Active Learning for Node Classification: The Additional Learning Ability from Unlabelled Nodes

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ABSTRACT

Node classification on graph data is an important task on many practical domains. However, it requires labels for training, which can be difficult or expensive to obtain in practice. Given a limited labelling budget, active learning aims to improve performance by carefully choosing which nodes to label. Our empirical study shows that existing active learning methods for node classification are considerably outperformed by a simple method which randomly selects nodes to label and trains a linear classifier with labelled nodes and unsupervised learning features. This indicates that existing methods do not fully utilize the information present in unlabelled nodes as they only use unlabelled nodes for label acquisition. In this paper, we utilize the information in unlabelled nodes by using unsupervised learning features. We propose a novel latent space clustering-based active learning method for node classification (LScale). Specifically, to select nodes for labelling, our method uses the K-Medoids clustering algorithm on a feature space based on the dynamic combination of both unsupervised features and supervised features. In addition, we design an incremental clustering module to avoid redundancy between nodes selected at different steps. We conduct extensive experiments on three public citation datasets and two co-authorship datasets, where our proposed method LSCALE consistently and significantly outperforms the state-of-the-art approaches by a large margin.

KEYWORDS

graph representation learning, active learning, node classification, unsupervised learning

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1 INTRODUCTION

Node classification on graphs has attracted much attention in the graph representation learning area. Existing methods [2, 7, 13, 31] for node classification are usually employed under the semi-supervised setting, where labels are only available for a few nodes.

In reality, labels, which are required for the semi-supervised node classification task, are often difficult and expensive to collect. To ease this problem, active learning aims to select the most informative nodes which can lead to a better classification accuracy using the same number of labelled nodes. In some applications such as medical image analysis and drug discovery, label acquisition requires intensive domain knowledge and costs a considerable amount of time. The effectiveness of active learning in these fields has been demonstrated in [9, 10, 21]. Recently, graph neural networks (GNNs) have also been used in medical and biological fields for many applications [4, 11, 19] including disease predictions and drug discovery. Thus, these applications motivate research into active learning for node classification on graphs.

Recently, a few active learning methods based on graph convolutional neural networks (GCNs) [13] have been proposed for node classification task on graphs [1, 3, 32]. However, their performance is still less than satisfactory. To demonstrate this, we present an unexpected experimental finding in Section 4. We show that the state-of-the-art active learning methods for node classification [1, 3, 32] can be outperformed by a simple method. This method, firstly obtains unsupervised features by a simple unsupervised model, i.e., Deep Graph Infomax (DGI) [30]; then it randomly selects nodes to label; finally it trains a logistic regression using labelled nodes with unsupervised features. This finding verifies that the performance of the existing active learning methods for node classification is still not good enough and this topic is still under-explored. More importantly, this finding demonstrates the potential power of unlabelled data in active learning for node classification.

Among existing approaches, AGE [1] and ANRMAB [3] select corresponding informative nodes to label based on the hidden representations of GCNs and graph structures. The hidden representations of GCNs can be updated only based on the labelled data. On the other hand, FeatProp [32] is a clustering-based algorithm which uses propagated node features to select nodes to label. However, these propagated node features are generated in a fixed manner based on the graph structure and node features, and are not learnable. In summary, the unexpected results in our finding indicates that all these existing approaches do not fully utilize the information present in unlabelled nodes. Using unsupervised graph
learning, nodes without labels can be used to directly generate node representations, which can be more informative and accurate. The more accurate representations can be further helpful for selecting more informative nodes in active learning.

Motivated by the limitations of the state-of-the-art methods and our experimental finding, in this work, we propose a novel and effective Latent Space Clustering-based Active Learning framework (LSCALE)\(^1\). In this framework, we first use DGI [30] on all nodes without label information to generate unsupervised learning features. We design a novel distance-based classifier to classify nodes, where supervised hidden representations are learned based on the classification loss. To select nodes for querying labels, we use the K-Medoids clustering algorithm to select cluster centers. The distances between different nodes used in clustering are calculated based on a dynamic combination of unsupervised learning features and learnable supervised representations. In this way, we can utilize the learned unsupervised features, while still deciding which nodes to query labels based on supervised features through the active learning process. In contrast, FeatProp [32], which is also a clustering-based active learning method, uses a fixed approach to propagate node features before clustering. Thus, it cannot learn a suitable space for classification and active learning, which is a drawback we address in this work.

As in [23, 32], we consider the batch setting in our method, where multiple nodes are selected in each node selection step. It is also conventional to consider multiple rounds of selection [23, 24]. However, other clustering-based active learning methods like [23, 32] only select nodes in multiple rounds with a myopic approach to propagate node features before clustering. Thus, it cannot learn a suitable space for classification and active learning, which is a drawback we address in this work.

The contributions in this paper are summarized as follows:

- We present an unexpected experimental finding, showing that the performance of state-of-the-art active learning methods for node classification is less than satisfactory and they can be outperformed by a simple unsupervised learning method.
- We propose a latent space clustering-based active learning framework (LSCALE) for node classification on graphs, which combines unsupervised learning features and supervised hidden representations throughout the whole process.
- We design an incremental clustering strategy to ensure that newly selected nodes are not redundant with previous nodes, which further improves the performance.
- We conduct comprehensive experiments on three public citation datasets and two co-authorship datasets. The results show that our method provides a consistent and significant performance improvement compared to the state-of-the-art active learning methods for node classification.

