Graph Representation Learning: A Survey

FENXIAO CHEN, YUNCHENG WANG, BIN WANG AND C.-C. JAY KUO

Research on graph representation learning has received a lot of attention in recent years since many data in real-world applications come in form of graphs. High-dimensional graph data are often in irregular form, which makes them more difficult to analyze than image/video/audio data defined on regular lattices. Various graph embedding techniques have been developed to convert the raw graph data into a low-dimensional vector representation while preserving the intrinsic graph properties. In this review, we first explain the graph embedding task and its challenges. Next, we review a wide range of graph embedding techniques with insights. Then, we evaluate several stat-of-the-art methods against small and large datasets and compare their performance. Finally, potential applications and future directions are presented.

I. INTRODUCTION

Research on graph representation learning has gained more and more attention in recent years since many real world data can be represented by graphs conveniently. Examples include social networks, linguistic (word co-occurrence) networks, biological networks and many other multimedia domain-specific data. Graph representation allows the relational knowledge of interacting entities to be stored and accessed efficiently. Analysis of graph data can provide significant insights into community detection, behavior analysis and other useful applications such as node classification, link prediction and clustering. Various graph embedding techniques have been developed to convert the raw graph data into a high-dimensional vector while preserving intrinsic graph properties. This process is also known as graph representation learning. With a learned graph representation, one can adopt machine learning tools to perform downstream tasks conveniently. Obtaining an accurate representation of a graph is challenging in three aspects. First, finding the optimal embedding dimension of a representation is not an easy task. A representation of a higher dimension tends to preserve more information of the original graph at the cost of storage and computation. A representation of a lower dimension is more resource efficient. It may reduce noise in the original graph as well. However, there is a risk in losing some critical information of the original graph. The dimension choice depends on the input graph type as well as the application domain. Second, choosing the proper graph property to embed is an issue of concern if a graph has a plethora of properties. Third, many graph embedding methods have been developed in the past. It is desired to have some guideline in selecting a good embedding method for a target application. In this work, we intend to provide an extensive survey on graph embedding methods with the following three contributions in mind.

• We would like to offer new comers in this field a global perspective with insightful discussion and an extensive reference list. Thus, a wide range of graph embedding techniques, including the most recent graph representation models, are reviewed.
• To shed light on the performance of different embedding methods, we conduct extensive performance evaluation on both small and large data sets in various application domains. To the best of our knowledge, this is the first survey paper that provides systematic evaluation of a rich set of graph embedding methods in domain-specific applications.
• We provide an open-source Python library, called the Graph Representation Learning Library (GRLL), to readers. It offers a unified interface for all graph embedding methods discussed in this paper. This library covers the largest number of graph embedding techniques up to now.

The rest of this paper is organized as follows. We first state the problem as well as several definitions in Sec. II. Then, traditional and emerging graph embedding methods are reviewed in Sec. III and IV, respectively. Next, we conduct extensive performance evaluation on a large number of embedding methods against different datasets in different application domains in Sec. V. The application of the learned graph representation and the future research directions are discussed in Sec. VI and Sec. VII, respectively. Finally, concluding remarks are given in Sec. VIII.

II. DEFINITION AND PRELIMINARIES

A) Notations

A graph, denoted by \( G = (V, E) \), consists of vertices, \( V = \{v_1, v_2, ..., v_n\} \), and edges, \( E = \{e_{i,j}\} \), where an edge \( e_{i,j} \) connects vertex \( v_i \) to vertex \( v_j \). Graphs are usually represented by an adjacency matrix or a derived vector space representation. The adjacency matrix, \( A \), of graph \( G \) contains non-negative weights associated with each edge, \( a_{ij} \geq 0 \). If \( v_i \) and \( v_j \) are not directly connected to one another, \( a_{ij} = 0 \). For undirected graphs, \( a_{ij} = a_{ji} \) for all \( 1 \leq i \leq j \leq n \).
Graph representation learning (or graph embedding) aims to map each node to a vector where the distance characteristics among nodes is preserved. Mathematically, for graph $G = (V,E)$, we would like to find a mapping:

$$f: v_i \rightarrow x_i \in \mathbb{R}^d,$$

where $d \ll |V|$, and $X_i = \{x_1, x_2, \ldots, x_d\}$ is the embedded (or learned) vector that captures the structural properties of vertex $v_i$.

The first-order proximity [14] in a network is the pairwise proximity between vertices. For example, in weighted networks, the weights of the edges are the first-order proximity between vertices. If there is no edge observed between two vertices, the first-order proximity between them is 0. If two vertices are linked by an edge with high weight, they should be close in the embedding space. This objective can be obtained by minimizing the distance between two vertices. Although there is no direct edge between two vertices of the second-order proximity, their representation vectors should be close in the embedded space if they share similar neighborhood structures.

The objective function of the second-order proximity can be defined as

$$O_2 = - \sum_{(i,j) \in E} w_{ij} \log p_2(v_i | v_j),$$

where $p_2(v_i | v_j) = \frac{1}{1 + \exp(-\bar{u}_i \cdot \bar{u}_j)}$

and where $\bar{u}_i \in \mathbb{R}^d$ is the low-dimensional vector representation of vertex $v_i$ and $w_{ij}$ is the weight. The second-order proximity [115] is used to capture the 2-step relationship between two vertices. Although there is no direct edge between two vertices of the second-order proximity, their representation vectors should be close in the embedded space if they share similar neighborhood structures.

The objective function of the second-order proximity can be defined as

$$O_2 = - \sum_{(i,j) \in E} w_{ij} \log p_2(v_i | v_j),$$

where $w_{i,j}$ is the edge weight between node $i$ and $j$ and

$$p_2(v_j | v_i) = \frac{\exp(\gamma \bar{u}_j^T \cdot \bar{u}_i)}{\sum_{k=1}^{|V|} \exp(\gamma \bar{u}_k^T \cdot \bar{u}_i)},$$

and where $\bar{u}_i \in \mathbb{R}^d$ is the representation of vertex $v_i$ when it is treated as a vertex and $\gamma \bar{u}_j \in \mathbb{R}^d$ is the vector representation of vertex $v_j$ when it is treated as a specific context for vertex $v_i$.

Graph sampling is used to simplify graphs [5]. They can be categorized into two types.

- **Negative Sampling [68, 96]**
  Negative sampling is proposed as an alternative to the hierarchical computation of the softmax, which reduces the runtime of the softmax computation on a large scale dataset. Graph optimization requires the summation over the entire set of vertices. It is computationally expensive for large-scale networks. Negative sampling is developed to address this problem. It helps distinguish the neighbors from other nodes by sampling multiple negative examples according to the noise distribution. In the training process, correct surrounding neighbors positive examples in contrast to a set of sampled negative examples (usually noise).

