Exploring Graph Learning for Semi-Supervised Classification Beyond Euclidean Data

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Abstract—Semi-supervised classification on graph-structured data has received increasing attention, where labels are only available for a small subset of data such as social networks and citation networks. This problem is challenging due to the irregularity of graphs. Graph convolutional neural networks (GCN) have been recently proposed to address such kinds of problems, which feed the graph topology into the network to guide operations such as graph convolution. Nevertheless, in most cases where the graphs are not given, they are empirically constructed manually, which tends to be sub-optimal. Hence, we propose Graph Learning Neural Networks (GLNN), which exploits the optimization of graphs (the adjacency matrix in particular) and integrates into the GCN for semi-supervised node classification. Leveraging on spectral graph theory, this essentially combines both graph learning and graph convolution into a unified framework. Specifically, we represent features of social/citation networks as graph signals, and propose the objective of graph learning from the graph-signal prior; sparsity constraint and properties of a valid adjacency matrix via maximum a posteriori estimation. The optimization objective is then integrated into the loss function of the GCN, leading to joint learning of the adjacency matrix and high-level features. Experimental results show that our proposed GLNN outperforms state-of-the-art approaches over widely adopted social network datasets and citation network datasets.

Index Terms—Graph learning, graph convolutional neural networks, adjacency matrix, semi-supervised node classification

I. INTRODUCTION

Graphs are natural and efficient representation for non-Euclidean data, such as social networks, citation networks, brain neural networks, 3D geometric data, etc. The nodes of a graph often represent the entities and the edges reflect the relationship between two nodes. Taking social networks as an example, nodes refer to individuals, edges describe their relationships, and labels may represent interests, affiliations, locations and so on. In various applications of graph data, due to the high cost of labeling, semi-supervised classification is crucial, where labels are only available for a small subset of nodes. For instance, the semi-supervised classification problem for social networks is to predict the label of every individual from only a few labels. This enables a variety of applications, such as suggesting new connections to individuals based on similar interests or experiences, sociological study of communities and detecting trends in academic research from a citation network [11], [2].

While semi-supervised learning has been studied extensively for Euclidean data, its extension to non-Euclidean domain is challenging due to the data irregularity. Recently, Graph Convolutional Networks (GCN) has been proposed to generalize CNNs to non-Euclidean domain [3], which has shown its efficiency in semi-supervised classification [4]. The key idea is to explore the convolution of graph data in the spectral domain, leveraging on spectral graph theory [5]. However, this requires the eigen-decomposition of graph Laplacian matrices [5], [5], which is computationally expensive. Hence, several methods propose to approximate the convolution in the spectral domain by spectrum-free filtering, such as Chebyshev polynomials [6], [7], Lanczos method [8], Cayley polynomials [9], etc. Also, spatial methods have been proposed to approximate graph convolution in the spatial domain via weighted averaging of neighboring nodes [10], [11], [3], [12], [13].

In the aforementioned methods, graphs are fed into the network for basic operations such as graph convolution, and thus play a vital role in feature extraction. Nevertheless, the graphs are not given in most cases. Previous works manually construct graphs from the input graph data before feeding them into the network. The performance is thus dependent on the

1\footnote{For instance, the extent to which communities form around particular interests or affiliations.}
way of graph construction, which tends to be sub-optimal with manual methods. Hence, this motivates us to learn the optimal graph in GCN so as to fully exploit the relationship in the data.

Several approaches have been proposed for graph learning in the field of graph signal processing [14], which optimize the graph Laplacian from data. Dong et al. [15], Kalofolias [16], and Egilmez et al. [17] propose to learn Laplacian matrices from the constraints of data structure and properties of a valid graph Laplacian. Segarra et al. [18] and Pasdeloup et al. [19] focus on learning graph shift or diffusion operators (such as adjacency and Laplacian matrices) from a set of diffused graph signals [20]. Sardellitti et al. [21] propose an approach to learn the graph topology from graph signals under a signal band-limited assumption, which corresponds to signals having clustering properties. However, these approaches need to solve complicated optimization problems with high computation complexity, which is unsuitable for large-scale graph learning and is hard to be integrated into a deep learning model.

There are some attempts to solve similar learning problems via machine learning methods, such as the estimation of the precision matrix (i.e., the inverse covariance matrix) for Gaussian graphical models from the observed data [22], [23], [24], [25], [26], [27], [28]. Nevertheless, these approaches focus on indirect representations of graph structures such as the precision matrix, which are related to various graph Laplacian under certain conditions but not always equivalent. Hence, this direction differs from exact graph learning, and is thus difficult to adapt to GCNs.

