

Semi-supervised Graph Embedding for Multi-label Graph Node Classification

Kaisheng Gao, Jing Zhang^(⊠), and Cangqi Zhou

School of Computer Science and Engineering, Nanjing University of Science and Technology, Nanjing 210094, China {kaisheng_gao, jzhang, cqzhou}@njust.edu.cn

Abstract. The graph convolution network (GCN) is a widely-used facility to realize graph-based semi-supervised learning, which usually integrates node, features, and graph topologic information to build learning models. However, as for multi-label learning tasks, the supervision part of GCN simply minimizes the cross-entropy loss between the last layer outputs and the ground-truth label distribution, which tends to lose some useful information such as label correlations, so that prevents from obtaining high performance. In this paper, we propose a novel GCN-based semi-supervised learning approach for multi-label classification, namely ML-GCN. ML-GCN first uses a GCN to embed the node features and graph topologic information. Then, it randomly generates a label matrix, where each row (i.e., label vector) represents a kind of labels. The dimension of the label vector is the same as that of the node vector before the last convolution operation of GCN. That is, all labels and nodes are embedded in a uniform vector space. Finally, during the model training of ML-GCN, label vectors and node vectors are concatenated to serve as the inputs of the relaxed skip-gram model to detect the node-label correlation as well as the label-label correlation. Experimental results on several graph classification datasets show that the proposed ML-GCN outperforms four state-of-the-art methods.

Keywords: Graph convolution network · Graph embedding · Graph node classification · Multi-label classification

1 Introduction

There exist many graph-structured datasets in the real world, such as social networks, academic citation networks, and knowledge graph. Graph Representation Learning (GRL) methods that aim to learn the vector representations for graphs has attracted much attention in recent years. Because the dimension of every node vector could be very large it may suffer from the high computational complexity and huge memory space usage, if we merely use the one-hot encoding methods or a discrete adjacency matrix to present the nodes. Therefore, we usually embed a graph into a low-dimensional space, which not only preserves the structural information but also significantly reduces the computational costs. Within this low-dimensional space, the distance between two nodes with a close relation in the original graph will also be close in a measure derived from the embedding presentation. Here, the close relation of two

nodes means that they are directly connected with each other or share a set of common neighbors, which is often used to define the similarity of two users in a social network.

There are several graph embedding methods proposed in recent years. For example, GF [1] factorizes the adjacency matrix and minimizes the L2-norm of the embedding matrix. LINE [2] defines two joint probability distributions for each pair of nodes, one using the adjacency matrix and the other using the embedding vector. Then, LINE minimizes the KL divergence of these two distributions. DeepWalk [3] uses a random walk to generate a node sequence. Then, for each node sequence, it applies the Word2Vec model [4] to get the node embedding by treating each sequence as a word sentence. All the above methods can be classified as the shallow model, compared with the methods using deep learning technology. Recently, a kind of deep learning models, namely graph neural networks (GNN), has attracted much attention, including some typical methods such as GraphSage [5], graph attention networks (GAT) [6], and graph convolutional networks (GCN) [7], which use neural networks to train classification models on graph-structured datasets.

GCN is a deep neural network model to catch structural information in a graph, which has been widely used in several machine learning paradigms, such as semantic role labeling [8], event extraction [9], and recommendation tasks [10]. In addition, the GCN model also obtains good performance in graph-based semi-supervised learning because its structure is robust to the missing information in training sets [7]. In a semi-supervised learning task, GCN uses a graph convolution operation to integrate each node and its one-hop neighbor information in each layer. After conducting several layers of convolution, each node in the network can gather its *k*-hop neighbor information in the final layer, which is the embedded feature presentation of such a node. Eventually, we can use some supervised information to train a classifier based on these embedded features.

Usually, multi-label classification models are trained in a semi-supervised manner, because not all labels on every instance are obtained values. In multi-label graph datasets, one node may have several labels. i.e. the correlation between this node and these labels are high, we called it node-label correlation. if two labels are highly correlated, the nodes with these labels should be close in the embedding space. For example, in movie genres dataset, the genres (labels) "Western" and "Adventure" always appear in the same movie. Thus, two movies with labels "Western" and "Adventure" respectively should also be close to each other. We called this *label-label correlation*. Because this correlation is not reflected in the graph structure it cannot be captured in the original GCN models. Accordingly, for a multi-label graph dataset, some nodes may have several specific labels. That is, one node and some labels may be highly correlated, which is called the *node-label correlation* in this study.

