Learning with Few Labeled Nodes via Augmented Graph Self-Training

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ABSTRACT
It is well known that the success of graph neural networks (GNNs) highly relies on abundant human-annotated data, which is laborious to obtain and not always available in practice. When only few labeled nodes are available, how to develop highly effective GNNs remains understudied. Though self-training has been shown to be powerful for semi-supervised learning, its application on graph-structured data may fail because (1) larger receptive fields are not leveraged to capture long-range node interactions, which exacerbates the difficulty of propagating feature-label patterns from labeled nodes to unlabeled nodes; and (2) limited labeled data makes it challenging to learn well-separated decision boundaries for different node classes without explicitly capturing the underlying semantic structure. To address the challenges of capturing informative structural and semantic knowledge, we propose a new graph data augmentation framework, AGST (Augmented Graph Self-Training), which is built with two new (i.e., structural and semantic) augmentation modules on top of a decoupled GST backbone. In this work, we investigate whether this novel framework can learn an effective graph predictive model with extremely limited labeled nodes. We conduct comprehensive evaluations on semi-supervised node classification under different scenarios of limited labeled-node data. The experimental results demonstrate the unique contributions of the novel data augmentation framework for node classification with few labeled data.

1 INTRODUCTION
Graphs serve as a common language for modeling a wide spectrum of structured and relational systems, ranging from social networks [43] to knowledge graphs [36], from financial transaction networks [35] to e-commerce product graphs [22]. To ingest the valuable information encoded in graph-structured data, graph learning algorithms have been proposed in the research community and made huge success in different domains. Recently, graph neural networks (GNNs), a generalized form of neural networks for graph-structured data, have become the prevailing paradigm due to their effectiveness and scalability [12, 14, 33].

As a fundamental graph analytical task, node classification has received continuous endeavors in the graph machine learning community. Existing GNNs developed for node classification usually focus on the canonical semi-supervised setting where relatively abundant gold-labeled nodes are provided. While this setting is often impractical since data labeling is extremely labor-intensive, especially when considering the heterogeneity of graph-structured data [9, 10]. To overcome the data scarcity issue, self-training or pseudo-labeling [16] has been explored to combine with GNNs and proven to be effective for solving semi-supervised node classification with fewer labels [10, 17, 31]. Specifically, a teacher GNN model is initially trained on the small labeled node set, and its predictions on unlabeled nodes are used as pseudo labels. The pseudo-labeled set will be included into the labeled set for training a student GNN model that shares the same architecture of the teacher model.

Existing GST methods, however, simply combine the idea of self-training with GNNs, which can be ineffective in handling graph data with few labeled nodes, or in exploiting numerous unlabeled nodes due to two limitations: (1) Structural Bottleneck. Given few labeled nodes, it is important for the GNN model to enable more propagation steps so the feature patterns of labeled nodes can be better propagated to the long-distance unlabeled nodes. However, recent work pointed out the distortion of information flowing from distant nodes (i.e., over-squashing [1, 32]) as a factor limiting the efficiency of message-passing for tasks relying on long-range node interactions. In addition, real-world graphs often come with a certain level of structure noise (e.g., “noisy” and “missing” edges), which could be generated by either adversaries [47] or the data collection process itself [44]. Such structure noise can easily interfere with the message-passing process and make it difficult to learn correct feature-label patterns with few labeled nodes. Hence, it is crucial to avoid over-squashing and reduce data noise in our endeavor to further improve the performance of GST with few labeled nodes; and (2) Semantic Bottleneck. It is challenging to learn well-separated decision boundaries between different node classes when labeled training data is severely scarce and the semantic manifold is complex. Though GST methods attempt to alleviate the data scarcity problem by adding pseudo labels, the nodes with pseudo-labels may introduce complex feature patterns and pseudo labels can be unreliable, which causes the model performance to deteriorate. We ask if novel ideas can be explored to optimize the usage of pseudo labels for capturing the underlying semantic structure of the sparsely-labeled graph.

In this paper, we propose an Augmented Graph Self-Training framework, namely AGST, for tackling semi-supervised node classification where few labeled nodes are available. We plan to address the limitations of conventional GST methods by proposing two original modules for structural and semantic data augmentations. Specifically, our framework employs a simple, decoupled GNN as the GST backbone, where the teacher model first performs high-order label propagation to generate pseudo labels on unlabeled nodes based on Personalized PageRank [27], and the student model conducts feature transformation by mapping the features of nodes to their gold/pseudo labels. From the structural data augmentation perspective, our framework not only enables large receptive fields to capture long-range node interactions, but also avoids the
weakly-supervised contrastive loss to encourage intra-class compac-
tness and inter-class separability in the latent feature space. As such, well-separated decision boundaries can be learned during the GST process even with few labeled nodes. The proposed AGST framework enables the two data augmentation modules to work seamlessly with the decoupled GST backbone and to quickly learn an effective graph predictive model even with few labeled nodes. To summarize, our key contributions are listed as follows:

- **Problem:** We investigate the problem of semi-supervised node classification under the limited labeled data setting where few labeled nodes are available, advancing the frontier of graph machine learning in practical scenarios.
- **Algorithm:** We propose a principled GST framework, which differs from the existing efforts and improves the performance with scarce labeled data by augmenting data from both structural and semantic perspectives.
- **Evaluation:** We conduct extensive experiments on various real-world datasets to evaluate the effectiveness of our approach. The experimental results demonstrate the unique contributions made by AGST to performance improvement over existing methods.

