Deep Active Graph Representation Learning

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Abstract

Graph neural networks (GNNs) aim to learn graph representations that preserve both attributive and structural information. In this paper, we study the problem of how to select high-quality nodes for training GNNs, considering GNNs are sensitive to different training datasets. Active learning (AL), whose purpose is to find the most informative instances to maximize the performance of the model, is a promising approach to solve this problem. Previous attempts have combined AL with graph representation learning by designing several selection criteria to measure how informative a node is. However, these methods do not directly utilize both the rich semantic and structural information and are prone to select sparsely-connected nodes (i.e., nodes having few neighbors) and low-purity nodes (i.e., nodes having noisy inter-class edges), which are less effective for training GNN models. To address these problems, we present a Deep Active Graph Representation Learning framework (DAGRL), in which three novel selection criteria are proposed. Specifically, we propose to measure the uncertainty of nodes via random topological perturbation. Besides, we propose two novel representativeness sampling criteria, which utilize both the structural and label information to find densely-connected nodes with many intra-class edges, hence enhance the performance of GNN models significantly. Then, we combine these three criteria with time-sensitive scheduling in accordance to the training progress of GNNs. Furthermore, considering the different size of classes, we employ a novel cluster-aware node selection policy, which ensures the number of selected nodes in each class is proportional to the size of the class. Comprehensive experiments on three public datasets show that our method outperforms previous baselines by a significant margin, which demonstrates its effectiveness.

1 Introduction

Recent years have witnessed a rapid development in graph representation learning, which aims to embed nodes into a low-dimensional space that preserves both structural and attributive features. Graph neural networks (GNNs), as a promising means of learning graph representations, attract a lot of research interests. (Kipf and Welling 2017; Veličković et al. 2018; Hu et al. 2019). In general, GNN models follow a common paradigm of information propagation by combining features from neighboring nodes—hence the name of the neighborhood aggregation scheme. Although most existing GNN models are trained in a semi-supervised manner, they still require high-quality labels. Moreover, even with the same amount of labeled data, training/test set splits strongly affect the performance of models. For example, Kipf and Welling (2017) have demonstrated that the model trained using a carefully-selected labelled set (aka., the public split) greatly outperforms the one trained using randomly-labelled sets.

To measure how informative an instance is, previous AL methods design various criteria, which can be roughly categorized into two lines, uncertainty- and representativeness-based strategies (Settles 2009). The former method queries the sample with the least confidence to the model, for instance, samples with a probability 50% of being positive in binary classification. The latter approach focuses on data instances that are representative of the data distribution. For example, a node in a graph is representative if its label almost conforms with its neighbors’ labels.

In the past few years, several active learning algorithms are proposed to operate on graphs by designing heuristics to calculate the informative score of each node (Cai, Zheng, and Chang 2017; Gao et al. 2018). The two approaches, following previous active learning paradigms, measure the uncertainty of nodes by calculating the entropy over its predicted label distribution. Then, they measure the representativeness of nodes from two aspects, one by computing the distance between one node and its cluster center, where the clusters are obtained via the k-means algorithm, and the other by calculating the centrality score of each node via the PageRank algorithm (Page et al. 1997).

Despite their effectiveness, we argue that these strategies do not consider semantic and structural information in a hybrid manner. Therefore, they may select sparsely-connected and low-purity nodes, which are less effective for training GNNs. First of all, the entropy-based uncertainty sampling method fails to consider the graph structure, which is prone to select nodes inferior to GNN training, e.g., sparsely-
connected nodes or low-purity nodes with noisy inter-class edges. These kinds of nodes are selected because they are the most uncertain to the neighborhood aggregation scheme of GNNs. Secondly, the two representativeness criteria consider the attributive and structural information separately. By utilizing the embeddings learned via GNNs, they calculate the distance between a node and its cluster center. This strategy simply considers the attributes of nodes that may result in selecting the low-purity nodes, whose embeddings are usually inaccurate since they are hard for GNNs to predict. Besides, they propose to select densely-connected nodes via the PageRank algorithm. However, this algorithm only considers the structural information. In other words, it is still likely to select low-purity nodes from the resulting densely-connected nodes. In summary, these three strategies tend to select sparsely-connected and low-purity nodes. Considering that sparsely-connected nodes are difficult to participate in information propagation due to insufficient neighbors, low-purity nodes are hard for GNN to predict (Yang et al. 2020; Zhu et al. 2020), these kinds of nodes may lead to suboptimal performance. Furthermore, previous methods simply select the same number of informative nodes for each class. We argue that this policy neglects the influence of the class bias, that is the number of nodes in different classes varies from each other, which may select some less informative nodes in the small-size cluster.