To address this issue, we propose a novel GCN-based model for semi-supervised multi-label graph node classification, namely ML-GCN. To capture the high non-linear correlations among nodes, we use a two-layer neural network model, on each of which we conduct a series of graph convolution operations. To preserve the label-label correlation, we treat each label as a vector so that we can measure the relationship between two labels. After labels are embedded, we can shorten the distance between two nodes whose labels are highly correlated in the embedding space. After obtaining the representation of all nodes in a graph, we can train a multi-label classifier to make

predictions to the unlabeled nodes. In the proposed ML-GCN method, we use a sigmoid layer as the downstream learning method. The contributions of this paper are three-fold:

- We first investigate the applicability of graph convolutional network applying to the
 multi-label learning and point out that the label-label correlation should be considered to improve the learning performance.
- We propose a novel learning method, namely ML-GCN, where labels on nodes and
 the nodes themselves are uniformly embedded into the same low-dimensional
 space. ML-GCN can capture both node-label and label-label correlations. To the
 best of our knowledge, it is the first that the labels of each node are embedded and
 fed into GCN.
- We conduct a comprehensive empirical study on three real-world multi-label graph node classification datasets, whose results demonstrate that ML-GCN outperforms four state-of-the-art methods.

The remainder of the paper is organized as follows: In Sect. 2, we briefly review the related work. Section 3 presents the novel ML-GCN method. In Sect. 4, we compare our ML-GCN with four state-of-the-art methods on three real-world datasets. Section 5 concludes the paper.

2 Related Work

A large number of application problems can be abstracted as a classification problem in a graph structure, where some attributes of nodes in the graph are being predicted. In recent years, various kinds of graph neural network models have been proposed [11], such as graph convolution networks (GCN) [7], graph attention networks (GAT) [6], graph autoencoder [12], graph generative networks [13], graph spatial-temporal networks [14], and so on. The principle of most of these approaches is the *neural message* passing proposed by Gilmer et al. [15]. In the message-passing framework, a GNN can be viewed as a message passing algorithm, where the representation of a node is iteratively computed from the features of its neighbor nodes using a differentiable aggregation function. For the identity of the principle, the GCN model can be considered as a fundamental structure of most GNN models [11], which aggregates each node with its neighbors and let the node receive messages from its neighbors. Therefore, in this paper, we mainly focus on GCN models. GCN models can be divided into two categories: spectral-based and spatial-based approaches. The spectral-based methods define convolution operations by introducing filters from the perspective of graph signal processing [16], where the convolution on the graph is interpreted as removing noise from graph signals and passing messages in the spectral domain. The spatial-based approaches formulate convolution operations on a node as aggregating feature derived from its neighbors and the information passing through it. In general, all the GNN-based methods attempt to embed the graph structural information into vectors and follow the same hypothesis that nodes with similar structure tend to be close in the embedding space.

Multi-label learning is usually semi-supervised because, in many situations, instances in the training set do not necessarily have all the potential labels been assigned values. The training process usually learns from fully-labeled, partly-labeled, and even unlabeled samples to form predictive models. For the multi-label learning in a graph structure, a straightforward method is to train multiple independent binary classifiers for each label. However, this simple method has several defects: It does not consider the correlations among labels: The number of labels to predict will grow exponentially as the number of label categories increases; It is essentially limited by ignoring the topological structure among nodes. In some recent studies, researchers attempted to capture label-label correlations in some classical deep learning models for multi-label classification. Gong et al. [17] used a ranking-based learning strategy to train deep convolutional neural networks for multi-label image recognition and found that the weighted approximated-ranking loss performs best. Wang et al. [18] utilized recurrent neural networks (RNNs) to transform labels into embedded label vectors so that the correlation between labels can be employed. Wang et al. [19] introduced a spatial transformer layer and long short-term memory (LSTM) units to capture label correlation.

In this study, our novel learning method is still based on the GCN model but first introduces the label matrix embedding to capture the label-label correlation among the graph nodes.

