Graph Embedding for Combinatorial Optimization: A Survey

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Abstract Graphs have been widely used to represent complex data in many applications, such as e-commerce, social networks, and bioinformatics. Efficient and effective analysis of graph data is important for graph-based applications. However, most graph analysis tasks are combinatorial optimization (CO) problems, which are NP-hard. Recent studies have focused a lot on the potential of using machine learning (ML) to solve graph-based CO problems. Using ML-based CO methods, a graph has to be represented in numerical vectors, which is known as graph embedding. In this survey, we provide a thorough overview of recent graph embedding methods that have been used to solve CO problems. Most graph embedding methods have two stages: graph preprocessing and ML model learning. This survey classifies graph embedding works from the perspective of graph preprocessing tasks and ML models. Furthermore, this survey summarizes recent graph-based CO methods that exploit graph embedding. In particular, graph embedding can be employed as part of classification techniques or can be combined with search methods to find solutions to CO problems. The survey ends with several remarks on future research directions.

Keywords Graph Processing · Graph Embedding · Graph Neural Network · Combinatorial Optimization

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1 Introduction

Graphs are ubiquitous and are used in a wide range of domains, from e-commerce [29], [23] to social networking [69], [36] to bioinformatics [77], [22]. Effectively and efficiently analyzing graph data is important for graph-based applications. However, many graph analysis tasks are combinatorial optimization (CO) problems, such as the traveling salesman problem (TSP) [67], maximum independent set (MIS) [18], maximum cut (MaxCut) [27], minimum vertex cover (MVC) [43], maximum clique (MC) [13], graph coloring (GC) [55], subgraph isomorphism (SI) [25], and graph similarity (GSim) [56]. These graph-based CO problems are NP-hard. In the existing literature on this subject, there are three main approaches used to solve a CO problem: exact algorithms, approximation algorithms, and heuristic algorithms. Given a CO problem on a graph $G$, exact algorithms aim to compute an optimal solution. Due to the NP-hardness of the problems, the worst-case time complexity of exact algorithms is exponential to the size of $G$. To reduce time complexity, approximation algorithms find a suboptimal solution, which has a guaranteed approximation ratio to the optimum, with a polynomial runtime. Nevertheless, many graph-based CO problems, such as General TSP [53], GC [37], and MC [31], are inapproximable with such a bounded ratio. Thus, heuristic algorithms are designed to efficiently find a suboptimal solution with desirable empirical performance. Despite having no theoretical guarantee of optimality, heuristic algorithms often produce good solutions in practice and are widely used for their efficiency.

The practice of applying machine learning (ML) to solve graph-based CO problems has a long history. For example, as far back as the 1980s, researchers were using the Hopfield neural network to solve TSP [33], [61]. Recently, the success of deep learning methods has led to an increasing attention being paid to this subject [6], [44], [18], [67]. Compared to manual algorithm designs, ML-based methods have several advantages in solving graph-based CO problems. First, ML-based methods can automatically identify distinct features from training data. In contrast, human algorithm designers need to study the heuristics with substantial problem-specific research based on trial-and-errors. Second, for a graph-based CO problem, ML has the potential to find useful features that it may be hard to specify using human algorithm designers, enabling it to develop a better solution [34]. Third, an ML-based method can adapt to a family of CO problems. For example, S2V-DQN [18] can support TSP, MVC, and MaxCut; GNNTS [43] can support MIS, MVC, and MC. In comparison, it is difficult for an algorithm that has been handcrafted specifically for one CO problem to be adapted so that it works with other CO problems. In this survey, we review recent studies that have used ML to solve graph-based CO problems.

In solving graph-based CO problems using ML-based methods, a graph has to be represented in numerical vectors, which is known as graph embedding [30]. Formally, given a graph $G$, graph embedding embeds $G$ and the nodes in $G$ to $d$-dimensional vectors, while preserving the structural properties of $G$. 
Existing graph embedding techniques can be classified into three categories: matrix factorization (MF)-based methods [73], graph neural network (GNN)-based methods [27, 29], and deep learning (DL)-based methods [68]. First, MF-based methods compute the embedding of $G$ by factorizing a proximity matrix of $G$. The proximity matrix is defined based on the important structural properties of $G$ to be preserved. Second, GNN-based methods use neural network models specially defined on graphs to embed $G$. Two widely used GNN models are i) generalized SkipGram, which is extended from the word embedding model SkipGram in natural language processing [41] and (ii) graph convolution, which is extended from the convolutional neural network (CNN) in computer vision [40]. Third, DL-based methods use the deep neural network (DNN) to extract features from graphs and regularize their objective function with the graph structural properties to be preserved. Since MF-based methods are seldom used to solve graph-based CO problems, this survey covers GNN-based and DL-based graph embedding methods only.

Most graph embedding studies follow a two-stage framework (e.g., [39, 29, 35, 57, 28, 76, 71, 15]), where the first stage is a preprocessing of the input graph and the second stage is model learning based on the preprocessing result. The preprocessing is crucial. For example, GNN-based methods sample the neighborhood for each node and construct positive and negative training samples in the preprocessing stage [29]; DL-based methods need to compute the node proximity in the preprocessing stage [11], which will be used in the objective function of model learning. Moreover, the preprocessing can dominate the overall time complexity of graph embedding. For example, for the well-known GCN model [39], if the GCN has $l$ layers, the preprocessing needs to find the $l$-hop neighbors for each node in the graph, which would be computationally prohibitive even for a small value of $l$ on large power-law graphs. However, existing surveys [30, 9, 14, 17, 78] mainly focus on the second stage and classify graph embedding studies on the basis of the ML model used. Classifying graph embedding studies from the perspective of the preprocessing tasks has not received the attention that it deserves. Therefore, besides considering the ML models used in graph embedding, this survey also takes into account the preprocessing tasks in order to classify graph embedding techniques.

There have been several previous surveys that have discussed ML-based CO methods [44, 6]. The present survey, however, has slightly different emphases from previous studies. [6] focuses on branch and bound (B&B) search techniques for the mixed-integer linear programming (MILP) problem. Although many graph-based CO problems can be formulated using MILP and solved using the B&B method, most existing ML-based methods for solving graph-based CO problems focus on graph-specific methods. [44] covers reinforcement learning (RL)-based CO methods. However, there are many ML-based CO methods that do not use RL. This survey is, therefore, not limited to RL approaches.

The rest of this survey is organized as follows. Section 2 presents the notations and preliminaries. Section 3 summarizes GNN-based and DL-based graph
embedding techniques. Section 4 discusses the use of ML to solve graph-based CO problems. Finally, Section 5 concludes this survey and suggests directions for potential future research efforts.

2 Notations and Preliminaries

In this section, we present some of the notations and definitions that are used frequently in this survey.

We denote a graph by $G = (V, E, X)$, where $V$ and $E$ are the node set and the edge set of $G$, respectively, $X$ is the matrix of initial features of all nodes, and $x_u = X[u, \cdot]$ denotes the initial features of node $u$. We may choose $u \in G$ or $u \in V$ to denote a node of the graph, when the choice is more intuitive. Similarly, we may use $(u, v) \in G$ or $(u, v) \in E$ to denote an edge of the graph. The adjacency matrix of $G$ is denoted by $A$. The weight of edge $(u, v)$ is denoted by $w_{u,v}$. We use $P$ to denote the transition matrix, where $P[u, v] = \sum_{v' \in G} w_{u,v'}$. $P^k = \prod_k P$ is the $k$-step transition matrix and $P$ is also called the 1-step transition matrix. We use $g$ to denote a subgraph of $G$ and $G \setminus g$ to denote the subgraph of $G$ after removing all nodes in $g$. For a node $u \in G$, we use $u \notin g$ to denote adding the node $u$ and the edges ${\{(u,v)|v \in g,(u,v) \in E\}}$ to $g$. $G$ can be a directed or undirected graph. If $G$ is directed, $(u,v)$ and $(v,u)$ may not present simultaneously in $E$. $N^o(u)$ and $N^i(u)$ denote the outgoing and incoming neighbors of $u$, respectively. If $G$ is undirected, $N(u)$ denotes the neighbors of $u$. For convention, we use a bold uppercase character to denote a matrix (e.g., $X$), a bold lowercase character to denote a vector (e.g., $x$), and a lowercase character to denote a scalar (e.g., $x$).

A graph-based CO problem has been formulated in Definition 1.

Definition 1 Given a graph $G$ and a cost function $c$ quantifying the subgraphs of $G$, a CO problem is to find the optimum value of $c$ and the corresponding subgraph that achieves that optimum value.

For example, for a graph $G$, the maximum clique (MC) problem is to find the largest clique of $G$, and the minimum vertex cover (MVC) problem is to find the minimum set of nodes that are adjacent to all edges in $G$.

2.1 Graph Embedding

This subsection presents the important terminologies and concepts of graph embedding. The embedding of $G$ is expected to preserve the structural properties of $G$. The structural properties are often quantified by the following proximities.

Definition 2 Given a graph $G = (V, E)$, the first-order proximity from $u$ to $v$ is the weight of $(u, v)$. If $(u, v) \in E$, $p^{(1)}(u, v) = w_{u,v}$; otherwise, $p^{(1)}(u, v) = 0$. 
The first-order proximity captures the direct relationship between nodes. The second-order proximity captures the similarity of the neighbors of two nodes.

**Definition 3** Given a graph $G$, the second-order proximity between $u$ and $v$ is $p^{(2)}(u, v) = sim(p^{(1)}(u), p^{(1)}(v))$, where $p^{(1)}(u)$ is the vector of the first-order proximity from $u$ to all other nodes in $G$, i.e., $p^{(1)}(u) = (p^{(1)}(u, v_1), p^{(1)}(u, v_2), ..., p^{(1)}(u, v_{|V|}))$, and $sim$ is a user-specified similarity function.

