
Graph Mask Convolutional Network

Bo Jiang, Beibei Wang, Jin Tang and Bin Luo

School of Computer Science and Technology, Anhui University
jiangbo@ahu.edu.cn

Abstract

Graph Convolutional Networks (GCNs) have been widely studied for graph data representation and learning. The graph convolution operation in GCNs can usually be regarded as a composition of feature aggregation/propagation and transformation. Existing GCNs generally conduct feature aggregation on a fixed neighborhood graph in which each node computes its representation by aggregating the feature representations of all its neighbors (biased by its own representation). However, this fixed aggregation strategy is not guaranteed to be optimal for GCN based graph learning and also can be affected by some graph structure noises, such as incorrect or undesired edge connections. To address these issues, we propose a novel Graph mask Convolutional Network (GmCN) in which nodes can adaptively select the optimal neighbors in their feature aggregation to better serve GCN learning. More importantly, GmCN can be theoretically interpreted by a unified regularization framework, based on which we derive a simple update algorithm to determine the optimal mask adaptively in GmCN training process. Experiments on several datasets demonstrate the effectiveness of GmCN.

1 Introduction

Recently, Graph Convolutional Networks (GCNs) have been widely studied to deal with graph-structured data representation and learning problems, such as semi-supervised learning, graph embedding, data clustering and so on [3, 8, 18, 19, 17, 22].

The core aspect of GCNs is to develop some effective graph convolution operations for layer-wise propagation. Based on spectral representation of graphs, Bruna et al. [1] propose to define graph convolution by using the eigen-decomposition of graph Laplacian matrix. Henaff et al. [6] define graph convolution by introducing a spatially constrained spectral filter. Defferrard et al. [3] propose to further approximate the spectral filters in graph convolution based on Chebyshev expansion to avoid the high complexity. Kipf et al. [8] propose a simple Graph Convolutional Network (GCN) for semi-supervised learning by exploring the first-order approximation of spectral filters. Li et al. [15] also present an adaptive graph CNNs. Monti et al. [13] recently propose a unified mixture model CNNs (MoNet) for graph data learning and analysis. Hamilton et al. [5] present a general inductive representation and learning framework (GraphSAGE) for graph embedding. By introducing the attention mechanism into graph convolution, Velickovic et al. [18] propose Graph Attention Networks (GAT). Petar et al. [19] propose Deep Graph Infomax (DGI), which provides a general unsupervised approach for learning node representation. Klicpera et al. [9] propose to combine GCN and PageRank together to derive an improved propagation scheme in layer-wise propagation.

In general, the graph convolution operation in the above GCNs can usually be regarded as a composition of feature aggregation/propagation and feature transformation. Existing GCNs generally conduct feature aggregation on a fixed structured graph in which each node obtains its representation recursively by aggregating/absorbing the feature representations of its all neighbors (biased by its own representation). However, this fixed ‘full’ aggregation strategy may be not guaranteed to be

optimal for GCN based graph learning tasks, such as semi-supervised classification. Also, it can be affected by the graph structure noises, such as incorrect or undesired edge connections.

To overcome these issues, in this paper, we propose a novel Graph mask Convolutional Network (GmCN) for graph data representation and learning. The key idea behind GmCN is that it learns how to aggregate feature information **selectively** from a node’s local neighborhood set. Specifically, in graph mask convolution (GmC) operation, each node can adaptively select the desirable/optimal neighbors from its full neighborhood set to conduct feature aggregation, which allows GmC to better serve the final graph learning tasks. GmC is achieved by employing an adaptive and learnable mask guided aggregation mechanism. More importantly, to determine the optimal selection mask in GmC, we derive a new unified regularization framework for GmC interpretation and thus develop a simple update algorithm to learn the optimal mask adaptively in GmCN training process. Overall, the main contributions of this paper are summarized as follows:

- We propose a novel graph mask convolution (GmC) operation which simultaneously learns the topological structure of each node’s neighborhood for feature aggregation as well as the linear (or nonlinear) transformation for feature representation.
- We develop a unified regularization framework for GmC interpretation and optimization.
- Based on the proposed GmC, we propose a novel Graph mask Convolutional Network (GmCN) for graph node representation and semi-supervised learning.

Experimental results on several datasets demonstrate the effectiveness of our GmCN on semi-supervised learning tasks.