To address the aforementioned problems, we proposed a novel Deep Active Graph Representation Learning (DAGRL) algorithm, which explicitly considers both attributes and structural information in the data selection criteria. Specifically, we propose a hybrid selection scheme consisting of uncertainty sampling and representativeness sampling. The framework of our proposed DAGRL method is presented in Figure 1.

For the uncertainty sampling, we propose to select the most sensitive node to random perturbation, which directly utilizes the structural information. Specifically, we make structural perturbation to the graph by randomly dropping edges and then obtain the node representations of these modified graphs. After that, we calculate the variances over representation vectors of all nodes and compute the uncertainty score as the maximum variance along the representation dimension.

Regarding the representativeness sampling, we design two criteria, namely degree-based sampling and purity-based sampling, which explicitly incorporate graph structures into consideration. As nodes with the larger degree will influence more neighboring nodes during message propagation, we firstly define the degree as a part of the representativeness score. To avoid selecting the outliers that have noisy inter-class edges like previous methods, we further consider the purity of each node, where the purity is defined as the ratio of one-hop neighbors belonging to the same class as the center node. Through this criteria, we are able to find the high-purity nodes with many intra-class edges. Then, we compute the informative score through a linear combination with time-sensitive scheduling (Cai, Zheng, and Chang 2017) of these three criteria. Finally, considering that there are probably more informative nodes in a large-size class, we design a class-aware node selection policy, which ensures that the number of selected nodes in the class is proportional to the class size.

In a nutshell, the main contribution of this paper can be summarized in threefold as follows:

- We propose three novel node selection criteria, which explicitly utilize the graph structure and semantic information in graph representation learning.
- We propose a novel cluster-aware node selection policy, which takes the class size into consideration and further improves the performance of model.
- We conduct comprehensive experiments on three real-world graph datasets. The results show that our method outperforms both traditional and graph-based baselines, achieving state-of-the-art performance.

2 Related Work

In this section, we briefly review related work in the field of graph neural networks and active learning.

2.1 Graph Neural Networks

In general, graph neural networks aggregate neighborhood information to learn graph representations. Based on the strategy of aggregating information, GNNs can be divided into two categories, i.e. spectral-based methods and spatial-based methods.

On the one hand, spectral-based methods are based on the graph theory to define the filters. Early spectral-based method (Bruna et al. 2014) defines the convolutional operation by computing the eigendecomposition of the graph Laplacian. However, it has a high computation complexity that limits it to operating on large-scale graphs. To address this problem, Defferrard, Bresson, and Vandergheynst (2016) use Chebyshev expansion of the graph Laplacian to design the filters instead of computing the eigenvectors of the Laplacian. Later,
further restricts the filters to operate on one-hop neighborhood.

On the other hand, spatial-based methods apply several strategies to directly operate aggregation on neighbors. GraphSAGE (Hamilton, Ying, and Leskovec 2017) samples fixed-size neighbors of nodes and then perform different aggregating strategies, such as long/short-term memory (LSTM), mean pooling, on them. Veličković et al. (2018) first introduce the attention mechanism to GNNs which obtains node representations by the self-attention strategy.

2.2 Active Learning

Different active learning algorithms propose various strategies to select the most informative instances from a large pool of unlabelled data, which have achieved promising performance in several tasks, e.g., text mining (Settles and Craven 2008) and visual representation learning (Gal, Islam, and Ghahramani 2017). Previous approaches can be roughly grouped into three categories (Settles 2009): heterogeneity-based methods, performance-based methods, and representativeness-based methods.

For the methods falling into the first category, (Settles and Craven 2008) propose uncertainty sampling, which calculate based on the sequence entropy on the label distribution. Bilgic, Mihalkova, and Getoor (2010) introduce a vote mechanism to choose the data, which models disagree the most. Regarding the performance-based algorithms, in the second group, Guo and Greiner (2007), Schein and Ungar (2007) explore the criteria directly related to the model performance including prediction error and variance reduction. The last group of methods focus on discover the instance that can be representative of the data distribution. Sener and Savarese (2018) regard the sampling process as a coreset problem, in which the representations of the last layer in deep neural networks are used for constructing the coreset. However, these methods can not be directly performed on graph-structural data since they are all designed for independent and identically distributed (i.i.d) data and do not consider rich structural information.