The first- and second-order proximities encode the local structures of a graph. Proximities to capture more global structures of a graph have also been proposed in the literature. For example, Cai et al. [9] propose to use $p^{(k)}(u, v)$ (recursively defined, similar to Definition 3) as the $k$-th-order proximity between $u$ and $v$, Cao et al. [10] use the $k$-step transition probability $P^k[u, v]$ to measure the $k$-step relationship from $u$ to $v$, Chen et al. [16] use the node centrality, Tsitsulin et al. [65] use the Personalized PageRank, and Ou et al. [52] use the Katz Index and Adamic-Adar to measure more global structural properties of $G$.

**Graph embedding** is to learn a mapping function $f$ that maps $G$ to $\mathbb{R}^d$, such that the proximities of $G$ are preserved. If $f$ embeds each node of $G$ into a $d$-dimensional vector, it is called node-level embedding. If $f$ embeds the entire $G$ into a $d$-dimensional vector, it is called graph-level embedding. We use $h_u$ and $h_G$ to denote the embedding vectors of node $u$ and graph $G$, respectively, and $H^{V \times d}$ to denote the matrix of the embeddings of all nodes.

### 2.2 Graph Embedding Models

In this subsection, we present the ML-based GNN models that are widely used to solve graph-based CO problems, including generalized SkipGram, graph spectral convolution, graph spatial convolution, and AutoEncoder.

#### 2.2.1 Generalized SkipGram

The generalized SkipGram model is extended from the well-known SkipGram model [46] for embedding words in natural language processing. The generalized SkipGram model relies on the neighborhood $\mathcal{N}_u$ of node $u$ to learn an embedding of $u$. The objective is to maximize the likelihood of the nodes in $\mathcal{N}_u$ conditioned on $u$.

$$\max P(v_1, v_2, ..., v_{|\mathcal{N}_u|}, v_i \in \mathcal{N}_u)$$

Assuming conditional independence, $P(v_1, v_2, ..., v_{|\mathcal{N}_u|}, u) = \prod_{v_i \in \mathcal{N}_u} P(v_i | h_u)$. $P(v_i | h_u)$ can be defined as $h_i^T h_u / \sum_{v \in \mathcal{N}_u} h_i^T h_u$. Maximizing $\prod_{v_i \in \mathcal{N}_u} P(v_i | h_u)$ is then equivalent to maximizing its logarithm. Hence, (1) becomes
max \sum_{v_i \in N_u} \log P(v_i | h_u) = \max \sum_{v_i \in N_u} \log \frac{h_v^T h_u}{\sum_{v \in G} h_v^T h_u} \tag{2}

Since computing the denominator of the softmax in (2) is time consuming, many optimization techniques have been proposed. Negative sampling [46] is one of the most well-known techniques. Specifically, the nodes in the neighborhood \(N_u\) of a node \(u\) are regarded as positive samples of \(u\). On the other hand, the nodes not in \(N_u\) are considered negative samples of \(u\). Then, maximizing the likelihood in Formula 2 can be achieved as follows:

\[ \max \log \sigma(h_v^T h_u) + \sum_{i=1}^{K} E_{\bar{v} \sim P_n} \log \sigma(-h_{\bar{v}}^T h_u), \tag{3}\]

where \(v\) is a positive sample of \(u\), \(\bar{v}\) is a negative sample, \(P_n\) is the probability distribution of negative samples, \(\bar{v} \sim P_n\) means sampling a node from the probability distribution \(P_n\), \(K\) is the number of negative samples, \(\sigma\) is the sigmoid activation function, and \(E\) is the expectation.

To conveniently adopt the gradient descent algorithms, maximizing an objective is often rewritten as minimizing its negative. Thus, the objective function of the generalized SkipGram model is to minimize the loss \(L\) as follows:

\[ \min L = \min -\log \sigma(h_v^T h_u) - \sum_{i=1}^{K} E_{\bar{v} \sim P_n} \log \sigma(-h_{\bar{v}}^T h_u) \tag{4}\]

Existing studies on the generalized SkipGram model define the neighborhood in different ways. For example, LINE [64] defines the 1-hop neighbors as the neighborhood in order to preserve the second-order proximity; DeepWalk [57] uses the random walk to define the neighborhood for preserving more global structural information of \(G\).

2.2.2 Graph Convolution

Graph convolution can be divided into two categories: i) spectral convolutions, defined using the spectra of a graph, which can be computed from the eigen-decomposition of the graph’s Laplacian matrix, and ii) spatial convolutions, directly defined on a graph by information propagation.

A) Graph Spectral Convolution

Given an undirected graph \(G\), \(L = I - D^{-1/2}AD^{-1/2}\) is the normalized Laplacian matrix of \(G\). \(L\) can be decomposed into \(L = U\Lambda U^T\), where \(U\) is the eigenvectors ordered by eigenvalues, \(\Lambda\) is the diagonal matrix of eigenvalues, and \(\Lambda[i, i]\) is the \(i\)-th eigenvalue \(\lambda_i\).

The graph convolution \(*_G\) of an input signal \(s \in \mathbb{R}^{|V|}\) with a filter \(g_\omega\) is defined as
\[ s \ast_G g_\theta = U g_\theta U^T s \] (5)

Existing studies on graph spectral convolution all follow Formula (5), and the differences are the choice of the filter \( g_\theta \) [70]. The \( u \)-th row of the output channel is the embedding \( h_u \) of a node \( u \).

### B) Graph Spatial Convolution

Graph spatial convolution aggregates the information from a node’s local neighborhood. Intuitively, each node sends messages based on its current embedding and updates its embedding based on the messages received from its local neighborhood. A graph spatial convolution model often stacks multiple layers, and each layer performs one iteration of message propagation. To illustrate this, we recall the definition given in GraphSAGE [29]. A layer of GraphSAGE is as follows:

\[ h^l_u = \sigma(W^l[h^{l-1}_u || h^{l}_{N_u}]) \] (6)

\[ h^{l}_{N_u} = AGG(\{h^{l-1}_v, v \in N_u\}), \] (7)

where \( l \) denotes the \( l \)-th layer, \( || \) denotes concatenation, \( N_u \) is a set of randomly selected neighbors of \( u \), and \( AGG \) denotes an order-invariant aggregation function. GraphSAGE suggests three aggregation functions: element-wise mean, LSTM-based aggregator, and max-pooling.

### 2.2.3 AutoEncoder

AutoEncoder is composed of an encoder and a decoder. For a graph-based CO problem, the encoder encodes the nodes in the graph into \( d \)-dimensional embedding vectors. The decoder then predicts a solution to the CO problem using the node embeddings (e.g., PointerNet [67]).

Formally, the encoder is a function

\[ enc : \mathbb{R}^d \to \mathbb{R}^d \]

\( enc(x_u) \) embeds node \( u \) into \( h_u \in \mathbb{R}^d \).

There are several different types of decoder. For instance, the inner product-based decoder, the reconstruction-based decoder, and the classification-based decoder are three widely-used decoders.

The inner product-based decoder is a function

\[ dec : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R} \]

\( dec(h_u, h_v) \) returns the similarity of \( h_u \) and \( h_v \). Let \( sim(u, v) \) denote the proximity of \( u \) and \( v \) in \( G \) (e.g., \( A[u,v] \) in [68]). The objective function of the inner product decoder is to minimize the loss

\[ L = \sum_{(u,v) \in D} dist(dec(h_u, h_v), sim(u, v)), \] (8)
where $D$ is the training dataset and $\text{dist}$ is a user-specified distance function.

The reconstruction-based decoder is a function

$$\text{dec} : \mathbb{R}^d \rightarrow \mathbb{R}^{d'}$$

$\text{dec}(h_u)$ outputs $x_u$ as the reconstruction of $x_u$. The objective function is to minimize the reconstruction loss

$$L = \sum_{u \in G} \|\text{dec}(h_u), x_u\|_2^2$$

The classification-based decoder is a function

$$\text{dec} : \mathbb{R}^d \rightarrow \mathbb{R}^{d'}$$

where $d'$ is the number of classes. $\text{dec}(h_u)$ outputs a vector $y_u$, where $y_u[i]$ is the probability that $u$ belongs to the $i$-th class. The objective function can be minimizing the cross-entropy between the prediction and the ground truth.

The encoder and the decoder can be implemented by different types of neural networks, e.g., the multi-layer perceptron (MLP) [68] or the recurrent neural network (RNN) [67].

2.3 Reinforcement Learning

When solving a graph-based CO problem, a widely used approach is to iteratively extend a partial solution. Each iteration can greedily select the “best” node and update the partial solution. Such a sequential decision process can be modeled as a Markov decision process (MDP) and solved by reinforcement learning (RL). Therefore, this subsection presents a brief review of RL.

In RL, an agent acts in an environment, collecting rewards and updating its policy to select future actions. It can be formulated as an MDP $(S, A, T, R, \gamma)$, where

- $S$ is the set of states, and some states in $S$ are end states;
- $A$ is the set of actions;
- $T : S \times A \times S \rightarrow [0, 1]$ is the transition function, $T(s, a, s')$ is the probability of transition to state $s'$ after taking action $a$ in state $s$;
- $R : S \times A \rightarrow \mathbb{R}$ is the reward of taking action $a$ in state $s$;
- $\gamma$ is a discount factor.

The agent uses a policy $\pi : S \rightarrow A$ to select an action for a state. RL is to learn an optimal policy $\pi^*$ that can return the optimal action for each state in terms of the overall reward. RL relies on the state-value function and the action-value function to optimize the policy. The state-value function $V^\pi(s)$ denotes the overall reward starting from the state $s$ following the policy $\pi$. The action-value function $Q^\pi(s, a)$ denotes the overall reward starting from the state $s$ and the action $a$ following the policy $\pi$. Formally,
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\[ V^\pi(s) = \mathbb{E}_\pi \left[ \sum_{t=0}^{T} \gamma^t R(s_t, a_t) | s_0 = s \right], \]

\[ Q^\pi(s, a) = \mathbb{E}_\pi \left[ \sum_{t=0}^{T} \gamma^k R(s_t, a_t) | s_0 = s, a_0 = a \right] \]

where \( \mathbb{E}_\pi \) denotes the expected value given that the agent follows the policy \( \pi \), \( t \) is the time step and \( T \) is the time step of reaching an ending state. The state-value function and the action-value function of the optimal policy \( \pi^* \) are denoted by \( V^* \) and \( Q^* \), respectively.