## 2 RELATED WORK

### 2.1 Graph Neural Networks

Graph neural networks (GNNs), a family of neural endeavors for learning latent node representations in a graph, have drawn much attention in the community of graph machine learning (GML) [2, 7, 14, 33]. In general, graph neural networks can be categorized into spectral [2, 7, 14, 37] and spatial approaches [12, 24, 39]. Originally inspired by graph spectral theory, spectral-based graph convolutional networks (GCNs) extend convolution operation in the spectral domain to graph-structured data. Among them, the model proposed by Kipf et al. [14] has become the most prevailing one by using a linear filter. Later on, SGC [37] is proposed to further reduce the computational complexity by removing the non-linearity of GCNs. As another line of work, spatial-based GNNs define graph convolutions based on a node’s spatial relations [12, 33, 39]. For example, GAT [33] incorporates trainable attention weights to specify fine-grained weights on neighbors when aggregating neighborhood information of a node. In essence, although spectral-based and spatial-based GNNs start on a different basis, both of them share the same propagation rule, which is the message-passing scheme. Those methods model the homophily principle [23] and learn node representations by iteratively transforming, and propagating/aggregating node features within graph neighborhoods. When long-range node interactions are needed, the over-squashing issue can largely undermine the model performance if we directly increase the model depth. Thus researchers try to solve this issue by proposing different techniques, such as sampling or rewiring edges [12, 24], decoupling the feature transformation and propagation steps [5, 8, 11, 15, 21] and many others [17, 40]. In particular, decoupled GNNs [11] have become a prevailing paradigm due to their simplicity and learning efficiency. For example, APPNP [15] propagates the neural predictions via personalized PageRank, which can preserve the node’s local information while increasing the receptive fields. Liu et al. [21] propose to decouple the propagation and transformation steps and then utilizes an adaptive adjustment mechanism to balance the information from local and global neighborhoods of each node. However, the aforementioned models neglect the additional supervision signals from unlabeled data, which has become a bottleneck for pushing the performance boundary of GNNs. Though CGPN [34] leverages poisson learning to propagate the labels to the entire graph, it cannot address the structure noise and explicitly capture the semantic structures of the input graph.

### 2.2 Node Classification with Few Labels

In real-world scenarios, labeled training samples are usually quite limited due to the intensive cost of data labeling. Albeit the great success of GNNs for graph-based semi-supervised learning, most of the existing efforts are designed as shallow models with a restricted receptive field, leading to their ineffectiveness in low-data scenarios [11, 19, 21]. Under the extreme cases when very few labels are given, shallow GNNs cannot effectively propagate the training labels and characterize the global information of the input graph [17]. Many advanced deep GNNs [5, 15, 21, 40, 41] have shown their advantages in leveraging large receptive fields for propagating label signals. However, the main concern in semi-supervised node classification, i.e., the shortage of supervision information, has not been directly addressed. To counter this issue, self-training [42], also known as pseudo-labeling [16], where one imputes labels on unlabeled data based on a teacher model trained with limited labeled data, has been applied to improve GNNs to solve the problem of semi-supervised node classification. Among those methods, Li et al. [17] first combine GCNs and self-training to expand supervision signals. Furthermore, MS3 [31] proposed multi-stage self-training and utilized clustering method to eliminate the pseudo labels that may be incorrect. Similar ideas can also be found in [6, 20, 46]. However, existing methods still adopt shallow GNNs to build the teacher and student models, which inherently restrict the effective propagation of label signals. Apart from the aforementioned methods, our AGST framework adopts a decoupled design, in which the teacher model is a label propagation module and the student model is a feature transformation module. As such, our framework is capable of leveraging both large receptive fields and pseudo supervision signals, making the learned model more label-efficient. In addition, we propose a weakly-supervised contrastive loss and graph topology augmentation function to further improve model performance during the self-training process.

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The difference between over-smoothing and over-squashing can be found in [1].
3 AUGMENTED GRAPH SELF-TRAINING

We start by introducing the notations used throughout this paper. We let bold uppercase letters represent matrices and bold lowercase letters denote vectors. Let $G = (V, E, X)$ denote an undirected graph with nodes $V$ and edges $E$. Let $n$ denote the number of nodes and $m$ the number of edges. The nodes in $G$ are described by the attribute matrix $X \in \mathbb{R}^{n \times f}$, where $f$ denotes the number of features per node. The graph structure of $G$ is described by the adjacency matrix $A \in \{0, 1\}^{n \times n}$, while $\tilde{A}$ stands for the adjacency matrix for a graph with added self-loops. We let $\tilde{D}$ be the diagonal degree matrix of $\tilde{A}$ and $S = \tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}}$ denote the symmetric normalized adjacency matrix with self-loops. The class (or label) matrix is represented by $Y \in \mathbb{R}^{n \times c}$, where $c$ denotes the number of classes.

Problem Definition. Given an input graph $G = (V, E, X)$, where the node set $V$ is divided to two disjoint node sets $V^L$ and $V^U$. In this paper we focus on the semi-supervised node classification task under the low-data settings. Specifically, suppose that the labels of the labeled training set $V^L$ are given, where each node class in $V^L$ only have few labeled nodes (could be either balanced or imbalanced for different classes), the goal is to predict the labels of the unlabeled nodes in $V^U$. Note that if each class has the same number of $K$-labeled nodes, the studied problem can be called few-shot semi-supervised node classification.

Architecture Overview. In this section, we propose an augmented graph self-training framework (AGST) to solve the problem of semi-supervised node classification with only a few labeled nodes. Compared to existing efforts, AGST is able to address the structural and semantic bottlenecks under the low-source setting by virtue of two focal designs: (1) a new GST backbone with a graph topology augmentation function that is able to leverage long-range node interactions while alleviating the structure noise; (2) a weakly-supervised contrastive loss that enhances the semantic structures of the input graph by aligning the semantic similarities between pseudo-labeled data and gold-labeled data. A detailed illustration of the proposed approach is provided in Figure 1.

3.1 Augmenting Structural Knowledge in GST

For semi-supervised node classification, graph neural predictors commonly have a large variance and easy to overfit when the labeled training data is extremely limited [17, 31]. Though previous GST methods partially alleviate this issue by expanding the labeled training set, they still suffer from the incapability of leveraging long-range node interactions and handling structure noise in nature: one the one hand, if the teacher and student model shares the same shallow GNN architecture, the over-squashing issue will largely impede the effective propagation of feature-label patterns when multiple layers are deployed; on the other hand, the missing or noisy edges in the input graph may also distort the information flow. To better exploit the useful graph structural knowledge, we go beyond the existing GST architectures and develop a decoupled GST backbone with a structural data augmentation module.

