Learning Graph Embedding with Limited Labeled Data: An Efficient Sampling Approach

Qirui Li1,∗, Xiaoming Liu1,∗,†, Chao Shen1, Xi Peng2, Yadong Zhou1 and Xiaohong Guan1
1Ministry of Education Key Lab for Intelligent Networks and Network Security, Xi’an Jiaotong University.
2Deep Robust and Explainable AI Lab, University of Delaware.
lqr1996@stu.xjtu.edu.cn, {xm.liu,chaoshen,ydzhou,xhguan}@xjtu.edu.cn,xipeng@udel.edu *
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Abstract

Semi-supervised graph embedding methods represented by graph convolutional network has become one of the most popular methods for utilizing deep learning approaches to process the graph-based data for applications. Mostly existing work focus on designing novel algorithm structure to improve the performance, but ignore one common training problem, i.e., could these methods achieve the same performance with limited labelled data? To tackle this research gap, we propose a sampling-based training framework for semi-supervised graph embedding methods to achieve better performance with smaller training data set. The key idea is to integrate the sampling theory and embedding methods by a pipeline form, which has the following advantages: 1) the sampled training data can maintain more accurate graph characteristics than uniformly chosen data, which eliminates the model deviation; 2) the smaller scale of training data is beneficial to reduce the human resource cost to label them; The extensive experiments show that the sampling-based method can achieve the same performance with only 10%-50% of the scale of training data. It verifies that the framework could extend the existing semi-supervised methods to the scenarios with the extremely small scale of labelled data.

1 Introduction

Graph is a natural way to represent and organize data with complicated relationships. But graph data is hard to processed by the machine learning methods directly, especially the deep learning [LeCun et al., 2015], which has achieved brilliant achievements in various fields. Learning a useful graph representation lies at the heart of many deep learning-based graph mining applications, such as node classification, link prediction, and community detection, etc.

It is now wildly adopted to embed the structure data into vectors for the well developed deep learning methods. Recently, Semi-supervised method represented by graph con-

volutional network has been a hot topic in graph embedding area, and massive outstanding works are proposed. Kipf[2017] came up with GCN, the one widely used today, has formally brought the field of graphs into neural networks’ era. Since then, plenty of work like GraphSAGE[Hamilton et al., 2017], Graph Attention Networks[Veličković et al., 2017] have been proposed.

However, there are two key challenges in applying these semi-supervised methods to specific fields: 1) extreme insufficient of labeled data; 2) out-of-distribution prediction, when the distribution of training set differs from the test set much. Works like GCN[Kipf and Welling, 2017], GAT[Veličković et al., 2017] tend to handly pick the training set in order to maintain the distribution-similarity. On the other hand, as this work is proceeding, there are some researchers seek to overcome the challenges by utilizing transfer learning[Hu et al., 2019; Yun et al., 2019]. But the ’pre-train’ methods needs extensive domain knowledge and pretty long training time.

To address the research gap, we proposed a sampling-based training framework for graph convolution network methods in this paper, which is more scalable and needless of domain knowledge. We integrate a random walk-based sampling strategy into the graph convolution network model training process. In this way, our framework utilizes the sampling algorithm to find out the most representative nodes of

*Both authors contributed equally to this work.
†Corresponding author.
a graph, which have proven successful in graph measurement, and graph structure estimating. The comparison between random walk-based sampled nodes and uniformly chosen nodes with limited ratio is shown in Fig. 1. When the sampling scale is small, the 'Law of Large Number' fails, and nodes chosen uniformly are more likely to be in a small sub-graph, which would lost much information during the training process. Several works[Hamilton et al., 2017; Chen et al., 2018] also utilize the thought of sampling, the difference between ours and them will be clarified in Section 2.

Our framework can improve the performance of existing graph convolution network methods significantly with the following advantages: 1) the random walk-based sampled training data can maintain more accurate graph characteristics than uniformly chosen data, which eliminate the model deviation; 2) the well-sampled training nodes can estimate the parameters in graph convolution network models effectively; 3) the smaller scale of training data to be labelled would make the existing models work with limited labelled data and save lots of human resource. To demonstrate the sampling method’s verification in training graph convolution network, we combine it with five state-of-the-art GCN-based methods, and evaluate its performance on challenging multi-label node classification problems with limited labelled training data. The result shows that each combined method can outperform its original one with the same scale of training data, or achieve the same accuracy with less labelled data.

The contribution of this paper is summarized as follows:

- To the best of our knowledge, this is the first work by utilizing the sampling strategy as a preprocess stage to improve the performance of graph convolution network algorithms. It can reduce the scale of labelled data and lower the human resource cost significantly without changing the original methods.