RL can learn \( \pi^* \) by iteratively optimizing the value functions, which is called as the value-based method. The value-based methods compute \( Q^* \) and output the optimal policy \( \pi^*(s) = \max_a Q^*(s, a) \). Q-learning is a well-known value-based RL method. Suppose \( Q \) is the current action-value function. At each state \( s_t \), Q-learning selects the action \( a_t \) by the \( \epsilon \)-greedy policy, which is selecting \( \max_a Q(s_t, a) \) with a probability \( 1 - \epsilon \) and selecting a random action with a probability \( \epsilon \), and updates \( Q \) as Formula 9.

\[ Q(s_t, a_t) = Q(s_t, a_t) + \alpha_t [R(s_t, a_t) + \gamma \max_a Q(s_{t+1}, a) - Q(s_t, a_t)], \quad (9) \]

where \( \alpha_t \) is the learning rate at the time step \( t \). Q-learning converges to \( Q^* \) with probability 1, if each state-action pair is performed infinitely often and \( \alpha_t \) satisfies \( \sum_{n=1}^{\infty} \alpha_t = \infty \) and \( \sum_{n=1}^{\infty} \alpha_t^2 < \infty \).

Q-learning needs a table, namely Q-table, to store the action values. The size of the Q-table is \( |S| \times |A| \), which can be too large to support the applications having a large number of states and actions. Therefore, many methods have been proposed to approximate the Q-table by parameterized functions. For example, deep Q-learning network (DQN) uses a deep neural network as the function approximation of the Q-table [47].

The value-based methods first optimize the value functions and then improve the policy based on the optimized value functions. There are also many methods that directly optimize the policy based on policy gradient. We refer the reader to [62] for more details of RL.

3 Graph Embedding Methods

In this section, we survey the graph embedding methods that have been applied to solve graph-based CO problems.

Most graph embedding methods have two stages. The first stage is preprocessing of the input graph, and the second stage is training a machine learning (ML) model. The following subsections summarize some representative graph embedding works from the perspective of the two stages. Specifically, the preprocessing tasks are node proximity computation, neighborhood expansion,
path or subgraph extraction, and graph coarsening. The ML models are the generalized SkipGram model, the graph convolution model, and AutoEncoder. A taxonomy of selected related papers is shown in Fig. 1.

3.1 Node Proximity Based Graph Embedding

The preprocessing of the graph embedding works in this category can be either directly computing the node proximity or computing a probability of neighborhood that can be used to measure the node proximity.

3.1.1 Generalized SkipGram Based Method

Zhou et al. \cite{80} propose an asymmetric proximity preserving method (APP) to preserve the rooted PageRank (RPR) in graph embedding using the generalized SkipGram model. Specifically, for each node \( u \) in \( G \), APP samples a set of random walks starting from \( u \). For a random walk, each step can go to a neighbor with a probability \( 1 - \alpha \) or stop with a probability \( \alpha \). The end nodes of the random walks are regarded as the neighborhood of \( u \). The objective function is to maximize the likelihood of the neighborhood stated in Formula \( 2 \). Zhou et al. theoretically prove that the graph embedding can preserve the RPR from \( u \) to other nodes.
3.1.2 Graph Convolution Based Method

Chen et al. [16] use node centrality as a high-order proximity, and propose a node-centrality based graph convolution framework (GraphCSC). GraphCSC is a framework and can support several different node centrality measures, such as Betweenness, PageRank, and Closeness.

The node-centrality based graph convolution is a spatial convolution, which is extended from the graph convolution of GraphSAGE, as shown in Formula 6. The extension is the determination of $\mathcal{N}_u$. GraphSAGE randomly selects $k$ neighbors of node $u$ as $\mathcal{N}_u$. However, GraphCSC selects $\mathcal{N}_u$ as the top-$k$ neighbors of $u$ ranked by the centrality scores. The exact centrality scores of all nodes need to be precomputed.

Besides the node-centrality based graph convolution, GraphCSC further enforces $h_u$, encoding the centrality information of $u$ by a ranking preserving loss. Specifically, GraphCSC uses an MLP $f$ to model the non-linear relationship between the node embedding and the centrality measure. Let $p(u|v)$ denote the probability that $u$ is ranked before $v$ w.r.t. a specific centrality measurement. $p(u|v)$ is computed from the node embeddings as follows.

$$p(u|v) = \sigma(f(h_u) - f(h_v)),$$

where $\sigma$ is the sigmoid function. The objective function of GraphCSC is to minimize the negative logarithm:

$$\mathcal{L} = - \sum_{(u,v) \in G} \log p(u|v)$$

As verified in experiments, GraphCSC can effectively preserve the centrality information in the node embedding.

3.1.3 AutoEncoder

Large-scale information network embedding (LINE) [64] preserves both the first- and second-order proximity in graph embedding using two AutoEncoders, respectively.

In order for AutoEncoder to preserve the first-order proximity, the encoder is a simple embedding lookup [12]. The decoder outputs the estimated adjacent matrix using the node embeddings, and the objective is to minimize the loss between the estimated adjacent matrix and the ground truth.

The decoder is designed as follows. Since adjacent nodes $u$ and $v$ in $G$ have high first-order proximity, they should be close in the embedding space. LINE uses the inner product of $h_u$ and $h_v$ to measure the distance between $u$ and $v$ in the embedding space, as shown below.

$$P_1(u, v) = \frac{1}{1 + exp(-h_u^T h_v)}$$ (10)
$P_1(\cdot, \cdot)$ defines the estimated distribution of the first-order proximity (i.e., the estimated adjacent matrix). LINE ensures that the estimated distribution $P_1(\cdot, \cdot)$ is close to the empirical distribution $\hat{P}_1(\cdot, \cdot)$ so as to preserve the first-order proximity.

$$\mathcal{L}_1 = \min \text{dist}(\hat{P}_1(\cdot, \cdot), P_1(\cdot, \cdot))$$ (11)

where $\hat{P}_1(u, v) = \frac{w_{u,u}}{\sum_{u',v' \in G} w_{u',v'}}$ and dist is the distance between two probability distributions. If the KL-divergence is used as dist, $\mathcal{L}_1$ becomes

$$\mathcal{L}_1 = \min - \sum_{(u,v) \in G} w_{u,v} \log P_1(u,v)$$ (12)

In order for AutoEncoder to preserve the second-order proximity, the encoder is also a simple embedding lookup [12]. The decoder outputs an estimated distribution between each node and its neighbors. The estimated distribution is reconstructed from the embeddings of the nodes. The objective is to minimize the reconstruction loss between the estimated distribution and the ground truth.

The decoder is designed as follows. Inspired by word embedding [41], the neighbors of $u$ are regarded as the “context” of $u$. LINE uses a conditional probability $P_2(v|u)$ defined in Formula 13 to model the estimated probability of $u$ generating a neighbor $v$.

$$P_2(v|u) = \frac{\exp(h'_v^T h_u)}{\sum_{v' \in G} \exp(h'_{v'}^T h_u)},$$ (13)

where $h'$ is the vector of a node when the node is regarded as context.

$P_2(\cdot|u)$ defines the estimated distribution of $u$ over the context. The nodes $u$ and $u'$ in $G$ that have high second-order proximity should have similar estimated distributions over the context, i.e., $P_2(\cdot|u)$ should be similar to $P_2(\cdot|u')$. This can be achieved by minimizing the distance between the estimated distribution $P_2(\cdot|u)$ and the empirical distribution $\hat{P}_2(\cdot|u)$, for each node $u$ in $G$. The empirical distribution $\hat{P}_2(\cdot|u)$ is defined as $\hat{P}_2(v|u) = \frac{w_{u,v}}{\sum_{u,v'} w_{u,v'}}$.

LINE preserves the second-order proximity as follows.

$$\mathcal{L}_2 = \min \sum_{u \in G} \text{dist}(\hat{P}_2(\cdot|u), P_2(\cdot|u)))$$ (14)

Using the KL-divergence for dist, Formula 14 will produce

$$\mathcal{L}_2 = \min - \sum_{(u,v) \in G} w_{u,v} \log P_2(v|u)$$ (15)

LINE trains the two AutoEncoders separately. The node embeddings generated by the two AutoEncoders are concatenated as the embeddings of the nodes. The model of LINE is also adopted by Tang et al. [63] to embed the words in a heterogeneous text graph.
Wang et al. [68] argue that LINE is a shallow model, in the sense that it cannot effectively capture the highly non-linear structure of a graph. Therefore, structural deep network embedding (SDNE) is proposed as a mean of using the deep neural network to embed the nodes. As with LINE, SDNE also preserves the first- and second-order proximity. Both the encoder and decoder of SDNE are MLPs. Given a graph $G$, the encoder embeds $x_u$ to $h_u$, where $x_u$ is the $u$-th row in the adjacent matrix $A$ of $G$, and the decoder reconstructs $\hat{x}_u$ from $h_u$.

SDNE preserves the first-order proximity by minimizing the distance in the embedded space for the adjacent nodes in $G$.

$$L_1 = \sum_{(u,v) \in G} A[u,v] \times ||h_u - h_v||_2^2$$

The second-order proximity is preserved by minimizing the reconstruction loss.

$$L_2 = \sum_{u \in G} ||\hat{x}_u - x_u||_2^2$$

SDNE combines $L_1$, $L_2$, and a regularizer term as the objective function and jointly optimizes them by means of a deep neural network. The first- and second-order proximity are preserved and the graph embedding learnt is more robust than LINE. As demonstrated in experiments, SDNE outperforms LINE in several downstream tasks (e.g., node classification and link prediction).

Versatile graph embedding method (VERSE) [65] shows that the first-and second-order proximity are not sufficient to capture the diverse forms of similarity relationships among nodes in a graph. Tsitsulin et al. [65] propose to use a function $\text{sim}(u,v)$ to measure the similarity between any two nodes $u$ and $v$ in $G$, where $\text{sim}(\cdot, \cdot)$ can be any similarity function. The similarity distribution of $u$ to all other nodes can be defined by $\text{sim}(u, \cdot)$. The encoder of VERSE is a simple embedding lookup. The decoder estimates the similarity distribution using the node embeddings, as in Formula 13. The objective is to minimize the reconstruction loss between the estimated similarity distribution and the ground truth.