In order to address the above problems, we propose a Graph Learning Neural Network (GLNN) for semi-supervised node classification, which combines graph learning and graph convolution into a unified framework as shown in Fig. 1. In particular, we exploit the learning of the direct representation of the underlying graph structure, i.e., the adjacency matrix, which encodes the connectivities and edge weights in the graph.

Specifically, we first represent features of network data (e.g., social/citation networks) as signals on the graph, and pose a Maximum a Posteriori (MAP) estimation on the underlying adjacency matrix. In the MAP estimation, we propose a likelihood function by modeling the data dependency via Gaussian Markov Random Fields (GMRF) and leveraging on spectral graph theory. Also, we propose a prior distribution from the sparsity constraint and properties of a valid adjacency matrix, considering a symmetric, normalized and loopless graph. The MAP estimation then leads to an optimization problem for the underlying adjacency matrix. Secondly, we integrate the optimization objective into the loss function of the GCN, which seamlessly optimizes the network model with graph learning. Finally, we design the framework of the proposed GLNN, which mainly consists of a Graph Learning Layer and Graph Convolution Layers. The input feature matrix will first go through the Graph Learning Layer, leading to a learned adjacency matrix. We then feed the learned graph into a two-layer GCN model [4] for the semi-supervised node classification task.

In summary, our main contributions are as follows:

- We propose a GLNN framework that integrates graph learning with graph convolution, which optimizes the network model by introducing a graph-signal prior, properties of valid adjacency matrices and sparsity constraints into the loss function.
- Extensive experimental results show that we outperform state-of-the-art approaches on widely used citation network datasets and social network datasets.

The rest of the paper is organized as follows. Section II reviews previous works on graph learning, GCNs and semi-supervised node classification. Next, we present the proposed graph learning in Section III and then elaborate on the proposed GLNN in Section IV. Finally, experimental results and conclusions are presented in Section V and Section VI respectively.

II. RELATED WORK

We first review previous works on graph learning and GCNs, which inspire the proposed method. Then we introduce related works on semi-supervised node classification.

A. Graph Learning

Previous graph learning methods can be divided into two main categories: optimization methods and machine learning methods.

Optimization methods. Since the graph representation is fundamental in the field of graph signal processing, several works have been proposed to address learning of different types of graph Laplacians from data. Tenenbaum et al. [29] propose to learn combinatorial graph Laplacians via the proposed sparse model. A regression framework is proposed in [30] to learn a graph Laplacian matrix based on a fitness metric between the signals and the graph, which essentially evaluates the smoothness of the signals on the graph. Dong et al. [15] and Kalofolias [16] propose to learn Laplacian matrices from the smoothness prior of the graph signal. Egilmez et al. [17] propose graph learning under the constraints of data structure and properties of a valid Laplacian.

Besides, some studies focus on inferring the graph topology (i.e., connectivity) information from signals assumed to be diffused on a graph. A fitness metric similar to the regression framework has been used in [31] to learn a valid graph topology (the adjacency matrix). In particular, Segarra et al. [18] and Pasdeloup et al. [19] focus on learning graph shift/diffusion operators (such as adjacency and Laplacian matrices) from a set of diffused graph signals [20]. Sardellitti et al. [21] propose to learn the graph topology from graph signals, under the assumption of band-limited signals, which corresponds to signals with clustering properties. Nevertheless, these approaches need to solve complex optimization problems, which is computationally expensive. Thus, they are unsuitable for large-scale graph learning problem and difficult to integrate with deep learning.
Machine learning methods. There have been some attempts to solve similar learning problems via machine learning approaches. One main focus in the research of learning graphical models is to estimate the precision matrix for Gaussian graphical models from the observed data [22], [23], [24], [25], [26], [27], [28], especially in cases where the number of observations is smaller than the sample dimension and the sample covariance becomes singular. Another similar problem is to infer the graph structure for discrete Markov Random Fields [32]. The key idea is that in case of a Gaussian graphical model, there is exact correspondence between the location of nonzero entries in the precision matrix and the existence of partial correlations between the random variables [33].

However, these approaches are based on indirect representations of graph structures, which are difficult to adapt to GCNs.

B. Graph Convolutional Neural Networks

GCN extends CNN by consuming data defined on irregular grids. The key challenge is to define convolution over graphs, which is difficult due to the unordered data. According to the definitions of graph convolution, most of these approaches can be classified into two main categories: spectral-domain methods and nodal-domain methods.

Spectral-domain methods. The convolution over graphs is elegantly defined in the spectral domain, which is the multiplication of the spectral-domain representation of signals. Specifically, the spectral representation is in the graph Fourier transform (GFT) [6] domain, where each signal is projected onto the eigenvectors of the graph Laplacian matrix [6], [34]. The computation complexity, however, is high due to the eigen-decomposition of the graph Laplacian matrix in order to get the eigenvector matrix. Hence, it is improved by [7] through fast localized convolutions, where the Chebyshev expansion is deployed to approximate GFT. Besides, Susnjara et al. introduce the Lanczos method for approximation [8]. Spectral GCN has shown its efficiency in various tasks such as segmentation and classification [4], [35].