The rest of this paper is organized as follows. In Section 2, we review existing work on active learning and unsupervised learning on graphs. In Section 3, we introduce the problem definition in this work and DGI method which we adopt in our framework. Our proposed latent space clustering-based active learning method (LSCALE) for node classification is elaborated in Section 5, followed by experimental results and analysis in Section 6. Finally, we conclude this paper in Section 7.

2 RELATED WORK

2.1 Active learning

Before the advances in deep learning of the past few years, active learning has been extensively studied and most of the early work are summarized in [24], which covers several types of methods such as uncertainty based methods [14, 29] and query-by-committee approaches [16, 25]. A comprehensive empirical study of different active learning methods for classification using the logistic regression model is provided in [34], which shows uncertainty sampling methods [14] perform exceptionally well on plenty of diverse datasets.

Some methods are designed for neural networks in recent years. Core-set [23] is proposed to select examples by core-set selection based on distances of the last-layer activation in a convolutional neural network. Inspired by adversarial learning, in [5, 27], a binary classifier is trained to make the labelled set indistinguishable with the unlabelled pool. These methods are not for graph data, while we only focus on graph data in this paper.

The effectiveness of using graph convolutional neural networks (GCNs) [13] on active learning for node classification are claimed in recent work [1, 3, 32], which are most closely related to our work. In AGE [1], they use the output of GCN to design three active learning metrics, namely the uncertainty metric, the graph centrality, and the information density metric. The uncertainty metric tends to select the node which the current model is least certain by using the entropy of the softmax output of the GCN model, while the information density metric aims to find a node which is “representative” in the embedded space. The graph centrality uses the pagerank scores [18] of nodes, which is independent with the GCN model. The active selecting strategy is based on a score which is a weighted sum of these three metrics. In each iteration, the node with the highest score is selected for querying the label and added to training set. During the whole process, the weights of different metrics change via time-sensitive parameters through. The same three metrics are also considered in ANRMB [3]. However, they design a multi-armed bandit method with a reward scheme to adaptively assign weights for the different metrics. They claim this method can satisfy different datasets with different characteristics. Inspired by the core-set approach [23], another clustering-based active learning method for graphs FeatProp is proposed in [32]. It calculates the distances between nodes by the last-layer representations of the simplified GCN model [31] and conducts a clustering algorithm for selecting representative nodes. Instead of using K-Center algorithm, it chooses K-Medoids as the clustering algorithm. Meanwhile, it claims that K-Medoids with propagated node features can achieve a lower loss bound than K-Center.

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\(^1\)The source code will be released upon acceptance.
2.2 Unsupervised learning on graphs

Many algorithms for unsupervised representation learning with graph data highly rely on random-walk based objectives [6, 7, 20, 28, 33]. The intuition of using random-walk based objectives is that nodes which are close in the original graph should also be close in the representation space. DeepWalk [20] and node2vec [6] only learn node representations on non-attributed graphs, while disparate nodes have highly distinct representations. Different from random-walk based methods, DGI [30] relies on maximizing the mutual information between node representations and the embedding vector of the whole graph.

3 PRELIMINARIES

In this section, we provide the problem definition of active learning for node classification. The main notations used in the paper are summarized in Table 1. Then we introduce Deep Graph Infomax (DGI) [30] which we adopt in our framework.

3.1 Problem Definition

We are given a graph $G = (V, E)$, where $V$ and $E$ represent the set of nodes and edges respectively. We define the input node attribute matrix as $X \in \mathbb{R}^{n \times d}$, $n = |V|$ denotes the number of nodes and $d$ is the number of dimensions of node attributes. In node classification, we have a one-hot label vector $y_v$ for each node $v$. The label matrix for labelled nodes are constructed as $Y$. For node classification, we are required to build a model $M$ which maps the inputs $(G, X)$ to the predictions $\hat{Y}$ and minimize a loss function $L(M|G, X, Y)$ over the inputs $(G, X, Y)$.

Initially given the graph $G$ and input feature matrix $X$, an active learning strategy $\mathcal{A}$ selects a node subset $S^t \subseteq U^{t-1}$ for querying the labels $y_v$ for each node $v \in S^t$ in each step $t$ ($t \geq 1$). After getting the new set of labelled nodes $S^t$, we obtain a set of all labelled nodes $L^t = S^t \cup L^{t-1}$ and a set of unlabelled nodes $U^t = U^{t-1} \setminus S^t$ prepared for the next iteration. Then $G$ and $X$ with labels $y_v$ of $v \in L^t$ are used as training data to train a model $M$ at the end of each step $t$. We define the labelling budget $b$ as the total maximum number of nodes which are allowed to be labelled. The eventual goal is to maximize the performance of the node classification task under the budget $b$. At each step $t$, the objective of graph active learning is to minimize the loss using all labelled nodes $L^t$: 

$$\min_{L^t} L(M, \mathcal{A}|G, X, Y)$$

(1)

3.2 Deep Graph Infomax

Deep Graph Infomax (DGI) maximizes local mutual information to learn node representations which capture the global information of the entire graph. The encoder is defined as a one-layer GCN to generate the node representations:

$$E(X, A) = \sigma(\hat{D}^{-\frac{1}{2}} A \hat{D}^{-\frac{1}{2}} X \Theta_{enc}),$$