2.3 Active Learning for Graphs

Active learning for graphs is more difficult than that for Euclidean data, since nodes in the graph are highly correlated to each other. Previous attempts (Bilgic, Mihalkova, and Getoor 2010, Gu et al. 2013a) regard active data selection and graph representation learning as two separate and independent processes. Later, Gu et al. (2013b), Gadde, Anis, and Ortega (2014) develop strategies based on the assumption that neighboring nodes are more possible to have the same label. Recently, researchers propose to combine the data selection process with graph representation learning, expecting that on the one hand, high-quality data selected in the active learning process can promote the predicted accuracy of the model, and on the other hand, more accurate model also support the data selection. AGE (Cai, Zheng, and Chang 2017) calculates the informativeness score by combining three designed criteria (i.e., entropy on the predicted label distribution, distance between the node and its cluster center and the centrality obtained via the PageRank algorithm (Page et al. 1997) linearly. ANRMB (Gao et al. 2018) uses the same selection criteria as AGE and further introduces a multi-armed bandit algorithm to adaptively decide weights of these three criteria in the final score. Though these methods have achieved the satisfied performance, they do not fully utilize the semantic and structural information.

3 The Proposed Method

In this section, we firstly introduce notations used throughout the paper and then describe the framework of the proposed deep active graph representation learning, followed by detailed introduction of three node selection criteria. Finally, we introduce the way to combine these criteria and a novel node selection policy.

3.1 Preliminaries

Problem definition. Active learning aims to train an accurate model with a limited budget of training data. Given a large unlabelled data pool \( U \) and a labelling budget \( b \), the target of our work is to select the top-\( b \) informative nodes via the designed selection criteria and add them to the labelling set \( L \) to maximize the accuracy of the model.

Graph representation learning. Let \( G = (V, E) \) be a graph with \( n \) nodes, where \( V = \{v_i\}_{i=1}^n \) is the vertex set and \( E = V \times V \) is the edge set. We denote \( A = \{0, 1\}^{n \times n} \) to be the adjacency matrix. Besides, the feature matrix of nodes is denoted as \( X \in \mathbb{R}^{n \times m} \), where \( m \) is the dimension of the feature vector, and \( x_i \in \mathbb{R}^m \) represents the feature vector of the \( i \)-th node in the graph.

In this paper, following previous work (Cai, Zheng, and Chang 2017, Gao et al. 2018), we choose the widely-used GCN (Kipf and Welling 2017) model to learn node representations. Mathematically, the layer-wise propagation rule in GCN can be formulated as:

\[
H^{(l+1)} = \sigma \left( \tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}} H^{(l)} W^{(l)} \right),
\]

where \( \tilde{A} = A + I_n \) is the adjacency matrix with self-loops and \( D_{ii} = \sum_j A_{ij} \), \( H^{(l)} \in \mathbb{R}^{n \times k_l} \) represents the node embedding matrix in the \( l \)-th layer, where \( k_l \) is the dimensionality of the node embedding. We set \( k_0 = m \) and feed the feature matrix to the model, i.e., \( H^{(0)} = X, W^{(l)} \in \mathbb{R}^{m \times k_l} \) is a learnable weight matrix of layer \( l \), which transforms the node representations into a low-dimensional space. \( \sigma(\cdot) \) is the nonlinear activation function, e.g., \( \text{ReLU}(\cdot) = \max(0, \cdot) \).

In this paper, we utilize a two-layer GCN model, denoted as \( f(A, X) \). For simplicity, we denote \( H = H^{(2)} \) as the output representations and \( k = k_2 \) as the dimension of output representations.

3.2 The Overall Framework

Our algorithm starts with a labelled budget \( b \), a graph \( G \), an unlabelled node pool \( U \), an empty training set \( L \), a node selection frequency \( c \), and a GCN model \( f \) with randomly initialized parameters. At first, we calculate informative scores for nodes in the unlabelled pool \( U \) according to the three
proposed criteria. After obtained informative scores, we select the node with the highest score in each class, and query the labels from the human annotators and add them into the labelled set \( L \). Then, based on the updated training set, we retrain the GCN for \( e \) epochs to obtain new node representations. Besides, considering there are probably more informative nodes in the large-size class, we set a label budget \( b_i \) to be proportional to the class size for every class. If the budget is reached, we will not select the node from this class in the following selection step. We repeat the above two steps until the size of the training set reaches the labelling budget \( b \).