Nodal-domain methods. Many techniques are introduced to implement graph convolution directly on each node and its neighbors, i.e., in the nodal domain. Gori et al. introduce recurrent neural networks that operate on graphs in [10]. Duvenaud et al. propose a convolution-like propagation to accumulate local features [11]. Bruna et al. deploy the multiscale clustering of graphs in convolution to implement multiscale representation [3]. Furthermore, Niepert et al. define convolution on a sequence of nodes and perform normalization afterwards [12]. Wang et al. propose edge convolution on graphs by incorporating local neighborhood information, which is applied to point cloud segmentation and classification [13]. Nodal-domain methods provide strong localized filters, but it also means it might be difficult to learn the global structure.

The above methods apply convolutional aggregators in the propagation step. Besides, there are other related works based on different aggregators, including attention aggregators [36], which incorporate the attention mechanism [37] into the propagation step, aiming to compute the hidden states of each node by attending over its neighbors; and gate aggregators [38], [39], [40], [41], [42], [43], which use the gate mechanism like GRU [44] or LSTM [45] in the propagation step to improve the long-term propagation of information across the graph structure.

C. Semi-Supervised Node Classification

Quite a few approaches for semi-supervised node classification have been proposed in recent years, most of which fall into three categories: graph Laplacian regularization methods, graph embedding based methods, and convolutional neural network methods.

Graph Laplacian regularization methods. This class of methods is based on the assumption that neighboring nodes tend to have the same labels. Belkin et al. [46] use a parameterized classifier in the Reproducing Kernel Hilbert Space (RKHS), which is inductive and naturally handles unobserved instances. Weston et al. [47] propose a deep semi-supervised embedding approach, which extends the regularization, and imposes stronger constraints on a neural network. Sen et al. [48] present an iterative classification algorithm (ICA), which uses a local classifier that takes the labels of neighboring nodes as the input. Also, an iterative process is designed between estimating the local classifier and assigning new labels.

Graph embedding based methods. This class of approaches are inspired by the skip-gram model [49]. Perozzi et al. [50] propose a DeepWalk model, which learns embeddings via the prediction of the local neighborhood of nodes, sampled from random walks on the graph. Yang et al. [51] alleviate the optimization step of DeepWalk by injecting label information in the process of learning embeddings. Tran et al. [52] present a novel autoencoder architecture (LoNGAE) capable of learning a joint representation of both local graph structure and available node features for the multitask learning of link prediction and node classification.

Convolutional neural network methods. This family of approaches typically use CNNs, GCNs, or their variants. Kipf et al. [4] propose a simplified graph convolution model for semi-supervised learning by employing a first-order approximation of spectral filters. Monti et al. [53] propose mixture model (MoNet) and provide a unified generalization of CNN architectures on graphs. Velickovic et al. [36] present Graph Attention Networks (GATs) for semi-supervised learning by designing an attention layer. Xu et al. [54] present graph wavelet neural network (GWNN) to implement efficient convolution on graph data, which takes graph wavelets instead of the eigenvectors of the graph Laplacian as a set of basis.

III. THE PROPOSED GRAPH LEARNING

In this section, we first introduce some basic graph concepts, then elaborate on the proposed learning of graph adjacency matrices, and finally describe the network model optimization.

A. Preliminaries

We consider an undirected graph $G = \{V, E, A\}$ composed of a node set $V$ of cardinality $|V| = n$, an edge set $E$ connecting nodes, and a weighted adjacency matrix $A$. $A$ is a real symmetric $n \times n$ matrix, where $a_{ij}$ is the weight assigned to the edge $(i, j)$ connecting nodes $i$ and $j$. 

B. Preliminaries

\[ \text{G} = \{V, E, A\} \]
The Laplacian matrix, defined from the adjacency matrix, can be used to unveil useful properties of a graph. Among different variants of Laplacian matrices, the combinatorial graph Laplacian used in [53], [56] is defined as
\[ \mathbf{L} = \mathbf{D} - \mathbf{A}, \] (1)
where \( \mathbf{D} \) is the degree matrix—a diagonal matrix where \( d_{i,i} = \sum_{j=1}^{n} a_{i,j} \).

Considering the numerical stability in a deep neural network model, we adopt the symmetric normalized Laplacian, which is defined as
\[ \mathbf{L} = \mathbf{D}^{-\frac{1}{2}} \mathbf{L} \mathbf{D}^{-\frac{1}{2}} = \mathbf{I} - \mathbf{D}^{-\frac{1}{2}} \mathbf{A} \mathbf{D}^{-\frac{1}{2}}, \] (2)
where \( \mathbf{I} \) is an identity matrix. \( \mathbf{L} \) will be used in the graph-signal prior in the next subsection.