- We develop a general framework by integrating a random walk sampling strategy with graph convolution network methods, which could make them obtaining better results and extent them to the application with extremely small scale of labelled data.

- We verify the validation of our idea by evaluating our framework on different real-world networks. The case study of multi-label node classification shows that our framework can make GCN-based methods outperform their original ones.

This work is organized as follows. In Section 2, we formulate the problem definition. In Section 3, we detail the sampling-based training framework for graph convolutional network related methods. We demonstrate our experiment settings and result in Section 4. Finally, we close with a discussion of related work in Section 5 and conclusions of our work in Section 6.

## 2 Problem Definition

In this paper, we are trying to solve the problem that most of the state-of-the-art graph convolution network methods need a large number of labelled nodes as the training set.

We seek to solve this problem by proposing one sampling-based training framework introduced in section 1, we only need to put labels on the tiny-scale nodes set we sampled out and train the graph convolution network model to the same level performance as usual.

The most related work is FastGCN[Chen et al., 2018] and GraphSAGE [Hamilton et al., 2017]. These two works also manage to utilize sampling method (we simplify it as F-sampling as feature sampling) to improve the performance. But it is necessary to clarified that their sampling strategies and ours mentioned in this paper are not the same concept. Specially, both FastGCN and GraphSAGE focus on how to downsize the data steam passing through layer to layer in the graph convolution network during the training process, either change the network structure or the neighbour’s information.

We, differently, use sampling strategy (we simplify it as N-sampling as training node sampling) as a pre-process method, and pronounce a general framework, which can be extented easily to almost every kind of node representation methods, without the requirement of knowing specific workflow of the inner methods.

In short, F-sampling strategy aims to select features for the training nodes by changing the workflow of original models, but N-sampling is determined to select the more representative training nodes without changing anything of the original model.

## 3 Methodology

We seek to build such sampling-based framework for training graph convolution networks. Our framework can be generalized into a three-stage algorithm. First, we need to perform a sampling process on the graph we are going to deal with.

\[ V_s, X_s, Y_s = f(V, X, Y, B) \] (1)

The function \( f \) is the sampling strategy. Respectively, \( V_s, X_s, Y_s \) represent the sampled nodes, the corresponding feature matrix and labeled vectors. While the \( B \) denotes the the expected sampling budget. The original training process will be carried on after the training set has been sampled out by equation 1.

Generally, we demonstrate the training strategy by a generalized equation 2,

\[ Model = F(V_s, X_s, Y_s) \] (2)

The function \( F \) represents the training process based on the sampling training dataset. After the model has been well trained, it can be functional as usual.
Our framework integrates these three stages in a pipeline, as shown in Fig. 2. The framework samples a small scale of data as training set, whose time complexity is lower than linear. What’s more, because of the independent of the stages for sampling and training, the framework can be implemented on different models and datasets easily.

3.1 Sampling Strategy

The randomly way for choosing training dataset can be seen as ‘uniformly randomly sampling’(a.k.a UR), which select a node by the probability of \( p(v) = \frac{1}{N} \). \( N \) refers to the number of nodes. Because of its randomness, the generalization performance of its correlated networks varies a lot.

In order to overcome the disadvantage of UR, we consider several common used sampling methods: Depth First Sampling(DFS), Breadth First Sampling(BFS), Random Walk.

DFS and BFS are common ways to explore the graph structure, but both has inherent defect. If we set the sample budget as a certain small number, DFS may sampled out a long way through the graph, loosing the information on its way deep into the graph. BFS, on the contrary, could sampled out nodes within a small part of the whole graph.

Regular random walk(RW) is one of the popular methods to explore the network structure by obtaining a series of nodes or edges. It starts from a root vertex \( v^1 \). Then push \( v^1 \) into the traversed node list \( L \), and choosing its next hop \( v^2 \) uniformly from the neighbours of \( v^1 \). The probability that \( v^{t+1} \) will be selected by the probability of \( v^{t+1} = \frac{\text{deg}(v^t)}{\sum_{v \in L} \text{deg}(v)} \), where \( \text{deg}(v^t) \) is the degree of node \( v^t \). Repeating this moving strategy for \( T \) times, we get the whole traversed node list. This makes the most common type of RW.

RW can be performed with low time cost, and it is a exploration and exploitation tradeoff, which overcomes the weakness of BFS and DFS.

But this type of random regular walk still suffers from several flaws. It has a relatively high demand for the structure of the graph. A necessary condition for a regular RW to reach stationary is that the graph must be symmetric, connected, and non-bipartite. When the graph is not connected, a regular random walk would only explore the sub-graph where it starts. This would severely damage the result of training a model random walker would only explore the sub-graph where it starts. This would severely damage the result of training a model.