3 The Proposed Method

The key idea behind the proposed ML-GCN is that it embeds multiple labels and nodes in the same space, where label-label correlations and label-node correlations can be simultaneously considered. In this section, we first introduce the problem statement and some preliminaries. Then, we present the label embedding scheme of ML-GCN. Finally, we present the optimization algorithm of the ML-GCN model.

3.1 Problem Statement

We define graph G = (V, E, X, Y) as an undirected graph, where $V = (V_l \cup V_u)$ is a finite node set that includes n_l labeled nodes (V_l) and n_u unlabeled nodes (V_u) . There are totally $n = n_l + n_u$ nodes on the graph. E is an edge set and $X \in \mathbb{R}^{n \times d}$ is a feature matrix of all the graph nodes. $Y \in \mathbb{R}^{n_l \times c}$ is a 0–1 matrix that presents the labels of n_l labeled nodes, where c is the number of different label types in the dataset. The adjacency matrix of the graph is denoted by $A = [a_{ij}] \in \mathbb{R}^{n \times n}$, where a_{ij} is the weight assigned on the edge between nodes i and j. The degree matrix of A is denoted by a diagonal matrix $D = diag(d_1, \ldots, d_n)$, where $d_i = \sum_j a_{ij}$ is the degree of node i. The

symmetric normalized Laplacian matrix is denoted by $L_{sym} = I - D^{-\frac{1}{2}}AD^{-\frac{1}{2}}$. Our goal is to build a multi-label classification model that can predict the labels of unlabeled graph nodes.

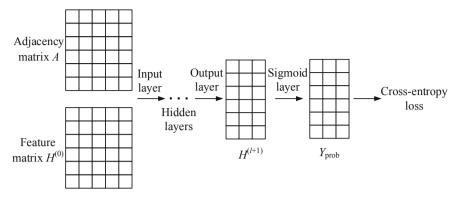


Fig. 1. The structure of graph convolutional networks (GCN).

3.2 Preliminaries: Graph Convolutional Network (GCN)

To embed features of nodes and their structural information, we first introduce the graph convolutional networks (GCN) [7]. Figure 1 shows a basic structure of graph convolutional networks. In particular, the core of GCN is the operation in each layer, which can be defined as follows:

$$H^{(l+1)} = \sigma \left(\tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}} H^{(l)} W^{(l)} \right). \tag{1}$$

Here, $\tilde{A} = A + I_{n_l + n_u}$ is an adjacency matrix with self-connections added. Matrix $I_{n_l + n_u}$ is an identity matrix. Diagonal matrix. Diagonal matrix $\tilde{D} = diag(\tilde{d}_1, \dots \tilde{d}_n)$ is a degree matrix of \tilde{A} , where $\tilde{d}_i = \sum_j \tilde{A}_{ij} \cdot W^{(l)} \cdot W^{(l)}$ trainable parameters of the l-th layer. Function σ is an activation function. In this paper, the activation function of each layer is defined as $\sigma(x) = \max(0, x)$ as it used in other studies [7]. In the first layer, we have $H^{(0)} = X$. That is, we take the graph feature matrix as the input of GCN. In the last layer, we have

$$Y_{prob} = \operatorname{sigmoid}\left(H^{(l+1)}\right) = 1/\left(1 + \exp\left(-H^{(l+1)}\right)\right), \tag{2}$$

where $H^{(l+1)} \in \mathbb{R}^{n \times c}$ and Y_{prob} is the probability distribution of labels for each node. Then, we minimize the cross-entropy loss between Y_{prob} and labeled nodes:

$$\min \sum_{i=1}^{n_l} y_i log\left(y_{prob}^{(i)}\right),\tag{3}$$

where y_i and y_{prob} denote the row vectors of Y and Y_{prob} , respectively. That is, we embed all nodes into a c-dimension space and use a sigmoid function to determine the predicted values of the labels. However, this simply model may be confronted with some drawbacks:

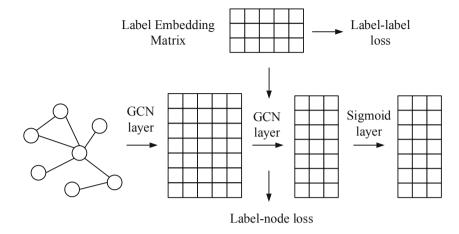


Fig. 2. The framework of the proposed ML-GCN.