**Graph signal** \( \mathbf{x} \in \mathbb{R}^n \) refers to data that resides on the nodes of a graph, such as social, transportation, sensor, and citation networks. In our context, we treat each person or paper as a node in a graph, and the relationship as the edge between each pair of nodes. Then we define the corresponding graph signal as the social information or paper information of each node.

**B. Optimization of Graph Adjacency Matrices**

As mentioned, we propose to exploit the learning of the direct representation of the underlying graph, i.e., the adjacency matrix. In particular, we pose a MAP estimation of the adjacency matrix, which leads to graph learning from the graph-signal prior, sparsity constraint and properties of a valid adjacency matrix.

1) **MAP Estimation of Graph Adjacency Matrices**: We first formulate a MAP estimation problem for the optimal graph adjacency matrix \( \hat{\mathbf{A}} \): given the observed graph signal \( \mathbf{x} \), find the most probable graph \( \hat{\mathbf{A}} \).

\[ \hat{\mathbf{A}}_{\text{MAP}}(\mathbf{x}) = \arg \max_{\mathbf{A}} f(\mathbf{x} | \hat{\mathbf{A}}) g(\hat{\mathbf{A}}), \] (3)

where \( f(\mathbf{x} | \hat{\mathbf{A}}) \) is the likelihood function, and \( g(\hat{\mathbf{A}}) \) is the prior probability distribution of \( \hat{\mathbf{A}} \). The likelihood function \( f(\mathbf{x} | \hat{\mathbf{A}}) \) is the probability of obtaining the observed graph signal \( \mathbf{x} \) given the graph \( \hat{\mathbf{A}} \), while the prior probability distribution \( g(\hat{\mathbf{A}}) \) provides the prior knowledge of \( \mathbf{A} \).

We propose a likelihood function assuming the GMRF model and propose the prior from the sparsity constraint and properties of a graph adjacency matrix, as discussed below separately.

2) **Proposed Likelihood Function**: We model the underlying spatial dependency of the structure via GMRFs. The definition of a GMRF is as follows:

**Definition**: A random vector \( \mathbf{x} = (x_1, x_2, ..., x_n)^\top \in \mathbb{R}^n \) is a GMRF with respect to a graph \( \mathcal{G} = \{ \mathcal{V}, \mathcal{E} \} \) with mean \( \mu \) and precision matrix \( \mathbf{Q} > 0 \), if its density has the form
\[ \pi(\mathbf{x}) = (2\pi)^{-\frac{n}{2}} |\mathbf{Q}|^{\frac{1}{2}} \exp \left( -\frac{1}{2} \mathbf{x}^\top \mathbf{Q} \mathbf{x} \right), \] (4)
and
\[ Q_{i,j} \neq 0 \iff \{i, j\} \in \mathcal{E}, \forall i \neq j. \] (5)

Here, the precision matrix \( \mathbf{Q} \) is the inverse of the covariance matrix in a typical multivariate Gaussian distribution [57], which provides the conditional dependency between variables [53].

Also, the conditional dependencies are represented via the corresponding graph, in which connected nodes are conditionally dependent as presented in Eq. (5). However, the precision matrix is difficult to estimate from statistics given small amounts of training data in practice. Hence, we interpret \( \mathbf{Q} \) as the graph Laplacian [57]:
\[ \mathbf{Q} = \delta \mathbf{L} = \delta (\mathbf{I} - \hat{\mathbf{A}}), \] (6)
where \( \delta \) is a scalar, \( \hat{\mathbf{A}} \) is the normalized adjacency matrix, and \( \mathbf{I} - \hat{\mathbf{A}} \) is the normalized Laplacian matrix introduced in Eq. (4). Compared with the statistical precision matrix \( \mathbf{Q} \), the graph Laplacian \( \mathbf{L} \) is much more efficient to compute as it is deterministic.

Assuming zero mean \( \mu = 0 \), we propose the likelihood function from Eq. (4) and (6) as
\[ f(\mathbf{x} | \hat{\mathbf{A}}) = \beta \exp \left( -\frac{1}{2} \mathbf{x}^\top \mathbf{Q} \mathbf{x} \right) \]
\[ = \beta \exp \left( -\frac{1}{2} \mathbf{x}^\top \delta \mathbf{L} \mathbf{x} \right) \] (7)
\[ = \beta \exp \left( -\lambda_0 \mathbf{x}^\top (\mathbf{I} - \hat{\mathbf{A}}) \mathbf{x} \right), \]
where \( \beta = (2\pi)^{-\frac{n}{2}} |\mathbf{Q}|^{\frac{1}{2}} \) and \( \lambda_0 = \frac{\delta}{2} \).