(2)

where $\hat{A} = A + I_N$ is the adjacency matrix with self-loops while $\Theta_{enc} \in \mathbb{R}^{d \times d'}$ is the weight matrix. The degree matrix $\hat{D}$ is constructed as a diagonal matrix: $\hat{D}_{ii} = \sum_j \hat{A}_{ij}$. The parametric ReLU [8] is used as the nonlinearity function $\sigma$. $E(X, A) = H = [h_1, h_2, ..., h_M]$ represents the node representation $h_i$ for each node $i$. The graph-level representation $s$ is obtained through a readout function $\mathcal{R}$:

$$s = \mathcal{R}(H) = \sigma\left(\frac{1}{N} \sum_{i=1}^{N} h_i\right)$$

(3)

To maximize the local mutual information, a discriminator $\mathcal{D}(h_i, s)$ outputs a score indicating the probability of this node representation is contained within the graph-level representation. It is defined by a simple bilinear function:

$$\mathcal{D}(h_i, s) = \sigma(h_i^T W s),$$

(4)

where $W$ is a trainable weight matrix and $\sigma$ is the sigmoid function.

In order to learn how to distinguish whether a node belongs to the graph, the model requires negative samples. Negative samples of node representations $\tilde{h}_i$ are obtained by passing the corrupted node attributes $\tilde{X}$ through the encoder $E$:

$$\tilde{H} = E(\tilde{X}, A) = [\tilde{h}_1, \tilde{h}_2, ..., \tilde{h}_M],$$

(5)

where the corrupted features $\tilde{X}$ are obtained by row-wise shuffling of $X$. The objective is a binary cross-entropy loss between the positive examples and the negative examples, defined as follows:

$$L_{DGI} = \frac{1}{N + M} \left(\sum_{i=1}^{N} \log \mathcal{D}(h_i, s) + \sum_{j=1}^{M} \log \left(1 - \mathcal{D}(\tilde{h}_j, s)\right)\right),$$

(6)

where $N, M$ are the numbers of positive and negative samples respectively. The model updates the parameters by maximizing the objective function and, resulting in unsupervised representations $H$.

4 INEFFECTIVENESS OF UTILIZING UNLABELLED NODES: AN EXPERIMENTAL FINDING

In this section, we share an unexpected experimental finding which suggests that current state-of-the-art active graph learning methods are not effective enough. This unexpected finding also inspires us to form a new method where we use a latent space for active learning, which combines unsupervised and supervised learning.

Unsupervised learning shares the similar motivation with active learning of mitigating the lack of labelled data. Due to this, we design experiments to compare the performance of an unsupervised
learning method which randomly selects nodes for labelling, and the state-of-the-art active graph learning methods on a same setting for node classification. In our designed method, we use Deep Graph Infomax (DGI) [30] to obtain unsupervised features; then randomly select nodes for labelling; finally train a logistic regression with labelled nodes and unsupervised features.

Through experiments, we surprisingly find that the designed method (DGI_Rand) already outperforms all current state-of-the-art methods [1, 3, 32] on Cora, Citeseer [22], Pubmed [17], and 2 co-authorship datasets. For simplicity, we only show the comparison on the Cora dataset in Figure 1. DGI_Rand performs much better than all three state-of-the-art active graph learning methods (FeatProp [32], AGE [1], ANRMAB [3]), especially in the early stages when the number of labelled nodes is relatively small. We postpone the details of experiments and datasets used in this finding to Section 6. Similar phenomena are found on other datasets, as shown in Section 6.

Based on the results, we conjecture that the inferior performance of previous graph active learning methods comes from not fully harnessing the unlabelled nodes. For previous graph active learning methods, they only use unlabelled nodes for selecting new nodes to label without considering representation power which can be obtained from unlabelled nodes alone. In contrast, unsupervised learning focuses on utilizing only unlabelled nodes and their attributes to generate good node representations, which can be useful for selecting nodes in active learning.

To conclude this unexpected finding, a desirable active graph learning method should at least outperform the sole DGI with randomly selected labelled nodes. So in this paper, we aim to design a method to learn a latent space, which combines unsupervised learning and supervised learning. Clustering is conducted based on the distances to select informative nodes. We also propose an incremental clustering method to prevent that the newly selected nodes are redundant with the previously selected nodes. After receiving the labels of selected nodes at each step, we train the classifier using all the labelled nodes.

5 METHODOLOGY

In this section, we introduce our active learning framework LSCALE for node classification in a top-down fashion. First, we describe the overview of LSCALE. Then we provide the details of each module used in LSCALE.

Figure 1: The comparison of the designed method (DGI_Rand) and other state-of-the-art active learning algorithms on the Cora dataset.

The overview of our latent space clustering-based active learning framework is shown in Figure 2. The framework contains a few main components:

- a unsupervised graph learning method to generate unsupervised node representations.
- a classifier for node classification. When the labels of selected nodes are collected, the classifier is trained for node classification based on all labelled nodes.
- a distance function to compute the feature distances between different nodes.
- a clustering method to select data points as centroids, which we use as the nodes to be labelled during active learning.