- **Edge Sampling [61, 74]**
  In the training stage, it is difficult to choose an appropriate learning rate in graph optimization when the difference between edge weights is large. To address this problem, one solution is to use edge sampling that unfolds weighted edges into several binary edges at the cost of increased memory. An alternative is treating weighted edges as binary ones with their sampling probabilities proportional to the weights. This treatment would not modify the objective function.

**B) Graph Input**

Graph embedding methods take a graph as the input, where the graph can be homogeneous graphs, heterogeneous graphs, with/without auxiliary information or constructed graphs [111]. They are detailed below.

- **Homogeneous graphs** refer to graphs whose nodes and edges belong to the same type. All nodes and edges of homogeneous graphs are treated equally.

- **Heterogeneous graphs** contain different edge types to represent different relations among different entities or categories. For example, their edges can be directed or undirected. Heterogeneous graphs typically exist in community-based question answering (cQA) sites, multimedia networks and knowledge graphs. Most social network graphs are directed graphs [85]. Only the basic structural information of input graphs is provided in real-world applications.

- **Graphs with auxiliary information** [38, 86] are those that have labels, attributes, node features, information propagation, etc. A label indicates node’s category. Nodes with different labels should be embedded further away than those with the same label. An attribute is a discrete or continuous value that contains additional information about the graph rather than just the structural information. Node features are shown in form of text information for each node. Information propagation indicates dynamic interaction among nodes such as post sharing or "retweet" while Wikipedia [104], DBpedia [8], Freebase [9], etc. provide popular knowledge bases.

- **Graphs constructed from non-relational data** are assumed to lie in a low dimensional manifold.

The input feature matrix can be represented as $X \in \mathbb{R}^{|V| \times N}$ where each row $X_i$ is a $N$-dimensional feature vector for the $i^{th}$ training instance. A similarity matrix, denoted by $S$, can be constructed by computing the similarity between $X_i$ and $X_j$ for graph classifications.
C) Graph Output

The output of a graph embedding method is a set of vectors representing the input graph. It could be node embedding, edge embedding, hybrid embedding or whole-graph embedding. The preferred output form is application-oriented and task-driven. We elaborate them below.

- Node embedding represents each node as a vector, which would be useful for node clustering and classification. For node embedding, nodes that are close in the graph are embedded closer together in the vector representations. Closeness can be first-order proximity, second-order proximity or other similarity calculation.
- Edge embedding aims to map each edge into a vector. It is useful for predicting whether a link exists between two nodes in a graph. For example, knowledge graph embedding can be used for knowledge graph entity/relation prediction.
- Hybrid embedding is the combination of different types of graph components such as node and edge embedding. Hybrid embedding is useful for semantic proximity search and subgraphs learning. It can also be used for graph classification based on graph kernels. Substructure or community embedding can also be done by aggregating individual node and edge embedding inside it. Sometimes, better node embedding is learned by incorporating hybrid embedding methods.
- Whole graph embedding is usually done for small graphs such as proteins and molecules. These smaller graphs are represented as one vector, and two similar graphs are embedded to be closer. Whole-graph embedding facilitates graph classification tasks by providing a straightforward and efficient solution in computing graph similarities.

D) History of Graph Embedding

The study of graph embedding can be traced back to 1900s when people questioned whether all planar graphs with $n$ vertices have a straight line embedding in an $n_k \times n_k$ grid. This problem was solved in [21] and [29]. The same result for convex maps was proved in [83]. More analytic work on the embedding method and time/space complexity of such a method were studied in [18] and [22]. However, a more general approach is needed since most real world graphs are not planer. A large number of methods have been proposed since then.

E) Overview of Graph Embedding Ideas

We provide an overview on various graph embedding ideas below.

- Dimensionality Reduction
  In early 2000s, graph embedding is achieved by dimensionality reduction. For a graph with $n$ nodes, each of which is of dimension $D$, these embedding methods aim to embed nodes into a $d$-dimensional vector space, where $d \ll D$. They are called classical methods and reviewed in Section A. Dimensionality reduction is less scalable.
- Random Walk
  One can trace a graph by starting random walks from random initial nodes so as to create multiple paths. These paths reveal the context of connected vertices. The randomness of these walks gives the ability to explore the graph, capture the global and local structural information by walking through neighboring vertices. Later on, probability models like skip-gram and bag-of-word are performed on the random sampled paths to learn node representations. The random walk based methods will be discussed in Section B.
- Matrix Factorization
  By leverage the sparsity of real-world networks, one can apply the matrix factorization technique that finds an approximation matrix for the original graph. This idea is elaborated in Section C.
- Neural Networks
  Neural network models such as convolution neural network (CNN) [57], recursive neural networks (RNN) [67] and their variants have been widely adopted in graph embedding. This topic will be described in Section A.
- Large Graphs
  Some large graphs are difficult to embed since CNN and RNN models do not scale well with the numbers of edges and nodes. New embedding methods are designed targeting at large graphs. They become popular due to their efficiency. This topic is reviewed in Section B.
- Hypergraphs
  Most social networks are hypergraphs. As social networks get more attention in recent years, hypergraph embedding becomes a hot topic, which will be presented in Section C.
- Attention Mechanism
  Attention mechanism can be added to existing embedding models to increase embedding accuracy, which will be examined in Section B.

An extensive survey on graph embedding methods will be conducted in the next section.

III. CLASSICAL METHODS

A) Dimension-Reduction-Based Methods

Classical graph embedding methods aim to reduce the dimension of high-dimensional graph data into a lower dimensional representation while preserving the desired properties of the original data. They can be categorized into linear and nonlinear two types. The linear methods include the following.

- Principal Component Analysis (PCA) [51]
  The basic assumption for PCA is that that principal components that are associated with larger variances represent the important structure information while those smaller variances represent noise. Thus, PCA computes
the low-dimensional representation that maximizes the data variance. Mathematically, it first finds a linear transformation matrix $W \in \mathbb{R}^{D \times d}$ by solving

$$W = \arg\max_{W} \text{Tr}(W^T \text{Cov}(X)W), \quad d = 1, 2, \ldots, D,$$

where $\text{Cov}(X)$ denotes the covariance of data matrix $X$. It is well known that the principal components are orthogonal and they can be solved by eigen decomposition of the covariance of data matrix \[90\].

- Linear Discriminant Analysis (LDA) \[105\]
  The basic assumption for LDA is that each class is Gaussian distributed. Then, the linear projection matrix, $W \in \mathbb{R}^{D \times d}$, can be obtained by maximizing the ratio between the inter-class scatter and intra-class scatters. The maximization problem can be solved by eigen decomposition and the number of low dimension $d$ can be obtained by detecting a prominent gap in the eigen-value spectrum.

- Multidimensional Scaling (MDS) \[75\]
  MDS is a distance-preserving manifold learning method. It preserves spatial distances. MDS derives a dissimilarity matrix $D$, where $D^{i,j}$ represents the dissimilarity between points $i$ and $j$, and produces a mapping in a lower dimension to preserve dissimilarities as much as possible.