Teacher Model. In a self-training framework, the teacher model serves the role of generating pseudo labels on unlabeled data to augment the limited training set. The teacher model in our decoupled GST framework is a Label Propagation (LP) module that enables long-range propagation of label signals for computing the pseudo labels. This way the pseudo labels preserve both local and global structural knowledge when further training the student model. Specifically, the objective of LP is to find a prediction matrix $\hat{Y} \in \mathbb{R}^{n \times c}$ that agrees with the label matrix $Y$ while being smooth on the graph such that nearby vertices have similar soft labels:

$$\hat{Y} = \arg \min_Y \left( \text{Tr}(\hat{Y}^T (I - S) \hat{Y}) + \mu \|\hat{Y} - Y\|_2^2 \right),$$

where $\mu$ is a positive parameter balances the trade-off between these two competing constraints. The smoothness term smooths...
each column of the prediction matrix along the graph structure, while the fitting term enforces the prediction matrix \( \hat{Y} \) to agree with the label matrix \( Y \).

By solving the above unconstrained optimization function, a closed-form solution can be computed as \( \hat{Y} = (1 - \alpha)(1 - \alpha S)^{-1} Y \), where \( \alpha = \frac{1}{F} \). As derived by Zhou et al. [45], the solution can be approximated via the following iteration:

\[
Y^{(t+1)} = \alpha SY^{(t)} + (1 - \alpha)Y^{(0)},
\]

where \( Y^{(0)} = Y \), which converges to \( \hat{Y} \) rapidly. Here \( 1 - \alpha \) can be naturally connected with the teleport probability in Personalized PageRank [15]. With an appropriate \( \alpha \), the smoothed labels can avoid losing the focus on local neighborhood [17] even using infinitely many propagation steps.

**Student Model.** Since the LP-based teacher model supports long-range propagation without losing its focus on the local neighborhood, both local and global structure knowledge will be captured in the computed soft pseudo labels. Next, we develop a Feature Transformation (FT) module as the student model to distill the knowledge from the teacher model and meanwhile learn the feature knowledge by transforming the node features to class labels. The student model is composed of an encoder network \( f_\theta(\cdot) \) followed by a prediction network \( g_\phi(\cdot) \). For node \( v_i \), the class prediction can be computed:

\[
\hat{p}_i = g_\phi(z_i), \quad z_i = f_\theta(x_i),
\]

where the predicted label \( \hat{p}_i \) is computed based on the node features \( x_i \). Specifically, the encoder network \( f_\theta(\cdot) \) is built with a 2-layer MLP and the prediction network \( g_\phi(\cdot) \) is a feed-forward layer followed by softmax, producing a vector of confidence scores.

To learn the student model, instead of using hard pseudo labels as previous GST methods, here we consider the soft pseudo labels generated by the LP-based teacher model as the ground-truth, and compute the standard cross-entropy loss on unlabeled nodes:

\[
\mathcal{L}_{\text{CE}} = - \sum_{v_i \in V, \ c=1} \sum_{y \in \mathbb{Y}} \hat{y}_i^c \log \hat{p}_i^c.
\]

In addition, we derive another cross-entropy loss for the nodes from the labeled training set:

\[
\mathcal{L}_{\text{CE}} = - \sum_{v_i \in V, \ c=1} \sum_{y \in \mathbb{Y}} y_i^c \log \hat{p}_i^c.
\]

By jointly optimizing the above losses, we are able to learn a simple yet effective student model for semi-supervised node classification with only few labels.

**Graph Topology Augmentation.** Real-world graphs commonly come with a certain level of structure noise, which could be induced by either partial observation, graph pre-processing, or even adversarial attacks [3, 44, 47]. Since labeled nodes are extremely limited, the feature patterns of labeled nodes will be even harder to propagate to unlabeled nodes due to the imperfect graph structure. Considering that message-passing is a type of Laplacian Smoothing [15], representations of nodes belonging to different classes will become inseparable due to the existence of many unnecessary inter-class edges. As such, we argue that it is helpful to eliminate potentially noisy edges and strengthen the connections between similar nodes for better preserving the graph structure knowledge and improve the effectiveness of message-passing.

To this end, after the student model converges in each self-training iteration, we in turn use it to refine the graph topology by strengthening intra-class edges and reducing inter-class connections. Specifically, given the predicted label matrix \( \hat{P} \), the edge probability matrix \( \hat{A} \) (symmetric) is computed by:

\[
\hat{A} = \sigma(\hat{P}^T \hat{P}), \quad \hat{P} = g_\phi(f_\theta(X)),
\]

where \( \hat{A}_{ij} \) denotes the probability that node \( v_i \) and \( v_j \) belong to a same class, \( \sigma \) is an element-wise sigmoid function.

Based on the Homophily principle [23] that assumes similar nodes are likely to be connected, thus we add/remove the edge \( e_{ij} \) in the original adjacency matrix \( A \) if the edge probability \( A_{ij} \) is larger/less than a threshold. Specifically, we add top \( \beta_A |E| \) non-exist (intra-class) edges with highest edge probabilities, and removes the \( \beta_r |E| \) existing (inter-class) edges with lowest edge probabilities, where \( \beta_A, \beta_r \in [0, 1] \).

**Design Discussion.** It is noteworthy that such a design has the following unique advantages: (1) it not only enables long-range propagation of feature-label patterns by decoupling the transformation and propagation steps, but also improve the propagation process by using the learned student model to augment the input graph structure; (2) different from standard self-training paradigm where teacher and student have the same architecture, our decoupled backbone uses a LP module as the teacher and a MLP as student, which is parameter-less and evidently efficient; and (3) previous GST methods need to select unlabeled samples with high confidence as training targets. However, many of these selected predictions are incorrect due to the poor calibration of neural networks [28]. Our approach uses propagated soft pseudo labels to circumvent the process of pseudo label selection.

### 3.2 Augmenting Semantic Knowledge in GST

Despite the effectiveness of the above design, the generated pseudo labels could introduce complex feature patterns and noisy training labels since the teacher model is trained with few labels, which exacerbates the difficulty of learning well-separated decision boundaries. Hence, how to enforce pseudo-labeled nodes to have aligned usage of gold-labeled ones is another important factor for improving the semantic knowledge of GST under the low-data regime.