2 Revisiting GCN

Recently, Graph Convolutional Networks (GCNs) have been widely studied for graph data representation and learning [3, 8, 6, 18]. The core aspect of GCNs is the specific definition of graph convolution operation in GCN layer-wise propagation. Here, we briefly review the widely used GCN model proposed in work [8]. Given a set of node features $\mathbf{H} = (\mathbf{h}_1, \mathbf{h}_2 \cdots \mathbf{h}_n) \in \mathbb{R}^{n \times d}$ and graph structure $\mathbf{A} \in \mathbb{R}^{n \times n}$, GCN [8] defines a kind of graph convolution as,

$$\mathbf{H}' = (\mathbf{D}^{-\frac{1}{2}} \mathbf{A} \mathbf{D}^{-\frac{1}{2}} + \mathbf{I}) \mathbf{H} \Theta \quad (1)$$

where \mathbf{D} is a diagonal matrix with elements $\mathbf{D}_{ii} = \sum_j \mathbf{A}_{ij}$ and $\Theta \in \mathbb{R}^{d \times \tilde{d}}$ is a layer-specific trainable weight matrix. Intuitively, the graph convolution operation Eq.(1) can be decomposed into two operations, i.e.,

$$\text{S1: } \mathbf{U} = \hat{\mathbf{A}} \mathbf{H} + \mathbf{H}, \quad \text{S2: } \mathbf{H}' = \mathbf{U} \Theta \quad (2)$$

where $\hat{\mathbf{A}} = \mathbf{D}^{-\frac{1}{2}} \mathbf{A} \mathbf{D}^{-\frac{1}{2}}$. The operation S1 provides a kind of feature aggregation on normalized graph $\hat{\mathbf{A}}$ while operation S2 presents a transformation for node features. Recent works [9, 10] also suggest to employ a more general T -step truncated random walk model to conduct feature aggregation in step S1 as

$$\mathbf{U}^{(t)} = \alpha \hat{\mathbf{A}} \mathbf{U}^{(t-1)} + (1 - \alpha) \mathbf{H} \quad (3)$$

where $t = 1, 2 \cdots T$ and $\mathbf{U}^{(0)} = \mathbf{H}$, and parameter $\alpha \in (0, 1)$ balances two terms. When $t = 1$, Eq.(3) degenerates to Eq.(2) by ignoring the weighting parameter α .

In each hidden layer of GCN, an activation function $\sigma(\cdot)$ is further conducted on \mathbf{H}' to obtain nonlinear representations. The last layer of GCN outputs the final representations of graph nodes, which can be used for many learning tasks, such as clustering, visualization and node classification etc. Here, we focus on semi-supervised classification. For this task, a softmax activation function is further used in the last layer to output the label predictions for graph nodes. The weight matrix Θ of each hidden layer is optimized by minimizing the cross-entropy loss defined on labelled nodes [8].

3 Graph Mask Convolutional Network

In this section, we present our Graph mask Convolutional Network (GmCN) model. Our GmCN is motivated by the aggregation operation Eq.(3) or Eq.(2), which is further analyzed as follows. Let

$\mathbf{U}^{(t)} = (\mathbf{u}_1^{(t)}, \mathbf{u}_2^{(t)} \cdots \mathbf{u}_n^{(t)})$ and $\mathbf{H} = (\mathbf{h}_1, \mathbf{h}_2 \cdots \mathbf{h}_n)$, then Eq.(3) is formulated as

$$\mathbf{u}_i^{(t)} = \alpha \sum_{j \in \mathcal{N}_i} \hat{\mathbf{A}}_{ij} \mathbf{u}_j^{(t-1)} + (1 - \alpha) \mathbf{h}_i \quad (4)$$

where \mathcal{N}_i denotes the neighborhood set of the i -th node. From Eq.(4), we can note that in GCN layer-wise propagation, each node aggregates the feature information from its *all neighboring* nodes on normalized graph $\hat{\mathbf{A}}$ (biased by its own feature \mathbf{h}_i) to obtain the context-aware representation, and $\alpha \in (0, 1)$ denotes the fraction of feature information that the i -th node receives from its neighbors.

However, first, this fixed ‘full’ aggregation strategy may be not guaranteed to be optimal for GCN based specific learning tasks, such as semi-supervised classification. Second, this ‘full’ aggregation can be affected by the graph structure noises, such as incorrect or undesired edge connections, disturbance of edge weights and so on. To overcome these issues, we propose to adaptively select some desired neighboring nodes from its neighborhood set \mathcal{N}_i to conduct feature aggregation. This can be achieved by using the mask weighted aggregation model as

$$\mathbf{u}_i^{(t)} = \alpha \sum_{j \in \mathcal{N}_i} \mathbf{M}_{ij} \hat{\mathbf{A}}_{ij} \mathbf{u}_j^{(t-1)} + (1 - \alpha) \mathbf{h}_i \quad (5)$$

where $\mathbf{M} \in \mathbb{R}^{n \times n}$, $\mathbf{M}_{ij} \in \{0, 1\}$ denotes the mask matrix in which $\mathbf{M}_{ij} = 1$ indicates that the j -th node in \mathcal{N}_i is selected and $\mathbf{M}_{ij} = 0$ otherwise. This mask matrix is learned adaptively, as discussed in Section 4 in detail. Based on this mask weighted aggregation, we then propose our *Graph mask Convolution* (GmC) operation as,