Dave et al. [20] propose Neural-Brane to capture both node attribute information and graph structural information in the embedding of the graph. Bonner et al. [7] study the interpretability of graph embedding models.

3.2 Neighborhood Expansion Based Graph Embedding

Most works in this category are graph convolution based methods. The main idea is stacking $L$ graph convolution layers to aggregation structural information from the $L$-hop neighborhood. To train such a $L$-layer model, each node needs to expand its $L$-hop neighbors. Considering a node may have a large number of $L$-hop neighbors, especially in a dense graph or a powerlaw graph,
several sampling techniques are proposed. In these sampling methods, only a small number of sampled $L$-hop neighbors are required in graph convolution. The efficiency of graph convolution is significantly improved.

### 3.2.1 Graph Convolution Based Method

Graph convolutional network (GCN) \cite{8} is a well-known graph spectral convolution model, which is an approximation of the original graph spectral convolution defined in Formula \ref{eq:5}. Given a graph $G$ and a one-channel input signal $s \in \mathbb{R}^{V}$, GCN can output a $d$-channel signal $H^{V \times d}$ as follows:

$$H = s *_{G} g_{\theta} = (\tilde{D}^{-1/2} \tilde{A} \tilde{D}^{-1/2})s_{\theta}, \quad (16)$$

where $\theta$ is a $1 \times d$ trainable parameter vector of the filter, $\tilde{A} = A + I$ and $\tilde{D}$ is a diagonal matrix with $\tilde{D}[i,i] = \sum_j \tilde{A}[i,j]$. The $u$-th row of $H$ is the embedding of the node $u$, $h_{u}$. To allow a $d'$-channel input signal $S^{V \times d'}$ and output a $d$-channel signal $H^{V \times d}$, the filter needs to take a parameter matrix $\Theta^{d' \times d}$. Formula \ref{eq:16} becomes

$$H = S *_{G} g_{\Theta} = (\tilde{D}^{-1/2} \tilde{A} \tilde{D}^{-1/2})S_{\Theta}. \quad (17)$$

Let $s_i$ denote the $i$-th channel (i.e., column) of $S$, $h_u$ can be written in the following way.

$$h_{u} = \Theta^{T}y, y[i] = \sum_{v \in N_{u} \cup \{u\}} \frac{1}{\sqrt{|N_{u}| \sqrt{|N_{v}|}}} s_{i}[v], 1 \leq i \leq d', \quad (18)$$

where $y$ is a $d'$-dimensional column vector.

When multi-layer models are considered, Formulas \ref{eq:17} and \ref{eq:18} are written as Formulas \ref{eq:19} and \ref{eq:20} respectively, where $l$ denotes the $l$-th layer.

$$H^{l} = (\tilde{D}^{-1/2} \tilde{A} \tilde{D}^{-1/2})H^{l-1} \Theta^{l} \quad (19)$$

$$h_{u}^{l} = \Theta^{l^{T}}y^{l} \quad (20)$$

$$y^{l}[i] = \sum_{v \in N_{u} \cup \{u\}} \frac{1}{\sqrt{|N_{u}| \sqrt{|N_{v}|}}} H^{l-1}[v,i]$$

$$= \sum_{v \in N_{u} \cup \{u\}} \frac{1}{\sqrt{|N_{u}| \sqrt{|N_{v}|}}} h^{l-1}_{v}[i]$$

From Formula \ref{eq:20} we can observe that GCN aggregates weighted information from a node’s neighbors. In particular, for a node $u$ and a neighbor $v$ of $u$, the information from $v$ is weighted by their degrees, i.e., $1/\sqrt{|N_{u}| |N_{v}|}$. Graph attention network (GAT) \cite{66} argues that the fixed weight approach of GCN may not always be optimal. Therefore, GAT introduces the attention mechanism to graph convolution. A learnable weight function $\alpha(\cdot, \cdot)$ is proposed, where $\alpha(u,v)$ denotes the attention weight of $u$ over its neighbor $v$. Specifically, the convolution layer of GAT is as follows.
\[ h_u' = \sigma \left( \sum_{v \in N(u)} \alpha_l(u, v) W_l h_v^{l-1} \right) \]  \hspace{1cm} (21)

\[ \alpha_l(u, v) = \frac{\exp(\text{LeakyReLU}(a_1^T [W_l h_u^{l-1} \| W_l h_v^{l-1}] ))}{\sum_{v' \in N(u)} \exp(\text{LeakyReLU}(a_1^T [W_l h_u^{l-1} \| W_l h_{v'}^{l-1}] ))} \]  \hspace{1cm} (22)

where \( \| \) denotes concatenation, \( a_1 \) and \( W_l \) are the trainable vector and matrix of parameters, respectively.

The attention mechanism enhances models’ capacity, and hence, GAT can perform better than GCN in some downstream tasks (e.g., node classification). However, when \( L \) layers are stacked, the \( L \)-hop neighbors of a node are needed to be computed. If the graph \( G \) is dense or a power-law graph, there may exist some nodes that can access almost all nodes in \( G \), even for a small value of \( L \). The time cost can be unaffordable.

To optimize efficiency, Hamilton et al. [29] propose a sampling-based method (GraphSAGE). GraphSAGE randomly samples \( k \) neighbors in each layer. Therefore, a model having \( L \) layers only needs to expand \( O(k^L) \) neighbors. Huang et al. [35] further improve the sampling process with an adaptive sampling method. The adaptive sampling in [35] samples the neighbors based on the embedding of \( u \), as illustrated in Fig. 2(a). The efficiency is further improved by layer-wise sampling, as shown in Fig. 2(b). These sampling techniques are experimentally verified effective regarding the classification accuracy.

Yang et al. [74] combine the ideas of attention and sampling and propose the shortest path attention method (SPAGAN). The shortest path attention of SPAGAN has two levels, as shown in Fig. 3. The first level is length-specific, which embeds the shortest paths of the same length \( c \) to a vector \( h_u^c \). The second level aggregates \( h_u^c \) of different values of \( c \) to get the embedding \( h_u \) of \( u \).

More specifically, let \( P_u^c \) be the set of shortest paths starting from \( u \) of the length \( c \) and \( p_{u,v} \) be a shortest path from node \( u \) to node \( v \). \( h_u^c \) is computed as follows.

\[ h_u^c = \sum_{p_{u,v} \in P_u^c} \alpha_{u,v} \phi(p_{u,v}), \]

where \( \alpha_{u,v} \) is the attention weight and \( \phi(p_{u,v}) \) is a mean pooling that computes the average of the embeddings of the nodes in \( p_{u,v} \).

\[ \alpha_{u,v} = \frac{\exp(\sigma(a_1([W h_u] \| \phi(p_{u,v})]))}{\sum_{p_{u,v} \in P_u^c} \exp(\sigma(a_1([W h_u] \| \phi(p_{u,v})])))}, \]

where \( a_1 \) and \( W \) are trainable parameters shared by all nodes, and \( \| \) is concatenation. The second level aggregates the paths with different lengths as follows.
Fig. 2 Adaptive sampling of ASGCN [35]: (a) the node-wise sampling and (b) the layer-wise sampling. In the node-wise sampling, each node in a layer samples its neighbors in the next layer independently. In particular, a node $v$ in the $l+1$-th layer samples its neighbors in the $l$-th layer by $p(u_j|v)$. In contrast, all nodes in a layer jointly sample the neighbors in the next layer. $u_j$ is sampled based on $p(u_j|v_1, v_2, ..., v_4)$. The layer-wise sampling is more efficient than the node-wise sampling.

Fig. 3 The two-level convolution of SPAGAN [74]

$$h_u = \sigma \left( \sum_{c=2}^{C} \beta_c h_u^c \right),$$

where $C$ is a hyperparameter of the path length limit and $\beta_c$ is the attention weight.
\[ \beta_c = \frac{\exp(\sigma(a_2[(Wh_u)||h'_u]))}{\sum_{c'=2}^C \exp(\sigma(a_2[(Wh_u)||h''_{c'}]))} \]

where \( a_2 \) is a trainable parameter vector.

### 3.2.2 AutoEncoder Based Method

Kipf and Welling [38] propose variational graph AutoEncoder (VGAE) to preserve the first-order proximity. In a nutshell, let \( x_u \) denote the input feature of the node \( u \) in \( G \). The encoder of VGAE does not directly compute the embedding \( h_u \) of \( x_u \). Instead, VGAE assumes that \( h_u \) follows a Gaussian distribution and the encoder needs to predict the mean and standard deviation of the Gaussian distribution. Then, \( h_u \) is sampled from the Gaussian distribution.

Specifically, the encoder has two GCNs. The first GCN predicts the mean of the node embedding \( h_u \).

\[
GCN_{\text{mean}}(X, A) = (\tilde{D}^{-1/2}\tilde{A}\tilde{D}^{-1/2})[(\tilde{D}^{-1/2}\tilde{A}\tilde{D}^{-1/2})X\Theta_0]\Theta_1,
\]

where \( \Theta_0 \) and \( \Theta_1 \) are matrices of trainable parameters. The second GCN predicts the standard deviation of the node embedding \( h_u \).

\[
GCN_{\text{std}}(X, A) = (\tilde{D}^{-1/2}\tilde{A}\tilde{D}^{-1/2})[(\tilde{D}^{-1/2}\tilde{A}\tilde{D}^{-1/2})X\Theta_0]\Theta_2,
\]

where \( \Theta_0 \) and \( \Theta_2 \) are matrices of trainable parameters. Note that \( \Theta_0 \) is shared by \( GCN_{\text{mean}} \) and \( GCN_{\text{std}} \).