To this end, we propose a weakly-supervised contrastive loss that mitigates pseudo label noise and enhances semantic structure learning. Specifically, a contrastive loss [4] encourages the similarity function to assign large values to the positive pairs and small values to the negative pairs. With similarity measured by dot product, a form of a contrastive loss function, called InfoNCE [13, 26] has been widely used in self-supervised learning:

\[
\mathcal{L}_{\text{InfoNCE}} = \sum_{i=1}^n - \log \frac{\exp(x_i \cdot \tilde{z}_i/\tau)}{\sum_{j=0}^n \exp(\tilde{z}_i \cdot \tilde{z}_j/\tau)},
\]

where \( \tilde{z}_j \) are positive embedding for \( z_i \), and \( \tilde{z}_j \) includes one positive embedding and \( r \) negative embedding for other instances. Here \( r \) is a temperature hyper-parameter.

Different from the unsupervised contrastive loss [26] which only preserves the local smoothness around each instance, our goal is to
improve the utility of pseudo-labeled nodes to learn better semantic structures of the input graph. To achieve this, we first compute the similarity distribution between pseudo-labeled samples and different class prototypes in the feature space:

\[ s_{ij} = \frac{\exp(z_i \cdot c_j / \tau)}{\sum_{c \in \mathcal{V}_c^U} \exp(z_i \cdot c / \tau)}, \quad c_c = \frac{1}{|\mathcal{V}_c^L|} \sum_{i \in \mathcal{V}_c^L} z_i, \]  

(8)

where \( \mathcal{V}_c^U \) denotes the labeled node set of class \( c \) and \( c_c \) is the corresponding class prototype computed as the average of the labeled examples in class \( c \).

Due to the existence of incorrect pseudo labels, there could be an inconsistency between the latent feature space and the pseudo label space. Here we apply the following rule to obtain a filtered set of pseudo-labeled nodes \( \mathcal{V}_c^U \):

\[ \hat{y}_i > 1/C, \quad \hat{y}_i = \arg \max_j s_{ij}, \]  

(9)

where \( \hat{y}_i \) is the hard pseudo label of node \( v_i \) with the maximum confidence score. For each pseudo-labeled node \( v_i \), we consider it trustworthy if its embedding similarity (to its pseudo-labeled prototype) \( s_{ij} \) is higher than uniform probability, this way we largely reduce the risk of noisy training on hard pseudo labels.

With the calibrated pseudo-labeled node set, next we try to enhance the intra-class compactness and inter-class separability of learned node representations. Specifically, our contrastive loss encourages each node clustering around their corresponding class prototypes, which can be formulated as follows:

\[ L_{CL} = \sum_{v_i \in \mathcal{V}_c^U} -\log \frac{\exp(z_i \cdot c_{\hat{y}_i} / \tau)}{\sum_{c \in \mathcal{V}_c^U} \exp(z_i \cdot c / \tau)}, \]  

(10)

where \( c_{\hat{y}_i} \) denotes the corresponding prototype of node \( v_i \). For any pseudo-labeled node \( v_i \), its embedding, \( z_i \), is treated as the anchor, the embedding of its corresponding class prototype \( c_{\hat{y}_i} \) forms the positive sample, and the embeddings of other class prototypes are naturally regarded as negative samples. This loss will be optimized to reduce the variance of pseudo-labeled nodes that share the same semantic, while pushing away instances from different classes.

For the sake of stable training, we follow the idea of MoCo [13] and use the node representations learned from a momentum encoder parameterized by \( f_p(x) \) to compute the momentum prototype of each class. Note that the momentum encoder has the same architecture as the encoder network, and its parameters are the moving-average of the encoder’s parameters. Formally:

\[ \theta'_i = m \cdot \theta'_{i-1} + (1 - m) \cdot \theta_i, \]  

(11)

where \( m, \theta \), and \( \theta' \) are momentum, encoder parameters, and the momentum encoder parameters, respectively.

### 3.3 Model Training

Given the above focal designs, we train the AGST framework with an iterative learning fashion. In each self-training iteration, the teacher model first generate pseudo labels and we then optimize the student model until converge. Afterwards, the graph structure will be refined by the topology augmentation function and fed to the next iteration.

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**Algorithm 1: The learning algorithm of AGST.**

**Input:** The input graph \( G = (V, E) \) with labeled node set \( V^L \) and unlabeled node set \( V^U \), self-training iterations \( I \)

**Output:** The well-trained student model

1. Initialize the parameters \( \theta \) and \( \phi \)

2. for \( i = 1, 2, \ldots, I \) do

   3. Label Propagation (Teacher)

   4. Generate soft pseudo labels on unlabeled nodes by Eq. (2);

   5. Feature Transformation (Student)

   while not converge do

   6. Compute the classification loss according to Eq. (4), Eq. (5);

   7. Compute the contrastive loss according to Eq. (10);

   8. Update the student model’s parameters by optimizing the joint loss in Eq. (12);

   9. Graph Topology Augmentation

   10. Compute the edge probability matrix using Eq. (6);

   11. Augment the input graph by adding/removing edges

12. return The student model

To train the student model end-to-end, we jointly optimize the classification losses and the weakly-supervised contrastive loss. The full training objective is defined as follows:

\[ L = L_{CE} + \lambda_1 L_{CE}' + \lambda_2 L_{CL}, \]  

(12)

where \( \lambda_1 \) and \( \lambda_2 \) are balancing parameters. According to our preliminary experiments, simply setting the parameters \( \lambda_1 \) and \( \lambda_2 \) as 1 and 0.1 can offer stable and strong performance in practice. By minimizing the training objective, the rich unlabeled data and the scarce yet valuable labeled data work collaboratively to provide additional supervision signals for learning discriminative prediction model.

The detailed learning process of AGST is presented in Algorithm 1. Note that in each iteration, we refine the graph topology based on the original graph structure instead of the previously refined graph, since informative edges might be accidentally removed at the early stage of the training procedure. To reduce computational complexity, we only consider the edge between node \( v_i \) and \( v_j \) as candidate only when they have the same hard labels when adding edges. Further, by refining the graph structure, it is essential to repeat training both the teacher and student models, which connects naturally to the iteration loops in conventional self-training.

### 4 EXPERIMENTS

In this section, we start by introducing the setup of our experiments. Then we conduct experiments on benchmark datasets to show the effectiveness of the proposed framework. Afterwards, we present quantitative results and analysis of different evaluations.