- If we utilize fewer layers to construct GCN, the difference between the dimension of the last layer and the second to the last layer may be quite large. It may cause hidden feature loss and make the model difficult to optimize. For example, on the dataset in [20], whose input feature dimension is 3703 and the number of labels is six, if we use a two-layer GCN, we cannot let the dimension decrease smoothly regardless of the settings of the hidden layer dimension.
- As the article [21] pointed out, if we simply stack more layers, the model will mix
 the features of nodes from different labels and make them indistinguishable. This is
 because each layer of GCN applies Laplacian smoothing [22] to features, and every
 two nodes with a connected path tend to be close with Laplacian smooth.
- A multi-label classification model with a sigmoid layer cannot capture the labellabel relationship because it treats each label individually. Thus, it may lose some information on the multi-label graph dataset.

To address these drawbacks, we propose a novel model ML-GCN for multi-label classification in the next subsection.

3.3 ML-GCN: Label Embedding Matrix

The ML-GCN introduces a label embedding matrix as well as the label-node coembedding to GCN. Let $Z_Y \in \mathbb{R}^{c \times l}$ denote the label embedding matrix, where c is the number of different label classes and l is the dimension of label vectors. We generate the label embedding matrix randomly at the beginning of training. The dimension of the matrix is the same as the dimension of node features before the last graph convolution operation. Here, we set $H^{(l+1)}$ as the last output before the sigmoid layer. That is, the dimension l of the label embedding matrix is the same as the dimension of $H^{(l)}$. Then, we can calculate the label-label correlation and the label-node correlation using the Z_Y and $H^{(l)}$, respectively. Figure 2 shows the framework of the proposed ML-GCN. Here, each grid represents a matrix. We feed a graph into the first GCN layer and obtain

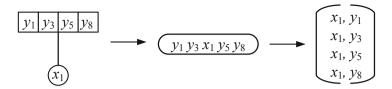


Fig. 3. Convert a node with several labels to a sentence.

the first embedding matrix as the output of this layer. Then, we use the randomly generated label embedding matrix to calculate the label-label loss, and together with the first embedding matrix to calculate the label-node loss. Then, we feed the first embedding matrix into the second GCN layer. Finally, we use the output of the sigmoid layer to calculate the cross-entropy loss against the ground truth.

Consider a node with several labels. Our goal is to maximize the occurrence probability of these labels given the node. The inputs are the node vectors and the corresponding label vectors. If we treat a node and its labels as a sentence, our goal also can be expressed as "given a center word (node), to predict the neighbor words (labels)," which is the essential idea of Skip-Gram [23]. For example, in Fig. 3, we have a node with four labels, and we can treat each element as a word and generate a sentence. Then, we utilize Skip-Gram for the next calculation.

In the Skip-Gram model, for a word w_i and window size c, we can extract w_i and its c-1 neighbors with w_i at the center. Word w_i and each of its neighbor can form a pair as (w_i, w_j) . The co-occurrence probability of w_j given w_i is defined as:

$$P(w_j|w_i) = \frac{\exp(w_j^T w_i)}{\sum_{t=1}^{M} \exp(w_t w_i)},$$
(4)

where M is all the words in the corpus. Thus, we can obtain the word embedding by maximize such co-occurrence probability for all the word pairs.

Consider the node-label sentences. Given a node x_i and its labels $Y_{x_i} = \{y_1, y_2, \ldots, y_c\}$, the vector representation of x_i is the *i*-th row of $H^{(l)}$, denoted by h_i . The label vector of y_j is z_{y_j} . We only consider the node as the center word and remove the window size. We use each label to form a pair with the node because there is no predefined order of its labels. Therefore, we have a set of node-label pairs, denoted by $\{(x_iy_1), (x_iy_2), \ldots, (x_iy_c)\}$. For any node x_i , we can optimize the node and its label embedding by maximize the object function as follows:

$$\max \frac{1}{c} \sum_{y_j \in Y_{x_i}} \log P(z_{y_j} | h_i)$$
 (5)

Since this function is operated in the second to the last layer of GCN and uses the features of layer $H^{(l)}$, we can better capture the node-label correlation in a high dimensional space before the feature dimension is reduced to the label-class wise. As we know GCN conducts the Laplacian smoothing on each node, whose consequence is

that the presentations of many nodes may tend to be the same at the final stage of training. Adding this function prevents the side-effort of the Laplacian smoothing in GCN. It hinders the Laplacian smoothing which aggregates each node to be hard to distinguish. Thus, it can accelerate the training process and prevent the model from over smoothing that makes each node converge to the same point.

