A Survey of Graph Embedding

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1 Introduction

Graph embedding is a structure-preserving dimensionality reduction problem. Input the graph, output low-dimension representation in the latent space(usually in vectors format), and feed it into downstream graph analytics tasks.

1.1 Graph Embedding Inputs

Graph embedding input can be divided into four categories: homogeneous graph, heterogeneous graph, graph with auxiliary information and constructed graph. Each category can be further classified as directed/undirected graphs, or weighed/unweighted graphs. Two nodes that share a higher-weight edge should be embedded closer.

Homogeneous graph is a graph that all nodes belong to a single type, so do all edges.

Heterogeneous graph, on contrary, allows the various types of nodes and edges. For example, in a film related knowledge graph constructed from Freebase (1), the types of entities can be "director", "actor", "film", etc. The types of relations can be "produce", "direct", "act in".

The third type is graphs with auxiliary information. In addition to the structural relations of node, it contains labels, affiliated attributes, information propagation, etc. One example can be Neo4J property graph.

The last type is graphs constructed from non-relational data. Imagine to convert a picture into a graph(2), where pixels are treated as nodes and the co-occurrence of spatial relations between pixels are as edges.

Insight: For heterogeneous graphs, like knowledge graph, the distributions of different types nodes/edges can be skewed, how to deal the imbalance can be a challenge. For graphs with auxiliary information, like the property graph, the embedding shall reflect both topological and unstructured auxiliary information sources.

1.2 Graph Embedding Outputs

The output of embedding can be either a deterministic low-dimension vector, or an uncertain multivariate Gaussian distribution, corresponding to Vector Point-Based embedding methods and Gaussian Distribution-Based embedding methods(3). Gaussian distribution-based graph embedding enables effective in-corporation of useful unstructured attribute information associated with each node. But let's focus on vector-based embedding mainly.

Based on the output granularity, graph embedding output can be divided into four categories, node embedding, edge embedding, hybrid embedding and whole-graph embedding. The choice to implement which level of granularity is task-driven.

Node embedding is used for node clustering, node classification.

Edge embedding is common in link prediction. For example knowledge graph embedding model(TransE(4)) can be used to conduct entity/relation prediction, where $< h, r, t >$ is a triplet, with head/tail entity nodes and their relationship both embedded into same vector space. The subtraction of head/tail entity embedded vectors is exactly the relationship embedded vector. By given two components of a triplet, the third component can be predicted.

Hybrid embedding contains sub-graph embedding, and community embedding. The latter requires the nodes embedding inside a community is similar to its community embedding, while two communities embedding should be disparate.

Whole-graph embedding provides a straightforward and efficient solution for graph classification. It's usually used in small graphs, such as proteins, molecules, etc. Two similar graphs should be embedded closer.

1.3 Linkage Between Embedding Inputs and Outputs

Node embedding is the most common task, let's take it as an example.

Nodes that are "close" in the graph are embedded to have "similar" vector representations.

There lays two questions, how to define the closeness of two nodes in original graph(see Chapter 2.4 on the following page), and how to define the similarity of two vectors in embedded space(see Chapter 2.3). Concerning whether two nodes are close in original graph, we shall consider to which extent we should include the node context information, for example, 1-hop neighbors, 2-hop neighbors, or even the whole graph structure.

The objective function is clear, that is to minimize the difference of original graph's node closeness and the embedded graph's vector similarity. By given the nodes information from original graph, the optimized node embedding vector will be output.

The way to mapping high-dimension node context to low-dimension vector is via an Encoder.

2 Mathematics Preliminaries

2.1 Original Graph

We consider a graph $G(V, E)$ as a mathematical data structure that contains a node (or vertex) set $V = \{v_1, v_2, v_3, ..., v_n\}$ and an edge (or link) set E. The edge set, one edge e_{ij} describes the connection between two adjacent nodes vi and v_j, and hence e_{ij} can be represented as (v_i, v_j).

2.2 Embedding Space

The task of learning its node/edge/hybrid/graph embedding (e.g., d dimension, $d \ll |V|$) can be mathematically formulated as finding a projection ϕ such that, take node embedding as an example,

$$\phi : v_i \to \begin{cases} z_i \in \mathbb{R}^d \quad (i = 1, 2, ..., |V|) \quad or, \\ P_i \sim (\mu_i, \Sigma_i), \mu_i \in \mathbb{R}^{d/2}, \Sigma_i \in \mathbb{R}^{d/2 \times d/2} \quad (i = 1, 2, ..., |V|) \end{cases}$$

is either Point Vector-based representation or Gaussian Distribution-based representation.

2.3 Similarity in Embedding Space

Representations	Similarity Measures
Point Vector	• Dot Product : $z_j^T z_i$ • Cosine similarity: $\frac{z_i \cdot z_j}{\|\|z_i\|\| \times \|\|z_j\|\|}$ • Euclidean distance: $\|\|z_i - z_j\|\|$
Gaussian Distribution	• Expected likelihood: $EL(P_i, P_j)$ • KL-divergence: $D_{KL}(P_j \|\| P_i))$ • Wasserstein distance: $W(P_i, P_j)^2$

2.4 Closeness in Original Graph

2.4.1 Adjacency Matrix

The most intuitive one is Adjacency Matrix(5), if an edge exist between two nodes v_i and v_j, then the weights between them w_{ij} is not 0.