In order to overcome these drawbacks, we utilize a technique called "Frontier Sampling"[Ribeiro and Towsley, 2010], which is an advanced sampling strategy based on random walk. It performs \( m \) dependent walkers at the same time, who share the candidate list \( L \) together.

Walkers" in "Frontier Sampling" are less likely to get stuck in a loosely connected part of the whole graph. And this kind of method can be easily parallelized. We would also carry out a comparison experiment in Section 4.5 on the sampling methods mentioned above, in order to verify the analyse.

3.2 Implementation

The sampling strategy provides a easy and effective way to decrease the scale of the training set scale. We intend to combine this kind of strategy as a preprocess stage of GCN-based methods in a pipel ine form.

The sampling stage takes the graph \( G \), sampling budget \( B \) and the number of the walkers \( m \) as input and generate the sampled list \( S \) by performing Line 1-13 in Algorithm1.

The nodes \( V_s \) in the sampled list \( S \), their correspond features \( X_s \) and the labels \( Y_s \) will be fed into GCN-based methods. The models then function as it used to be. We formulate the whole structure of our framework as Algorithm 1, which is a typical three-stage framework.

3.3 Feasibility

The node sequence sampled in Algorithm 1 can maintain more accurate graph structure than that by uniformly randomly sampled, which overcomes the second drawback we mentioned in Section 1: out-of-distribution prediction. Considering a important graph characteristic – label density, we assume that each vertex \( v \) is associated with a label \( Y(v) \in \{y_1, ... , y_j \} \). The label density on graph \( G \) is \( \theta = \{\theta_1, ..., \theta_j \} \), \( \theta_i \) is defined by equation 3, \( \mathbb{1} \) is the indicator function.

\[
\theta_i = \frac{1}{n} \sum_{v \in V} \mathbb{1}(Y(v) = y_i), j \geq i \geq 1
\]
Utilizing the same unbiased estimator came up by Zhao [2019], which is depicted as equation 4.

$$\hat{\theta}_i = \frac{1}{C} \sum_{v \in S} x(v), \quad C = \sum_{v \in S} \frac{1}{\pi(v)} \quad (4)$$

$\pi(v)$ is the probability that node $v$ is sampled, which equals to $\frac{1}{n}$ in uniformly randomly sampling, and equals to $\frac{d_v}{m}$ in random walk at steady state, where $d_v$ is the degree of node $v$, and $m$ is the number of edges in the graph.

**Theorem 1:** For a single random walker, $(\hat{\theta}_i^{RW} - \theta_i)^2 \leq (\hat{\theta}_i^{UR} - \theta_i)^2$

**Proof.** For notation convenience, we depict $\sum_{v \in V} x(v)$ as $q$, $\sum_{v \in SU} x(v)$ as $p$. The length of sampled nodes is $B$. Combining the equation 3 and 4, the original inequality can be written as:

$$(\hat{\theta}_i^{RW})^2 - 2 \frac{p^2}{B^2} \leq \frac{2qp}{NB} \quad (5)$$

When $B\hat{\theta}_i^{RW} - p > 0$ we have:

$$N(\hat{\theta}_i^{RW}) \leq 2Bq \quad (6)$$

Equation 6 can be simplified and scaled as $2q - n\hat{\theta}_i^{RW} > 0$.

The situation also suits the condition that $B\hat{\theta}_i^{RW} - p \leq 0$.

Theorem 1 tells that the label density estimated by node sequence $S^{RW}$ sampled by random walk $\hat{\theta}_i^{RW}$ is closer to $\theta_i$ than $\hat{\theta}_i^{UR}$ estimated by uniformly randomly sampled sequence $S^{UR}$.

**Lemma 1:** The M-dimensional random walk process is equivalent to the process of a single random walker over $G^m$.

**Theorem 1** is proved by Ribeiro[2012], combining with Theorem 1, we can deduced Theorem 2.

**Theorem 2:** Estimating label density with nodes sampled by ‘Frontier Sampling’ can performs better than nodes sampled uniformly.

Theorem 2 prove the assumption we make before theoretically, and ensures the performance of the Algorithm 1.

### 3.4 Time Complexity

We come up with the framework to mainly reduce the training dataset scale, then reduce the labor force and compute consumption. So the first stage, i.e., sampling process, should not have a high time complexity. Or the data prepossessing stage may contrary to our original idea.