The key purpose of our framework is to effectively utilize unlabelled nodes for active learning on graphs. To achieve this, we design a learned latent space, which combines unsupervised learning and supervised learning, to select nodes for labelling. We first use DGI to learn unsupervised features $H$ based on graphs and node attributes. Then with $H$, we design a novel distance-based classifier to generate output predictions. In the classifier, we apply a learnable linear transformation on $H$ to obtain hidden representations $Z$. The distances between nodes are calculated based on both $Z$ and $H$ in order to consider both information from unsupervised and supervised learning. Clustering is conducted based on the distances to select informative nodes. We also propose an incremental clustering method to prevent that the newly selected nodes are redundant with the previously selected nodes. After receiving the labels of selected nodes at each step, we train the classifier using all the labelled nodes.

5.1 Distance-based Classifier

A classifier is trained by using all labelled nodes at each step after receiving the labels of selected nodes. In previous work [1, 3, 32], they use a 2-layer GCN as the classifier. In our framework, we design a novel distance-based classifier, in which firstly DGI features $H$ is mapped to another features $Z$ by a linear transformation:

$$Z = HW_c, \quad (7)$$

where $W_c \in \mathbb{R}^{d' \times K}$ is the trainable linear transformation matrix. Then we define a set of learnable class representations $c_1, c_2, ..., c_K$, where $K$ is the number of classes. The distance vector of node $i$ is defined as:

$$a_i = \|z_i - c_1\|_2 \oplus \|z_i - c_2\|_2 \oplus ... \oplus \|z_i - c_K\|_2, \quad (8)$$
where @ is the concatenation operation and || · ||₂ is the $L_2$ norm. The $j$-th element $\hat{y}_{ij}$ in the output prediction $\hat{y}_i$ of node $i$ is obtained by the softmax function:

$$\hat{y}_{ij} = \text{softmax}(a_{ij}) = \frac{\exp(||z_i - c_j||_2)}{\sum_{k=0}^{K} \exp(||z_i - c_k||_2)} \quad (9)$$

For training the classifier, suppose the labelled node set at step $t$ is $L_t$. Then the cross-entropy loss function for node classification over the labeled node set is defined as:

$$\mathcal{L} = \sum_{i \in L_t} y_i \ln \hat{y}_i \quad (10)$$

With the guide of labelled nodes and their labels, we can update the transformation matrix $W$ based on the classification loss. Through the classification loss, new features $Z$ can capture the supervised information from labelled data.

### 5.2 Distance Function

In LSCALE, the distance function determines the distances between nodes for further clustering. We define our distance function as:

$$d(v_i, v_j) = ||g(X_i) - g(X_j)||_2 \quad (11)$$

where $g(X)$ is a mapping from node attributes $X$ to new distance features. As argued in Section 4 that previous methods do not effectively utilize the unlabelled nodes, we take advantage of unsupervised learning features and supervised information from labelled data. To this end, we combine unsupervised learning features $H$ and supervised hidden representations $Z$ in the distance function. A straightforward way to combine them is using concatenation of $H$ and $Z$: $g(X) = H \oplus Z$. Noted that $H$ and $Z$ are in different space and may have different magnitudes of row vectors. We define the distance features as follows:

$$g(X) = \alpha \cdot H' \oplus \beta \cdot Z' \quad (12)$$

where $H'$ and $Z'$ are $L_2$-normalized $H$ and $Z$ respectively to make sure they have same euclidean norms of rows. $\alpha$ and $\beta$ can be treated as two parameters for controlling the dynamic combination of unsupervised features and supervised features.

Intuitively, $Z$ can be unstable in the early stages as there are relatively few labelled nodes in the training set. So, in the early stages, we would like to focus more on unsupervised features $H$, which are much more stable than $Z$. As the number of labelled nodes increases, the focus should be shifted to hidden representations $Z$ in order to emphasize supervised information. Thus, to achieve this, we design a simple heuristic way to assign $\alpha$ and $\beta$:

$$\alpha = \lambda_L |L_t|; \quad \beta = 1.0 - \alpha \quad (13)$$

where $|L_t|$ is the number of labelled nodes at step $t$. $\lambda$ can be set as a number close to 1.0, e.g., 0.99. By using this dynamic combination of unsupervised learning features $H$ and supervised hidden representations $Z$, we can effectively capture information from both of them to facilitate selecting informative nodes in the clustering module.

### Discussion

Recall that FeatProp [32] uses propagated node features as representations for calculating distances. The propagated node features are fixed and not learnable throughout the whole active learning process, which makes the node selection less effective. By contrast, most importantly, our distance function uses learned feature space which is learned based on supervised signals from the classification loss. In addition, our distance function can also gradually shift the focus to emphasize supervised signals by the dynamic combination of unsupervised and supervised features.

### 5.3 Clustering Module

At each step, we use the K-Medoids clustering as in [32] to obtain cluster representatives. In K-Medoids, medoids have to be the data points themselves, which makes them can be used for active learning. So, after clustering, we directly select medoids for labelling. This ensures that the chosen centers are well spread out and provide good coverage of the remaining data, which matches the intuition of active learning, since we want the chosen centers to help us classify as much as possible of the rest of the data. At each step $t$, the objective of K-Medoids is:

$$\sum_{i=1}^{n} \min_{j \in S_t} ||g(X)_i - g(X)_j||_2 \quad (14)$$

Besides K-Medoids, common clustering methods used in the previous work are K-Means [1, 3], K-Centers [23]. K-Means cannot be directly used for selecting nodes in active learning as it does not return real sample nodes as cluster representatives.