The decoder of VGAE is the inner product decoder \( \sigma(h_u^T h_v) \), where \( h_u \) and \( h_v \) are sampled from the Gaussian distribution and \( \sigma \) is the sigmoid activation function. The objective of VGAE is to minimize the loss from \( \sigma(h_u^T h_v) \) to \( A \) and a regularizer term on the predicted Gaussian distribution.

GAE [38] is a simplified version of VGAE, where the encoder just has one GCN and the objective function has no regularizer term on the predicted Gaussian distribution.

### 3.3 Path/Subgraph Based Graph Embedding

The preprocessing of the graph embedding works in this category are mainly either sampling a set of paths or computing a subgraph matching on the input graph.
3.3.1 Generalized SkipGram Based Method

This subsection reviews the path based graph embedding methods DeepWalk [57], Node2Vec [28], and Struc2Vec [59]; and the subgraph based graph embedding methods DeepGK [71], Subgraph2Vec [49], RUM [76], Motif2Vec [19], and MotifWalk [51].

DeepWalk [57] was one of the earliest works to introduce the generalized SkipGram model to graph embedding. The main idea of DeepWalk is to sample a set of truncated random walks of the graph $G$, and the nodes in a window of a random walk are regarded as co-occurrence. The neighborhood of a node is the nodes that co-occurred with it. DeepWalk uses the generalized SkipGram model with the negative sampling (refer to Formula 4) to learn the graph embedding.

To incorporate more flexibility into the definition of node neighborhood, Node2Vec [28] introduces breadth-first search (BFS) and depth-first search (DFS) in neighborhood sampling. The nodes found by BFS and DFS can capture different structural properties. Node2Vec uses the second-order random walk to simulate the BFS and DFS. (“second-order” means that when the random walk is at the step $i$, the random walk needs to look back to the step $i - 1$ to decide the step $i + 1$.) Two parameters $p$ and $q$ are introduced to control the random walk. $p$ controls the probability of return to an already visited node in the following two steps; and $q$ controls the probability of visiting a close or a far node in the following two steps. Let $u_i$ denote the current node in the walk and $u_{i-1}$ denote the previous node. The probability of the random walk to visit the next node $u_{i+1}$ is defined as below.

$$P(u_{i+1}|u_i) = \begin{cases} \alpha_{u_{i-1},u_{i+1}} \times w_{u_i,u_{i+1}} & \text{if } (u_i, u_{i+1}) \in G \\ 0 & \text{otherwise} \end{cases}$$  \hspace{1cm} (23)

$$\alpha_{u_{i-1},u_{i+1}} = \begin{cases} 1/p & \text{if } \text{dist}(u_{i-1}, u_{i+1}) = 0 \\ 1 & \text{if } \text{dist}(u_{i-1}, u_{i+1}) = 1 \\ 1/q & \text{if } \text{dist}(u_{i-1}, u_{i+1}) = 2 \end{cases}$$

where $\text{dist}(u_{i-1}, u_{i+1})$ is the shortest distance from $u_{i-1}$ to $u_{i+1}$ and $w_{u_i,u_{i+1}}$ is the weight of the edge $(u_i, u_{i+1})$. An example is shown in Fig. 4. The current node of the random walk is $u_i$. There are four nodes $u_{i-1}$, $v_1$, $v_2$ and $v_3$ that can be the next node of the random walk. The probability of selecting each of them as the next node is shown in Fig. 4.

Struc2Vec [59] argues that the random walks of Node2Vec cannot find nodes that have similar structures but are far away. Struc2Vec builds a multi-layer graph $G'$ for the input graph $G$. The layer $l$ is a complete graph $G'_l$, where each node in $G$ is a node in $G'_l$ and each edge $(u, v) \in G'_l$ is weighted by the structural similarity of the $l$-hop neighborhoods of $u$ and $v$ in $G$. In this way, two nodes that are far away in $G$ can reach each other by just one hop in $G'_l$. The nodes in $G'_l$ can have directed edges to the nodes in $G'_{l-1}$ and
Fig. 4 An example of selecting the next node by the second-order random walk of Node2Vec [28]. $u_i$ is the current node of the random walk and $u_{i-1}$ is the previous node. $u_{i-1}$, $v_1$, $v_2$, and $v_3$ can be selected as the next node with the corresponding probabilities, respectively.

$G'_{t+1}$. Random walks are sampled on $G'$, and the generalized SkipGram model is used to learn the node embedding.

Besides using paths to sample the neighborhood, many works use representative subgraphs of the input graph. The representative subgraphs may be termed motifs, graphlets or kernels in different studies. Yanardag and Vishwanathan [71] propose DeepGK, which is the earliest work embedding the motifs. The neighborhood of a motif $g$ is defined as the motifs within a small distance from $g$. The generalized SkipGram model is used to learn the embeddings for the motifs.

Yu et al. [76] propose a network representation learning method using motifs (RUM). RUM builds a motif graph $G'$ for the input graph $G$, where each node in $G'$ is a motif of $G$ and two nodes have an edge in $G'$ if the corresponding motifs share common nodes. Triangle is used as the graph motif in RUM. RUM uses random walks on the motif graph $G'$ to define the neighborhood of a motif. Then, the generalized SkipGram model is used to learn the embedding of the motif. An original node $u$ of $G$ may occur in multiple motifs of $G'$. RUM uses the average of the embeddings of the motifs as the embedding of $u$.

Dareddy et al. [19] propose another type of motif graph. Given a graph $G = (V,E)$, for each motif $g$, Motif2Vec builds a motif graph $G' = (V,E')$, where the weight of an edge $(u,v) \in E'$ is the number of motif instances of $g$ in $G$ that contain node $u$ and $v$. Then, Motif2Vec simulates a set of random walks on each motif graph and uses Node2Vec [28] to learn the embeddings
of the nodes in $G$. A similar idea is also proposed in the MotifWalk method of\,[51]. Narayanan et al.\,[49] propose Subgraph2Vec to compute the embeddings of the neighboring subgraphs of the nodes in the input graph. Let $g_u$ denote the neighboring subgraph of a node $u$, Subgraph2Vec computes $h_{g_u}$ using the generalized SkipGram model. The neighborhood of $g_u$ is defined as the neighboring subgraphs of the neighbors of $u$, i.e., \{$g_v | v \in N(u)$\}.

3.3.2 AutoEncoder Based Method

Meng and Zhang\,[45] propose an isomorphic neural network (IsoNN) for learning graph embedding. The encoder has three layers: a convolution layer, a min-pooling layer, and a softmax layer. The encoder is shown in Fig.\,5. The decoder is an MLP to predict the binary class of $G$, and the loss is the cross-entropy between the prediction and the ground truth.

Specifically, the encoder of IsoNN is designed as follows. Given a set of motifs, the convolution layer of the encoder extracts a set of isomorphism features from $G$ for each motif. Suppose $K_i$ is the adjacent matrix of the $i$-th motif that has $k$ nodes. The L2-norm between $K_i$ and a $k$ by $k$ submatrix $A_{x,y,k}$ of the adjacent matrix $A$ of $G$ is an isomorphism feature extracted by $K_i$, with respect to $A_{x,y,k}$, where $x$ and $y$ denote the top-left corner of the submatrix in $A$. IsoNN examines $k!$ permutations of $K_i$ and extracts $k!$ isomorphism features for $A_{x,y,k}$. The smallest one is regarded as the optimal isomorphism feature extracted by $K_i$ for $A_{x,y,k}$, which is computed by the min-pooling layer. Since the optimal isomorphism features for $A_{x,y,k}$ extracted by
different motifs can have different scales, the softmax layer is used to normalize them. Finally, the normalized isomorphism features extracted by all motifs for all values of $x$ and $y$ are concatenated as the embedding of $G$.

Motif-based attentional graph convolutional neural network model (MA-GCNN) [54] presents a 2-hop path motif matching based graph embedding method. The encoder is a deep convolutional neural network. The decoder is a self-attention layer that predicts the class label of $G$. The loss is the cross-entropy between the prediction and the ground truth. The input to the encoder is computed by the 2-hop path matching. Specifically, given a graph $G$, MA-GCNN firstly selects the top-$k$ nodes of the largest closeness centrality as $k$ central nodes (Fig. 6 Step1). Secondly, for each central node $c_i$, a neighboring subgraph $g_{c_i}$ is extracted (Fig. 6 Step2). Thirdly, matchings of the 2-hop path on $g_{c_i}$ are computed (Fig. 6 Step3). In Fig. 6 Step3, each node in $g_{c_i}$ is given a unique label for illustration purpose. The matching results are sorted by the distance from $c_i$ and stored in a matrix $M_{c_i}$ of several blocks. For a matching,
if the shortest distance between the matched node to the $c_i$ is $j$, the matching is inserted to the $j$-th block. For example, $a_2, a_4, a_6$ is a matching between the 2-hop path and $g_{c_1}$. Since its shortest distance from $c_1$ is 1, $a_2, a_4, a_6$ is inserted to the 1-st block. The matrices of the neighboring subgraphs of all the central nodes are concatenated as $M_G$ and input to the encoder.

In [72], Yang et al. propose NEST as a method for embedding a graph in different granularities, i.e., node-level, motif-level and graph-level embeddings. The encoder is an MLP, the decoder is a softmax layer, and the loss is cross-entropy. For the node embedding, given a graph $G = (V, E, X)$, NEST uses an MLP to learn the embedding $h_u$ from $x_u$ for each node $u$. For the motif embedding, given a motif $g$, NEST uses $\sigma(W||_{u \in g} h_u)$ as the embedding of $g$. The embeddings of all the motifs of $G$ are fed into an MLP to compute the embedding of $G$. A similar idea involves the use of heterogeneous graph embedding [26], where each meta-path can be regarded as a motif. In a heterogeneous graph, the nodes have types (e.g., Author type and Paper type in a scholar network). A metapath is an ordered sequence of node types (e.g., Author-Paper-Author in a scholar network).

3.4 Graph Coarsening Based Graph Embedding

There are many graph embedding works based on graph coarsening. In a nutshell, for the input graph $G = (V, E, X)$, we first cluster the nodes in $G$ to supernodes and obtain a coarsened graph. Then, we embed the coarsened graph using the methods presented in previous subsections. Finally, the embedding of $G$ can be derived from the embedding of the coarsened graph. The advantage of this method is that the number of pairwise relationships in the coarsened graph is much smaller than $G$, such that the training samples can have fewer variations. Therefore, the objective function can be smoother and easier to optimize [15].