The above three-mentioned methods are referred to as “subspace learning” \[100\] under the linear assumption. However, linear methods might fail if the underlying data are highly non-linear \[78\]. Then, non-linear dimensionality reduction (NLDR) \[24\] can be used for manifold learning. The objective is to learn the nonlinear topology automatically. The NLDR methods include the following.

- Isometric Feature Mapping (Isomap) \[77\]
  The Isomap finds low-dimensional representation that most accurately preserves the pairwise geodesic distances between feature vectors in all scales as measured along the submanifold from which they were sampled. Isomap first constructs neighborhood graph on the manifold, then it computes the shortest path between pairwise points. Finally it constructs low-dimensional embedding by applying MDS.

- Locally Linear Embedding (LLE) \[76\]
  LLE preserves the local linear structure of nearby feature vectors. LLE first assign neighbors to each data point. Then it compute the weights $W^{i,j}$ that best linearly reconstruct $X_i$ from its neighbors. Finally it compute the low-dimensional embedding that best reconstructed by $W^{i,j}$. Besides NLDR, kernel PCA is another dimension reduction technique that is comparable to Isomap, LLE.

- Kernel Methods \[49\]
  Kernel extension can be applied to algorithms that only need to compute the inner product of data pairs. After replacing the inner product with kernel function, data is mapped implicitly from the original input space to higher dimensional space and then apply linear algorithm in the new feature space. The benefit of kernel trick is data that are not linearly separable in the original space could be separable in new high dimensional space. Kernel PCA is often used for NLDR with polynomial or Gaussian kernels.

B) Random-Walk-Based Methods

Random-walk-based methods sample a graph with a large number of paths by starting walks from random initial nodes. These paths indicate the context of connected vertices. The randomness of walks gives the ability to explore the graph and capture global as well as local structural information by walking through neighboring vertices. After that, probability models such as skip-gram and bag-of-word can be performed on these randomly sampled paths to learn the node representation.

- DeepWalk \[73\]
  DeepWalk is the most popular random-walk-based graph embedding method. In DeepWalk, a target vertex, $v_t$, is said to belong to a sequence $S = \{v_1, \ldots, v_{|S|}\}$ sampled by random walks if $v_t$ can reach any vertex in $S$ within a certain number of steps. The set of vertices, $V_s = \{v_{t-1}, v_{t-2}, v_{t+1}, \ldots, v_{t+j}\}$, is the context of center vertex $v_t$ with a window size of $t$. DeepWalk aims to maximize the average logarithmic probability of all vertex context pairs in random walk sequence $S$. It can be written as

$$\frac{1}{|S|} \sum_{i=1}^{|S|} \sum_{t \leq j \leq t \neq 0} \log p(v_{i+j}|v_i),$$

where $p(v_j|v_i)$ is calculated using the softmax function. It is proven in \[101\] that DeepWalk is equivalent to factoring a matrix

$$M = W^T \times H,$$

where $M \in \mathbb{R}^{k \times [V]}$ whose entry, $M_{ij}$, is the logarithm of the average probability that vertex $v_i$ can reach vertex $v_j$ in a fixed number of steps and $W \in \mathbb{R}^{k \times [V]}$ is the vertex representation. The information in $H \in \mathbb{R}^{k \times [V]}$ is rarely utilized in the classical DeepWalk model.

- node2vec \[40\]
  node2vec is a modified version of DeepWalk. In DeepWalk, sampled sequences are based on DFS (Depth-first Sampling) strategy. They consist of neighboring nodes sampled at increasing distances from the source node sequentially. However, if the contextual sequences are sampled by the DFS strategy alone, only few vertices close to the source node will be sampled. Consequently, the local structure will be easily overlooked. In contrast with the DFS strategy, the BFS (Breadth-first Sampling) strategy will explore neighboring nodes with a restricted maximum distance to the source node while the global structure may be neglected.

As a result, node2vec proposes a probability model in which the random walk has a certain probability, $\frac{1}{n}$, to revisit nodes being traveled before. Furthermore, it uses an in-out parameter $q$ to control the ability of exploring
the global structure. When return parameter $p$ is small, the random walk may get stuck in a loop and capture the local structure only. When in-out parameter $q$ is small, the random walk is more similar to a DFS strategy and capable of preserving the global structure in the embedding space.

C) Matrix-Factorization-Based Methods

To obtain node embedding, matrix-factorization-based embedding methods, also called Graph Factorization (GF) [3], was the first one to achieve graph embedding in $O(|E|)$ time. To obtain the embedding, GF factorizes the adjacency matrix of a graph. It corresponds to a structure-preserving dimensionality reduction process. There are several variations as summarized below.

- **Graph Laplacian Eigenmaps [6]**
  This technique minimizes a cost function to ensure that points close to each other on the manifold are mapped close to each other in the low-dimensional space to preserve local distances.

- **Node Proximity Matrix Factorization [31]**
  This method approximates node proximity in a low-dimensional space via matrix factorization by minimizing the following objective function:

  $$Y = \text{argmax} \min |W - YY^T|,$$

  where $W$ is the node proximity matrix, which can be derived by several methods. One way to obtain $W$ is to use Eq. [6].

- **Text-Associated DeepWalk (TADW) [101]**
  TADW is an improved DeepWalk method for text data. It incorporates the text features of vertices in network representation learning via matrix factorization. Recall that the entry, $m_{ij}$, of matrix $M \in \mathbb{R}^{|V| \times |V|}$ denotes the logarithm of the average probability that vertex $v_i$ randomly walks to vertex $v_j$. Then, TADW factorizes $M$ into three matrices

  $$M = W^T \times H \times T,$$

  where $W \in \mathbb{R}^{k \times |V|}$, $H \in \mathbb{R}^{k \times f_t}$, and $T \in \mathbb{R}^{f_t \times |V|}$ is the text feature matrix. In TADW, $W$ and $HT$ are concatenated as the representation for vertices.

- **Homophily, Structure, and Content Augmented (HSCA) Network [111]**
  The HSCA model is an improvement upon the TADW model. It uses Skip-Gram and hierarchical Softmax to learn a distributed word representation. The objective function for HSCA can be written as

  $$\min_{W,H} (||M - W^THT||^2_F + \frac{\lambda}{2} (||W||^2_F + ||H||^2_F)) + \mu(R_1(W) + R_2(H))),$$

  where $||.||_2$ is the matrix $l_2$ norm and $||.||_F$ is the matrix Frobenius norm. In Eq. (9), the first term aims to minimize the matrix factorization error of TADW. The second term imposes the low-rank constraint on $W$ and $H$ and uses $\lambda$ to control the trade-off. The last regularization term enforces the structural homophily between connected nodes in the network. The conjugate gradient (CG) optimization technique can be used to update $W$ and $H$. We may consider another regularization term to replace the third term; namely,

  $$R(W, H) = \frac{1}{4} \sum_{i,j=1}^{|V|} A_{i,j} \left( \frac{w_i}{|H|_{1,i}} - \frac{w_j}{|H|_{1,j}} \right)^2.$$  

  This term will make connected nodes close to each other in the learned network representation [17].