According to Algorithm 1, the whole sampling process’s time complexity $T$ depends only on the scale of the sampling budget $B$,

$$T \propto B, \quad B = \frac{n}{k}, \quad k \in (1, +\infty), \quad (7)$$

where $n$ represents the number of nodes in the graph $G$. Thus, the time complexity of sampling algorithm is lower than $O(n)$. Compared with the graph convolutional network methods’ time complexity, the linear time complexity for sampling is acceptable.

### 4 Evaluation

We verify our proposal by the multi-class classification task on three real-world datasets, including two citation networks and one social network. In the citation networks, the nodes are papers and the edges are the citation relationship. Each paper has a feature vector that contains the information of its contents. Classes implicate the kind of the categories among the papers. And for social network, the nodes represent users using the social media, and an edge between two users means the follower-followed relation. And the details for these datasets are presented in Table 1.

| Dataset       | Type      | Node     | Edges    | Classes |
|---------------|-----------|----------|----------|---------|
| Cora          | Citation  | 2,707    | 5,429    | 7       |
| Pubmed        | Citation  | 19,717   | 44,338   | 3       |
| BlogCatalog   | Social    | 10,312   | 333,983  | 10      |

### 4.1 Experimental Settings

We utilize our framework on five GCN-based methods to verify the validation of our proposal. For the sampling strategy, we set $m = 3$. For the training data scales(sampling budget), we range it in $[0.5\%, 1\%, 5\%, 10\%]$ nodes for each dataset. For the baseline algorithms, we choose the same scale of training data from the graphs uniformly randomly; 100 nodes are randomly selected from training set as the validation part. The prediction accuracy is evaluated on another randomly selected 1000 nodes for each dataset. We use the ‘Cross Entropy Loss’ as our loss function during the experiments. For the methods combined with our framework, we use ‘SS-’ with the original method name to represent them. We performs each experiment 10 times and take the average results as the final results. The experiment on FastGCN is based on the code released by the original author\(^3\), and all the other algorithms are implemented based on the the Deep Graph Library (DGL)\(^4\).

### 4.2 Baseline Methods

To validate the improvement of the sampling strategy to GCN-related methods, we evaluate it on several state-of-the-art GCN-related baselines:

- **GCN** [Kipf and Welling, 2017]: This is the first wildly used graph convolutional network method to embed the graph structure. It takes the graph structure and a few number of labeled nodes as input and output the node embedding vector.
- **GraphSAGE** [Hamilton et al., 2017]: This method is built on GCN, which utilizes the neighbours’ features to represent one node. In this way, the framework can deal with dynamic graph structure.
- **SGC** [Wu et al., 2019]: This method speeds up the GCN’s training time by removing nonlinearities and collapsing weight matrices between consecutive layers.

\(^3\)https://github.com/matenure/FastGCN
\(^4\)https://github.com/dmlc/dgl
4.3 Results

We now validate the effectiveness of our framework by combining it with 5 GCN-related baseline algorithms and compare them with the original ones. Specifically, we use the task of node classification for evaluation. The experimental results are shown in Table 2. We bold the better result for each comparison pair, the detailed analyse for the table are as follows.

When we fix the training set at 0.5% and evaluate the performance of each algorithm, we can tell that the ones with sampling strategy can outperform the original ones 4% – 60%. This simulates the extreme situation that the labeled data are scarcely little. We can get a lift of 10% on average, which is significant. And the greatest improvement happens with GCN and SS-GCN on the Pubmed dataset.

As the training set scale raises, although the improvement gets smaller, it still exists. We can get an improvement of 4% when the training scale is set as 10%. In some cases, under the relatively larger training set, because of the powerful structure of the original algorithm, it can get the same result with its 'SS-' competitor. The trend that the gap shrinks with the growing of the training set scale is reasonable, because the large data scale makes sure that uniformly sampling can explore as much as the 'Frontier Sampling' we utilize.

If we take another perspective, we can get more meaningful observations. Take the accuracy of SS-SGC on the Pubmed with 0.5% dataset – 0.81 as a goal. We notice that the original SGC can achieve this accuracy on the same dataset with up to 5% of the training data, which is 10 times of SS-SGC. In other words, sampling strategy can save 90% need of labelled data to get the same accuracy. This observation benefits more in real-world scenarios, the saving of labelled data can significantly improve the efficiency of labelling process and cross-validate among different models or datasets.

4.4 Algorithm Efficiency

The training data with well distribution would help the model to quickly converge, which is a common way to reduce the training time. The sampling method we utilized is a simple but effective way to achieve the target of well-distributed training data.