#### 4.1 Experimental Setup

**Evaluation Datasets.** We adopt six graph benchmark datasets to demonstrate the effectiveness of the proposed approach for semi-supervised node classification. Specifically, Cora [29], Citeseer [29], and PubMed [25] are three most widely used citation networks. Coauthor-CS [30] and Coauthor-Physics [30] are two co-authorship graphs based on the Microsoft Academic Graph.
Amazon-Photo [30] is an Amazon product co-purchase networks. The detailed statistics of the datasets are summarized in Table 1.

To provide a robust and fair comparison between different models on each dataset, we conduct evaluation under two low-data settings with different data splitting protocols as follows:

- **Balanced training setting.** Similar to the setting in [21, 30], for each dataset, we sample few (i.e., $K$-shot) labeled nodes per class as the training set, 30 nodes per class as the validation set, and the rest as the test set. We conduct 100 runs for random training/validation/test splits to ensure a fair comparison.

- **Imbalanced training setting.** In this setting, we strictly follow the setup in [17, 31] and randomly split the data into one small sample subset for training, and the test sample subset with 1000 samples. Following this line of work, we report the mean accuracy of 10 runs without validation to make fair comparison.

### Compared Methods

In the experiments, we compare our approach AGST with both classic and state-of-the-art methods for evaluating the semi-supervised node classification task, including:

- **LP** (Label Propagation) [45] is a classical semi-supervised learning algorithm. It iteratively assigns labels to the unlabeled nodes by propagating the labels through the graph.

- **GCN** [14] is a widely used graph neural network, and it learns node representations based on the first-order approximation of spectral graph convolutions.

- **GAT** [33] employs parameterized attention mechanism to specify fine-grained weights for neighborhood aggregation.

- **SGC** [37] is a linear model reduces the unnecessary complexity of GCN by successively collapsing the convolution functions between consecutive layers into a linear transformation.

- **APPNP** [15] decouples prediction and propagation with performing personalized propagation of neural predictions.

- **GLP and IGCN** [18] are two models combine label propagation and GCN from a unifying graph filtering perspective.

- **PTA** [11] is a LP-based graph self-training method with a dynamic and adaptive weighting strategy.

- **Co-train and Self-train** [17] are two frameworks that leverage pseudo labels on unlabeled nodes. Co-train uses ParWalks [38] to select the most confident nodes and add their pseudo labels to the labeled data to train GCN. While Self-train selects the pseudo node labels from GCN to boost the model performance. Moreover, **Union and Intersection** takes the union or intersection of the pseudo labels generated by Co-train and Self-train, respectively. For simplicity, here we use ST-GCNs to represent the best performing model of those four variants.

- **MSS** [31] leverages clustering method to select confident pseudo labels assigned by GCN for training the student model.

It is noteworthy that GCN, GAT, SGC are three conventional GNN baselines, while GLP, IGCN and APPNP can be categorized as deep GNN models. In addition, and PTA, ST-GCNs (and its variants), and MSS are GST methods, which are the most related to our work. We didn’t include some very recent works in evaluation such as [34] and [20] since their codes are not released.

### Parameter & Implementation

For the label propagation module in AGST, we use $T = 10$ propagation steps and set $\alpha = 0.9$ by default. As suggested by [11, 15], we use $\alpha = 0.8$ for the two co-authorship graphs due to their structural difference. We use a 2-layer MLP with 64 hidden units to build the student model. The learning rate is set to 0.01 and we apply L2 regularization with $\lambda = 0.005$ on the weights of the first neural layer and set the dropout rate for both neural layers to be 0.5. A momentum of 0.9 is used in the momentum encoder, and the temperature $\tau$ in contrastive loss is 0.2. The self-training iteration of AGST is set to 3 for all the datasets. We apply grid search for the augmentation hyper-parameters $\beta_0, \beta_r \in [0, 1]$ with a constant interval of 0.1. All hyper-parameters are fine-tuned based on the validation set unless otherwise specified. For other baseline methods, we adopt their public code and tune hyper-parameters for the best performance. All the results are reported as the mean accuracy of multiple runs for a fair comparison. More details about baselines and the implementation can be found in Appendix A.1.

### 4.2 Main Results

In our experiments, we evaluate the proposed framework AGST and all the baseline methods on semi-supervised node classification task in low-data settings, which aims to predict the missing node labels with only a few labeled nodes.

#### Balanced Training Setting

We first compare the proposed framework AGST with baseline methods under the canonical few-shot semi-supervised setting, in which each node class is provided with few labeled samples. We run each model with 3, 5, 10 labeled nodes per class (i.e., 3-shot, 5-shot, and 10-shot) and report the average test accuracy under such balanced training setting in Table 2. According to the reported results, we are able to make the following in-depth observations and analysis:

- Overall, AGST significantly outperforms all the baseline methods on each dataset based on the paired $t$-tests with $p < 0.05$. For example, AGST improves the best performing baseline model (i.e., APPNP) on Cora obtains an 5.92% improvement in 5-shot evaluation. This observation further proves that the design of AGST is effective for tackling the node classification problem when only few labels per class are given.

- Both deep GNNs and GST methods can achieve better performance over the shallow GNNs such as GCN and GAT when training data is extremely scarce. While compared to the deep GNNs, existing GST methods cannot achieve better performance in most cases, which verifies our claim that their shallow backbones largely restrict the effective propagation of label signals. Our framework AGST adopts a decoupled backbone that inherits the advantages of both deep GNN models and GST methods, which is more data-efficient.

### Table 1: Summary statistics of the evaluation datasets.

| Dataset       | # Nodes | # Edges | # Features | # Classes |
|---------------|---------|---------|------------|-----------|
| Cora          | 2,708   | 5,278   | 1,433      | 7         |
| CiteSeer      | 3,327   | 4,552   | 3,703      | 6         |
| PubMed        | 19,717  | 44,324  | 500        | 3         |
| Coauthor-CS   | 18,333  | 81,894  | 6,805      | 15        |
| Coauthor-Physics | 34,493 | 247,962 | 8,415      | 5         |
| Amazon-Photo  | 7,487   | 119,043 | 745        | 8         |

#### Accuracy Comparison

In the experiments, we compare our approach AGST with both classic and state-of-the-art methods for evaluating the semi-supervised node classification task, including:

- **MSS** [31] leverages clustering method to select confident pseudo labels assigned by GCN for training the student model.