- **GraRep [13]**
  GraRep aims to preserve the high order proximity of graphs in the embedding space. While the random-walk based methods have a similar objective, their probability model and objective functions used are difficult to explain how the high order proximity are preserved. GraRep derives a $k$-th order transition matrix, $A^k$, by multiply the adjacency matrix to itself $k$ times. The transition probability from vertex $w$ to vertex $c$ is the entry in the $w$-th row and $c$-th column of the $k$-th order transition matrix. Mathematically, it can be written as

  $$p_k(c|w) = A^k_{w,c}.$$  

  With the transition probability defined in (11), the loss function is defined by the skip-gram model and negative sampling. To minimize the loss function, the embedding matrix can be expressed as

  $$Y_{i,j} = W^k_i \cdot C_{j} = \log\left(\frac{A^k_{i,j}}{\sum_{i'} A^k_{i',j}}\right) - \log(\beta),$$

  where $\beta$ is a constant $\frac{1}{N}$, $\lambda$ is the negative sampling parameter, and $N$ is the number of vertices. The embedding matrix, $W$, can be obtained by factorizing matrix $Y$ in (12).

- **HOPE [72]**
  HOPE preserves asymmetric transitivity in approximating the high order proximity, where asymmetric transitivity indicates a certain correlation among directed graphs. Generally speaking, if there is a directed edge from $u$ to $v$, it is likely that there is a directed edge from $v$ to $u$ as well. Several high order proximities such as the Katz Index [53], the Rooted PageRank, the Common Neighbors, and the Adamic-Adar were experimented in [72]. The embedding, $\hat{v}_i$, for node $i$ can be obtained by factorizing the similarity matrix, $S$, derived from these proximities. To factorize $S$, SVD is adopted and only the top-$k$ eigenvalues are chosen.
IV. EMERGING METHODS

A) Neural-Network-Based Methods

Neural network models become popular again since 2010. Being inspired by the success of recurrent neural networks (RNNs) and convolutional neural networks (CNNs), researchers attempt to generalize and apply them to graphs. Natural language processing (NLP) models often use the RNN to find a vector representation for words. The Word2Vec \[66\] and the skip-gram models \[68\] aim to learn the continuous feature representation of words by optimizing a neighborhood preserving likelihood function. By following this idea, one can adopt a similar approach for graph embedding, leading to the Node2vec method \[46\]. Node2Vec utilizes random walks \[82\] with a bias to sample the neighborhood of a target node and optimizes its representation using stochastic gradient descent (SGD). Another family of neural-network-based embedding methods adopts CNN models. The input is either paths sampled from a graph or the whole graph itself. Some use the original CNN model designed for the Euclidean domain and reformat the input graph to fit it. Others generalize the deep neural model to non-Euclidean graphs.

Several neural-network-based Methods based graph embedding methods are presented below.

- **Graph Convolutional Network (GCN)** \[56\]: GCN allows end-to-end learning of the graph with arbitrary size and shape. This model uses convolution operators on the graph and iteratively aggregates the embedding of neighbors for nodes. This approach is widely used for semi-supervised learning on graph-structured data that is based on an efficient variant of convolutional neural networks that operates directly on graphs and it learns hidden layer representations that encode both local graph structure and features of nodes. In the first step of the GCN, a node sequence will be selected. The neighborhood nodes will be assembled, then the neighborhood might be normalized to impose order of the graph, then convolutional layers will be used to learn representation of nodes and edges. The propagation rule used is

\[
f(H^{(l)}, A) = \sigma(D^{-\frac{1}{2}}AD^{-\frac{1}{2}}H^{(l)}W^{(l)}),
\]

where \(A\) is the identity matrix, with enforced self loops to include the node features of itself we get \(^*A= A + I\), \(I\) is the identity matrix and \(^*D\) is the diagonal node degree matrix of \(^*A\) to normalize the neighbors of \(A\). Under spectral graph theory of CNNs on graphs, GCN is equivalent to Graph Laplacian in the non-euclidean domain \[23\]. The decomposition of eigenvalues for the Normalized Graph Laplacian data can also be used for tasks such as classification and clustering. However, GCN usually only uses two convolutional layer and why it works its not well explained. One recent work showed that GCN model is a special form of Laplacian smoothing \[63\] [32]. This is the reason that GCN works, and also more than two convolutional layers will lead to over-smoothing, therefore making making the features of nodes similar to each other and more difficult to separate from each other.

- **Signed Graph Convolutional Network (SGCN)** \[25\]: Most GCNs operate on unsigned graphs, however, many links in real world have negative links. To solve this problem, signed GCNs aims to learn graph representation with the additional signed link information. Negative links usually contains semantic information that is different from positive links, also the principles are inherently different from positive links. The signed network will have a different representation as \(G = (V, E^+, E^-)\) where the signs of the edges are differentiated. The aggregation for positive and negative links are different. Each layer will have two representations, one for the balanced user where the number of negative links is even and one for the unbalanced user where the number of negative links is odd. The hidden states are

\[
h^{B(1)}_i = \sigma(W^{B(l)} \sum_{j \in N^{(i)}_{+}} h^0_j \frac{1}{|N^+_i|}, h^{(0)}_i),
\]

\[
h^{U(1)}_i = \sigma(W^{U(l)} \sum_{j \in N^{(i)}_{-}} h^0_j \frac{1}{|N^-_i|}, h^{(0)}_i),
\]

where \(\sigma()\) is the non-linear activation function, \((W^{B(l)})\) and \((W^{U(l)})\) are the linear transformation matrices for balanced and unbalanced sets.

- **Variational Graph Auto-Encoders (VGAE)** \[55\]: An autoencoder minimizes the reconstruction error of the input and the output using an encoder and a decoder. The encoder maps input data to a representation space. Then, it is further mapped to a reconstruction space that preserves the neighborhood information. VGAE uses GCN as the encoder and an inner product decoder to embed graphs.

- **GraphSAGE** \[47\]: GraphSAGE uses a sample and aggregate method to conduct inductive node embedding with node features such as text attributes, node profiles, etc. It trains a set of aggregation functions that integrate features of local neighborhood and pass it to the target node \(i\). Then, the hidden state of node \(i\) is updated by

\[
h^{(k+1)}_i = ReLU(W^{(k)}h^{(k)}_i, \sum_{n \in N(i)}(ReLU(Q^{(k)}h^{(k)}_n))))
\]

where \(h^{(0)}_i = X_i\) is the initial node attributes and \(\sum(...\) denotes a certain aggregator function, e.g., average, LSTM, max-pooling, etc.