**Algorithm 1:** Deep active graph representation learning

| Data: Graph \( G \), unlabelled set \( U \), label budget \( b \), node selection frequency \( e \), class number \( c \), randomly initialized GCN model \( f \) |
|---|
| Result: Training set \( L \) containing selected informative nodes |
| 1. Initialize the empty labelled set \( L = \emptyset \) |
| 2. Initialize a counter to all zeros \([r_1, \ldots, r_c] = 0\) |
| 3. Initialize unlabelled set to be the vertex set \( U = V \) |
| /* Calculate representativeness */ |
| 4. Obtain pseudo-labels \( l_p \) using the unsupervised clustering algorithm |
| 5. Calculate the budget of each class \( b_i \) using Eq. (10) |
| 6. Calculate degree scores \( s_d \) by counting one-hop neighbors of each node in graph \( G \) |
| 7. Calculate purity scores \( s_p \) using Eq. (8) |
| 8. while labelling budget \( b \) is not reached do |
| 9. for every \( e \) epochs do |
| /* Calculate uncertainty */ |
| 10. Calculate uncertainty scores \( s_u \) using Eq. (6) |
| /* Calculate informative scores \( s \) using Eq. (9) */ |
| /* Rank scores in each cluster respectively */ |
| 11. for each cluster \( i \) do |
| 12. if \( r_i = b_i \) then |
| 13. continue |
| 14. Sort \( s \) in descending order |
| 15. Pick out the node with the largest score in cluster \( i \) and add it into \( L \) |
| 16. \( r_i = r_i + 1 \) |
| 17. Train \( f \) using the current labelled set \( L \) |
| 19. return \( L \) |

### 3.3 Node Selection Criteria

Previous work only considers the graph structure and attributes separately and do not take abundant semantic information (e.g., class information) into account. To address these problems, we introduce three novel node selection criteria to measure the uncertainty and representativeness of nodes, explicitly utilizing both structural and semantic information in a hybrid manner.

**Variance-based uncertainty sampling.** Previous uncertainty sampling methods on the graph only take label prediction into account, which tend to select the sparsely-connected and low-purity nodes, especially at the beginning of training. Based on this observation, we design a variance-based uncertainty sampling method, which straightly considers the graph structure.

In every active node selection epoch, we first randomly drop edges for several times. After that, we obtain a series of topology-modified graphs, which are denoted as \( \{G_j\}_{j=1}^{n_d} \). Then, these graphs are fed into GCN to obtain corresponding node representations \( \{H_j\}_{j=1}^{n_d} \), where \( n_d \) is the number of graphs. Finally, we calculate the variance along the dimension of representation vectors of each node and obtain the variance matrix \( V \in \mathbb{R}^{|U| \times k} \), where \( |U| \) is the current number of unlabelled nodes and \( v_i \in V \) is the variance vector of each node. Then the uncertainty scores \( s_u \in \mathbb{R}^{|U|} \) are defined as the maximum variance among each entry of \( V \). Formally, it can be written as follows:

\[
H_i = f(G_i), \quad i = 1, \ldots, n_d, \tag{2}
\]

\[
H = [H_1, H_2, \ldots, H_{n_d}], \tag{3}
\]

\[
v_i = \text{var}(H_i,:), \tag{4}
\]

\[
V = [v_1, v_2, \ldots, v_{n_d}], \tag{5}
\]

\[
s_i^u = \max(V[,i]), \tag{6}
\]

where \( H \in \mathbb{R}^{n_d \times n \times k} \) is a tensor, which contains feature matrices from \( n_d \) graphs and \( \text{var}() \) takes the rows of node representation matrix as input and calculate variance along the second dimension of the matrix. \( s_i^u \) denotes the uncertainty score of \( j \)-th node, which is obtained via max pooling along the row of the variance matrix \( V \).