Ying et al. propose a differentiable graph pooling method (DIFFPOOL) [75] to find $h_G$ using a hierarchy of coarsened graphs. In the hierarchy, each level is a graph coarsened from the graph of the previous level. The graph at the final level has only one node, and its embedding is used as $h_G$. The hierarchy is illustrated in Fig. 7.

Assume $G^l$ is the graph at the $l$-th level of the hierarchy. DIFFPOOL uses the embedding of $G^l$ to generate $G^{l+1}$. Let $n_l$ and $n_{l+1}$ denote the numbers of nodes in $G^l$ and $G^{l+1}$, respectively. $n_l$ and $n_{l+1}$ can be hyperparameters. DIFFPOOL stacks two GNNs and a pooling layer to generate $G^{l+1}$ from $G^l$, as illustrated in Fig. 8. Specifically, we provide some highlights of DIFFPOOL below.

- A GNN $GNN_{emb}$ is used to learn the embeddings of the nodes in $G^l$, denoted by $H^l$, from the adjacent matrix $A^l$ and the input feature matrix $X^l$ of $G^l$. $X^0 = X$ and $A^0 = A$. 

Fig. 7 Graph embedding using the hierarchy of coarsened graphs

Fig. 8 The GNNs and pooling layer for the t-th level of the hierarchy

- The other GNN $GNN_{cluster}$ is used to learn the cluster assignment matrix $M^t \in \mathbb{R}^{n_t \times n_{t+1}}$, where each row corresponds to a node in $G^t$ and each column corresponds to a node in $G^{t+1}$.
- The pooling layer generates the input feature matrix $X^{t+1}$ and the adjacent matrix $A^{t+1}$ for $G^{t+1}$. 
Chen et al. propose a hierarchical representation learning method (HARP) \[15\] to build a hierarchy of coarsened graphs. The hierarchy of HARP is constructed by heuristics: edge compression and star compression. As shown in Fig. 9(a), the edge compression means that if two edges are not incident to the same node, the end nodes of the two edges can be merged to two supernodes, respectively. Considering that the peripheral nodes of a star have the same neighborhood, the star compression is to merge two peripheral nodes of a star to a supernode as shown in Fig. 9(b). The number of nodes can be approximately reduced by 1/2 using the edge and star compression. In this way, a hierarchy of \(\log_2 |V|\) levels can be constructed from the input graph \(G\).

![Fig. 9 Edge compression and star compression of HARP](image)

HARP computes the embedding of \(G\) in the top-down manner. Let \(G^l\) denote the coarsened graph at the \(l\)-th level of the hierarchy and \(G^0 = G\). Suppose the embedding of \(G^l\) has been computed. If \(v^{l-1} \in G^{l-1}\) maps to \(u^l \in G^l\), \(v^{l-1}\) uses \(h_{ul}\) as the input feature to the GNN at the \(l-1\)-th level. The GNN at the \(l-1\)-th level generates the node embeddings for \(G^{l-1}\). Finally, we can obtain the node embeddings of \(G\).

Akbas and Aktas \[2\] propose the method NECL, different from the edge and star compression of HARP, that coarsens the graph based on neighborhood similarity. Nodes that have a similar neighborhood are merged to a supernode. The neighborhood similarity between two nodes is defined as \(sim(u, v) = \frac{2|N_u \cap N_v|}{|N_u| + |N_v|}\). The random walk based graph embedding method (e.g., DeepWalk) is used on the coarsened graph to find the embedding of the supernodes. The embedding of a supernode is given to the original nodes within the supernode.
Table 1 Summary of selected CO methods using graph embedding

| Method            | CO Problem | Model                      |
|-------------------|------------|----------------------------|
| Ptr-Net [67]      | TSP        | AutoEncoder + Classification|
| DTSPGNN [38]      | TSP        | GNN + Classification       |
| GPNNGNN [60]      | MDS, MM, MVC | GNN + Classification      |
| GAP [66]          | Graph Partition | GNN + Classification |
| GNN [42]          | GED        | GNN + Classification       |
| SimGNN [3]        | GED        | GNN + Classification       |
| GRAPHStudent [7]  | GED        | GNN + Classification       |
| GNNNTS [43]       | MIS, MVC, MC | GNN + Searching   |
| S2V-DQN [18]      | MVC, MaxCut, TSP | GNN + Searching |
| CombOptZero [1]   | MVC, MaxCut, MC | GNN + Searching |
| RLMCS [7]         | MCS        | GNN + Searching            |

Fahrbach et al. [23] propose coarsening the graph using the Gaussian elimination method. It has been proved that the coarsened graph can preserve the random walk transition probabilities of the original graph. Fahrbach et al. prove that the graph embedding found on the coarsened graph is equivalent to the embedding found on the original graph, but that the latter works with greater efficiency.

Graph coarsening is also employed in spectral convolution works for graph embedding. For example, for the merging of the nodes of the input graph, Defferrard et al. [21] and Monti et al. [48] adopt the Graclus clustering algorithm; agglomerative clustering is used by Bruna et al. [8]; and multi-resolution spectral clustering is used by Henaff et al. [32].

4 Combinatorial Optimization Methods

In this section, we review the works that solve CO problems using graph embedding. These works can be classified into two categories. The first category is based on classification techniques. The embeddings of the nodes are used to predict the probability of belonging to a solution. The second category is based on searching, which constructs a solution by iteratively extending a partial solution to a final solution. Graph embedding is used within a searching procedure to select the node to extend the partial solution. Table 1 lists the selected CO methods using graph embedding.

4.1 CO Methods Based on Classification Techniques

Most works in this category use classification techniques to predict the class label of the nodes in the input graph. For a graph $G$, the prediction result is a $|V| \times K$ matrix $Y$, where $K$ is the number of classes. The $u$-th row $y_u$ of $Y$ is the prediction result for the node $u$, where $y_u[i]$ is the probability that $u$ is of the $i$-th class, for $1 \leq i \leq K$. For example, for the minimum vertex cover (MVC) problem, the classification is binary (i.e., $K = 2$), and $\{u|y_u[1] > y_u[0]\}$ is the predicted solution. For the graph partition problem, $K$ is the number of parts, and a node $u$ is classified to the part with the largest
predicted probability. There are some works that predict a score for the input graphs. For example, for the graph similarity problem, the similarity score between two graphs is predicted.

A. Travelling Salesman Problem

The pointer network (Ptr-Net) proposed by Vinyals et al. [67] is a seminal work in this category. It uses an RNN-based AutoEncoder to solve the travelling salesman problem (TSP) on a Euclidian graph. The encoder of Ptr-Net is an RNN taking the nodes of the graph \( G \) as input and outputting an embedding of \( G \), where the order of the nodes is randomly chosen. The decoder of Ptr-Net is also an RNN. In each time step, the decoder computes an attention over the input nodes, and selects the input node that has the largest attention weight as output.

Specifically, given a graph \( G \), suppose the nodes of \( G \) are sequentially input as \( v_1, v_2, ..., v_{|V|} \) to the encoder, and the decoder sequentially outputs \( v_{j_1}, v_{j_2}, ..., v_{j_{|V|}} \). Let \( a_1, a_2, ..., a_{|V|} \) and \( b_1, b_2, ..., b_{|V|} \) denote the sequences of the hidden states of the encoder and the decoder, respectively. For the \( k \)-th time step of the decoder, the decoder selects one node in \( v_1, v_2, ..., v_{|V|} \) as \( v_{j_k} \) by an attention weight vector \( \alpha^k \) over \( a_1, a_2, ..., a_{|V|} \). \( \alpha^k \) is defined as:

\[
\alpha^k[j] = c^T[tanh(W_1a_j + W_2b_k)], 1 \leq j \leq |V|
\]

where \( c, W_1, \) and \( W_2 \) are trainable parameters. Then, the decoder outputs \( v_{j_k} = v_i \), where \( i = \text{argmax} \alpha^k \).

For example, Fig. 10(a) shows a Euclidean graph \( G \) with four nodes and a solution \( v_1, v_3, v_2, v_4 \). Fig. 10(b) shows the procedure of Ptr-Net for computing the solution. The hollow arrow marks the node that has the largest attention weight at each time step of the decoder.

Prates et al. [58] use GNN to solve the decision version of TSP, which is to decide if a given graph admits a Hamiltonian route with a cost no greater than a given threshold \( C \). Since the weights of edges are closely related to the cost of a route, Prates et al. compute edge embedding in the graph convolution. Specifically, given a graph \( G = (V, E) \), an auxiliary bipartite graph \( G' = (V' \cup V', E') \) is constructed, where for each edge \((u, v) \) in \( G \), \( G' \) has a node \( n_{u,v} \) in \( V' \) and edges \((n_{u,v}, u) \) and \((n_{u,v}, v) \) are added to \( E' \). The embeddings of the nodes and edges of \( G' \) can be computed by a GNN on the auxiliary graph \( G' \). Finally, the embeddings of the edges of \( G \) are fed into an MLP to make a binary classification. If the class label of \( G \) is predicted to be 1, \( G \) has a Hamiltonian route with a cost no greater than \( C \); otherwise, \( G \) has no such route.

B. Graph Partition

Nazi et al. [50] propose GAP as a method for computing a balanced partition of a graph. GAP is composed of a graph embedding module, which uses a GNN model to determine the embedding of the input graph, and a graph
partition module, which uses an MLP to predict the partition of nodes. The architecture of GAP is illustrated in Fig. 11. The normalized cut size and the balancedness of the partition is used as the loss. GAP trained on a small graph can be generalized at inference time on unseen graphs of larger size.

Specifically, suppose $G = (V, E, X)$ is to be partitioned to $K$ disjoint parts and $V_1, V_2, \ldots, V_K$ denote the sets of nodes in the parts, respectively. A GNN first computes the embeddings of the nodes in $G$. Then, the MLP uses the node embeddings to predict the partition probability $Y$ for the nodes, where $Y[u, i]$ is the probability that node $u$ is partitioned to $V_i$. Finally, each node can be partitioned to the partition of the largest probability.