$$\mathbf{U}^{(t)} = \alpha (\mathbf{M} \odot \hat{\mathbf{A}}) \mathbf{U}^{(t-1)} + (1 - \alpha) \mathbf{H}, \quad t = 1, 2 \cdots T \quad (6)$$

$$\mathbf{H}' = \mathbf{U}^{(T)} \Theta \quad (7)$$

where $\mathbf{U}^{(0)} = \mathbf{H}$ and \odot represents element-wise multiplication. Parameters $\{\mathbf{M}, \Theta\}$ denote the layer-specific trainable mask matrix and weight matrix, respectively. Similar to GCN [8], in layer-wise propagation, an activation function $\sigma(\cdot)$ is further conducted on \mathbf{H}' to obtain nonlinear representations. Note that, when $T = 1$, our GmC has a simple formulation as

$$\mathbf{H}' = (\alpha \mathbf{M} \odot \hat{\mathbf{A}} + (1 - \alpha) \mathbf{I}) \mathbf{H} \Theta \quad (8)$$

Remark. In contrast to GCN which only has weight parameter Θ in each layer to conduct feature transformation, GmCN has two kinds of parameters $\{\mathbf{M}, \Theta\}$ in which \mathbf{M} is employed to select the desired neighbors for feature aggregation while Θ is used to conduct feature transformation. We will present the detail comparisons between GmCN and other related GCN works in Section 5. In the following, we first propose an effective algorithm to learn \mathbf{M} . We summarize the complete architecture and parameter training of our GmCN network in Section 5.

4 Regularization Framework and Mask Optimization

4.1 Regularization framework

Our mask optimization is motivated based on our re-interpretation of feature aggregation in GCN by using a regularization framework. Formally, we can show that, Eq.(3) provides a T -step power iteration solution to the following regularization framework [21]¹,

$$\min_{\mathbf{U}} \mathcal{R}_{\text{GCN}}(\mathbf{U}) = \text{Tr}[\mathbf{U}^T (\mathbf{I} - \hat{\mathbf{A}}) \mathbf{U}] + \mu \|\mathbf{U} - \mathbf{H}\|_F^2 \quad (9)$$

where $\mu = \frac{1}{\alpha} - 1$ is a replacement parameter of α . $\text{Tr}(\cdot)$ denotes the trace function and $\|\cdot\|_F$ denotes the Frobenius norm of matrix. Using this representation, we can thus derive a regularization framework for our GmCN (Eq.(6) or Eq.(8)) as

$$\min_{\mathbf{M}, \mathbf{U}} \mathcal{R}_{\text{GmCN}}(\mathbf{M}, \mathbf{U}) = \text{Tr}[\mathbf{U}^T (\mathbf{I} - \mathbf{M} \odot \hat{\mathbf{A}}) \mathbf{U}] + \mu \|\mathbf{U} - \mathbf{H}\|_F^2 + \gamma \|\mathbf{M}\|_F^2 \quad (10)$$

$$s.t. \quad \mathbf{M}_{ij} \in \{0, 1\} \quad (11)$$

¹When T is large enough, the update Eq.(3) converges to the optimal solution as $\mathbf{U}^* = (\mathbf{I} - \alpha \hat{\mathbf{A}}) \mathbf{H}$. It is identical to the optimal solution of this problem Eq.(9) given as $\mathbf{U}^* = (1 - \alpha)(\mathbf{I} - \alpha \hat{\mathbf{A}}) \mathbf{H}$ by ignoring the scaling coefficient, as proved in work [21].

where $\gamma > 0$ and the last term is used to control the sparsity (number of non-zeros) of mask matrix \mathbf{M} , i.e., larger parameter γ leads to more sparse \mathbf{M} . From optimization aspect, the discrete constraints $\mathbf{M}_{ij} \in \{0, 1\}$ make the problem be combinational and thus hard to be optimized. Therefore, we first relax the discrete constraints to continuous ones and solve

$$\min_{\mathbf{M}, \mathbf{U}} \mathcal{R}_{\text{GmCN}}(\mathbf{M}, \mathbf{U}) = \text{Tr}[\mathbf{U}^T(\mathbf{I} - \mathbf{M} \odot \hat{\mathbf{A}})\mathbf{U}] + \mu \|\mathbf{U} - \mathbf{H}\|_F^2 + \gamma \|\mathbf{M}\|_F^2 \quad (12)$$

$$s.t. \quad \mathbf{M}\mathbf{1}^T = \mathbf{1}^T, \mathbf{M} \geq 0 \quad (13)$$

where $\mathbf{1} = (1, 1 \cdots 1)$. Then, we utilize a post-discretization step to obtain the final discrete mask \mathbf{M} , as summarized in Algorithm 1.

4.2 Mask optimization

The optimal \mathbf{M} and \mathbf{U} can be obtained via a simple algorithm which alternatively conducts the following **Step 1** and **Step 2** until convergence.