- **Structural Deep Network Embedding (SDNE)** \[92\]: SDNE learns a low-dimensional network-structure-preserving representation by considering both the first-order and the second-order proximities between vertexes using CNNs. To achieve this objective, it adopts a semi-supervised model to minimize the following objective
function:
\[
||((\hat{X} - X) \odot B)||^2_F + \alpha \sum_{i,j=1}^n s_{i,j}||y_i - y_j||^2_F + vL_{reg},
\]
where \(L_{reg}\) is an \(L_2\)-norm regularizing term to avoid overfitting, \(S\) is the adjacency matrix, and \(B\) is the bias matrix.

B) Large Graph Embedding Methods

To address the scalability issue, several embedding methods targeting at large graphs have been proposed recently. They are examined in this subsection.

Fig. 1. Illustration of a learnable graph convolutional layer (LGCL) method [35].

• Learnable graph convolutional layer (LGCL) [35]

For each feature dimension, every node in the LGCL method selects a fixed number of features from its neighboring nodes with value ranking. Fig. 1 serves as an example. Each node in this figure has a feature vector of dimension \(n = 3\). For the target node (in orange), the first feature component of its six neighbors takes the values of 9, 6, 5, 3, 0, 0. If we set the window size to \(k = 4\), then the four largest values (i.e., 9, 6, 5, 3) are selected. The same process is repeated for the two remaining features. By including the feature vector of the target node itself, we obtain a data matrix of dimension \((k + 1) \times n\). This results in a grid-like structure. Then, the traditional CNN can be conveniently applied so as to generate the final feature vector. To embed large-scale graphs, a sub-graph selection method is used to reduce the memory and resource requirements. As shown in Fig. 2, it begins with \(N_{init} = 3\) randomly sampled nodes (in red) that are located in the center of the figure. At the first iteration, the breadth-first-search (BFS) is used to find all first-order neighboring nodes of initial nodes. Among them, \(N_m = 5\) nodes (in blue) are randomly selected. At the next iteration, \(N_m = 7\) nodes (in green) are randomly selected. After two iterations, 15 nodes are selected as a sub-graph that serves as the input to LGCL.

Graph partition neural networks (GPNN) [70]

GPNN extends graph neural networks (GNNs) to embed extremely large graphs. It alternates between local (propagate information among nodes) and global information propagation (messages among subgraphs). This scheduling method can avoid deep computational graphs required by sequential schedules. The graph partition is done using a multi-seed flood fill algorithm, where nodes with large out-degrees are sampled randomly as seeds. The subgraphs grow from seeds using flood fill, which reaches out unassigned nodes that are direct neighbors of the current subgraph.

• LINE [85]

LINE is used to embed graphs of an arbitrary type such as undirected, directed and weighted graphs. It utilizes negative sampling to reduce optimization complexity. This is especially useful in embedding networks containing millions of nodes and billions of edges. It is trained to preserve the first- and second-order proximities, separately. Then, the two embeddings are merged to generate a vector space to better represent the input graph. One way to merge two embeddings is to concatenate embedding vectors trained by two different objective functions at each vertex.

C) Hypergraph Embedding

Research on social network embedding grows quickly. A simple graph is not powerful enough in representing the information of social networks. The relation of vertices in social networks is far more complicated than the vertex-to-vertex edge relationship. Being different from traditional graphs, edges in hypergraphs may have a degree larger than two. All related nodes are connected by a hyperedge to form a supernode. Mathematically, an unweighted hypergraph is defined as follows. A hypergraph, denoted by \(G = (V, E)\), consists of a vertex set

\[V = \{v_1, v_2, ..., v_n\} \]
and a hyperedge set,
\[ E = \{e_1, e_2, \ldots, e_m \}. \]

A hyperedge, \( e \), is said to be incident with a vertex \( v \) if \( v \in e \). When \( v \in e \), the incidence function \( h(v, e) = 1 \). Otherwise, \( h(v, e) = 0 \). The degree of a vertex \( v \) is defined as
\[ d(v) = \sum_{e, v \in e} h(v, e). \]

Similarly, the degree of a hyperedge \( e \) is defined as
\[ d(e) = \sum_{v \in V} h(v, e). \]

A hypergraph can be represented by an incidence matrix \( H \) of dimension \(|V| \times |E|\) with entries \( h(v, e) \).

Hyperedges possess the properties of edges and nodes at the same time. As an edge, hyperedges connect multiple nodes that are closely related. A hyperedge can also be seen as a supernode. For each pair of two supernodes, their connection is established by shared incident vertices. As a result, hypergraphs can better indicate the community structure in the network data. These unique characteristics of hyperedges make hypergraphs more challenging. An illustration of graph and hypergraph structures is given in Fig. [3]. It shows how to express a hypergraph in table form. The hyperedges, which are indecomposable [89], can express the community structure of networks. Furthermore, properties of graphs and hypergraphs are summarized and compared in Table [1]. Graphs and hypergraphs conversion techniques have been developed. Examples include clique expansion and star expansion. Due to indecomposibility of hyperedges, conversion from a hypergraph to a graph will result in information loss.

Since hypergraphs provide a good tool for social network modeling, and hypergraph embedding is a hot research topic nowadays. On one hand, hypergraph modeling has a lot of applications that are difficult to achieve by graph modeling such as multi-modal data representation. On the other hand, hypergraphs can be viewed as a variant of simple graphs and many graph embedding methods could be applied onto the hypergraphs with minor modifications. There are embedding methods proposed for simple graphs and they can be applied to hypergraphs as well as reviewed below.

- **Spectral Hypergraph Embedding [117]**
  Hypergraph embedding can be treated as a k-way partitioning problem and solved by optimizing a combinatorial function. It can be further converted to a real-valued minimization problem by normalizing the hypergraph Laplacian. Its solution is any lower dimension embedding space spanned by orthogonal eigenvectors of the hypergraph Laplacian, \( \Delta \), with the \( k \) smallest eigenvalues.

- **Hyper-Graph Neural Network (HGNN) [31]**
  Being inspired by the spectral convolution on graphs in GCN [56], HGNN applies the spectral convolution to hypergraphs. By training the network through a semi-supervised node classification task, one can obtain the node representation at the end of convolutional layers. The architecture is depicted in Fig. [4].

\[
f(X, W, \Theta) = \sigma(D_v^{-\frac{1}{2}} H W D_e^{-1} H^T D_v^{-\frac{1}{2}} X \Theta),
\]

where \( X \) is the hidden embedding in each layer, \( \Theta \) is the filter response, and \( D_v \) and \( D_e \) are diagonal matrices with entries being the degree of the vertices and the hyperedges, respectively.
first order proximity is preserved in the embedding space by defining an $N$-tuplewise similarity function. That is, if $N$ nodes are in the same hyperedge, the similarity of these nodes in the embedding space should be high. Based on similarity, one can predict whether $N$ nodes are connected by a single hyperedge. However, the $N$-tuplewise similarity function should be non-linear; otherwise, it will lead to contradicted predictions. The local information of a hypergraph can be preserved by shortening the distance of connected vertices in the embedding space.