Furthermore, the quadratic term \( \mathbf{x}^\top \mathbf{L} \mathbf{x} \) in Eq. (7) is usually considered as a smoothness measure of the signal \( \mathbf{x} \) with respect to the graph with \( \mathbf{L} \) [53], i.e.,
\[ \mathbf{x}^\top \mathbf{L} \mathbf{x} = \sum_{i \sim j} a_{i,j} (x_i - x_j)^2, \] (8)
where \( a_{i,j} \) represents the edge weight between \( x_i \) and \( x_j \), and \( i \sim j \) denotes \( i \) and \( j \) are one-hop neighbors. This prior is coined graph-signal smoothness prior, as the graph signal has to follow the topology indicated by the edge weights in order to minimize Eq. (3). Therefore, the proposed likelihood function can be also interpreted as the graph-signal smoothness prior.

Hence, the graph learning problem becomes learning the conditional dependency from data, which is reflected in graph connectivities (dependent or not) and graph weights (the extent of dependency).

3) **Proposed Prior Probability Distribution**: The prior probability distribution \( g(\hat{\mathbf{A}}) \) provides the prior knowledge of \( \mathbf{A} \). We propose the prior knowledge of an adjacency matrix from two aspects: 1) the sparsity constraint \( g_s(\hat{\mathbf{A}}) \); 2) the property constraint of a valid adjacency matrix \( g_p(\hat{\mathbf{A}}) \). Since the two prior constraints are independent, we have
\[ g(\hat{\mathbf{A}}) = g_s(\hat{\mathbf{A}}) g_p(\hat{\mathbf{A}}). \] (9)
We elaborate on the sparsity constraint and property constraint separately as follows.

**Sparsity Constraint**: One key of the GMRF model is the sparsity of the precision matrix [53] due to the Markov property. As we interpret the precision matrix by the graph Laplacian, the corresponding adjacency matrix should be also...
sparse. Hence, we pose the sparsity constraint on \( \hat{A} \), leading to

\[
g_s(\hat{A}) = \exp\left(-\lambda_1 \|\hat{A}\|_1\right),
\]

where \( \|\cdot\|_1 \) denotes the \( l_1 \)-norm of a matrix, and \( \lambda_1 \) is a weighting parameter.

**Property Constraint.** The properties of a valid normalized adjacency matrix include:

- Symmetry. In our model, we only consider undirected graphs, in which any edge \((x_i, x_j) \in \mathcal{E}\) is identical to the edge \((x_j, x_i) \in \mathcal{E}\). Hence, the corresponding adjacency matrix \( \hat{A} \) is symmetric. The mathematical description is

\[
\hat{A}^\top = \hat{A}.
\]

- Normalized. We consider normalized adjacency matrices in order to avoid numerical instabilities and exploding or vanishing gradients when used in a deep neural network architecture. The mathematical description is

\[
\hat{A} \mathbf{1} = \mathbf{1},
\]

where \( \mathbf{1} \) denotes the vector with all the elements equal to one.

- Loopless. Since it is unnecessary to link a node with itself, we consider graphs without self loop. The mathematical description is

\[
\text{tr}(\hat{A}) = 0,
\]

where \( \text{tr}(\cdot) \) denotes the trace of a matrix.

Combining the above properties, we propose the following prior probabilistic distribution of \( \hat{A} \):

\[
g_p(\hat{A}) = \exp\left(-\lambda_2\|\hat{A}^\top - \hat{A}\|^2_F - \lambda_3\|\hat{A} \mathbf{1} - \mathbf{1}\|^2_F - \lambda_4\|\text{tr}(\hat{A})\|^2\right),
\]

where \( \|\cdot\|^2_F \) is the Frobenius norm of a matrix, and \( \lambda_2, \lambda_3, \) and \( \lambda_4 \) are all weighting parameters.

4) **Final MAP Estimation:** Having discussed the proposed likelihood function and prior, we arrive at our final MAP estimation of the graph adjacency matrix. Combining Eq. (3), (7), (9), (10), and (14), we have

\[
\max_{\hat{A}} \exp\left(-\lambda_0 x^\top (I - \hat{A}) x\right) \cdot \exp\left(-\lambda_1 \|\hat{A}\|_1\right) \\
\cdot \exp\left(-\lambda_2 \|\hat{A}^\top - \hat{A}\|^2_F - \lambda_3\|\hat{A} \mathbf{1} - \mathbf{1}\|^2_F - \lambda_4\|\text{tr}(\hat{A})\|^2\right).
\]