To evaluate the contribution to reduce the training time, we carried out a case study on GraphSAGE and SS-GraphSAGE with the Pubmed dataset. We set 10% of the dataset as the training data, and the number of training epochs is set as 200. The converge speed of GraphSAGE and SS-GraphSAGE is

![Figure 3](image-url)

Figure 3: (a) shows the training process of GraphSAGE and SS-GraphSAGE; (b) compare the SS-GraphSAGE with the original one; Fig. 3b does the comparison among several sampling strategies.
Figure 4: Figure 4a depicts the gap from the steady accuracy with different sampling scale for SS-GraphSAGE; Figure 4b depicts the accuracy and memory cost with different number of walkers.

A box figure shows the sampling-based methods can easily approach the steady performance with about 1% to 3% of nodes as training sampling data. It reveals the power of sampling strategy added to the GCN-related methods.

4.5 Sampling Strategy Comparison
We have discussed about several sampling strategies in Section 3.1. We have done a case study on the 'cora' dataset with GraphSAGE to verify our analyse before. We replace the 'Frontier Sampling' we used in Algorithm 1 by 'Uniform sampling', 'Regular Random Walk', 'DFS', and 'BFS'. Experiment setting is the same as the one in Section 4.1. From the result shown in Fig 3b (We take the Natural logarithm of the training set scale for clarity display), we can tell the sampling method we use outperforms the others theoretically and experimentally. Regular random walk performs the worst when the sampling scale is shrink to 0.5%, caused by its nature of 'easily been trapped', but its accuracy raises dramatically when the scale get a little bit larger, which is consistent with our analyse. To be noticed, when the training scale get larger, uniformly sampled data can get close accuracy with ours, which meets the 'Law of Large Number'.

4.6 Parameter Influence
We take a numerical evaluation on the influence of sampling scale $B$ and the number of random walk dimensions $m$ with SS-GraphSAGE on the Cora dataset.

Sampling Scale
Fig. 4a shows the accuracy distance from the steady performance with different sampling budget $B$ on multi-label classification task. The steady accuracy is obtained through taking 50% of the nodes as training data. From the result, we can observe that the sampling-based methods can easily approach the steady performance with about 1% to 3% of nodes as training sampling data. It reveals the power of sampling strategy added to the GCN-related methods.

Number of Walkers
The sampling scheme performs a $m$ dimensional random walks. Fig. 4b shows the influence of the number of walkers $m$ on the accuracy and memory cost. The box figure shows the distribution of accuracy, the green line is the median accuracy, and the yellow line across the boxes connects the average accuracy. It shows small fluctuations with the changing value of $m$. The memory cost is also plotted in the same figure, which stays at about the same level when the $m$ ranges.

5 Related Work
Two lines of research are related to our work, which are summarized as follows.

5.1 GCN-based Methods
Graph neural networks have drawn a lot of attention recently. It has been proposed since 2014[Bruna et al., 2014], and been modified by[Defferrard et al., 2016; Duvenaud et al., 2015]. Kipf’s GCN[2017] has brought it under the spotlight. Since then researchers seek to build more effective network structure. Like the GraphSAGE[Hamilton et al., 2017] is proposed to deal with the dynamic graphs, Graph Attention Network[Velickovic et al., 2017] is proposed to weight the node’s neighbours. Some works also focus on the problem of training efficiency, FastGCN[Chen et al., 2018] is one of the pioneers to accelerate the training process by eliminating part of neurons. SGC[Wu et al., 2019] steps further by simplifying convolutional computation.

5.2 Graph Sampling Based on Random Walks
Sampling methods, especially random walk-based graph sampling methods, have been widely studied[Avrachenkov et al., 2010][Ribeiro et al., 2012][Xu et al., 2014]. Leskovec[2006] has came up with an efficient way to down-size the sampling scale based on random walk. And Wei[2004] has worked out how to make the sampling by random walk more efficient. Random-walk based sampling can also be used in overlay networks[Massoulié et al., 2006]. Based on the prior knowledge about the graph structure, Zhao et al. [2019] proposed a graph sampling strategy by random walk with indirect jumps.

6 Conclusion and Future Work
Faced with the challenge of limited labeled data for semi-supervised methods, we propose a sampling-based model to improve their performance without changing original model. The evaluation of our proposal on real-world datasets show that our framework could achieve better results with smaller scale of training data, and it surpasses the original ones 4% - 60%.

In this paper, we take a small step to improve the performance of semi-supervised methods represented by GCN in the condition of limited labeled data. But limited labeled data is a very common problem in graph embedding method study, and we would try to develop a more general framework working for all of them. What’s more, we would like to study the problem of lowering the training time complexity with smaller scale of training data.

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