It is noteworthy that GCN, GAT, SGC are three conventional GNN baselines, while GLP, IGCN and APPNP can be categorized as deep GNN models. In addition, and PTA, ST-GCNs (and its variants), and MSS are GST methods, which are the most related to our work. We didn’t include some very recent works in evaluation such as [34] and [20] since their codes are not released.

#### Parameter & Implementation

For the label propagation module in AGST, we use $T = 10$ propagation steps and set $\alpha = 0.9$ by default. As suggested by [11, 15], we use $\alpha = 0.8$ for the two co-authorship graphs due to their structural difference. We use a 2-layer MLP with 64 hidden units to build the student model. The learning rate is set to 0.01 and we apply L2 regularization with $\lambda = 0.005$ on the weights of the first neural layer and set the dropout rate for both neural layers to be 0.5. A momentum of 0.9 is used in the momentum encoder, and the temperature $\tau$ in contrastive loss is 0.2. The self-training iteration of AGST is set to 3 for all the datasets. We apply grid search for the augmentation hyper-parameters $\beta_0, \beta_r \in [0, 1]$ with a constant interval of 0.1. All hyper-parameters are fine-tuned based on the validation set unless otherwise specified. For other baseline methods, we adopt their public code and tune hyper-parameters for the best performance. All the results are reported as the mean accuracy of multiple runs for a fair comparison. More details about baselines and the implementation can be found in Appendix A.1.

### 4.2 Main Results

In our experiments, we evaluate the proposed framework AGST and all the baseline methods on semi-supervised node classification task in low-data settings, which aims to predict the missing node labels with only a few labeled nodes.

#### Balanced Training Setting

We first compare the proposed framework AGST with baseline methods under the canonical few-shot semi-supervised setting, in which each node class is provided with few labeled samples. We run each model with 3, 5, 10 labeled nodes per class (i.e., 3-shot, 5-shot, and 10-shot) and report the average test accuracy under such balanced training setting in Table 2. According to the reported results, we are able to make the following in-depth observations and analysis:

- Overall, AGST significantly outperforms all the baseline methods on each dataset based on the paired $t$-tests with $p < 0.05$. For example, AGST improves the best performing baseline model (i.e., APPNP) on Cora obtains an 5.92% improvement in 5-shot evaluation. This observation further proves that the design of AGST is effective for tackling the node classification problem when only few labels per class are given.

- Both deep GNNs and GST methods can achieve better performance over the shallow GNNs such as GCN and GAT when training data is extremely scarce. While compared to the deep GNNs, existing GST methods cannot achieve better performance in most cases, which verifies our claim that their shallow backbones largely restrict the effective propagation of label signals. Our framework AGST adopts a decoupled backbone that inherits the advantages of both deep GNN models and GST methods, which is more data-efficient.

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**Table 1: Summary statistics of the evaluation datasets.**

| Dataset       | # Nodes | # Edges | # Features | # Classes |
|---------------|---------|---------|------------|-----------|
| Cora          | 2,708   | 5,278   | 1,433      | 7         |
| CiteSeer      | 3,327   | 4,552   | 3,703      | 6         |
| PubMed        | 19,717  | 44,324  | 500        | 3         |
| Coauthor-CS   | 18,333  | 81,894  | 6,805      | 15        |
| Coauthor-Physics | 34,493 | 247,962 | 8,415      | 5         |
| Amazon-Photo  | 7,487   | 119,043 | 745        | 8         |
Table 2: Results of semi-supervised node classification with few labels (balanced training setting): mean accuracy (%) with 95% confidence interval.

| Method | Coauthor CS | Coauthor Physics | Amazon Photo |
|--------|-------------|------------------|-------------|
|        | 3-shot | 5-shot | 10-shot | 3-shot | 5-shot | 10-shot | 3-shot | 5-shot | 10-shot |
| LP     | 57.7 ± 0.77 | 62.09 ± 0.60 | 66.18 ± 0.36 | 73.46 ± 0.93 | 76.94 ± 0.61 | 80.55 ± 0.41 | 69.24 ± 0.92 | 73.43 ± 0.72 | 77.78 ± 0.61 |
| GCN    | 77.17 ± 0.79 | 84.09 ± 0.59 | 89.01 ± 0.98 | 82.49 ± 0.88 | 87.50 ± 0.69 | 90.78 ± 0.38 | 69.54 ± 0.99 | 74.42 ± 0.97 | 80.30 ± 0.78 |
| GAT    | 79.66 ± 0.75 | 85.11 ± 0.49 | 89.34 ± 0.19 | 86.07 ± 1.16 | 89.35 ± 0.48 | 91.64 ± 0.48 | 70.47 ± 1.19 | 77.89 ± 1.05 | 82.93 ± 1.11 |
| SGC    | 84.93 ± 0.57 | 88.11 ± 0.85 | 90.13 ± 0.99 | 87.55 ± 0.64 | 87.68 ± 0.39 | 91.38 ± 0.31 | 75.05 ± 0.88 | 78.73 ± 0.69 | 84.14 ± 0.45 |
| GLP    | 84.58 ± 0.61 | 87.36 ± 0.61 | 91.59 ± 0.15 | 89.34 ± 0.99 | 91.52 ± 0.32 | 93.02 ± 0.20 | 75.11 ± 1.19 | 81.99 ± 0.97 | 85.33 ± 0.38 |
| IGCN   | 84.26 ± 0.47 | 86.45 ± 0.33 | 90.82 ± 0.13 | 89.82 ± 0.57 | 91.33 ± 0.29 | 92.78 ± 0.21 | 75.36 ± 0.98 | 82.10 ± 0.89 | 85.50 ± 0.32 |
| APPNP  | 88.96 ± 0.37 | 90.14 ± 0.27 | 91.37 ± 0.14 | 90.00 ± 0.48 | 91.76 ± 0.33 | 92.56 ± 0.22 | 82.25 ± 0.99 | 84.74 ± 0.63 | 87.78 ± 0.44 |
| PTA    | 86.56 ± 0.46 | 89.43 ± 0.31 | 90.72 ± 0.18 | 88.62 ± 0.60 | 90.36 ± 0.53 | 92.15 ± 0.32 | 77.43 ± 0.89 | 82.63 ± 0.76 | 85.51 ± 0.74 |
| ST-GCNs| 88.34 ± 0.46 | 89.68 ± 0.45 | 91.39 ± 0.14 | 87.61 ± 0.69 | 90.23 ± 0.39 | 91.75 ± 0.21 | 73.86 ± 1.53 | 81.93 ± 1.09 | 85.54 ± 0.67 |
| M3S    | 84.11 ± 0.46 | 86.96 ± 0.41 | 91.08 ± 0.11 | 89.12 ± 0.55 | 91.27 ± 0.31 | 92.91 ± 0.25 | 74.96 ± 0.97 | 81.88 ± 0.93 | 85.42 ± 0.37 |
| AGST   | 90.29 ± 0.33 | 91.31 ± 0.37 | 92.76 ± 0.12 | 92.86 ± 0.62 | 93.04 ± 0.47 | 94.37 ± 0.24 | 85.08 ± 0.89 | 86.53 ± 0.92 | 89.27 ± 0.62 |