Taking the logarithm of Eq. (15) and multiplying by \(-1\), we have

\[
\min_{\hat{A}} \lambda_0 x^\top (I - \hat{A}) x + \lambda_1 \|\hat{A}\|_1 + \lambda_2\|\hat{A}^\top - \hat{A}\|^2_F \\
+ \lambda_3\|\hat{A} \mathbf{1} - \mathbf{1}\|^2_F + \lambda_4\|\text{tr}(\hat{A})\|^2.
\]

where the first term is the graph-signal smoothness prior, the second term is the sparsity constraint of the adjacency matrix, and the rest are the property constraints of a valid adjacency matrix. Hence, the above problem formulation is to learn such a valid and sparse adjacency matrix \( \hat{A} \) that the graph signal \( x \) is smooth with respect to the learned graph.

**C. The Network Model Optimization**

It is time consuming to solve the optimization problem in Eq. (16) given multiple observations of \( x \), which is not amenable to the integration with the GCN architecture. Instead, we propose to integrate the optimization objective in Eq. (16) into the loss function of the GCN, which seamlessly optimizes the network model with graph learning. Accordingly, the proposed overall loss in graph learning \( L_{\text{GL}} \) includes three components: the loss in graph-signal smoothness \( L_{\text{smooth}} \), the loss in sparsity \( L_{\text{sparsity}} \), and the loss in property constraints \( L_{\text{properties}} \):

\[
L_{\text{GL}} = L_{\text{smooth}} + L_{\text{sparsity}} + L_{\text{properties}}.
\]

In accordance with Eq. (16), \( L_{\text{smooth}} \) is defined as

\[
L_{\text{smooth}} = \lambda_0 \|x^\top (I - \hat{A}_{\text{out}}) x\|^2_2.
\]

**Fig. 2.** The architecture of the proposed GLNN for semi-supervised node classification. Our proposed network takes a feature map and a ground-truth graph (optional) as the input in the training phase. We then employ the Graph Learning Layer to obtain an optimal graph, and feed the learned graph and feature map to Graph Convolution Layers to generate the output node classification scores. We add classification loss and the proposed graph learning loss together for backward propagation.
where $\hat{A}_{\text{out}}$ is the final output adjacency matrix at each epoch. We see that $L_{\text{smooth}}$ is a quadratic form, which is differentiable.

$L_{\text{sparsity}}$ is accordingly defined as

$$L_{\text{sparsity}} = \lambda_1 \|\hat{A}_{\text{out}}\|_1. \tag{19}$$

The $l_1$-norm is non-differentiable since it is not continuous everywhere. In the backward propagation algorithm of machine learning, the gradient of the $l_1$ regularizer is solved using the sub-gradient \[59\].

$$\frac{\partial L_{\text{sparsity}}}{\partial \hat{A}_{\text{out}}} = \text{sgn}(\hat{A}_{\text{out}}), \tag{20}$$

where

$$\text{sgn}(x) = \begin{cases} -1 & x < 0, \\ 0 & x = 0, \\ 1 & x > 0. \end{cases} \tag{21}$$

Finally, we define $L_{\text{properties}}$ as

$$L_{\text{properties}} = \lambda_2 \|\hat{A}_{\text{out}}^T - \hat{A}_{\text{out}}\|_2^2 + \lambda_3 \|\hat{A}_{\text{out}}1 - 1\|_2^2 + \lambda_4 |\text{tr}(\hat{A}_{\text{out}})|^2. \tag{22}$$

The three terms of this function are all $l_2$ norms, so the function is differentiable.

Hence, we are able to compute the gradient of the proposed loss function, which is suitable to guide the optimization of the network model.

### IV. THE PROPOSED GLNN

Having discussed the proposed graph learning, we elaborate on its integration with GCN, which leads to the proposed GLNN architecture. As shown in Fig. 2, given graph-structured networks as the input, GLNN consists of two major procedures: graph learning and graph convolution. The graph learning layer aims to produce an optimal adjacency matrix for the subsequent graph convolution. The graph convolution has two layers, with the same parameter setting as in \[4\]. Besides, the classification loss measures the classification performance of our model, whose value is a probability between 0 and 1. The graph learning loss is for the optimization of the adjacency matrix during the network training. We train the entire network using gradient descent, in which the gradient is calculated by using the backward propagation of both the classification loss and graph learning loss. We discuss each module in detail as follows.

#### A. Graph Learning Layer

The graph learning layer aims to construct an optimal graph structure from the input graph signals. In this layer, we first randomly initialize the adjacency matrix before training the network, and then train the graph using gradient descent from the backward propagation of the proposed loss function introduced in Eq. \[17\].