Step 1. Solving \mathbf{M} while fixing \mathbf{U} , the problem becomes

$$\min_{\mathbf{M}} \text{Tr}[\mathbf{U}^T(\mathbf{I} - \mathbf{M} \odot \hat{\mathbf{A}})\mathbf{U}] + \gamma \|\mathbf{M}\|_F^2 \quad s.t. \quad \mathbf{M}\mathbf{1}^T = \mathbf{1}^T, \mathbf{M} \geq 0 \quad (14)$$

It is rewritten as

$$\min_{\mathbf{M}} \sum_{i,j} -(\mathbf{M} \odot \hat{\mathbf{A}})_{ij}(\mathbf{U}\mathbf{U}^T)_{ij} + \gamma \|\mathbf{M}\|_F^2 \quad s.t. \quad \mathbf{M}\mathbf{1}^T = \mathbf{1}^T, \mathbf{M} \geq 0 \quad (15)$$

Let $\mathbf{Z} = \hat{\mathbf{A}} \odot (\mathbf{U}\mathbf{U}^T)$, then Eq.(15) is equivalent to

$$\min_{\mathbf{M}} \left\| \mathbf{M} - \frac{1}{2\gamma} \mathbf{Z} \right\|_F^2 \quad s.t. \quad \mathbf{M}\mathbf{1}^T = \mathbf{1}^T, \mathbf{M} \geq 0 \quad (16)$$

This is a constrained projection problem which can be solved efficiently via a successive projection algorithm, as discussed in work [20]. The algorithm is summarized in Algorithm 1. Note that, in practical, we use a T -step truncated iteration to obtain an approximate solution. We will show this in Algorithm 2 in detail.

Algorithm 1 Mask optimization

- 1: Initialize $\mathbf{M} = \frac{1}{2\gamma} \mathbf{Z}$
 - 2: **while** not convergence **do**
 - 3: $\tilde{\mathbf{M}} \leftarrow \mathbf{M} - \frac{1}{n} \mathbf{1}^T \mathbf{1} \mathbf{M} + \left(\frac{1}{n} \mathbf{I} + \frac{1}{n^2} \mathbf{1} \mathbf{M}^T \mathbf{1} - \frac{1}{n} \mathbf{M} \right) \mathbf{1}^T \mathbf{1}$
 - 4: $\mathbf{M}_{ij} \leftarrow \max\{\tilde{\mathbf{M}}_{ij}, 0\}$
 - 5: **end while**
 - 6: Discretization: Set $\mathbf{M}_{ij} = 1$ when $\mathbf{M}_{ij} > \epsilon$, and $\mathbf{M}_{ij} = 0$ otherwise
 - 7: Return \mathbf{M}
-

Step 2. Solving \mathbf{U} while fixing \mathbf{M} , the problem becomes

$$\min_{\mathbf{U}} \text{Tr}[\mathbf{U}^T(\mathbf{I} - \mathbf{M} \odot \hat{\mathbf{A}})\mathbf{U}] + \mu \|\mathbf{U} - \mathbf{H}\|_F^2 \quad (17)$$

This problem can be solved approximately via a T -step truncated power iteration algorithm (Eq.(6)) [21] as follows,

$$\mathbf{U}^{(t)} = \alpha(\mathbf{M} \odot \hat{\mathbf{A}})\mathbf{U}^{(t-1)} + (1 - \alpha)\mathbf{H}, \quad t = 1, 2 \cdots T \quad (18)$$

where $\mathbf{U}^{(0)} = \mathbf{H}$ and $\alpha = \frac{1}{1+\mu}$. One can also use a simple one-step iteration ($T = 1$) to obtain an approximate solution efficiently as,

$$\mathbf{U} = \alpha(\mathbf{M} \odot \hat{\mathbf{A}})\mathbf{H} + (1 - \alpha)\mathbf{H} \quad (19)$$

which is similar to the feature aggregation used in GCN [8].

5 GmCN Architecture

5.1 Layer-wise propagation

The overall layer-wise propagation of GmCN is summarized in Algorithm 2, where $\sigma(\cdot)$ used in the last step denotes an activation function, such as $\text{ReLU}(\cdot) = \max(0, \cdot)$. Considering the efficiency of GmCN training, we employ a truncated iteration algorithm to optimize the \mathbf{M} -problem approximately in GmCN architecture. GmCN can be used in many graph learning tasks. In this paper, we use it for semi-supervised classification. Similar to many other works [8, 18], the optimal weight matrix Θ of each hidden layer in GmCN is trained by minimizing the cross-entropy loss via an Adam algorithm [7] which is initialized by using Glorot initialization [4].