To capture the label-label correlation, we utilize the same model but get rid of the node vectors. That is, we only use the labels of a node to construct the sentence. For example, given a node x_i with labels $\{y_1, y_2, \ldots, y_c\}$, we only use labels to construct a sentence, which forms a set of label-label pairs with the combinations of all different labels, denoted by $\{(y_1y_2), (y_1y_3), \ldots, (y_cy_{c-1})\}$. Note that the pairs of (y_iy_j) and (y_jy_i) are different. similar to Eq. (5), we have the objective function as follows:

$$\max \frac{1}{c} \sum_{y_i, y_j \in Y_{x_i, i \neq j}} \log P(z_{y_j} | z_{y_i}). \tag{6}$$

If the node only has one label, we omit the label-label relation and only calculate Eq. (5) on this node. To maximize the Eqs. (5) and (6), we can reserve the node-label correlation as well as label-label correlation in the embedding space.

3.4 Co-optimization and Negative Sampling

To calculate Eqs. (5) and (6), we need to calculate $P(z_{y_j}|h_i)$ and $P(z_{y_j}|z_{y_i})$, which requires the summation over all the labels. The calculation may cost too much running time because some multi-label graph datasets may have abundant label types. To accelerate the calculation of these two co-occurrence probabilities, we use a trick of negative sampling in the Skip-Gram model. First, we rewrite Eq. (1) as follow:

$$\min -\log \sigma(z_{y_i}h_i) - \sum_{t=1}^{K} \mathbb{E}_{y_t \sim P(y)} \log \sigma(-z_{y_t}h_i), \tag{7}$$

where K is a hyperparameter that represents the number of sampled labels for one nodelabel pair. Therefore, the task becomes to distinguish the target label y_j from the K labels drawn from the noise distribution P(y). The idea behind the negative sampling is: We will maximize the co-occurrence probability of z_{y_j} given h_i and minimize the probability of a randomly sampled labels z_{y_t} given the same node h_i . In practice, we define a noise distribution as chosen to be $U(y)^{3/4}/\sum_y U(y)^{3/4}$, where U(y) is the unigram distribution of the labels. Here, we only consider the co-occurrence times of each label type on labeled data as the unigram distribution. If the sample process obtains the positive label $y_t = y_j$, we just resample y_t until the condition $y_t \neq y_j$ is satisfied.

Similar to Eq. (5), we sample K labels as the negative labels and rewrite Eq. (6) as follows:

$$\min -\log \sigma(z_{y_j}z_{y_i}) - \sum_{t=1}^K \mathbb{E}_{y_t \sim P(y)} \log \sigma(-z_{y_t}z_{y_i}). \tag{8}$$

The goal is to distinguish the label y_j from K sampled negative labels on the condition of given y_i . To calculate Eqs. (7) and (8) in each labeled node, we can obtain the loss function L_{n-l} denoting the node-label loss calculated by Eq. (7) and l_{l-l} denoting the label-label loss calculated by Eq. (8). With the sigmoid loss of the last layer, we can have the final objective for optimization:

```
Algorithm 1: ML-GCN (Training and Predicting)
```

```
Input: Graph G, feature X, label Y_L, number of GCN layers l+I

Output: labels of unlabeled nodes Y_U

1: randomly generate the label matrix Z_Y

2: H^{(0)} = X

3: for epoch = l, ..., n do:

3: For i = 0, l, ..., l do:

4: calculate the output of i+I GCN layer H^{(i+1)} using H^{(i)}

5: L_{sigmoid} = \text{crossentropy}\left(Y_L, \text{sigmoid}\left(H^{(l+1)}\right)\right)

6: calculate Eq. (7) using Z_Y and H^{(l)}, and obtain L_{n-l}

7: calculate Eq. (8) using Z_Y, and obtain L_{l-l}

8: optimize to minimize L_{sum} = \lambda_1 L_{l-l} + \lambda_2 l_{n-l} + l_{sigmoid} using Adam [24]

9: return 1 if Y_{prob} = \text{sigmoid}(H^{(l+1)}) > 0.5, else 0, given Y_U
```

