jensen’s inequality, the first inequality of Eq. (6) holds.

\[\mathbb{E}[X] = \mathbb{E}[X|A]P(A) \leq P(A)\mathbb{E}[\|X\| |A].\]

The second inequality is from the bounded gradient norm assumption and the triangle property of the norm, such that

\[\|\nabla_\theta L(\tilde{Y}_i, F_i) - \nabla_\theta L(Y_i, F_i)\| \leq \|\nabla_\theta L(\tilde{Y}_i, F_i)\| + \|\nabla_\theta L(Y_i, F_i)\| \leq 2\Theta\]

Then we have

\[
\frac{|\mathcal{U}| \cdot P(A)}{|\mathcal{L}|} \cdot \mathbb{E} \left[ \|X\| |B \right] \leq 2\Theta |\mathcal{U}| \cdot P(A) = \frac{2\Theta |\mathcal{U}|}{|\mathcal{L}|} \cdot P_{\eta, U}(\mathcal{L}) (\tilde{Y}_i \neq Y_i)
\]

Thus Eq. (6) holds. 

\[\square\]

B REPRODUCIBILITY

In what follows, we explain the details for reproducibility, including details of datasets, hardware and software versions used in our experiments, and hyper-parameter settings.

Our source code is at link: https://anonymous.4open.science/r/e7aca211-0d8d-4564-8f3f-0ef24b01941e/

We get the Cora, CiteSeer, PubMed, and Cora-full datasets from the following links provided by others. Our code will check these links and automatically download the data.

Cora, CiteSeer, and PubMed datasets at link: https://github.com/kimyoung/planetoid/raw/master/data
Cora-full dataset at link: https://github.com/abojchevski/graph2gauss/raw/master/data/

B.1 Details of Datasets

Cora [39], CiteSeer [39], PubMed [39], and Core-full [1] are representative networks, widely used in existing studies [30, 31, 40] to benchmark the performance of semi-supervised learning tasks. For instance, in Cora, a node represents an article, and if two articles (nodes) have citation relationship, there is an edge between the two nodes in the corresponding graph. Every node has a bag-of-words (Cora, CiteSeer, Cora-full) or TF-IDF (PubMed) representation as the features of the node. Moreover, every node has a class label, representing the research area that the corresponding article belongs..
### Table 5: Hyper parameters and search space

| Parameters | Search Space |
|-----------|--------------|
| Balancing | {True, False} |
| \( \lambda \) | [0.1, 1] |
| \( \beta \) | [0.1, 0.9] with step 0.1 |
| \( \lambda_1 \) | [0, 0.1, 0.3, 1, 3] |
| \((|I|, |J_i|)\) | {(1, 10), (2, 5), (5, 2), (10, 1)} |
| \( L_2 \) regularization | {1e-2, 5e-3, 1e-3, 5e-4, 1e-4} |
| Early Stopping | {True, False} |
| \( k \) in ABN\( \_D \) | [10, 15, 20] |
| Dropout rate | [0.5, 0.8] |

to. For instance, The class labels in Cora include Case Based Study, Genetic Algorithms, Neural Networks, Probabilistic Methods, Reinforcement Learning, Rule Learning, and Theory. The class labels in Citeseer include Agents, AI, DB, IR, ML, HCI. The Cora-full dataset in [1] is an extended version of Cora with more nodes, edges, and classes.

### B.2 Hardware and Software

In this section, we explain the hardware and software versions used in our experiments.

**Hardware.** We use a linux machine powered by a Intel(R) Xeon(R) E5-2603 v4 @ 1.70GHz CPU, associated with 131GB RAM, and installed with 4 Nvidia Geforce 1080Ti GPU Cards. Each 1080Ti card has 11GB GPU memory.

**Software versions.** The operating system is 16.04.1-Ubuntu SMP on x86_64. The Cuda version is 10.2.89. We use Python 3.7.4, and also use PyTorch 1.7.1 and Pytorch Geometric 1.6.0. In addition, we use the python packages including NetworkX, tdqm, DGL (cuda 10.2 version).

### B.3 Hyper Parameters and Search Space

In this section, we explain the hyper parameters of ABN\( \_G \) and ABN\( \_D \) when instantiated over base models GCN and DAGNN respectively, and also introduce the search space of these parameters.

Table 5 summarizes the hyper parameters and their corresponding search space. We first tune the parameters of base models, and then tune the parameters of ABN. In particular, in terms of base models, we tune the following parameters: a \( L_2 \) regularization rate with search space in \{1e-2, 5e-3, 1e-3, 5e-4, 1e-4\}, an early stopping enabler in \{True, False\}, a dropout rate in \{0.5, 0.8\}. In addition, for ABN\( \_D \), the level \( k \) of propagation after MLP is searched in \{10, 15, 20\}.