#### 5.3.1 Incremental Clustering

Despite these advantages of K-Medoids for active learning on graphs, a crucial drawback is that it is possible to select similar nodes for querying during multiple iterations. That is, newly selected nodes may be close to previously selected ones, making them redundant and hence worsening the performance of active learning. For example, after selecting 10 nodes in the first iteration, the algorithm is required to select 10 more nodes in the second iteration. These 10 nodes are the medoids of clusters which are directly generated by K-Medoids on the whole space. Some of these nodes are likely close to the previous selected 10 nodes, making less informative. The reason is that the clustering algorithm only generates the representative nodes in the whole representation space without the awareness of previous selected nodes. In order to overcome this problem, we design a simple yet effective incremental clustering algorithm for K-Medoids to avoid selecting redundant nodes.

The goal of our incremental clustering method is to prevent the selection of redundant nodes. Selecting some nodes which are very close to the previous selected nodes in the representation space can be less effective and waste the budget. A desirable selection algorithm should have the ability to avoid this.

In our incremental clustering method, the key idea is that fixing previous selected nodes as some medoids can force the K-Medoids algorithm to select additional medoids that are dissimilar with the previous ones. We illustrate our incremental clustering method in Algorithm 1.

In the beginning of step $t$, we pre-define the budget of current step $b^t$ and provide $L^{t-1}$ to obtain desirable $k$ for clustering (Line 1). We randomly initialize the medoids and replace the first few
Algorithm 1: Incremental K-Medoids clustering

Input: the set of previous labelled nodes \( L^{t-1} \),
the set of unlabelled nodes \( U^{t-1} \) as the pool,
the budget \( b' \) of the current step

1. \( k \leftarrow |L^{t-1}| + b' \);
2. Randomly select \( k \) medoids for clustering;
3. Set nodes in \( L^{t-1} \) as the first \( |L^{t-1}| \) medoids;
4. Compute the distances \( d(v_i, v_j) \) for every pair \( (v_i, v_j) \) in \( G \);
5. repeat
6. foreach node \( u \in U^{t-1} \) do
7. Assign \( u \) to the cluster with the closest medoid;
8. end
9. foreach cluster \( C \) with medoid \( m \) do
10. if \( m \notin L^{t-1} \) then
11. Find the node \( m' \) which minimize the sum of
distances to all other nodes within cluster \( C \);
12. Update node \( m' \) as the medoid of cluster \( C \);
13. end
14. end
15. until all the medoids are not changed;
16. Construct selected node set \( S' \) using the medoids \( m \notin L^{t-1} \);
17. \( L^t \leftarrow S' \cup L^{t-1} \);
18. \( U^t \leftarrow U^{t-1} \setminus S' \);
19. return \( L^t, U^t \)

medoids with the previous labelled nodes (Line 2 and 3). After
calculating the distances for every node pair (Line 4), incremental
K-Medoids is conducted (Line 5 to Line 15). Compared to the original
K-Medoids, the most important modification is that only clusters
with a medoid, which is not in the previous labelled nodes set
(i.e., \( m \notin L^{t-1} \)), can update the medoid (Line 10-13). When all the
medoids are the same as those in the previous iteration, the K-
Medoids algorithm stops and keeps the medoids. For the medoids
which are not the previous selected nodes, we put them in selected
node set \( S' \), meanwhile we set labelled node set \( L' \) and unlabelled
node set \( U' \) using \( S' \) accordingly.

6 EXPERIMENTS
The goal of our experiments is to verify the effectiveness of our
proposed method LSCALE as compared to the baselines. We first clarify
the datasets we use and the baselines we compare with. Secondly,
we introduce the experimental setting including the data split,
and baseline methods, etc. Next, we present the experimental results
of LSCALE and different baselines, meanwhile we illustrate the effec-
tive improvements achieved by LSCALE on different datasets under
different budgets. Finally we conduct ablation studies to show the
influence of different components in LSCALE.

6.1 Datasets
To evaluate the effectiveness of LSCALE, we conduct the exper-
iments on Cora, Citeseer [22], Pubmed [17], Coauthor-CS (short
as Co-CS) and Coauthor-Physics (short as Co-Physics) [26]. The
first three are citation networks, which are undirected networks
and contain unweighted edges among different publications. Node
attributes in Cora and Citeseer are provided as bag-of-word features,
while node attributes of Pubmed are TF/IDF weighted word vectors.
Co-CS and Co-Physics are two co-authorship networks where nodes are authors, which are connected by an edge if they
coauthor a paper. Node attributes in these datasets are bag-of-word
encoded paper keywords. We summarize the dataset statistics for
different datasets in Table 2.

6.2 Baselines
To demonstrate the effectiveness of LSCALE, we compare our pro-
posed method LSCALE with the following active learning strategies:

- Random: Select the nodes uniformly from the unlabelled
node pool.
- Degree: Select the nodes with the largest degrees from the unla-
labelled node pool.
- Uncertainty: Select the nodes with the max information entropy
according to the current model.
- Featprop [32]: Perform the K-Medoids clustering on the propa-
gated features obtained by simplified GCN [31]. After getting the
K clusters, select the medoids to query their labels.
- AGE [1]: A graph neural network based method. Construct the
scores to choose a query node by linear weighted combining
different datasets in Table 2.

| Dataset | # Nodes | # Edges | # Classes | # Attributes |
|---------|---------|---------|-----------|-------------|
| Cora    | 2,708   | 5,429   | 7         | 1,433       |
| Citeseer| 3,327   | 4,732   | 6         | 3,703       |
| Pubmed  | 19,717  | 44,338  | 3         | 500         |
| Co-CS   | 18,333  | 81,894  | 15        | 6,805       |
| Co-Physics | 34,493  | 247,962 | 5         | 8,415       |

As suggested in [1, 3, 32], all methods, except LSCALE and
DGI_Rand, use GCNs as the prediction model, which is trained
after receiving the labelled nodes at each step.