Algorithm 2 GmCN layer-wise propagation

```

1: Input: Feature matrix  $\mathbf{H} \in \mathbb{R}^{n \times d}$ , normalized graph  $\hat{\mathbf{A}} \in \mathbb{R}^{n \times n}$  and weight matrix  $\Theta$ , parameter  $\gamma, \alpha$  and  $\epsilon$ , maximum iteration  $K, L$  and  $T$ 
2: Output: Feature map  $\mathbf{H}'$ 
3: Initialize  $\mathbf{U} = \mathbf{H}$ 
4: for  $k = 1, 2 \dots K$  do
5:   Compute  $\mathbf{M} = \frac{1}{2\gamma} \hat{\mathbf{A}} \odot (\mathbf{U}\mathbf{U}^T)$ 
6:   for  $l = 1, 2 \dots L$  do
7:     Update  $\mathbf{M}$  as
           
$$\tilde{\mathbf{M}} \leftarrow \mathbf{M} - \frac{1}{n} \mathbf{1}^T \mathbf{1} \mathbf{M} + \left( \frac{1}{n} \mathbf{I} + \frac{1}{n^2} \mathbf{1} \mathbf{1}^T \mathbf{I} - \frac{1}{n} \mathbf{M} \right) \mathbf{1}^T \mathbf{1}$$

           
$$\mathbf{M}_{ij} \leftarrow \max\{0, \tilde{\mathbf{M}}_{ij}\}$$

8:   end for
9:   Discretize  $\mathbf{M}$  as: Set  $\mathbf{M}_{ij} = 1$  when  $\mathbf{M}_{ij} > \epsilon$ , and  $\mathbf{M}_{ij} = 0$  otherwise
10:  for  $t = 1, 2 \dots T$  do
11:    Update  $\mathbf{U}$  as
           
$$\mathbf{U} \leftarrow \alpha(\mathbf{M} \odot \hat{\mathbf{A}}) \mathbf{U} + (1 - \alpha) \mathbf{H}$$

12:  end for
13: end for
14: Return  $\mathbf{H}' = \sigma(\mathbf{U}\Theta)$ 
```

5.2 Complexity analysis

The main computational complexity of GmCN involves mask \mathbf{M} optimization and feature aggregation. First, in \mathbf{M} -optimization, each update has a simple solution which can be computed efficiently. In particular, since $\mathbf{1}^T \mathbf{1}$ is a $n \times n$ matrix of ones, thus the computational complexity is $\mathcal{O}(n^2)$ in the worst case (for the dense graph). Second, we adopt a similar feature aggregation used in GCN [8] (as discussed in Section 3). Each update has the computational complexity as $\mathcal{O}(n^2 d)$ in the worst case, where d denotes the feature dimension of \mathbf{H} . Note that, in practical, both $\hat{\mathbf{A}}$ and \mathbf{M} are usually sparse and thus the computations of these operations become more efficient. Also, the maximum iterations $\{K, L, T\}$ are set to $\{4, 3, 3\}$ respectively and thus the overall propagation in GmCN is not computationally expensive.

5.3 Comparison with related works

First, in contrast to GCN [8], the key idea behind GmCN is that it learns how to *selectively* aggregate feature information from a node's local neighborhood set and thus conduct both neighborhood learning and graph convolution simultaneously. Second, our graph mask convolution (GmC) has some similarities with graph attention aggregation (GAT) [18]. The main differences are follows. (1) GmC aims to select some neighbors for feature aggregation while GAT tries to assign different importances to nodes within the same neighborhood. (2) We derive a unified regularization framework for the mask optimization and feature aggregation. In contrast, in GAT, it employs a single-layer feedforward neural network for graph attention optimization. Third, neighborhood selection techniques in graph neural network training and learning have also been studied via some neighborhood sampling strategies [5, 2]. For example, in GraphSAGE [5], it samples a fixed-size set of neighbors in feature

aggregation. Chen et al [2] propose a more optimal sampling technique with convergence analysis in GCN training. Differently, in our GmCN, we derive neighborhood selection from a regularization framework and also conduct neighborhood selection and feature aggregation simultaneously in a unified manner.

6 Experiments

6.1 Datasets

We evaluate GmCN on five widely used datasets including Cora [16], Citeseer [16], Cora-ML [12], Amazon Computers and Amazon Photo [11]. In Cora, Citeseer and Cora-ML, nodes denote documents and edges encode the citation relationships between documents. Amazon Computers and Amazon Photo are segments of the Amazon co-purchase graph [11], in which nodes represent products and edges indicate that two products are frequently bought together. Each node is represented as bag-of-words encoded product reviews and its class label is given by the product category. The detail usages of these datasets are introduced below.

- **Cora** contains 2708 nodes and 5429 edges. Each node is represented by a 1433 dimension feature descriptor and all the nodes are falling into six classes.
- **Citeseer** contains 3327 nodes and 4732 edges. Each node is represented by a 3703 dimension feature descriptor and all nodes are classified into six classes.
- **Amazon Computers** contains 13381 nodes and 259159 edges. Each node is represented by a 767 dimension feature descriptor and all the nodes are falling into ten classes.
- **Amazon photo** contains 7487 nodes and 126530 edges. Each node is represented by a 745 dimension feature descriptor and all the nodes are falling into eight classes.
- **Cora-ML** contains 2810 nodes and 7981 edges. Each node is represented by a 2879 dimension feature descriptor and all the nodes are falling into seven classes.