Further, we have the following parameter settings in our experiments: the number of hidden units of GCN and MLP (in DAGNN) is 64 units without bias; the number of layers of GCN and MLP (in DAGNN) is 2 layers; the learning rate of Adam Optimizer is 0.01; the activation function is RELU; the maximum number of training epochs is 1000. Moreover, early stopping is triggered when the validation loss is smaller than the average validation loss of previous 100 epochs, and the current epoch is beyond 500 epochs.

After finding the best hyper parameters of the base models on each classification task, we then tune the parameters of the three techniques in ABN. In particular, adaptive pseudo labeling has a parameter \( \beta \) with search space in range \{0.1, 0.9\} with step 0.1, and a parameter \( \lambda \) controlling the weight of adaptive pseudo labels, with search space \{0.1, 1\}. Pseudo label balancing enabler searches values in \{True, False\}. Negative sampling regularization weight \( \lambda_1 \) is searched in \{0, 0.1, 0.3, 1, 3\}, and the number of positive and negative samples \((I, J_i)\) is searched in \{(1, 10), (2, 5), (5, 2), (10, 1)\}.

For instance, \((2, 5)\) means that we sample 2 positive nodes and then for each positive node, we sample 5 negative nodes.

### B.4 Searched Hyper Parameters of ABN

In Tables 6 and 7, we present the searched hyper parameters of ABN\( \_G \) and ABN\( \_D \) on Cora and CiteSeer datasets respectively, in order to reproduce our results reported in Table 3 when varying the number of labels per class in \{1, 3, 5, 10, 20\}. Due to space limit, we only list the searched parameters on Cora and CiteSeer. Please find the searched parameters of ABN\( \_G \) and ABN\( \_D \) on all datasets including PubMed and Cora-full in our source code, to reproduce the results in experiments.
Table 6: The searched hyper parameters of ABN on Cora dataset

| Parameters                  | ABNG | ABND |
|-----------------------------|------|------|
| # of labels per class      | 1    | 3    | 5    | 10   | 20   | 1    | 3    | 5    | 10   | 20   |
| Balancing                  | True | True | True | False | False | True | True | True | False | False |
| $\lambda$                  | 1    | 1    | 1    | 1    | 1    | 1    | 1    | 1    | 1    | 1    |
| $\beta$                    | 0.2  | 0.5  | 0.5  | 0.5  | 0.8  | 0.4  | 0.5  | 0.6  | 0.6  | 0.9  |
| $\lambda_1$                | 1    | 0    | 1    | 1    | 0    | 1    | 1    | 1    | 0    | 1    |
| $|I|$                        | 5    | 0    | 5    | 2    | 0    | 5    | 2    | 10   | 0    | 10   |
| $|J_i|$                      | 2    | 0    | 2    | 5    | 0    | 2    | 5    | 1    | 0    | 1    |
| $L_2$ regularization        | 0.0005 | 0.001 | 0.001 | 0.001 | 0.001 | 0.005 | 0.005 | 0.005 | 0.005 | 0.005 |
| Early stopping              | True | True | True | True | True | True | True | True | True | True |
| $k$ in ABND                 | -    | -    | -    | -    | -    | 15   | 15   | 15   | 15   | 10   |
| Dropout rate                | 0.8  | 0.8  | 0.8  | 0.8  | 0.8  | 0.8  | 0.8  | 0.8  | 0.8  | 0.8  |

Table 7: The searched hyper parameters of ABN on CiteSeer dataset

| Parameters                  | ABNG | ABND |
|-----------------------------|------|------|
| # of labels per class      | 1    | 3    | 5    | 10   | 20   | 1    | 3    | 5    | 10   | 20   |
| Balancing                  | True | True | True | True | True | True | True | True | True | True |
| $\lambda$                  | 1    | 1    | 1    | 1    | 1    | 1    | 1    | 1    | 1    | 1    |
| $\beta$                    | 0.2  | 0.4  | 0.6  | 0.6  | 0.6  | 0.2  | 0.5  | 0.6  | 0.6  | 0.6  |
| $\lambda_1$                | 0    | 3    | 3    | 1    | 1    | 1    | 0    | 0    | 0    | 0    |
| $|I|$                        | 0    | 5    | 5    | 2    | 2    | 5    | 2    | 0    | 0    | 0    |
| $|J_i|$                      | 0    | 2    | 2    | 5    | 5    | 2    | 5    | 0    | 0    | 0    |
| $L_2$ regularization        | 0.0005 | 0.002 | 0.002 | 0.002 | 0.002 | 0.005 | 0.005 | 0.005 | 0.005 | 0.02  |
| Early stopping              | True | True | True | True | True | True | True | True | True | True |
| $k$ in ABND                 | -    | -    | -    | -    | -    | 15   | 15   | 15   | 15   | 10   |
| Dropout rate                | 0.8  | 0.5  | 0.5  | 0.8  | 0.5  | 0.8  | 0.5  | 0.5  | 0.8  | 0.8  |