The loss of GAP has two components. The first component is to minimize the normalized cut size of the partition:

$$\sum_{i=1}^{K} \frac{\text{cut}(V_i, \bar{V}_i)}{\text{vol}(V_i)},$$

where $\bar{V}_i$ denotes the nodes not in $V_i$, $\text{cut}(V_i, \bar{V}_i)$ denotes the number of edges crossing $V_i$ and $\bar{V}_i$, and $\text{vol}(V_i)$ denotes the total degree of the nodes in $V_i$. The second component is to minimize the distance from the balanced partition:

$$\sum_{i=1}^{K} \sum_{u \in G} (Y[u, i] - \frac{|V|}{K})^2,$$
where $\frac{|V_i|}{K}$ is the part size of the balanced partition. The objective function of GAP is as follows.

$$\min \sum_{i=1}^{K} \frac{\text{cut}(V_i, \bar{V}_i)}{\text{vol}(V_i)} + \sum_{i=1}^{K} \sum_{u \in G} (Y[u, i] - \frac{|V|}{K})^2$$

C. Graph Similarity

Bai et al. [3] propose SimGNN as a method for predicting the similarity between two graphs. SimGNN combines two strategies for predicting the similarity between two graphs $G_1$ and $G_2$. The first strategy compares $G_1$ and $G_2$ by comparing their global summaries $h_{G_1}$ and $h_{G_2}$. The second strategy uses the pair-wise node comparison to provide a fine-grained information as a supplement to the global summaries $h_{G_1}$ and $h_{G_2}$. The architecture of SimGNN is shown in Fig. 12.

As shown in Fig. 12, SimGNN first computes the node embeddings of the two input graphs $G_1$ and $G_2$ using GCN. For the first strategy, SimGNN computes $h_{G_1}$ and $h_{G_2}$ from the node embeddings by means of an attention mechanism that can adaptively emphasize the important nodes with respect to a specific similarity metric. Then, $h_{G_1}$ and $h_{G_2}$ are input to a neural tensor network (NTN) to compute a similarity score vector for $G_1$ and $G_2$.
The attention mechanism to compute $h_G$ is defined as follows. For a graph $G$, SimGNN introduces a context vector $c = \text{tanh}(W \sum_{u \in G} h_u)$ to encode the global information of $G$. $c$ is adaptive to the given similarity metric via $W$. Intuitively, nodes that are close to the global context should receive more attention. Therefore, the attention weight $\alpha_u$ of a node $u$ is defined based on the inner product of $c$ and $h_u$, $\alpha_u = \sigma(c^T h_u)$, where $\sigma$ is the sigmoid function. The embedding of $G$, $h_G$, is computed as $h_G = \sum_{u \in G} \alpha_u h_u$.

For the second strategy, SimGNN constructs a pair-wise node similarity matrix $M$ by computing the inner product of $h_u$ and $h_v$ for each $u \in G_1, v \in G_2$. SimGNN uses a histogram of $M$ to summarize the pair-wise node similarity.

Finally, the similarity score vector outputed by NTN and the histogram are input to a fully connected neural network to predict the similarity between $G_1$ and $G_2$. The mean squared error between the predicted similarity with the ground truth is used as the loss of SimGNN. In the follow-up work GRAPHSIM [4], a CNN-based method is used to replace the histogram of SimGNN.

Li et al. [42] propose the graph matching network (GMN) to solve the graph similarity problem. Instead of embedding each graph independently, GMN embeds two graphs $G_1$ and $G_2$ jointly by examining the matching between

![Diagram](image-url)
they. The matching used in GMN is soft matching, which means that a node of \( G_1 \) can match to all nodes of \( G_2 \) yet with different strengths. The embedding of \( G_1 \) can change based on the other graph it is compared against. At inference time, GMN can predict if the distance between two graphs is smaller than a given threshold \( \gamma \).

Given two graphs \( G_1 = (V(G_1), E(G_1)) \) and \( G_2 = (V(G_2), E(G_2)) \), the \( l \)-th convolution layer of GMN is defined as below.

\[
\begin{align*}
\mathbf{m}_{j \rightarrow i} &= \text{MLP}(h_i^l, h_j^l), \forall (i, j) \in E(G_1) \\
\mathbf{m}_{j' \rightarrow i'} &= \text{MLP}(h_{i'}^l, h_{j'}^l), \forall (i', j') \in E(G_2) \\
\mathbf{\mu}_{j \rightarrow i} &= f_{\text{match}}(h_i^l, h_j^l), \forall i \in V(G_1), j \in V(G_2) \\
\mu_{i \rightarrow j'} &= f_{\text{match}}(h_i^l, h_{j'}^l), \forall i \in V(G_1), j' \in V(G_2) \\
\mathbf{h}_i^{l+1} &= \text{MLP}(h_i^l, \sum_{j \in G_1} \mathbf{m}_{j \rightarrow i}, \sum_{j' \in G_2} \mu_{j' \rightarrow i}) \\
\mathbf{h}_{j'}^{l+1} &= \text{MLP}(h_{j'}^l, \sum_{i' \in G_2} \mathbf{m}_{i' \rightarrow j'}, \sum_{i \in G_1} \mu_{i \rightarrow j'}),
\end{align*}
\]

where \( \mathbf{m} \) denotes the message aggregation for a node from its neighbors in the same graph, \( \mu \) is the cross-graph matching vector that measures the difference between a node in a graph and all the nodes in the other graph, and \( f_{\text{match}} \) can be defined by the following attention based method.

\[
\begin{align*}
\mathbf{\mu}_{j' \rightarrow i} &= \alpha_{j' \rightarrow i}(h_i^l - h_{j'}^l), \forall i \in V(G_1), j' \in V(G_2) \\
\alpha_{j' \rightarrow i} &= \frac{\exp(\text{dist}(h_i^l, h_{j'}^l))}{\sum_{j' \in G_2} \exp(\text{dist}(h_i^l, h_{j'}^l))} \\
\mathbf{\mu}_{i \rightarrow j'} &= \alpha_{i \rightarrow j'}(h_i^l - h_{j'}^l), \forall i \in V(G_1), j' \in V(G_2) \\
\alpha_{i \rightarrow j'} &= \frac{\exp(\text{dist}(h_i^l, h_{j'}^l))}{\sum_{i' \in G_1} \exp(\text{dist}(h_i^l, h_{j'}^l))},
\end{align*}
\]

where \( \text{dist} \) is the Euclidean distance.

Suppose GMN stacks \( L \) layers. The embedding of a graph \( G \) is computed as below.

\[
\mathbf{h}_G = \text{MLP}((\mathbf{h}_i^L)_{i \in G}),
\]

where \( \mathbf{h}_i^L \) is the embedding of node \( i \) output by the last convolution layer.

The objective function of GMN is to minimize the margin-based pairwise loss \( \mathcal{L} = \max\{0, \gamma - t \times (1 - \text{dist}(G_1, G_2))\} \), where \( \gamma > 0 \) is the given margin threshold, \( \text{dist}(G_1, G_2) = ||h_{G_1} - h_{G_2}||_2 \) is the Euclidean distance, and \( t \) is the ground truth of the similarity relationship between \( G_1 \) and \( G_2 \), i.e., if \( G_1 \) and \( G_2 \) are similar, \( t = 1 \); otherwise, \( t = -1 \).

**D. Minimum Vertex Cover**

Sato et al. [60], from a theoretical perspective, study the power of GNNs in learning approximation algorithms for the minimum vertex cover (MVC) problem. They prove that no existing GNN can compute a \((2 - \epsilon)\)-approximation
for MVC, where \( \epsilon > 0 \) is any real number and \( \Delta \) is the maximum node degree. Moreover, Sato et al. propose a more powerful consistent port numbering GNN (CPNGNN), which can return a 2-approximation for MVC. The authors theoretically prove that there exists a set of parameters of CPNGNN that can be used to find an optimal solution for MVC. However, the authors do not propose a method for finding this set of parameters.

CPNGNN is designed based on graph port numbering. Given a graph \( G \), the ports of a node \( u \) are pairs \((u, i)\), \( 1 \leq i \leq |N_u| \), where \( i \) is the port number. A port numbering is a function \( p \) such that for any edge \((u_1, u_2)\) \( \in G \), there exists a port \((u_1, i)\) of \( u_1 \) and a port \((u_2, j)\) of \( u_2 \) satisfying \( p(u_1, i) = (u_2, j) \).

Intuitively, \( u_1 \) can send messages from the \( i \)th port of \( u_1 \) to the \( j \)th port of \( u_2 \).

An example of port numbering is shown in Fig. 13.

CPNGNN stacks \( L \) convolution layers, and the \( l \)-th layer is defined as follows.

\[
h_u^l = \text{ReLU}(W_l[h_u^{l-1}||x_u^{l-1}||x_u^{l-1}||\ldots||x_u^{l-1}])
\]

where \( W_l \) is the trainable parameter matrix and \( || \) is concatenation.

Let \( h_u^L \) denote the embedding of \( u \) outputed by the last layer of CPNGNN. An MLP takes \( h_u^L \) as input and outputs the prediction \( y_u \) for \( u \), where \( y_u[1] \) and \( y_u[0] \) are the probabilities that \( u \) is in an MVC or not, respectively. Then, the nodes \( \{u|y_u[1] > y_u[0]\} \) are output as an MVC of \( G \). The approximation ratio of CPNGNN is 2 for MVC. CPNGNN can also solve the minimum dominating set (MDS) problem and the maximum matching (MM) problem with approximation ratio \( \frac{\Delta + 1}{2} \).
4.2 CO Methods Based on Search Techniques

To find the node to extend a partial solution, graph embedding is combined with a search method. The search methods can be conducted using heuristic-based or reinforcement learning (RL)-based methods. These methods have been shown to be capable of finding better solutions than existing heuristic algorithms.