$$L_{sum} = \lambda_1 L_{l-l} + \lambda_2 l_{n-l} + l_{sigmoid}, \tag{9}$$

where $\lambda_1, \lambda_2 \in \mathbb{R}$ are the hyper parameters to weight three terms in the objective functions. We optimize the function with Adam optimizer [24]. We summarize all above contents with a pseudocode and list in Algorithm 1 (ML-GCN).

4 Experiments

In this section, we first present the datasets used in our experiments, methods in comparisons, and the experimental settings. Then, we focus on discussing the experimental results.

4.1 Datasets

Compared with the plenty of single-label classification datasets, there are only a few real-world multi-label graph node classification datasets that can be used in our experiments. We evaluate our ML-GCN model on three datasets collected from different domains of biology, movie, and social media. These datasets are chosen not only because they belong to different domains but also, they have different network topologic structures. The details of the datasets are listed in Table 1.

Dataset	Domain	Nodes	Edges	Classes	Features
Facebook	Social	347	5038	24	224
Yeast	Biology	1240	1674	13	831
Movie	Movie	7155	404241	20	5297

Table 1. The details of the datasets used in our experiments

The *Facebook* dataset [25] is a social network. The nodes represent users of Facebook and the edges represent the fan following relation. The feature of each node is the personal information of the corresponding user. The task is to determine the 'circles' tags of each user (node). One user can belong to multiple circles.

The *Yeast* dataset is part of the KDD Cup 2001 challenge¹. The graph is constructed based on the interactions between proteins. Each node represents a gene. The gene code information is set as the feature of nodes. The task is to predict the function of these genes.

We constructed a movie dataset from Movielens-2k dataset². The Movielens-2k dataset contains movies information such as actors, genres, and tags information. We set the tags information as the feature of movies and set a common director as an edge. For example, if two movies share the same director, we added an edge between these two movies, and set the weight of this edge to 1. The task is to predict the genres of the movies.

4.2 Methods in Comparison and Experimental Settings

Method in Comparison: We compared our ML-GCN with the following state-of-the-art methods:

- Multilayer perception (MLP) is a classical label classifier takes only node feature as input and ignores the graph structure.
- Deepwalk [3] learns node features by treating random walks in a graph as the equivalent of sentences.
- GCN [7] takes both node feature and graph structure as the input.
- Partly ML-GCN is a simpler ML-GCN without the calculation of the label-label loss. This method is added to evaluate the impact of the loss function on the performance of the learning models.

Experimental Settings: For fair comparisons, all the methods (MLP, GCN, Partly ML-GCN and ML-GCN) use two-layer models. For dataset *Facebook*, we set the middle layer dimension to 64 and use 100 nodes for training and 150 nodes for testing. For dataset *Yeast*, we set the middle layer dimension to 256 and use 200 nodes as training nodes and 500 nodes as testing nodes. For dataset Movie, we set the middle

¹ http://pages.cs.wisc.edu/~dpage/kddcup2001/.

² http://ir.ii.uam.es/hetrec2011/datasets.html.

layer dimension to 512 and use 500 nodes as training data and 2000 nodes as testing nodes. For all datasets, we set the number of negative sample to 5, set walk length to 40 for DeepWalk and set the window size to 10. All models are trained using Adam with a learning rate of 0.01. The parameters λ_1 and λ_2 are both equal to 0.25. We use the micro-F1 score (in percentage) as the evaluation metric in the paper.