In order to further simplify the implementation, we perform the following symmetrization on the adjacency matrix $\hat{A}$ before the output of the graph learning layer, which aims to ensure the symmetry property:

$$\hat{A}_{\text{out}} = \frac{1}{2} \left( \hat{A}^T + \hat{A} \right), \tag{23}$$

where $\hat{A}_{\text{out}} \in \mathbb{R}^{n \times n}$ is the final output adjacency matrix of the graph learning layer at each epoch. It is a real symmetric matrix by definition. Thus, we can remove the symmetric term in Eq. \[22\].

The graph obtained from the graph learning layer is then fed into the GCN architecture for the subsequent semi-supervised node classification task.

#### B. Graph Convolution and Feature Transfer

As introduced in \[4\], the graph convolution to a signal $X \in \mathbb{R}^{n \times C}$ with $C$ input channels (i.e., a $C$-dimensional feature vector for every node) and $F$ filters are defined as follows:

$$Z = \sigma \left( \hat{A}_{\text{out}} X W \right), \tag{24}$$

where $W \in \mathbb{R}^{C \times F}$ is a matrix of filter parameters, $Z \in \mathbb{R}^{n \times F}$ is the convoluted signal matrix, and $\sigma(\cdot)$ is an activation function.

We consider a two-layer GCN with the learned adjacency matrix $\hat{A}_{\text{out}}$. The forward model takes the form:

$$Z = f(X, \hat{A}_{\text{out}})$$

$$= \text{softmax} \left( \hat{A}_{\text{out}} \text{ReLU} \left( \hat{A}_{\text{out}} X W^{(0)} \right) W^{(1)} \right), \tag{25}$$

where $W^{(0)} \in \mathbb{R}^{C \times H}$ is an input-to-hidden weight matrix for a hidden graph convolutional layer with $H$ output feature channels, and $W^{(1)} \in \mathbb{R}^{H \times F}$ is a hidden-to-output weight matrix for an output layer with $F$ classes. The softmax($\cdot$) and ReLU($\cdot$) are two activation functions.

#### C. The Overall Loss Function

For the semi-supervised node classification task, we need to evaluate the cross-entropy loss (the Classification Loss in Fig. 2) over the labeled data:

$$L_{\text{GCN}} = - \sum_{l \in \mathcal{L}_L} \sum_{f=1}^F Y_{lf} \ln Z_{lf}, \tag{26}$$

where $\mathcal{L}_L$ is a set of labeled nodes, $Y_l$ denotes the label for the $l$th labeled node, and $Z_l$ is the predicted label for the $l$th node.

Further, in cases where the ground truth graph of training samples is available, we add the following loss function to ensure the learned graph is closer to the ground truth:

$$L_{\text{gt}} = \|\hat{A}_{\text{out}} - \hat{A}_{\text{gt}}\|_2, \tag{27}$$

where $A_{\text{gt}}$ is a ground truth adjacency matrix.

Hence, the overall loss function of our proposed GLNN framework is

$$L_{\text{overall}} = L_{\text{GCN}} + L_{\text{GL}} + L_{\text{gt}}. \tag{28}$$

### V. EXPERIMENTAL RESULTS

In order to evaluate the performance of GLNN, we carry out extensive experiments for semi-supervised node classification in terms of the classification accuracy, and provide comparison with the state-of-the-art methods. Further, we evaluate the robustness of GLNN under different label rates. Finally, we visualize the learned graph adjacency matrix from GLNN and provide analysis.
A. Datasets

We consider two social networks: TerroristRel and Terror Attack [60], and three citation networks: Citeseer, Cora, and Pubmed [48]. The five datasets are available at https://linqs.soe.ucsc.edu/data. We represent the relationship between terrorists and citation links as undirected edges, and construct a binary and symmetric matrix as introduced in [4] as the ground truth adjacency matrix. Dataset statistics are summarized in Table I.

| Dataset          | Nodes | Edges | Classes | Features | Rate     |
|------------------|-------|-------|---------|----------|----------|
| TerroristRel     | 848   | 8,592 | 4       | 1,224    | 0.189    |
| Terror Attack    | 1,293 | 3,172 | 6       | 106      | 0.090    |
| Citeseer         | 3,327 | 4,732 | 6       | 3,703    | 0.036    |
| Cora             | 2,708 | 5,429 | 7       | 1,433    | 0.052    |
| Pubmed           | 19,717| 44,338| 3       | 500      | 0.003    |

TerroristRel. This dataset contains information about terrorists and their relationships. We treat each terrorist as a node, and describe the relationship between each pair of terrorists via an edge in the graph. Further, we employ 160 nodes as labeled data to train our model, and leave the rest of 150 nodes for testing.

Terror Attack. This dataset consists of 1,293 terrorist attacks, each of which is assigned one of 6 labels to indicate the attack type. We treat terrorist attacks as nodes, and describe their relationship via edges. We deploy 120 nodes for training and leave 200 nodes for testing.