6.2 Experimental setup

Parameter setting. Similar to experimental setting of GCN [8, 18], we use a two-layer graph convolutional network and the number of units in hidden layer is set to 16. We train our GmCN using an ADAM algorithm [7] with 10000 maximum epochs and learning rate of 0.01. We stop training if the validation loss does not decrease for 100 consecutive epochs, as suggested in [8]. All the network weights are initialized using Glorot initialization [4]. The parameters $\{\alpha, \gamma\}$ are set to 0.8 and 0.001 respectively to obtain the best average performance. Note that, GmCN is not insensitive to these parameters. We provide additional experiments under different settings of parameters $\{\alpha, \gamma\}$ and network depth in §6.4. The maximum iterations $\{K, L, T\}$ in Algorithm 2 are set to $\{4, 3, 3\}$, respectively.

Data setting. For all datasets, we select 10%, 20% and 30% nodes as labeled data and use the remaining nodes as unlabeled data. For unlabeled data, we also use 10% nodes for validation purpose to determine the convergence criterion, and use the remaining 80%, 70% and 60% nodes respectively as testing samples. All the reported results are averaged over five runs with different data splits of training, validation and testing.

6.3 Comparison with state-of-the-art methods

Comparison methods. We compare our GmCN method against some other recent graph neural network methods including DeepWalk [14], Graph Convolutional Network (GCN) [8], Graph Attention Networks (GAT) [18], CVD+PP [2], GraphSAGE [5], APPNP [9] and Deep Graph Informax (DGI) [19]. For GraphSAGE, we use the mean aggregation rule. Note that, both GraphSAGE [5] and CVD+PP [2] also utilize neighborhood sampling techniques and thus are related with our GmCN. The codes of these methods were provided by authors and we use them in our experiments.

Results. Table 1-3 summarize the comparison results on these benchmark datasets. Overall, one can note that, GmCN obtains the best results on all datasets. In particular, we can note that (1) Comparing with the baseline model GCN [8], GmCN obtains obviously better learning results on all

datasets, which demonstrates the higher predictive ability of GmCN on semi-supervised classification by incorporating the proposed neighborhood selection and optimization in GCN training. (2) GmCN performs better than GAT [18] which utilizes an attention weighted feature aggregation in layer-wise propagation. (3) GmCN performs better than other sampling GNNs including GraphSAGE [5] and CVD+PP [2]. This demonstrates the more effectiveness of the proposed neighborhood selection technique on selecting the useful neighbors for GCN learning. (4) GmCN outperforms recent graph network APPNP [9] and DGI [19], which demonstrates the advantages of GmCN on graph data representation and semi-supervised learning.

Table 1: Comparison results of different methods on Cora and Citeseer datasets.

Dataset	Cora			Citeseer		
Ratio of label	10%	20%	30%	10%	20%	30%
Deep Walk	74.83±0.45	78.58±1.22	79.34±1.45	45.26±2.21	48.16±1.93	48.75±0.89
APPNP	72.87±1.31	78.37±0.81	80.52±0.69	66.27±1.49	70.00±0.81	72.19±0.97
DGI	81.22±0.92	82.19±0.87	83.32±0.76	68.25±1.13	69.69±0.35	71.41±0.56
GraphSAGE	82.14±0.32	84.81±0.78	86.56±0.46	71.48±0.73	73.63±0.73	74.60±0.55
CVD+PP	80.21±0.88	84.03±0.77	85.48±0.45	71.91±0.74	73.29±0.99	74.71±0.31
GCN	80.23±0.66	84.28±0.50	85.53±0.40	71.49±1.00	72.99±0.77	74.31±0.35
GAT	82.51±1.15	84.42±0.85	85.70±0.83	69.08±0.84	69.61±0.84	72.64±0.44
GmCN	83.07±0.56	85.70±0.56	87.29±0.42	72.30±0.37	74.13±0.74	74.92±0.34

Table 2: Comparison results of methods on Amazon Computers and Amazon Photo datasets.

Dataset	Amazon Computers			Amazon Photo		
Ratio of label	10%	20%	30%	10%	20%	30%
Deep Walk	87.01±0.53	87.91±0.13	88.31±0.15	90.47±0.38	91.63±0.43	91.84±0.14
APPNP	85.52±0.67	86.99±0.56	87.21±0.53	91.57±0.44	92.91±0.25	92.97±0.49
DGI	85.32±0.47	86.31±0.28	86.30±0.42	92.53±0.24	92.80±0.30	92.64±0.23
GraphSAGE	82.75±0.57	83.88±0.97	84.75±0.41	89.78±0.83	91.51±0.62	91.96±0.34
CVD+PP	83.71±1.53	85.72±0.43	81.14±1.12	91.52±0.40	92.53±0.38	92.27±0.28
GCN	85.51±0.49	85.28±1.29	84.67±0.76	92.58±0.25	92.65±0.44	92.64±0.37
GAT	83.64±5.21	86.10±2.50	85.70±3.05	90.53±2.91	91.26±1.14	91.93±1.11
GmCN	89.14±0.70	89.43±0.74	89.88±0.52	93.80±0.18	94.20±0.21	94.31±0.28

Table 3: Comparison results of different methods on Cora-ML dataset.