**Representativeness sampling.** Representativeness is also a significant criterion for revealing the most representative nodes and avoiding trivial solutions. However, previous methods compute the embedding distance and use the PageRank algorithm to obtain the centrality score, which consider the graph structure and attributive information separately. This may make the algorithm difficult to find high-purity nodes. To address this weakness, we design two structure-aware criteria, which are simple but efficient to find the informative nodes.

- **Degree-based criteria.** The degree reflects the importance of a node in the graph. A node of larger degree will interact with more neighbors during message propagation. To find the densely-connected nodes, we simply calculate the degree of each node. Then, we normalize the degrees of nodes via softmax function to obtain the degree-based score \( s_d \).

- **Purity-based criteria.** While the degree-based strategy considers structural information directly, it does not utilize rich attributive features contained in the graph. For example, it ignores the label information, which may mislead the algorithm to select nodes with noisy inter-class edges. To alleviate this problem, we further propose a purity-based criterion to capture semantic information of nodes. The purity of a node is defined as the ratio of its one-hop neighbors, whose labels are the same as the center node’s label.
For example, if a node has five one-hop neighbors and four neighbors have the same label as it, the purity of the node is 0.8.

Since labels are unavailable for those unselected nodes in the setting of AL, to calculate the purity, we first apply clustering algorithm introduced in Zhang et al. (2019) on the representations to obtain the pseudo-labels for calculating purity, due to its simplicity and effectiveness. The clustering algorithm first performs high-order graph convolution to obtain a new feature matrix and calculate the similarity matrix according to the feature matrix. Finally, the cluster partition (i.e. pseudo-label information) is obtained by applying spectral clustering on the similarity matrix. After obtaining the pseudo-labels, the purity-based criteria can be written in the following equations:

\[
s_p = \frac{\#(y_j \in \mathcal{N}(i) = y_i)}{|\mathcal{N}(i)|}, \quad s = \text{softmax}([s_1, s_2, \ldots, s_{|\mathcal{U}|}]^T),
\]

where \(|\mathcal{N}(i)|\) is the number of one-hop neighbors of node \(i\), \(|\mathcal{U}|\) is the size of unlabelled set, and \(y_i\) is the pseudo-label of each node. It is worth noting that we only calculate the purity score once since the clustering algorithm is parameter-free which directly applies the clustering on input graphs.

In summary, the two strategies explicitly consider the structural (i.e. connected relationship) and semantic information (i.e. label information) of graph, which helps the algorithm directly find the densely-connected and high-purity nodes, beneficial for training GNNs.

### 3.4 Combination Strategy of Criteria and Node Selection Policy

**Combination strategy of three criteria.** To combine the aforementioned criteria, we can simply employ a linear combination with fixed weights. However, as mentioned in Cai, Zheng, and Chang (2017), the uncertainty criterion depends on the output representations of networks, which are inaccurate at the beginning of training and node selection process. Therefore, its weight should be small and more attention should be paid to the representativeness of nodes at the beginning. During the progress, those nodes that are easy for model to classify have been already selected, so the weight of the uncertainty criterion should be increased. Based on the above observations, we employ the time-sensitive scheduling to adaptively adjust the weights of three criteria. Formally, it can be written as follows:

\[
s = \alpha \times s_u + \beta \times s_p + \gamma \times s_d,
\]

where \(\alpha = -\frac{|\mathcal{L}|}{|\mathcal{L}| + |\mathcal{U}|}\) and \(\beta = \gamma = 0.5 \times \left(1 - \frac{|\mathcal{L}|}{|\mathcal{L}| + |\mathcal{U}|}\right)\), \(|\mathcal{L}|\) is the ratio of selected nodes to the budget.

**Node selection policy.** After obtaining the scores, previous methods simply select the most informative node from each class or the whole unlabelled data pool in each node selection step, which may fail to select some informative nodes in the large-size class. We therefore propose a novel selection policy which ensures that the budget of selected nodes in a class is proportional to nodes in this class. To be specific, nodes in each class are sorted according to the informative score \(s\). Then, the node with the highest score in each class are selected and added into training set \(\mathcal{L}\) if the budget is not reached. Once the budget of a class is reached, this class is no longer considered in the node selection stage. Overall, the budget of each class can be formulated as:

\[
b_i = b \times \frac{c_i}{n},
\]

where \(b_i\) is the budget of the \(i\)-th class, \(b\) is the budget of all nodes, and \(c_i\) is the number of nodes in the \(i\)-th class.