4.3 Experimental Results

Experiment 1 (Overall Performance): The classification results of five methods on three datasets in terms of the micro-F1 score are summarized in Table 2. The best performance is in bold in the table. We have the following observations. Overall, our proposed ML-GCN method consistently outperforms the other methods on all datasets. Compared with the original GCN, on dataset *Facebook*, our ML-GCN achieves the improvement of 1.72 points, and on the datasets with stronger label-label correlations (i.e., datasets *Yeast* and *Movie*), the improvement of ML-GCN archived as high as 3 points. Thus, ML-GCN successfully captures the label-label correlations. Furthermore, our ML-GCN also outperforms the Partly ML-GCN on all dataset, which shows that the calculation of the label-label loss in the model training indeed improves the performance of the learning models.

Method	Facebook	Yeast	Movie	
MLP	58.13	63.79	33.62	
DeepWalk [3]	58.89	53.40	33.94	
GCN [7]	58.13	63.16	35.72	
Partly ML-GCN	59.51	65.27	37.75	
ML-GCN	59.85	66.06	37.96	

Table 2. Experimental results in terms of micro-F1 score (in percentage)

Experiment 2 (Performance Under Different Training Set Sizes): To investigate whether our ML-CGN is consistently superior to GCN under different training set sizes, we randomly selected different proportions of the instances from the original datasets to form the training sets. The experimental results are summarized in Table 3. We have the following observations. Overall, the proposed ML-GCN outperforms GCN under all different training set sizes on all datasets. On the *Movie* dataset, the advantage of ML-GCN over GCN will increase as the proportion of the training sets increases. That means, when the training instances increase, our ML-GCN is easier to capture the label-label correlations. On the *Yeast* dataset, the exceeding of ML-GCN to GCN is around 2 pinots, which is similar to that on the Movie dataset but better than that on the Facebook dataset. Again, it shows that on the datasets with stronger label-label correlations (i.e., datasets *Yeast* and *Movie*), our ML-GCN performs much better.

Dataset	Method	10%	20%	30%	40%
Facebook	GCN [7]	57.25	58.45	59.95	60.05
	ML-GCN	58.13	59.63	60.14	60.98
Yeast	GCN [7]	61.23	62.45	62.73	63.68
	ML-GCN	63.03	64.54	64.04	65.77
Movie	GCN [7]	36.82	37.64	38.06	38.23
	ML-GCN	38.04	39.92	40.64	40.76

Table 3. Experimental results under different training set sizes in terms of micro-F1 score

5 Conclusion

In this paper, we present a novel ML-GCN method for semi-supervised multi-label graph node classification. By embedding the label and node information into the same low-dimensional space, ML-GCN can jointly capture both node-label and la-bel-label correlations, which improves the performance of the learning models, com-pared with the state-of-the-art methods. In the future, we will consider embedding the contents of nodes to the learning models.

Acknowledgments. This work has been supported by the National Natural Science Foundation of China under grants 91846104 and 61603186, the Natural Science Foundation of Jiangsu Province, China, under grants BK20160843 and BK20180463, and the China Postdoctoral Science Foundation under grants 2017T100370.

References

- Ahmed, A., Shervashidze, N., Narayanamurthy, S., Josifovski, V., Smola, A.J.: Distributed large-scale natural graph factorization. In: Proceedings of the 22nd International Conference on World Wide Web, pp. 37–48. ACM (2013)
- Tang, J., Qu, M., Wang, M., Zhang, M., Yan, J., Mei, Q.: LINE: large-scale information network embedding. In: Proceedings of the 24th International Conference on World Wide Web, pp. 1067–1077. International World Wide Web Conferences Steering Committee (2015)
- Perozzi, B., Al-Rfou, R., Skiena, S.: Deepwalk: online learning of social representations. In: Proceedings of the 20th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, pp. 701–710. ACM (2014)
- Mikolov, T., Chen, K., Corrado, G., Dean, J.: Efficient estimation of word representations in vector space. arXiv preprint arXiv:1301.3781 (2013). https://arxiv.org/abs/1301.3781
- Hamilton, W., Ying, Z., Leskovec, J.: Inductive representation learning on large graphs. In: Advances in Neural Information Processing Systems, pp. 1024–1034 (2017)
- Veličković, P., Cucurull, G., Casanova, A., Romero, A., Lio, P., Bengio, Y.: Graph attention networks. arXiv preprint arXiv:1710.10903 (2017). https://arxiv.org/abs/1710.10903
- Kipf, T.N., Welling, M.: Semi-supervised classification with graph convolutional networks. arXiv preprint arXiv:1609.02907 (2016). https://arxiv.org/abs/1609.02907