Dataset	Cora-ML		
Ratio of label	10%	20%	30%
Deep Walk	79.13±1.60	81.51±0.89	82.36±0.90
APPNP	76.96±0.46	80.02±0.93	81.43±0.42
DGI	84.45±0.49	86.23±0.62	86.74±0.45
GraphSAGE	84.75±0.76	86.62±0.55	87.67±0.81
CVD+PP	84.97±0.40	87.00±0.40	87.25±0.74
GCN	85.17±0.70	86.92±0.32	87.23±0.77
GAT	81.53±1.78	83.46±0.99	83.89±0.57
GmCN	86.02±0.48	87.41±0.65	88.05±0.81

6.4 Parameter analysis

In this section, we evaluate the performance of GmCN model with different settings of network parameters. We first investigate the influence of GmCN model depth (number of convolutional layers). Figure 1 (a) shows the performance of GmCN model across different number of hidden layers on Cora dataset. As a baseline, we also report the results of GCN model with the same depth setting. Note that, GmCN maintains better performance under different model depths and consistently performs better than GCN, which indicates the insensitivity of the GmCN w.r.t. model depth. We then investigate the influence of the network parameter α and γ . Table 4 and 5 show the performance of GmCN with different parameter settings of parameter α and γ , respectively, which indicate the insensitivity of the GmCN w.r.t. parameter α and γ .

Table 4: Results of GmCN across different parameter α values on Cora and Citeseer datasets.

α	0.6	0.7	0.8	0.9
Cora	78.45 \pm 0.93	80.06 \pm 1.01	83.07 \pm 0.56	82.66 \pm 0.72
Citeseer	72.45 \pm 0.33	73.46 \pm 0.53	72.52 \pm 0.63	71.12 \pm 0.44

Table 5: Results of GmCN across different parameter γ values on Cora and Citeseer datasets.

γ	0.0001	0.0005	0.001	0.005
Cora	83.21 \pm 0.81	83.34 \pm 0.68	83.13 \pm 0.80	83.00 \pm 0.97
Citeseer	72.09 \pm 0.42	72.50 \pm 0.26	72.76 \pm 0.25	72.85 \pm 0.54

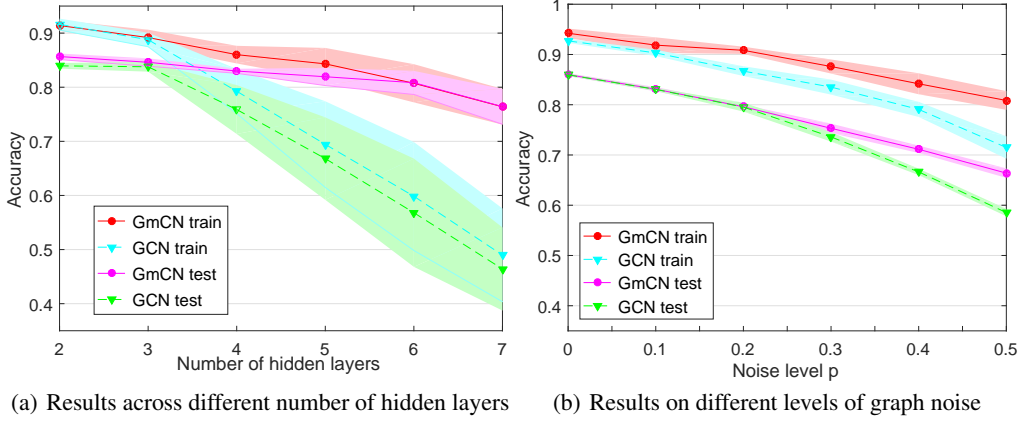


Figure 1: Results of GmCN on different parameters and graph noise levels on Cora dataset.

6.5 Perturbation analysis

To evaluate the robustness of the proposed GmCN w.r.t. graph noises, we test our method on graph data with different perturbation noise levels. The perturbation is built as follows. We first randomly cut each edge and then connect each pair of randomly selected nodes with probability p . Thus, parameter p controls the level of structure perturbation. For each level p , we generate ten noisy graphs and then compute the average performances including both training and testing accuracy. As a baseline, we also list the results of GCN model on the same noise data. Figure 1 (b) shows the comparison results on Cora dataset. We can note that GmCN performs more robustly on noisy graph, which further demonstrates that the proposed mask selection mechanism is helpful for capturing important information and thus avoiding noisy graph information.