A. Heuristic Search

Li et al. [43] propose a GNNTS model that combines GNN and heuristic search to compute the maximum independent set (MIS) of a graph. GNNTS trains a GCN $f$ using a set of training graphs, where the MISs of a graph can be used as the ground truth labels of the graph. For a graph $G = (V,E)$, the prediction result of $f$ is a $|V| \times 2$ matrix $Y$, where $Y[:, 1]$ and $Y[:, 0]$ are the probabilities of the nodes being in or not in an MIS of $G$, respectively.

The basic idea of GNNTS is to use $f$ as the heuristic function within a greedy search procedure. Specifically, in each iteration, the nodes of $G$ are sorted by $Y[:, 1]$. The greedy algorithm picks the node $u$ with the largest value in $Y[:, 1]$, marks $u$ as 1, and adds $u$ to a partial solution $U$. All neighbors of $u$ are marked as 0. $u$ and its neighbors are removed from $G$, and the remaining graph is input to $f$ for the next iteration. Once all nodes in $G$ are marked, $U$ is returned as the MIS of $G$.

The basic method described above has the disadvantage that it cannot support the case in which $G$ has multiple solutions. For the example shown in Fig. 14 the square graph of four nodes has two MISs and the basic method predicts that each node has a probability 0.5 of belonging to an MIS, which is not useful.

To address this disadvantage, the GNN $f$ is extended to output multiple prediction results, i.e., $f(G) = \{f^1(G), f^2(G), ..., f^m(G)\}$, where $f^i(G)$ is a $|V| \times 2$ matrix $Y^i$, $1 \leq i \leq m$, and $m$ is a hyperparameter. Then, the GNN
if is used in a tree search procedure. Specifically, GNNTS maintains a tree of partial solutions, where each leaf is a partial solution to be extended. At each step, GNNTS randomly picks a leaf \( n_{leaf} \) from the search tree and uses \( f \) to output \( m \) prediction results \( Y^1, Y^2, \ldots, Y^m \). Then, for each \( Y^i \), GNNTS uses the basic method to compute an extension of \( n_{leaf} \). The \( m \) newly obtained partial solutions are inserted to the search tree as the children of \( n_{leaf} \). If a leaf of the search tree cannot be extended anymore, the leaf is a maximal independent set. The largest of the computed maximal independent sets is output. GNNTS can also solve the minimum vertex cover (MVC) and maximal clique (MC) problems by reducing to MIS.

**B. RL-Based Searching**

Since extending a partial solution iteratively is inherently a sequential decision process, several works use reinforcement learning (RL) to extend the partial solution. The partial solution and the input graph together determine the state of RL, whereas the node that can be added to the partial solution is the action. RL can learn an optimal policy to find the optimal node for a partial solution.

Dai et al. propose S2V-DQN \[18\] that combines GNN and deep Q-learning to tackle the MVC problem. Given a graph \( G \), let \( U \) denote the current partial solution and \( \bar{U} = V \setminus U \). The RL task for MVC can be formulated as follows.

- A state \( s \) is determined by \( G \) and \( U \), \( s = f_{state}(G, U) \). If \( U \) is a vertex cover of \( G \), the state is an end state;
- An action \( a_v \) is adding a node \( v \in \bar{U} \) to \( U \);
- The transition \( T(f_{state}(G, U), a_v) = f_{state}(G, U \cup \{v\}) \); and
- The reward of an action \( R(s, a_v) = -1 \), as we wish to minimize the vertex cover.

The representation of state \( s \) can be computed by embedding \( G \) and \( U \) using a GNN as follows.

\[
f_{state}(G, U) = \sum_v h_u^L \tag{27}
\]

\[
h_u^l = ReLU(\theta_1 x_u + \theta_2 \sum_{v \in N_u} h_v^{l-1} + \theta_3 \sum_{v \in N_u} ReLU(\theta_7 w_{u,v})),
\]

where \( L \) is the total number of layers of the GNN, \( x_u = 1 \) if \( u \in U \) and otherwise, \( x_u = 0 \), \( w_{u,v} \) is the weight of the edge \((u,v)\), and \( \theta_1, \theta_2, \) and \( \theta_3 \) are trainable parameters.

We can use the embedding of \( v, h_v \) to represent the action \( a_v \). The representations of the state \( s \) and the action \( a_v \) are fed into an MLP to compute \( Q(s, a_v) \) as below.

\[
Q(s, a_v) = \theta_4 ReLU(\text{Concat}(\theta_5 \sum_{u \in V} h_u^L, \theta_6 h_v^L)), \tag{28}
\]

where \( \theta_4, \theta_5, \) and \( \theta_6 \) are trainable parameters.
Then, deep Q-learning is used to optimize the parameters. After the MLP and the GNN are trained, they can be generalized to compute MVC for unseen graphs. S2V-DQN can also solve the MaxCut and TSP problems.

Bai et al. [5] propose to compute the maximum common subgraph (MCS) of two graphs using GNN and Q-learning. Given two graphs $G_1$ and $G_2$, the partial solution is a subgraph $g_1$ of $G_1$ and a subgraph $g_2$ of $G_2$ satisfying $g_1$ and $g_2$ are isomorphic. The RL task for MCS is formulated as follows.

- A state $s$ is determined by $G_1$, $G_2$, $g_1$, and $g_2$, $s = f_{state}(G_1, G_2, g_1, g_2)$. If $g_1$ and $g_2$ cannot be extended, the state is an end state;
- A action $a_{u,v}$ is to select a node $u$ from $G_1 \setminus g_1$ and a node $v$ from $G_2 \setminus g_2$ and add them to $g_1$ and $g_2$, respectively;
- The transaction $T(f_{state}(G_1, G_2, g_1, g_2), a_{u,v}) = f_{state}(G_1, G_2, g_1 \cup \{u\}, g_2 \cup \{v\})$. The isomorphism between $g_1 \cup \{u\}$ and $g_2 \cup \{v\}$ needs to be assured; and
- The reward $R(s, a_{u,v}) = 1$.

The representation of the state $s$ can be computed by a GNN on an auxiliary graph $G'$. $G'$ is constructed by adding a pseudo node $n_s$ connecting to the nodes in $g_1$ and the nodes in $g_2$. Then, a GNN is used to compute the node embeddings for $G'$. Note that the node embeddings change with the extension of the partial solution $g_1$ and $g_2$. $h_{G_1}$ and $h_{G_2}$ can be computed by the summation of the embeddings of the nodes in $G_1$ and $G_2$, respectively. The concatenation of $h_{n_s}$, $h_{G_1}$, and $h_{G_2}$ is the representation of the state $s$. 

Fig. 15 Overview of RLMCS
The action $a_{u,v}$ is represented by the concatenation of $h_u$ and $h_v$. The representations of the states and the actions are fed into an MLP to predict $Q$. Fig. 15(a)-(b) show an example.

Rather than just selecting one node with the largest Q-value as in [18], Bai et al. [5] propose to select $k$ nodes utilizing the Beam search. At each time step, the agent of RL is allowed to transit to at most $k$ best next states. The Beam search actually builds an exploration tree, where each node of the tree is a state and each edge of the tree is an action. Fig. 15(c) shows an example of $k = 3$. If a partial solution cannot be extended, a maximal independent set is computed. The largest of the computed maximal independent sets is output.

Inspired by AlphaGo Zero, which has surpassed human in the game Go, Abe et al. [1] propose CombOptZero, combining GNN and Monte Carlo tree search (MCTS)-based RL to solve the MVC problem. The formulation of the RL task is as S2V-DQN [18]. The key difference is that CombOptZero uses the MCTS-based searching for the next action. For a state $s$, suppose $U$ is the partial solution, a GNN embeds $G$ and $U$ and outputs two vectors $p$ and $v$, where $p[a]$ is the probability of taking the action $a$ for the state, and $v[a]$ is the estimated overall reward from the state $s$ with action $a$. $p$ and $v$ are input to a MCTS, which can produce a better action prediction $p'$ than $p$. $\text{argmax}_a p'[a]$ is outputed as the optimal action selected for $s$. CombOptZero can also solve the MaxCut problem.

5 Conclusion and Future Work

In this survey, we provided a thorough overview of the recent graph embedding methods that have been used to solve graph-based CO problems. Most graph embedding methods have two stages. The first stage involves a preprocessing of the input graph, such as node proximity computation, neighborhood expansion, path or subgraph extraction, and graph coarsening. The second stage involves training model learning models, such as the generalized SkipGram model, the graph convolution model, and AutoEncoder. This survey classifies graph embedding works from the perspective of graph preprocessing tasks and ML models. This survey also summarizes recent graph-based CO methods that use graph embedding. For a graph-based CO problem, graph embedding can be used by classification techniques to predict the probabilities of the nodes belonging to a solution. Graph embedding can also be used within a searching procedure to iteratively extend a partial solution to a final solution.

There are at least two possible directions for future research. Firstly, for graph embedding, precomputing node proximities (e.g., PageRank, Betweenness) that can capture more global structures of graphs has a high time cost. Considering that some proximities can be computed iteratively, one potential direction for further research is to integrate the iteration of the node proximity computation with the iteration of model training, such that the overall time cost can be reduced. Secondly, for graph embedding based CO methods, existing works are mainly focused on processing one or two graphs. Another
possible future direction is to find ways to support a large number of graphs, for example, by optimizing the query evaluation on a large graph database.

6 List of abbreviations

ML, machine learning; GNN, graph neural network; DL, deep learning; RL, reinforcement learning; CNN, convolutional neural network; DNN, deep neural network; RNN, recurrent neural network; MLP, multi-layer perceptron; MDP, Markov decision process; MCTS, Monte Carlo tree search; CO, combinatorial optimization; MVC, minimum vertex cover; MIS, maximum independent set; TSP, travelling salesman problem; GC, graph coloring; MDS, minimum dominating set; MM, maximum matching; MaxCut, maximum cut; MC, maximum clique; SI, subgraph isomorphism; GSim, graph similarity; MF, matrix factorization; B&B, branch and bound; MILP, mixed-integer linear programming; BFS, breadth-first search; DFS, depth-first search.

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