- 8. Marcheggiani, D., Titov, I.: Encoding sentences with graph convolutional networks for semantic role labeling. In: Proceedings of the 2017 Conference on Empirical Methods in Natural Language Processing, pp. 1506–1515 (2017)
- Nguyen, T.H., Grishman, R.: Graph convolutional networks with argument-aware pooling for event detection. In: Thirty-Second AAAI Conference on Artificial Intelligence, pp. 5900– 5907. AAAI (2018)
- Ying, R., He, R., Chen, K., Eksombatchai, P., Hamilton, W.L., Leskovec, J.: Graph convolutional neural networks for web-scale recommender systems. In: Proceedings of the 24th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining, pp. 974–983. ACM (2018)
- 11. Wu, Z., Pan, S., Chen, F., Long, G., Zhang, C., Yu, P.S.: A comprehensive survey on graph neural networks. arXiv preprint arXiv:1901.00596 (2019). https://arxiv.org/abs/1901.00596
- 12. Kipf, T.N., Welling, M.: Variational graph auto-encoders. arXiv preprint arXiv:1611.07308 (2016). https://arxiv.org/abs/1611.07308
- 13. You, J., Ying, R., Ren, X., Hamilton, W., Leskovec, J.: GraphRNN: generating realistic graphs with deep auto-regressive models. In: International Conference on Machine Learning, pp. 5694–5703 (2018)
- Yan, S., Xiong, Y., Lin, D.: Spatial temporal graph convolutional networks for skeletonbased action recognition. In: Thirty-Second AAAI Conference on Artificial Intelligence, pp. 7444–7452. AAAI (2018)
- Gilmer, J., Schoenholz, S.S., Riley, P.F., Vinyals, O., Dahl, G.E.: Neural message passing for quantum chemistry. In: Proceedings of the 34th International Conference on Machine Learning, pp. 1263–1272 (2017). http://www.JMLR.Org
- Shuman, D., Narang, S., Frossard, P., Ortega, A., Vandergheynst, P.: The emerging field of signal processing on graphs: extending high-dimensional data analysis to networks and other irregular domains. IEEE Signal Process. Mag. 3(30), 83–98 (2013)
- 17. Gong, Y., Jia, Y., Leung, T., Toshev, A., Ioffe, S.: Deep convolutional ranking for multilabel image annotation. In: International Conference on Learning Representations (2014). https://arxiv.org/abs/1312.4894
- Wang, J., Yang, Y., Mao, J., Huang, Z., Huang, C., Xu, W.: CNN-RNN: a unified framework for multi-label image classification. In Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition, pp. 2285–2294 (2016)
- 19. Wang, Z., Chen, T., Li, G., Xu, R., Lin, L.: Multi-label image recognition by recurrently discovering attentional regions. In: Proceedings of the IEEE International Conference on Computer Vision, pp. 464–472 (2017)
- Sen, P., Namata, G., Bilgic, M., Getoor, L., Galligher, B., Eliassi-Rad, T.: Collective classification in network data. AI Mag. 29(3), 93 (2018)
- Li, Q., Han, Z., Wu, X.M.: Deeper insights into graph convolutional networks for semisupervised learning. In: Thirty-Second AAAI Conference on Artificial Intelligence, pp. 3538–3545. AAAI (2018)
- Taubin, G.: A signal processing approach to fair surface design. In: Proceedings of the 22nd Annual Conference on Computer Graphics and Interactive Techniques, pp. 351–358. ACM (1995)
- Mikolov, T., Sutskever, I., Chen, K., Corrado, G.S., Dean, J.: Distributed representations of words and phrases and their compositionality. In: Advances in Neural Information Processing Systems, pp. 3111–3119 (2013)
- 24. Kingma, D.P., Ba, J.: Adam: a method for stochastic optimization. arXiv preprint arXiv: 1412.6980 (2014). https://arxiv.org/abs/1412.6980
- 25. Leskovec, J., Mcauley, J.J.: Learning to discover social circles in ego networks. In: Advances in Neural Information Processing Systems, pp. 539–547 (2012)