D) Attention Graph Embedding

An attention mechanism can be used in machine learning to allow the learning process to focus on parts of a graph that are relevant to a specific task. One advantage of applying attention to graphs is to avoid the noisy part of a graph so as to increase the signal-to-noise (SNR) ratio [60] in information processing. Attention-based node embedding aims to assign an attention weight, $\alpha$, to the neighbors of a target node $t$, where $\sum_{i \in N(t)} \alpha_i = 1$ and $N(t)$ denotes the set of neighboring nodes of $t$.

- **Graph Attention Networks (GAT)** [91]
  GAT utilizes masked self-attentional layers to limit the shortcomings of prior graph convolutional based methods. They aim to compute the attention coefficients

$$
\alpha_{ij} = \frac{\exp(\text{LeakyReLU}(d^TW_h||W_h j)))}{\sum_{k \in N_i} \exp(\text{LeakyReLU}(d^TW_h||W_h j)))},
$$

where $W$ is the weight matrix for the initial linear transformation, then the transformed information on each neighbor’s feature are concatenated to obtain the new hidden state, which will be passed through a LeakyReLU activation. The above attention mechanism is a single-layer feedforward neural network parameterized by the above weight vector.

- **AttentionWalks** [1, 2]
  Generally speaking, one can use the random walk to find the context of the node. For a graph, $G$, with corresponding transition matrix $T$ and window size $c$ the parameterized conditional expectation after a $k$-step walk can be expressed as

$$
E[D|q_1, q_2, ..., q_c] = I_n \sum_{k=1}^c q_k T^k,
$$

where $I_n$ is the size-$n$ identity matrix, $q_k$, $1 \leq i \leq c$, are the trainable weights, $D$ is the walk distribution matrix whose entry $D_{uv}$ encodes the number of times node $u$ is expected to visit node $v$. The trainable weights are used to steer the walk towards a broader neighborhood or restrict it within a smaller neighborhood. Following this idea, AttentionWalks adopts an attention mechanism to guide the learning procedure. This mechanism suggests which part of the data to focus on during the training process.

The weight parameters are called the attention parameters in this case.

- **Attentive Graph-based Recursive Neural Network (AGRNN)** [97]
  AGRNN applies attention to a graph-based recursive neural network (GRNN) [98] to make the model focus on vertices with more relevant semantic information. It builds subgraphs to construct recursive neural networks by sampling a number of $k$-step neighboring information. AGRNN finds a soft attention, $\alpha_r$, to control how neighbor information should be passed to the target node. Mathematically, we have

$$
\alpha_r = \text{Softmax}(x^TW(a)h_r),
$$

where $x_k$ is the input, $W(a)$ is the weight to learn and $h_r$ is the hidden state of the neighbors. The aggregated representation from all neighbors is used as the hidden state of the target vertex

$$
h_k = \sum_{v_i \in N(v_k)} \alpha_r h_r,
$$

where $N(v_k)$ denotes the set of neighboring nodes of vertex $v_k$. Although attention has been shown to be useful in improving some neural network models, it does not always increase the accuracy of graph embedding [16].

E) Others

- **GraphGAN** [93]
  GraphGAN employs both generative and discriminative models for graph representation learning. It adopts adversarial training and formulates the embedding problem as a minimax game by borrowing the idea from the Generative Adversarial Network (GAN) [43]. To fit the true connectivity distribution $p_{true}(v|v_c)$ of vertices connected to target vertex $v_c$, GraphGAN models the connectivity probability among vertices in a graph with a generator, $G(v|v_c; \theta_G)$, to generate vertices that are most likely connected to $v_c$. A discriminator $D(v, v_c; \theta_D)$ outputs the edge probability between $v$ and $v_c$ to differentiate the vertex pair generated by the generator from the ground truth. The final vertex representation is determined by alternately maximizing and minimizing the value function $V(G, D)$ as

$$
\min_{\theta_G} \max_{\theta_D} V(G, D) = \sum_{c=1}^V (g_{v_c} \log D(v, v_c; \theta_D)) + \mathbb{E}_{v \sim G(\cdot|v_c; \theta_G)} \log (1 - D(v, v_c; \theta_D))
$$

- **GenVector** [104]
  GenVector leverages large-scale unlabeled data to learn large social knowledge graphs. It is cast as a weakly supervised problem and solved by unsupervised techniques with a multi-modal Bayesian embedding model.
GenVector can serve as a generative model in applications. For example, it uses latent discrete topic variables to generate continuous word embeddings and graph-based user embeddings and integrates the advantages of topic models and word embeddings.

V. EVALUATION

We study the evaluation of various graph representation methods in this section. Evaluation tasks and datasets will be discussed in Secs. A and B respectively. Then, evaluation results will be presented and analyzed in Sec. C.

A) Evaluation Tasks

The two most common evaluation tasks are vertex classification and link prediction. We use vertex classification to compare different graph embedding methods and draw insights from the obtained results.

- Vertex Classification
  Vertex classification aims to assign a class label to each node in a graph based on the information learned from other labeled nodes. Intuitively, similar nodes should have the same label. For example, closely-related publications may be labeled as the same topic in the citation graph while individuals of the same gender, similar age and common interests may have the same preference in social networks. Graph embedding methods embed each node into a low-dimensional vector. Given an embedded vector, a trained classifier can predict the label of a vertex of interest, where the classifier can be SVM (Support Vector Machine) [42], logistic regression [94], kNN (k nearest neighbors) [59], etc. The vertex label can be obtained in an unsupervised or semi-supervised way. Node clustering is an unsupervised method that groups similar nodes together. It is useful when labels are unavailable. The semi-supervised method can be used when part of the data are labeled. The F1 score is used for evaluation in binary-class classification while the Micro-F1 score is used in multi-class classification. Since accurate vertex representations contribute to high classification accuracy, vertex classification can be used to measure the performance of different graph embedding methods.

- Link Prediction [36]
  Link prediction aims to infer the existence of relationship or interaction among pairs of vertices in a graph. The learned representation should help infer the graph structure, especially when some links are missing. For example, links might be missing between two users and link prediction can be used to recommend friends in social networks. The learned representation should preserve the network proximity and the structural similarity among vertices. The information encoded in the vector representation for each vertex can be used to predict missing links in incomplete networks. The link prediction performance can be measured by the area under curve (AUC) or the receiver operating characteristic (ROC) curve. A better representation should be able to capture the connections among vertices better.

B) Evaluation Datasets

Citation datasets such as Citeseer [39], Cora [10] and PubMed [12] are examples of small datasets. They can be represented as directed graphs in which edges indicate author-to-author or paper-to-paper citation relationship and text attributes of paper content at nodes.

First, we describe several representative citation datasets below.

- Citeseer [39]
  It is a citation index dataset containing academic papers of six categories. It has 3,312 documents and 4,723 links. Each document is represented by a 0/1-valued word vector indicating the absence/presence of the corresponding word from a dictionary of 3,703 words. Thus, the text attributes of a document is a binary-valued vector of 3,703 dimensions.