### 4 Experiments

In this section, we conduct experiments on three graph datasets to answer the following questions:

- **RQ1:** How is the performance of our proposed method compared with existing active graph embedding approaches?
- **RQ2:** How do different node sampling criteria affect the performance of the model?
- **RQ3:** What are the differences between the data selected via our variance-based uncertainty sampling criteria and the previous entropy-based method?
- **RQ4:** How do different node selection policies affect the performance of model?

#### 4.1 Experimental Setup

**Datasets.** Following the previous work (Cai, Zheng, and Chang 2017; Gao et al. 2018), we use three citation network datasets: Citeseer, Cora and Pubmed. Each dataset contains a graph in which nodes represent articles and edges illustrate the citation relationship between two articles. The initial representation of nodes are the sparse bag-of-words feature vectors. Detailed statistics of datasets are summarized in Table I.

**Baselines.** To evaluate the performance of our proposed approach, we compare it with several representative baselines:

- **Random:** All training data are randomly selected.
- **Label entropy:** At each training epoch, we select a node which has the maximum cross entropy on the predicted label distribution.
- **AGE** (Cai, Zheng, and Chang 2017): It designs three simple node selection criteria, i.e., calculating uncertainty via the entropy of the predicted label distribution, measuring node centrality via the PageRank algorithm, and obtaining node density by calculating the distance between a node and the cluster center in the latent space.
- **ANRMAB** (Gao et al. 2018): It uses the same criteria as AGE and applies a multi-armed bandit mechanism to adaptively change the importance of these criteria in node selection.
Table 1: Statistics of datasets used in experiments.

| Dataset | # Nodes | # Edges | # Classes | # Features |
|---------|---------|---------|-----------|------------|
| Cora    | 2,708   | 5,429   | 7         | 1,433      |
| Citeseer| 3,327   | 4,732   | 6         | 3,703      |
| Pubmed  | 19,717  | 44,338  | 3         | 500        |

Implementation details. For a fair comparison, we closely follow the experiment setting in previous work (Cai, Zheng, and Chang 2017; Gao et al. 2018). For each dataset, we use 500 nodes for validation and 1,000 nodes for testing. The remaining nodes are set as the initial unlabelled data pool $U$. Besides, we randomly sample 500 nodes for validation to ensure that the performance variation is due to different active learning strategies. We actively select nodes every 4 epochs for Cora, 6 epochs for Citeseer, and 8 epochs for Pubmed due to different sizes of the graphs. We train two-layer GCN with 16 hidden units for a maximum of 200 epochs using the Adam optimizer (Kingma and Ba 2015) with a learning rate of 0.01 and early stopping with a window size of 10. The hyperparameters (i.e. the hidden units of GCN, the node selection frequency and the edge dropout rate) are tuned on the validation set using grid search. We repeat this process for 10 times on 10 different validation sets and report the averaged performance.

All experiments are conducted using PyTorch on a computer server with eight NVIDIA Titan Xp GPUs (with 12GB memory each) and fourteen Intel Xeon E5-2660 v4 CPUs.

4.2 Model Comparison (RQ1)

To evaluate the performance of our proposed method, we compare it with several baselines on three widely-used graph dataset in terms of Micro-F1. The results are shown in Table 2, with the highest performance highlighted in boldface. We make the following observations regarding the experimental results: at first, our method outperforms all baselines with a significant margin. Specifically, it improves the performance by 1.2%, 2.2% and 0.5% on Cora, Citeseer, and Pubmed respectively, compared to the current state-of-the-art method ANRMAB, which demonstrates the superiority of the proposed method.

As the GCN model is known to be sensitive to the dataset split (Kipf and Welling 2017), we further compare our method with the public split, trained with a semi-supervised manner. The results are presented in Table 3 where it is found that the performance of GCN model advances by a significant margin using the split selected via DAGRL, compared to the public split used in (Kipf and Welling 2017) and the random split.

The reasons for the improvement of the performance can be analyzed as follows:

- Previous uncertainty sampling methods may select sparsely-connected nodes, which are less effective for training, while our variance-based method is able to find nodes connecting two clusters which are effective for training.

- Two representativeness methods both explicitly utilize the graph structure information and the purity-based method further captures the attributive information, which avoids selecting nodes with noisy inter-class edges.