• Though LP only relies on structure information, it can perform competitively with shallow GNNs on some datasets when training labels are extremely limited, such as Cora and PubMed. However, we also notice that LP become the worst performing method on datasets like CiteSeer and Coauthor CS. The main reason behind is that noisy graph structure could easily lead to incorrect propagation of label signals, which verifies the rationality and necessity of refining the graph topology in GST.

Imbalanced Training Setting. Furthermore, we follow the imbalanced training setting used in [17, 31] and conduct another set of experiments where each model is trained with different label rates, i.e., 0.5%, 1%, 2%, 3% on Cora and CiteSeer, 0.03%, 0.05%, 0.1% on PubMed. Composed to the balanced training setting, this evaluation setting is more challenging since the training labels for each class could varies a lot. We report the average accuracy on three datasets in Table 3. For a fair comparison, the results of baseline methods are borrowed from the previous work [31].

• Similar to the balanced training setting, GCN that only uses limited receptive fields cannot achieve satisfactory results when labeled data is scarce and imbalanced. By incorporating pseudo labels into the learning process, methods including Co-train, Self-train, Union and Intersection are able to improve the performance of GCN with only few labels.

• However, the performance of those baselines based on pseudo-labeling varies a lot under different datasets, which shows that it is practically difficult to select informative pseudo labels and mitigate the pseudo label noise. Though M3S partially address this by using the clustering methods, it still largely falls behind our approach due to the inability of leveraging large receptive fields and handling structure noise.

• Compared to the original LP, the teacher model in the proposed AGST framework achieves better performance, even though they both use the same label propagation algorithm. It demonstrates that the graph structure can be well refined by our graph topology augmentation function. Based on both labeled and unlabeled data, the student model further pushes forward the performance by performing feature transformation and weakly-supervised contrastive learning.

Standard (20-shot) Training Setting. To make our evaluation more comprehensive, we then examine the performance of AGST under the standard semi-supervised node classification tasks. Specifically, we randomly sample 20 labeled nodes for each class (i.e., 20-shot) as the training set and test the performance of different methods. According to the average performance reported in Table 4, we can observe that: (1) the performance gain of GST methods over the vanilla GNNs decreases since the standard training setting has more labeled data; (2) though AGST is mainly proposed for few-shot
Table 4: Test accuracy on standard (20-shot) node classification: mean accuracy (%) with 95% confidence interval.

| Method   | Cora-ML | CiteSeer | PubMed | MS-CS |
|----------|---------|----------|--------|-------|
| LP       | 67.04 ± 0.41 | 45.29 ± 0.34 | 69.78 ± 0.54 | 72.24 ± 0.24 |
| GCN      | 77.85 ± 0.33 | 65.95 ± 0.42 | 76.33 ± 0.47 | 90.92 ± 0.11 |
| GAT      | 76.85 ± 0.34 | 65.12 ± 0.72 | 73.20 ± 0.49 | 90.39 ± 0.98 |
| SGC      | 71.19 ± 0.29 | 69.20 ± 0.37 | 72.13 ± 0.66 | 91.03 ± 0.21 |
| GLP      | 79.33 ± 0.27 | 68.94 ± 0.28 | 78.49 ± 0.39 | 82.53 ± 0.29 |
| IG-CN    | 80.11 ± 0.31 | 67.89 ± 0.29 | 78.64 ± 0.39 | 83.30 ± 0.23 |
| APPNP    | 80.58 ± 0.35 | 69.08 ± 0.38 | 78.81 ± 0.39 | 91.99 ± 0.10 |
| ST-GCNs  | 79.75 ± 0.24 | 70.26 ± 0.23 | 78.12 ± 0.30 | 91.61 ± 0.11 |
| M3S      | 78.11 ± 0.39 | 70.42 ± 0.29 | 77.98 ± 0.29 | 91.90 ± 0.18 |
| PTA      | 81.54 ± 0.35 | 69.84 ± 0.25 | 78.66 ± 0.44 | 92.51 ± 0.15 |
| Meta-PN  | 82.57 ± 0.22 | 71.52 ± 0.11 | 79.92 ± 0.27 | 93.27 ± 0.13 |

4.3 Ablation Study

In this section, we further conduct ablation studies to demonstrate the contribution of each component in AGST and justify our architectural design choice. Here *AGST-base* denotes the decoupled GST backbone of our framework. Meanwhile, we include another two variants by removing each of the other two key designs in the proposed framework. Specifically, *w/o contrast* represent the variant of AGST that excludes the weakly-supervised contrastive loss, and *w/o augment* is the variant without the graph topology augmentation function. Compared to the complete framework AGST, *w/o contrast* loses part of the semantic knowledge and *w/o augment* loses part of the structural knowledge.