7 Conclusion

This paper proposes a novel Graph mask Convolutional Network (GmCN) for graph data representation and semi-supervised learning. GmCN learns an optimal graph neighborhood structure that better serves GCN based semi-supervised learning. A new unified regularization framework is derived for GmCN interpretation, based on which we provide an effective update algorithm to achieve GmCN optimization. Experimental results on several benchmarks demonstrate the effectiveness and robustness of GmCN on semi-supervised learning tasks. In the future, we will explore GmCN on some other unsupervised learning tasks, such as clustering, embedding etc.

References

- [1] J. Bruna, W. Zaremba, A. Szlam, and Y. LeCun. Spectral networks and locally connected networks on graphs. In *International Conference on Learning Representations*, 2014.
- [2] J. Chen, J. Zhu, and L. Song. Stochastic training of graph convolutional networks with variance reduction. In *International Conference on Machine Learning*, pages 942–950, 2018.

- [3] M. Defferrard, X. Bresson, and P. Vandergheynst. Convolutional neural networks on graphs with fast localized spectral filtering. In *Advances in Neural Information Processing Systems*, pages 3844–3852, 2016.
- [4] X. Glorot and Y. Bengio. Understanding the difficulty of training deep feedforward neural networks. In *International conference on artificial intelligence and statistics*, pages 249–256, 2010.
- [5] W. Hamilton, Z. Ying, and J. Leskovec. Inductive representation learning on large graphs. In *Advances in Neural Information Processing Systems*, pages 1024–1034, 2017.
- [6] M. Henaff, J. Bruna, and Y. LeCun. Deep convolutional networks on graph-structured data. *arXiv preprint arXiv:1506.05163*, 2015.
- [7] D. P. Kingma and J. Ba. Adam: A method for stochastic optimization. In *International Conference on Learning Representations*, 2015.
- [8] T. N. Kipf and M. Welling. Semi-supervised classification with graph convolutional networks. *arXiv preprint arXiv:1609.02907*, 2016.
- [9] J. Klicpera, A. Bojchevski, and S. Günnemann. Predict then propagate: Graph neural networks meet personalized pagerank. 2019.
- [10] Y. Li, R. Yu, C. Shahabi, and Y. Liu. Diffusion convolutional recurrent neural network: Data-driven traffic forecasting. In *International Conference on Learning Representations (ICLR '18)*, 2018.
- [11] J. McAuley, C. Targett, Q. Shi, and A. Van Den Hengel. Image-based recommendations on styles and substitutes. In *Proceedings of the 38th International ACM SIGIR Conference on Research and Development in Information Retrieval*, pages 43–52, 2015.
- [12] A. K. McCallum, K. Nigam, J. Rennie, and K. Seymore. Automating the construction of internet portals with machine learning. *Information Retrieval*, 3(2):127–163, 2000.
- [13] F. Monti, D. Boscaini, J. Masci, E. Rodola, J. Svoboda, and M. M. Bronstein. Geometric deep learning on graphs and manifolds using mixture model cnns. In *IEEE Conference on Computer Vision and Pattern Recognition*, pages 5423–5434, 2017.
- [14] B. Perozzi, R. Al-Rfou, and S. Skiena. Deepwalk: Online learning of social representations. In *Proceedings of the 20th ACM SIGKDD international conference on Knowledge discovery and data mining*, pages 701–710, 2014.
- [15] F. Z. J. H. Ruoyu Li, Sheng Wang. Adaptive graph convolutional neural networks. In *AAAI Conference on Artificial Intelligence*, pages 3546–3553, 2018.
- [16] P. Sen, G. Namata, M. Bilgic, L. Getoor, B. Galligher, and T. Eliassi-Rad. Collective classification in network data. *AI magazine*, 29(3):93, 2008.
- [17] O. Shchur, M. Mumme, A. Bojchevski, and S. Günnemann. Pitfalls of graph neural network evaluation. *arXiv preprint arXiv:1811.05868*, 2018.
- [18] P. Velickovic, G. Cucurull, A. Casanova, A. Romero, P. Lio, and Y. Bengio. Graph attention networks. *arXiv preprint arXiv:1710.10903*, 2017.
- [19] P. Veličković, W. Fedus, W. L. Hamilton, P. Liò, Y. Bengio, and R. D. Hjelm. Deep graph infomax. In *ICLR*, 2019.
- [20] R. Zass and A. Shashua. Doubly stochastic normalization for spectral clustering. In *Advances in neural information processing systems*, pages 1569–1576, 2007.
- [21] D. Zhou, O. Bousquet, T. N. Lal, J. Weston, and B. Schölkopf. Learning with local and global consistency. In *Advances in neural information processing systems*, pages 321–328, 2004.
- [22] J. Zhou, G. Cui, Z. Zhang, C. Yang, Z. Liu, and M. Sun. Graph neural networks: A review of methods and applications. *arXiv preprint arXiv:1812.08434*, 2018.