6.3 Experimental setting
We evaluate LSCALE and other baselines on node classification
task following the experimental setup as in [1, 3, 13] for a fair
comparison. In the experiments, we report the average results over
20 trials with different data splits and initial labelled sets. Note that
all the experiments are conducted with a single GeForce RTX 2080
Ti GPU.
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Table 4: The averaged Micro-F1 (%) and standard deviations at different budgets on citation networks.

| Dataset | Co-Physics | Co-CS |
|---------|------------|-------|
| Budget | 10 | 30 | 60 | 10 | 30 | 60 | 10 | 30 | 60 |
| Random | 74.80 ± 2.6 | 86.48 ± 3.8 | 90.70 ± 3.8 | 49.72 ± 9.8 | 69.98 ± 7.3 | 78.15 ± 3.6 |
| Uncertainty | 71.42 ± 2.9 | 85.29 ± 2.0 | 92.04 ± 2.0 | 42.38 ± 7.3 | 57.43 ± 9.5 | 65.66 ± 9.9 |
| Degree | 61.39 ± 5.4 | 62.22 ± 5.6 | 58.61 ± 5.6 | 55.16 ± 6.6 | 65.61 ± 6.6 | 73.70 ± 2.9 |
| AGE [1] | 63.96 ± 7.2 | 84.47 ± 9.1 | 91.30 ± 9.1 | 27.20 ± 7.2 | 72.20 ± 7.2 | 76.51 ± 3.6 |
| ANRMAB [3] | 68.47 ± 4.9 | 84.19 ± 8.4 | 89.35 ± 8.4 | 43.48 ± 9.9 | 69.98 ± 7.5 | 75.51 ± 2.4 |
| FeatProp [32] | 80.23 ± 9.5 | 86.83 ± 9.5 | 90.82 ± 9.5 | 52.45 ± 7.0 | 78.83 ± 7.0 | 76.60 ± 3.5 |
| DGL_Rand | 82.81 ± 9.5 | 90.35 ± 9.5 | 92.44 ± 9.5 | 64.07 ± 7.8 | 83.83 ± 7.8 | 84.28 ± 2.7 |
| LSCALE | 90.38 ± 9.5 | 92.75 ± 9.5 | 93.70 ± 9.5 | 73.07 ± 8.9 | 82.96 ± 8.9 | 86.70 ± 1.7 |

Table 4: The averaged Micro-F1 (%) and standard deviations at different budgets on co-authorship networks.

| Dataset | Co-Physics | Co-CS |
|---------|------------|-------|
| Budget | 10 | 30 | 60 | 10 | 30 | 60 |
| Random | 74.80 ± 2.6 | 86.48 ± 3.8 | 90.70 ± 3.8 | 49.72 ± 9.8 | 69.98 ± 7.3 | 78.15 ± 3.6 |
| Uncertainty | 71.42 ± 2.9 | 85.29 ± 2.0 | 92.04 ± 2.0 | 42.38 ± 7.3 | 57.43 ± 9.5 | 65.66 ± 9.9 |
| Degree | 61.39 ± 5.4 | 62.22 ± 5.6 | 58.61 ± 5.6 | 55.16 ± 6.6 | 65.61 ± 6.6 | 73.70 ± 2.9 |
| AGE [1] | 63.96 ± 7.2 | 84.47 ± 9.1 | 91.30 ± 9.1 | 27.20 ± 7.2 | 72.20 ± 7.2 | 76.51 ± 3.6 |
| ANRMAB [3] | 68.47 ± 4.9 | 84.19 ± 8.4 | 89.35 ± 8.4 | 43.48 ± 9.9 | 69.98 ± 7.5 | 75.51 ± 2.4 |
| FeatProp [32] | 80.23 ± 9.5 | 86.83 ± 9.5 | 90.82 ± 9.5 | 52.45 ± 7.0 | 78.83 ± 7.0 | 76.60 ± 3.5 |
| DGL_Rand | 82.81 ± 9.5 | 90.35 ± 9.5 | 92.44 ± 9.5 | 64.07 ± 7.8 | 83.83 ± 7.8 | 84.28 ± 2.7 |
| LSCALE | 90.38 ± 9.5 | 92.75 ± 9.5 | 93.70 ± 9.5 | 73.07 ± 8.9 | 82.96 ± 8.9 | 86.70 ± 1.7 |

Dataset Splits. For each citation dataset, we use the same testing set as in [13, 35], which contains 1000 nodes. For coauthor datasets, we randomly sample 20% nodes as the testing sets, which include 3666 nodes for Coauthor-CS and 6898 nodes for Coauthor-Physics respectively. From the non-testing set in each dataset, we randomly sample 500 nodes as a validation set and fix it for all the methods to ensure the fairness of evaluation. Under the label budget, the remaining nodes are free to be selected by active learning strategies and trained by the model later. We set the different budgets of labelled nodes for different datasets.