We report the accuracy results of each variant (balanced training) on two datasets Cora, CiteSeer in Figure 2. Similar results are observed for other datasets and we omit here due to the space limit. It is apparent that the classification accuracy will decrease when any one of the focal components is removed, which reveals that both the weakly-supervised contrastive loss and the graph topology augmentation function make essential contributions to boosting the model performance. Meanwhile, compared to the conventional GNNs in Table 3, the backbone of AGST, i.e., *AGST-base* is able to achieve better classification performance. Meanwhile, by comparing *w/o augment* with *AGST-base*, we can see that our contrastive loss brings further improvements. Notably, the importance of the topology augmentation function varies on different datasets, it usually have larger contribution on datasets with noisy graph structures, such as CiteSeer.
4.4 Parameter Analysis

We explore the sensitivity of the model performance in terms of two important hyper-parameters $\lambda_1$ and $\lambda_2$, which are in the final objective function of AGST. $\lambda_1$ controls the contribution of the cross-entropy loss on pseudo labels (i.e., $L^{CE}$) and $\lambda_2$ controls the contribution of weakly-supervised contrastive loss (i.e., $L^{CL}$). Specifically, we vary the values of $\lambda_1$ and $\lambda_2$ as $\{0.005, 0.01, 0.05, 0.1, 0.5, 1, 5\}$ on the Cora and Citeseer datasets and report the results of AGST in Figure 3. As we can see from the figure, the performance of AGST goes up when we increase the value of $\lambda_1$ and reach the peak when $\lambda_1 = 1$. For $\lambda_2$, the best-performing value is 0.1. The performance will decrease if the value is either too large or too small. We have aligned observations with other datasets. The analysis about other hyper-parameters is presented in the Appendix A.2.

5 CONCLUSION

In this paper, we introduce an augmented graph self-training framework (AGST) to solve the problem of semi-supervised node classification under the low-resource setting. Specifically, our approach goes beyond the existing GST architectures and improve the model performance by augmenting the structural and semantic knowledge using only few labeled nodes. The empirical results over various benchmark datasets demonstrate the effectiveness of our proposed framework versus the baseline methods in node classification with few labels. For future work, one challenging direction is to explore other graph augmentation methods in our AGST framework for non-homophily graphs.

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A APPENDIX

A.1 Implementation Details

AGST. We implement the proposed AGST in PyTorch with a 12 GB Titan Xp GPU. Specifically, we use two-layer MLP with 64 hidden units for the feature transformation module. We optimize the model with Adam optimizer and grid search for the edge addition/removal ratio in \( \{0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0\} \). The optimal values are selected when the model achieve the best performance for validation set. The early stopping criterion uses a patience of \( p = 100 \) and an (unreachably high) maximum of \( n = 10,000 \) epochs. The patience is reset whenever the accuracy increases or the loss decreases on the validation set.

Baselines. In our experiments, we compare our approach with different methods including, LP, GCN, GAT, SGC, GLP, IGCN, APPNP, ST-GCNs, M3S and PTA. For the baseline methods, we adopt their public implementations and the details are as follows:

- LP [45]: For fair comparison, we use the same propagation step \( T = 10 \) and the teleport probability as Meta-LP.
- GCN\(^2\) [14]: We build the GCN model with two graph convolutional layers (64 dimensions) for learning node representations in the graph.
- GAT\(^3\) [33]: The model consists of two graph attentional layers with 8 heads and the negative input slope of the LeakyReLU function is 0.2 as suggested in the paper.
- SGC\(^4\) [37]: After the feature pre-processing step, it learns the node representations with 2-layer feature propagation with 64 hidden units.
- GLP & IGCN\(^5\) [18]: It uses a two-layer structure (64 hidden units) in which the filter parameters \( k \) and \( \alpha \) is set to be 5 and 10 for 20-shot, and is set to be 10 and 20 for all the other tasks. The results with the best performing filter (i.e., RNM or AR) are reported.
- APPNP\(^6\) [15]: Similar to Meta-LP, we use the 2-layer MLP (64 hidden units), with 10 steps of propagation. For the best performance, we set the teleport probability \( \alpha = 0.1 \) for the citation graphs and use \( \alpha = 0.2 \) for the co-authorship graph due to their structural difference.
- PTA\(^7\) [11]: For fair comparison, we use the same neural network model as AGST, which is a two-layer MLP with 64 hidden units.
- ST-GCNs\(^8\) [17]: It represents four variants: Co-train, Self-train, Union and Intersection. We use ST-GCNs to report the results of the best performing framework.
- M3S\(^9\) [31]: We fix the number of clusters as 200 and select the best number of layers and stages as suggested by the authors.

A.2 Additional Results

Propagation Steps. To demonstrate the effects of using different propagation steps, we compare our approach with two baselines (i.e., LP and GCN) under the 5-shot setting with varying number of \( T \). As shown in Figure 4, we can clearly see that GCN encounters performance degradation if we largely increase the number of propagation steps. Though LP is a naive baseline, its performance increases by using larger propagation steps. Our framework AGST adopts a decoupled backbone where label propagation serves as the teacher model, thus it is able to address the oversquashing issue and leverage large receptive fields. AGST achieve stable performance when the propagation step \( T > 5 \).

Topology Augmentation. We further examine the impact of two hyper-parameters in our graph topology augmentation module, i.e. the edge addition ratio \( \beta_a \) and the edge removal ratio \( \beta_r \) for refining the graph structure. Figure 5 shows the performance change (5-shot) on the Cora dataset by varying the value of each parameter, with a constant interval of 0.1. We also add the performance of AGST as reference. We observe that our graph topology augmentation function improves performance by either adding or removing edges within an appropriate range to mitigate the structure noise. For instance, the accuracy is first boosted by adding edges, then it reaches the peak until \( \sim 40\% \) and become stable throughout the range. Similarly, edge removal improves performance until \( \sim 20\% \), then the accuracy decreases quickly. One explanation is that a higher threshold may result in the accidental removal of possibly useful intra-class edges.

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1. https://github.com/tkipf/pygcn
2. https://www.dgl.ai/
3. https://github.com/Tiiiger/SGC
4. https://github.com/ligmai/Efficient-SSL
5. https://github.com/klicperajo/ppnp
6. https://github.com/LiangMa/AGST
7. https://github.com/Tiiiger/SGC
8. https://github.com/datake/M3S
9. https://github.com/DongHande/PT_propagation_then_training

Figure 4: Parameter analysis for propagation steps T.

Figure 5: Parameter analysis \((\beta_a, \beta_r)\) on Cora (5-shot).