Citation networks. We consider three widely used citation network datasets: Citeseer, Cora, and Pubmed. In these datasets, nodes are documents and edges are citation links. In particular, we sample 3,000 nodes to evaluate our model for the Pubmed dataset. In addition, we select 60 nodes as labeled data to train each model and test the performance on 1,000 nodes. For the Citeseer and Cora dataset, we follow the experimental setup in [51].

B. Implementation Details

We implemented the proposed model with the TensorFlow framework, while the network architecture was trained on NVIDIA RTX 2080Ti GPU. We employed Adam [62] to train the entire network with the learning rate 0.01. Before the first epoch of the training step in the graph learning layer, we generate a random matrix that follows a uniform distribution, which serves as the initial graph representation. This matrix is then optimized in the subsequent training epochs. In the graph learning loss function, we set \( \lambda_0 = 0.01, \lambda_1 = 0.1, \lambda_3 = 0.1, \) and \( \lambda_4 = 0.001. \) Note that \( \lambda_2 \) is set to 0 with the symmetricization operation introduced in Eq. (23). In the graph convolutional layers, we follow the same experimental settings in [4], i.e., two graph convolutional layers with 16 hidden units.

C. Node Classification Results

Table II lists the comparison results on the five datasets. Reported numbers denote the classification accuracy in percentage, and the best results are marked as bold in the table. Note that the underlying graphs of TerroristRel and Terror Attack datasets are not connected, so the Planetoid [51] cannot be executed properly.

First, we see that our GLNN outperforms the baseline method GCN [4] on all the datasets. This validates the effectiveness of the proposed graph learning for semi-supervised classification. In addition, GLNN performs better than the recently proposed network GWNN [54], which indicates the benefit of the GLNN on graph data representation and learning. Further, GLNN achieves better performance than other semi-supervised learning methods, which demonstrates the superiority of our model on conducting semi-supervised classification tasks on graph data.

D. Robustness Test

Further, we test the robustness of our model on citation networks under low label rates. We adopt five different label rates in \{0.005, 0.010, 0.015, 0.020, 0.025\} to train our model and three representative baseline methods (ChebNet [7], GCN [4] and GWNN [54]). Fig. 3 presents the classification accuracy under five different label rates for GCN, ChebNet, GWNN, and our method on the Citeseer and Cora datasets respectively. We see that while the performance of the other methods drops quickly with decreasing label rate, the proposed GLNN is much more robust, with the classification accuracy of 51.8% and 58.0% on the Citeseer and Cora datasets even when the label rate is lower than 0.01.

The robustness of the GLNN gives credits to the graph-signal smoothness prior in the loss function. This prior is important in practical applications, since graphs in real life are often unlabeled or have few labels.

E. Visualization and Analysis

We also provide some visualization results of the learned graph adjacency matrix obtained from the GLNN in Fig. 4. From the left to right columns, we show the ground truth adjacency matrix, the learned adjacency matrix after the 1st, 5th, 15th, and 50th epoch, respectively. Note that, the adjacency matrix at the 1st epoch is an initialized random matrix that follows a uniform distribution. In order to ensure clear visualization, we select a sub-matrix with size 30 \times 30 from the entire adjacency matrix.

We see that for all the three datasets, as the epoch increases, the learned graph adjacency matrix becomes more and more similar with the ground truth one. At the 50th epoch, the learned adjacency matrix is almost the same as the ground truth, thus validating the effectiveness of the proposed graph learning. Also, the learned adjacency matrix becomes sparser as the epoch increases, due to the sparsity constraint in the proposed graph learning loss.

VI. CONCLUSION

In this paper, we propose a novel Graph Learning Neural Network (GLNN) for semi-supervised node classification.
task, aiming to learn an optimal graph structure that best guides basic operations such as graph convolution in graph convolutional neural networks. Our GLNN model combines both graph learning and graph convolution into a unified framework, in which we integrate the optimization objective of graph learning into the loss function. In particular, the optimization objective for the underlying graph includes the graph-signal prior, sparsity constraint and properties of a valid adjacency matrix. Experimental results on widely adopted citation network datasets and social network datasets validate the effectiveness and robustness of the proposed GLNN. In the future, we will extend our GLNN to other applications such as 3D point cloud classification and segmentation, where there is no ground truth graph provided for training data.

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Fig. 4. The learned graph adjacency matrix (submatrix with size $30 \times 30$). The columns from the left to the right are the ground truth adjacency matrix, the learned adjacency matrix after the 1st, 5th, 15th and 50th epoch, respectively. The rows from the top to the bottom are for the TerroristsRel, Terror Attack, and Cora datasets, respectively.
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