Initial labelled nodes sampling. Each active learning strategy is provided a small set of labelled nodes as an initial pool. In [1, 3], to consider the label balance, a few nodes are randomly selected for each label class. However, it is usually not realistic as we do not have any label information at the beginning of a real-world active learning problem. So, as in [32], we randomly select 5 nodes regardless of the class as an initial pool.

Experiment Procedure. In the experiments, we set the budget sizes differently for different datasets and we focus on the “batched” multi-step setting as in [23]. The whole active learning process is as follows: (1) we first train the prediction model with initial labelled nodes, (2) we use the active learning strategy to select new nodes for labelling and add them to the labelled node pool, (3) we train the model based on the labelled nodes again. We repeat Step (2) and Step (3) until we run out of budgets and train the model based on the final labelled node pool. For AGE and ANRMAB, only one node is selected to query in each iteration according to their papers. For LSCALE and FeatProp, 10 nodes are selected for labelling in each iteration as these two methods depend on selecting medoids to label.

Hyper-parameter settings. For hyper-parameters of other baselines, e.g., the number of layers of GCNs, the number of hidden units of GCNs, the optimizer, the learning rate, we set them as suggested in their papers. For the embedding dimensionality $d'$ of DGI model in LSCALE, on three citation datasets, we set them as suggested in the original paper [30]. On two co-authorship datasets, we set it as 128 due to GPU memory limitations. Other hyper-parameters of DGI model are set as the same in the paper. For the dimensionality $l'$ of hidden representation $Z$, we set as 100 for all datasets. By default, we set $\lambda = 0.99$ in Equation 13 to determine $\alpha$ and $\beta$ at different steps. To train the classifier in LSCALE, we use the Adam [12] optimizer with the learning rate 0.2 and the weight decay $5 \times 10^{-6}$ for maximum 300 epochs and early stopping with a window size of 10.

6.4 Results and Discussion

We evaluate the performance by using Micro-F1 and Macro-F1 scores. We report the results over 20 runs with 10 different random data splits. Due to space limitations, the results of Macro-F1 scores are demonstrated in Appendix A.3. In Table 3, Table 4, we show Micro-F1 scores of different methods when the number of labelled nodes is less than 60. Generally, our method LSCALE always significantly outperforms the baselines on the varying datasets while LSCALE provides relatively lower standard deviations on most datasets. When the number of labelled nodes is relatively small (shown in Table 3 and Table 4), LSCALE significantly outperforms other methods on all presented datasets. Specially, when the total budget is only 10, LSCALE provides remarkable improvements compared with FeatProp by absolute values 19.0%, 26.0%, 20.5%, 20.7%, 23.0%, 20.5%, 19.0%, 26.0%, 20.5%, 19.0%, 26.0%, 20.5% for Coauthor-CS, Citeseer, and Co-CS respectively. When the budget size is less than 30, the Uncertainty baseline always performs worse than the Random baseline for all datasets, meanwhile AGE and ANRMAB do not have much higher Micro-F1 scores on most datasets compared with the Random baseline. Note that AGE, ANRMAB and the Uncertainty baseline all rely on GCN representations for

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Note: Refer to Appendix A.2 for detailed settings.
selecting nodes. So, both of the above two results indicate that GCN representations are inaccurate when having only a few labelled nodes. All other methods except our method LSCALE are outperformed by DGI_Rand on all presented datasets, which supports the unexpected finding mentioned in Section 4. Meanwhile, LSCALE consistently provides performance improvements up to 9.14% over DGI_Rand on different datasets, which verifies the effectiveness of LSCALE.

In Figure 3, we focus on how Micro-F1 scores of different methods change as the number of labelled nodes increases on Cora, Citeseer, Co-Physics, and Co-CS. We omit Pubmed in Figure 3 because of space limitations and also the similar performance as other datasets. Comparing AGE and Featprop on Cora, Co-Physics, and Co-CS, Featprop initially outperforms AGE. However, AGE outperforms Featprop as more labelled node obtained, showing that supervised information is indeed helpful for effectively selecting informative nodes. Recall that Featprop only uses propagated node features without considering supervised information during the node selection process, which makes it less effective as the number of labelled nodes increases on some datasets. Figure 3 clearly shows that LSCALE consistently outperforms other methods under different budgets, which thanks to the proposed dynamic combination of unsupervised learning features and supervised hidden representations.

In Figure 4, we present t-SNE visualization [15] of FeatProp features, DGI features, and our proposed distance features. Our distance features are obtained by dynamically combining DGI features and supervised hidden representations on 20 labelled nodes. Recall that FeatProp uses propagated node features as distance features and DGI features are learned based on an additional loss. Compared with others, the distance features used in LSCALE have clearer boundaries between different classes, which potentially facilitates selecting informative nodes in the clustering algorithm.