- The novel cluster-aware node selection policy takes the class size into consideration, which can select more informative nodes in larger-size classes.

4.3 Ablation Studies (RQ2)

We further conduct ablation studies on different selection criteria. To be specific, we design the following active learning strategy variants: (1) variance-based sampling only (DAGRL–$\text{pd}$), (2) purity-based sampling only (DAGRL–$\text{ud}$), (3) degree-based sampling only (DAGRL–$\text{up}$), (4) variance-based plus degree-based sampling (DAGRL–$\text{p}$), and (5) variance-based plus purity-based sampling (DAGRL–$\text{d}$).

As illustrated in Figure 2, it can be apparently seen that the hybrid node selection criteria used by DAGRL reaches the
best performance on all datasets, which verifies the importance of considering both structural and attributive information again. Besides, only using the variance-based uncertainty sampling also achieves the promising performance, revealing that the informative nodes (i.e., nodes which are hard for the model to classify) are selected via variance-based criteria. It is worth noting that applying degree-based method alone on Citeseer and Pubmed leads to the worse performance because this method does not consider any semantic information and some nodes which have noisy inter-class edges are selected.

4.4 A Case Study: the Karate Club Network (RQ3)

In this section, we conduct a case study on a well-known graph dataset, the Karate Club Network (Zachary 1977), to give qualitative difference between previous entropy-based uncertainty sampling criteria and our variance-based criteria. The Karate Club Network contains 34 nodes and 156 edges, corresponding to the social relationship among members in a university karate club. It is worth noting that, in this graph, nodes of the number of 0 and 33 represent two coaches who lead a group of members respectively.

In our experiment, we actively select 10 nodes by applying entropy-based sampling and variance-based sampling respectively. The selected nodes are marked in green in Figure 3. From the two figures, it is shown that our proposed variance-based method is able to find two coach nodes, which represent two hub nodes in this network. Contrary to our proposed scheme, most of nodes selected by the entropy-based method are sparsely-connected, which may contribute little to the learning process. The reason why entropy-based methods tend to select these sparsely-connected nodes is that the entropy-based criteria only selects nodes that the model is least confident to, ignoring the graph structures. In our proposed variance-based method, to find those influential nodes, we make random perturbation to the graph, where these sparsely-connected nodes tend to be more isolated, preventing them from information propagation in the graph. Therefore, the embeddings of these nodes tend to remain stable during random perturbation, i.e., the variance of these embeddings are relatively small, which will not be selected by our scheme.

4.5 Discussions on the Node Selection Policy (RQ4)

In this section, we discuss how do three different node selection policies affect the performance of model. Direct selection policy (Direct) selects the most informative node from the whole unlabelled data pool, cluster-balanced policy (Cluster-balanced) selects a node from each class at each step, and our proposed cluster-aware policy (Cluster-aware) sets the budget of each class to be proportional to the class size. Once the number of selected nodes in a class reaches the budget, we will no longer pick a node from this class.

The performance of model using these policies are summarized in Table 4. It is clear that our proposed cluster-aware policy outperforms the other two methods on all datasets. Direct selection policy performs the worst mainly because it does not consider any class information. Though cluster-balanced policy, which is used in previous benchmark AL algorithms (Cai, Zheng, and Chang 2017; Gao et al. 2018) achieves better performance than the direct policy, it still regards all classes equally and some informative nodes in the large-size class may not be selected via this policy. However, the cluster-aware policy takes the class size into account, which further explores the rich semantic information contained in the graph, helping the algorithm to find the most informative nodes in each class, hence enhances the performance of the model.

5 Conclusion

In this paper, we have proposed a novel active learning algorithm for graph representation learning named DAGRL. Firstly, by employing variance-based uncertainty criteria, our algorithm explicitly utilize the structural information to select nodes which are sensitive to the graph structure perturbation. Secondly, we have designed two simple but effective representativeness sampling criteria (i.e. degree- and purity-based criteria), through which they fully utilize the structural and semantic information to select dense-connected and high-purity
nodes, which are effective for training GNNs. Then, we combine these three criteria with the time-sensitive scheduling in accordance to the training progress. At last, considering that there are probably more informative nodes in the large-size class, we have applied a novel cluster-aware node selection policy, which adaptively select nodes from each class according to the class size. Experiments on several public datasets demonstrates the effectiveness of our algorithm.

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