- Cora [10]
  It consists of 2,708 scientific publications of seven classes. The graph has 5,429 links that indicate citation relations between documents. Each document has text attributes that are expressed by a binary-valued vector of 1,433 dimensions.

- WebKB [88]
  It contains seven classes of web pages collected from computer science departments, including student, faculty, course, project, department, staff, etc. It has 877 web pages and 1,608 hyper-links between web pages. Each page is represented by a binary vector of 1,703 dimensions.

- KARATE [109]
  Zachary’s karate network is a well-known social network of a university karate club. It has been widely studied in social network analysis. The network has 34 nodes, 78 edges and 2 communities.

- Wikipedia [19]
  The Wikipedia is an online encyclopedia created and edited by volunteers around the world. The dataset is a word co-occurrence network constructed from the entire set of English Wikipedia pages. This data contains 2405 nodes, 17981 edges and 19 labels.

Next, we present several commonly used large graph datasets below.

- Blogcatalog [84]
  It is a network of social relationships of bloggers listed in the BlogCatalog website. The labels indicate blogger’s
interests inferred from the meta-data provided by bloggers. The network has 10,312 nodes, 333,983 edges and 39 labels.

- **Youtube** [95]
  It is a social network of Youtube users. This graph contains 1,157,827 nodes, 4,945,382 edges and 47 labels. The labels represent groups of users who enjoy common video genres.

- **Facebook** [62]
  It is a set of postings collected from the Facebook website. This data contains 4039 nodes, 88243 edges and no labels. It is used for link prediction.

- **Flickr** [80]
  It is an online photo management and sharing dataset. It contains 80513 nodes, 5899882 edges and 195 labels.

Finally, parameters of the above-mentioned datasets are summarized in Table 2.

|          | Node | Edge | Labels |
|----------|------|------|--------|
| Citeseer | 3312 | 4723 | 6      |
| Cora     | 2708 | 5429 | 7      |
| WebKB    | 877  | 1608 | 7      |
| KARATE   | 34   | 78   | N/A    |
| Wiki     | 2405 | 17981| 19     |
| Blogcatalog | 10312 | 333983 | 39 |
| Youtube  | 1157827 | 4945382 | 47 |
| Facebook | 4039 | 88243| N/A    |
| Flickr   | 80513 | 5899882 | 195 |

Table 2. Summary of representative graph datasets.

C) Evaluation Results and Analysis

Since evaluations were often performed independently on different datasets under different settings in the past, it is difficult to draw a concrete conclusion on the performance of various graph embedding methods. Here, we compare the performance of graph embedding methods using a couple of metrics under the common setting and analyze obtained results. In addition, we provide an open-source Python library, called the Graph Representation Learning Library (GRLL), to readers in the Github. It offers a unified interface for all graph embedding methods that were experimented in this work. To the best of our knowledge, this library covers the largest number of graph embedding techniques up to now.

1) **Vertex Classification**

We compare vertex classification accuracy of seven graph embedding methods on Cora and Wiki. We used the default hyper-parameter setting provided by each graph embedding method. For the classifier, we adopted linear regression for all methods. We split samples equally into the training and the testing sets (i.e. 50% and 50%). The vertex classification results are shown in Table 3. DeepWalk and node2vec offer the highest accuracy for Cora and Wiki, respectively. The random-walk-based methods (e.g., DeepWalk, node2vec and GraRep) are the top three performers for both Cora and Wiki. DeepWalk and node2vec are preferred among them since GraRep usually demands much more memory and it is difficult to apply GraRep to larger graphs.

|          | Cora | Wiki |
|----------|------|------|
| DeepWalk | 0.829| 0.670|
| node2vec | 0.803| 0.680|
| GraRep   | 0.788| 0.650|
| HOPE     | 0.646| 0.608|
| SDNE     | 0.573| 0.510|
| LINE     | 0.432| 0.520|
| GF       | 0.399| 0.465|

Table 3. Performance comparison of seven graph embedding methods in vertex classification on Cora and Wiki.

2) **Clustering Quality**

We compare various graph embedding methods by examining their clustering quality in terms of the Macro- and Micro-F1 scores. The K-means++ algorithm is adopted for the clustering task. Since the results of K-means++ clustering are dependent upon seed initialization, we perform 10 consecutive runs and report the best result. We tested them on three large graph datasets (i.e., YouTube, Flickr and BlogCatalog). The experimental results are shown in Table 4. YouTube and Flickr contain more than millions of nodes and edges and we can only run DeepWalk, node2vec and LINE on them with the 24G RAM limit as reported in the table. We see that DeepWalk and node2vec provide the best results. They are both random-walk based methods with different sampling scheme. Also, they demand less memory as compared with others. In general, random walk with the skip-gram model is a good baseline for unsupervised graph embedding. GraRep offers comparable graph embedding quality for BlogCatalog. However, its memory requirement is huge so that it is not suitable for large graphs.

3) **Time Complexity**

Time complexity is an important factor to consider, which is especially true for large graphs. The time complexity of three embedding methods against three datasets is compared in Table 5. We see that the training time of DeepWalk is significantly lower than node2vec and LINE for larger graph datasets such as YouTube and Flickr. DeepWalk is an efficient graph embedding method with high accuracy by considering embedding quality as well as training complexity.

4) **Influence of Embedding Dimensions**

As the embedding dimension decreases, less information of the input graph is preserved so that the performance drops. However, some drops faster than others. We show the node classification accuracy as a function of the embedding
dimension for the Wiki dataset in Fig. 5. We compare six graph embedding methods (node2vec, DeepWalk, LINE, GraRep, SDNE and GF) and their embedding dimensions vary from 4, 8, 16, 32, 64 to 128. We see that the performance of the random-walk based embedding methods (node2vec and Deep-Walk) degrades slowly. Only about 20% drop in performance when the embedding dimension size goes from 128 to 4. In contrast, The performance of the structural preserving methods (LINE and GreRep) and the graph factorization method (GF) drops significantly (as much as 45%) when the embedding size goes from 128 to 4. One explanation is that the structural preserving methods optimize the representation vectors in the embedding space so that a small information loss will result in substantial difference. Random-walk based methods obtain embedding vectors by selecting paths from the input graph randomly. Yet, the relationship between nodes is still preserved when the embedding dimension is small. SDNE adopts the auto-encoder architecture to preserve the information of the input graph so that its performance remains about the same regardless of the embedding dimension.