6.5 Visualization
In Figure 4, we present t-SNE visualization [15] of FeatProp features, DGI features, and our proposed distance features. Our distance features are obtained by dynamically combining DGI features and supervised hidden representations on 20 labelled nodes. Recall that FeatProp uses propagated node features as distance features and DGI features are learned based on an additional loss. Compared with others, the distance features used in LSCALE have clearer boundaries between different classes, which potentially facilitates selecting informative nodes in the clustering algorithm.
We study the effect of varying the parameters in our method, including the number of hidden units $l'$ in our classifier and $\lambda$ for controlling the dynamic feature combination (Equation 13). The results are demonstrated in Figure 6 and 7. We alter the number of hidden units $l'$ among $\{25, 50, 100, 200, 400\}$ and $\lambda$ among $\{0.7, 0.8, 0.9, 0.95, 0.99\}$. As we can see in Figure 6, changing $l'$ has no much difference in terms of performance on Co-CS, while $l' = 25$ performs best on Cora when the number of labelled nodes is less than 60. However, when it is larger than 60, different $l'$ generate similar performances on Cora. These results show that our method is not sensitive to the number of hidden units $l'$.

For the parameter $\lambda$, increasing $\lambda$ from 0.7 to 0.99 generally increases the Micro-F1 score on Cora, especially when the number of labelled nodes is small. In the meantime, $\lambda = 0.99$ still provides slight better performance than $\lambda = 0.7$ on Co-CS. To conclude, we should avoid relatively low $\lambda$, e.g., lower than 0.8, to prevent inferior performance when the labelling budget is small.

7 CONCLUSION

In this paper, we first show the unexpected results of an empirical study, where the existing approaches of active learning for node classification can be outperformed by a simple unsupervised method. Motivated by this, we study how to effectively utilize the information present in nodes without labels. We propose LSCALE, a latent space clustering-based active learning method for node classification that selects nodes to label through k-Medoids clustering on the dynamically combined features of both unsupervised features and supervised features. We also design an incremental clustering module to prevent redundancy between nodes selected at different steps. Extensive experiments demonstrate that our method provides the superior performance over the state-of-the-art models.

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A SUPPLEMENT

In the supplement, we describe more details about experiments to facilitate the reproducibility. We also provides more additional experimental results to support the conclusion in our paper.

A.1 Experiment Environments

All the experiments are conducted on the settings as follows:

- Operating System: Ubuntu 18.04.2 LTS
- CPU: Intel(R) Xeon(R) Gold 6240 CPU @ 2.60GHz
- GPU: GeForce RTX 2080 Ti
- Software versions: CUDA 10.1; Python 3.7.6; PyTorch 1.4.0; TensorFlow 1.15.3; NumPy 1.18.1; SciPy 1.4.1.

A.2 Datasets and Baselines

The datasets used in the experiments can be found on the following websites:

- Cora, Citeseer, Pubmed: https://github.com/tkipf/gcn
- Co-CS, Co-Physics: https://github.com/rusty1s/pytorch_geometric

We refer to the following websites when implementing the baselines included in our experiments:

- AGE: https://github.com/vwz/AGE
- DGI_Rand: https://github.com/PetarV-/DGI

ForFeatProp and ANRMAB, we refer to the original source code received from the authors ofFeatProp via email.

**AGE and ANRMAB.** When implementing AGE in our experiments, on citation networks, the time-sensitive parameter is set as suggested in [1], i.e., 0.995 for Cora and Pubmed, 0.9 for Citeseer. On co-authorship datasets, which are not used in [1], we set the time-sensitive parameter to 0.995. A 2-layer GCN is used for classification. The number of hidden units is 16. The dropout is applied to the hidden representations of the first layer; the dropout rate is set to 0.5. The Adam optimizer is used with learning rate 0.01. The $L_2$ regularization weight is $5 \times 10^{-4}$. The Xavier uniform initialization is used for all variables. We adopt the early stopping training strategy: stop the training when the current validation cost is larger than the average of validation costs of the last 10 epochs. We set the maximum number of epoch as 300. For ANRMAB, we use the same settings as the above settings of AGE. Note that these setting used in our experiments can be found in the original implementations of authors or mentioned in the original paper.

**FeatProp.** When implementing FeatProp in our experiments, a 2-layer GCN is used for classification. The number of hidden units is 16 while the dropout is applied to the hidden representations of the first layer. The dropout rate is 0.5. We use the Adam optimizer with a learning rate of 0.01 and weight decay of $5 \times 10^{-4}$. The Xavier uniform initialization is used for all variables. We adopt the early stopping training strategy: stop the training when the validation accuracy does not improve for 100 epochs. We set the maximum number of epoch as 300.

**DGI_Rand.** When implementing DGI_Rand in our experiments, firstly we train the DGI model to obtain the unsupervised features. The embedding dimensionality is set to 512 for Cora and Citeseer, 256 for Pubmed, and 128 for Co-Physics and Co-CS. The parametric ReLU is used as the nonlinearity in the encoder. We use the Adam optimizer with learning rate 0.001. After obtaining the unsupervised features, we train a logistic regression for classification. In the logistic regression classifier, we use the Adam optimizer with learning rate 0.2 and weight decay $5 \times 10^{-4}$. We adopt the early stopping training strategy: stop the training when the validation accuracy does not improve for 100 epochs. We set the maximum number of epoch as 300.

A.3 Additional Experimental Results

In this section, we report Macro-F1 scores of different methods on all datasets used in the experiments. In Figure 8, it is clear that our proposed method LSCALE still outperforms other baselines in terms of Macro-F1 scores.
Figure 8: Macro-F1 scores comparison of different active learning algorithms on citation and co-authorship datasets.