### Table 4. Comparison of clustering quality of six graph embedding methods in terms of Macro- and Micro-F1 scores against three large graph datasets.

| Dataset     | Method       | Macro-F1 | Micro-F1 |
|-------------|--------------|----------|----------|
| YouTube     | DeepWalk     | 0.206    | 0.221    |
|             | node2vec     | 0.293    | 0.301    |
|             | LINE         | 0.170    | 0.266    |
|             | GraRep       | N/A      | N/A      |
|             | GF           | N/A      | N/A      |
|             | HOPE         | N/A      | N/A      |
| Flickr      | DeepWalk     | 0.212    | 0.203    |
|             | node2vec     | 0.313    | 0.311    |
|             | LINE         | 0.162    | 0.289    |
|             | GraRep       | N/A      | N/A      |
|             | GF           | N/A      | N/A      |
|             | HOPE         | N/A      | N/A      |
| BlogCatalog | DeepWalk     | 0.247    | 0.250    |
|             | node2vec     | 0.393    | 0.400    |
|             | LINE         | 0.194    | 0.356    |
|             | GraRep       | 0.230    | 0.393    |
|             | GF           | 0.072    | 0.236    |
|             | HOPE         | 0.143    | 0.308    |

### Table 5. Comparison of time used in training (seconds).

| Dataset     | DeepWalk | node2vec | LINE | Wiki |
|-------------|----------|----------|------|------|
| YouTube     | 37366    | 3636.14  | 37.23|
| Flickr      | 41626.94 | 40779.22 | 27.53|
| BlogCatalog | 185153.29| 31707.87 | 79.42|

5) **Influence of Training Sample Ratio**

By the training sample ratio, we mean the percentages of total graph samples that are used for the training purpose. When the ratio is high, the classifier could be overfit. On the other hand, if the ratio is too low, the offered information may not be sufficient for the training purpose. Such analysis is classifier dependent, and we adopt a simple linear regression classifier from the python sklearn toolkit in the experiment. The node classification accuracy as a function of the training sample ratio for the Cora dataset is shown in Fig. 6. Most methods have consistent performance for the training data ratio between 0.2 and 0.8 except for the machine learning based methods (SDNE and GCN). Their accuracy drops when the training data ratio is low. They need a larger number of training data.

### VI. EMERGING APPLICATIONS

Graphs offer a powerful modeling tool and find a wide range of applications. Since many real-world data have certain relationship between entities, they can be conveniently modeled by graphs. Multi-modal data can also be embedded into the same space through graph representation learning and, as a result, the information from different domains can be represented and analyzed in one common setting.

In this section, we examine three emerging areas that benefit from graph embedding techniques.
• Community Detection
Graph embedding can be used to predict the label of a node given a fraction of labeled node [15, 26, 108], [113]. Thus, it has been widely used for community detection [27], [71]. In social networks, node labels might be gender, demography or religion. In language networks, documents might be labeled with categories or keywords. Missing labels can be inferred from labeled nodes and links in the network. Graph embedding can be used to extract node features automatically based on the network structure and predict the community that a node belongs to. Both vertex classification [40] and link prediction [20] [114] can facilitate community detection [33], [102].

• Recommendation System
Recommendation is an important function in social networks and advertising platforms [48], [106], [112]. Besides the structure, content and label data [54], some networks contain spatial and temporal information. For example, Yelp may recommend restaurants based on user’s location and preference. Spatial-temporal embedding [110] is an emerging topic in mobile applications.

• Graph Compression and Coarsening
By graph compression (graph simplification), we refer to a process of converting one graph to another, where the latter has a smaller number of edges. It aims to store a graph more efficiently and run graph analysis algorithms faster. For example, a graph is partitioned into bipartite cliques and replaced by trees to reduce the edge number in [50]. Along this line, one can also aggregate nodes or edges for faster processing with graph coarsening [64], where a graph is converted into smaller ones repeatedly using a hybrid matching technique to maintain its backbone structure. The Structural Equivalence Matching (SEM) method [45] and the Normalized Heavy Edge Matching method (NHEM) [52] are two examples.

VII. FUTURE RESEARCH DIRECTIONS
Several future research opportunities in graph embedding are discussed below.

• Deep Graph Embedding
GCN [50] has drawn a lot of attention due to its superior performance. However, the number of graph convolutional layers in typically not greater than two. When there are more graph convolutional layers in cascade, it is surprising that the performance drops significantly. It was argued in [63] that each GCN layer corresponds to graph Laplacian smoothing since node features are propagated in the spectral domain. When a GCN is deeper, the graph Laplacian is over-smoothed and the corresponding node features become obscure. Yet, each layer of GCN only learns one-hop information, and two GCN layers learn the first and second-order proximity in the graph. It is difficult for a shallow structure to learn the global information. The receptive field of each filter in GCN is global since graph convolution is conducted in the spectral domain. One solution to fix this problem is to conduct the convolution in the spatial domain. For example, one can convert graph data into grid-structure data as proposed in [35]. Then, the graph representation can be learned using multiple CNN layers. Another way to address the problem is to down-sample graphs and merge similar nodes together. Then, we can build a hierarchical network structure, which allows to learn both local and global graph data in a hierarchical manner. Such a graph coarsening idea was adopted by [34] [50], [107] to build deep GCNs.

• Semi-supervised Graph Embedding
Classical graph embedding methods such as PCA, DeepWalk and matrix factorization are unsupervised learning methods. They use topological structures and node attributes to generate graph representations. No labels are required in the training process. However, labels are useful since they provide more information about the graph. In most real world applications, labels are available in a subset of nodes, leading to a semi-supervised learning problem. The feasibility for semi-supervised learning on graphs was discussed in [103], [116]. A large number of graph embedding problems belong to the semi-supervised learning paradigm, and it deserves our attention.

• Dynamic Graph Embedding
Social graphs such as the twitter are constantly changing. Another example is graphs of mobile users whose location information is changing along with time. To learn the representation of dynamic graphs is an important research topic and it finds applications in real-time and interactive processes such as the optimal travel path planning in a city at traffic hours.

• Scalability of Graph Embedding
We expect to see graphs of a larger scale and higher diversity because of the rapid growth of social networks, which contain millions and billions of nodes and edges. It is still an open problem how to embed very large graph data efficiently and accurately.

• Interpretability of Graph Embedding
Most state-of-the-art graph embedding methods are built upon CNNs, which are trained with backpropagation (BP) to determine their model parameters. However, the training complexity is very high. Besides, CNNs are mathematically intractable. Research was done to lower the training complexity such as quickprop [28]. Furthermore, there is new work [58] that attempts to explain CNNs using an interpretable and feedforward (FF) design without any BP. The work in [58] adopts a data-centric approach to network parameters of the current layer based on data statistics from the output of the previous layer in a one-pass manner.

VIII. CONCLUSION
A comprehensive survey of the literature on graph representation learning techniques was conducted in this paper.
We examined various graph embedding techniques that convert the input graph data into a low-dimensional vector representation while preserving intrinsic graph properties. Besides classical graph embedding methods, we covered several new topics such as neural-network-based embedding methods, hypergraph embedding and attention graph embedding methods. Furthermore, we conducted an extensive performance evaluation of several state-of-the-art methods against small and large datasets. For experiments conducted in our evaluation, an open source Python library, called the Graph Representation Learning Library (GRLL), was provided to readers. Finally, we presented some emerging applications and future research directions.

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