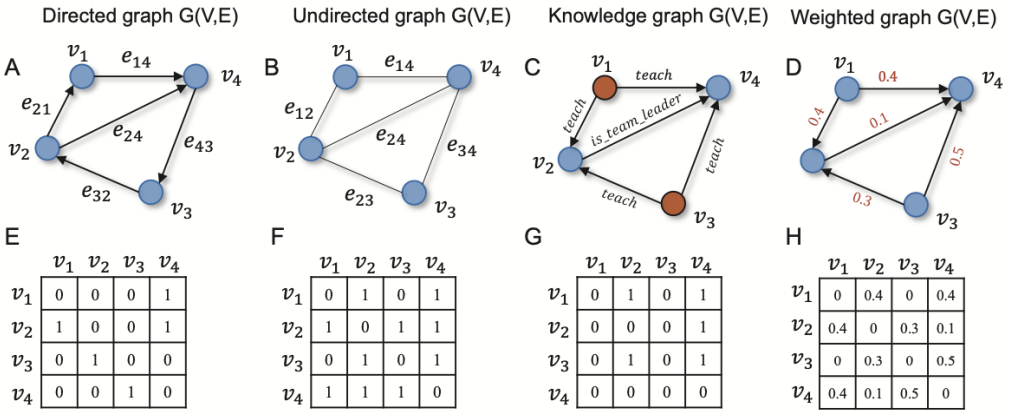

Figure 1: Adjacency Matrix

2.4.2 Proximity Graph and Proximity Matrix

Compared to Adjacency Matrix, which is a matrix derived from the original graph, a proximity graph is a new graph generated from the original graph, that only contains similar nodes and the edges between them.

The way to define the similar nodes can be very flexible. For example, we can say in Figure.2, s_1 and a_1 are similar because they are linked by one edge. And we can also define that s_2 and t_1 are similar because they share common neighbors, as illustrated in Shared Nearest Neighbor algorithm(SNN)(14), which defines proximity between two vertices in terms of k common neighbors (i.e., directly connected vertices). Similarly, algorithm kNN preserves only the nearest k neighbors in proximity graph.

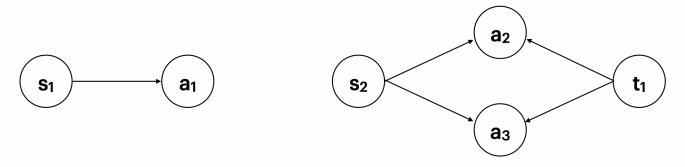

Figure 2: Smilar Nodes

Further, proximity measures take into account not only the adjacent, but also long distance connections. The Neumann Kernel uses a tunable decay parameter γ to control how much weight is given to the more distant connections, which can produce results based entirely on the immediate neighbors or results that take the full structure of the graph into consideration(14).

Based on Proximity Graph, the nodes' Proximity Matrix can be generated as an input of the embedding problem.

3 Graph Embedding Methods

We focus on Vector-based Graph Embedding Methods.

3.1 Matrix Factorization Method

There are two types of matrix factorization based graph embedding. One is to factorize graph Laplacian eigenmaps, and the other is to directly factorize the node proximity matrix.

3.1.1 Graph Laplacian Eigenmaps

Theory: Let $z = (z_1, ..., z_n)$ represent the d dimension embedding of the n nodes. We then formulate the following problem,

$$\min_{z \in \mathbb{R}^d} \sum_{i,j} \frac{1}{2} w_{ij} (z_i - z_j)^2$$

where w_{ij} is the similarity weights between node v_i and v_j in original graph. The higher the w_{ij} is, the smaller the $(z_i - z_j)^2$ should be. Further scale the embedding vector as $\sum_i (z_i)^2 = 1$.

Considers the Laplacia matrix of G, defined as,

$$L = D - W$$

where D is the diagonal matrix whose entries are the sum weights of each node. Then the objective function can be written as,

$$\min_{z \in \mathbb{R}^d} \sum_{i,j} \frac{1}{2} w_{ij} (z_i - z_j)^2 = \min_{z \in \mathbb{R}^d} z^T L z$$

Finally the optimal z is given by the second smallest eigenvector of L.

Insight: The differences of existing studies mainly lie in how they calculate the pairwise node similarity w_{ij}.

The initial study MDS(21) adopted Euclidean distance of two nodes v_i and v_j as w_{ij}. Later, it's proposed to construct a proximity graph first, which considers mainly local structure. As in Epsilon-ball approach, only nodes whose distance $||v_i - v_j|| <= \epsilon$ are considered as nearby nodes; or in the kNN approach, only k nearest neighbors are reserved in the proximity graph(6)(7)(8)(9). Nodes distance is the value of w_{ij}.

Recent Works: Some more advanced models are designed recently. For example, AgLPP(10) introduces an anchor graph to significantly improve the efficiency of earlier matrix factorization model LPP. LGRM(11) learns a local regression model to grasp the graph structure and a global regression term for out-of- sample data extrapolation. LSE(12) uses local spline regression to preserve global geometry.

3.1.2 Node Proximity Matrix Factorization

Theory: Proximity measures are applicable to weighted structures and could take into account not only the shortest, but also long-distance connections(14). Given the node proximity matrix W(as mentioned in Chapter 2.4.2 on the preceding page), the objective is,

$$min||W - ZZ^{cT}||$$

where $Z \in R^{|V| \times d}$ is the node embedding, and $Z^c \in R^{|V| \times d}$is the embedding for the context nodes. One popular solution is to apply SVD (Singular Value Decomposition) on W. Formally,

$$W = \sum_{i=1}^{|V|} \sigma_i \mu_i \mu_i^{cT} \approx \sum_{i=1}^{d} \sigma_i \mu_i \mu_i^{cT}$$

where $\{\sigma_1, \sigma_2, ..., \sigma_{|V|}\}$ are the singular values sorted in descending order, μ_i and μ_i^c are singular vectors of σ_i. The optimal embedding is obtained using the largest d singular values and corresponding singular vectors as follows,

$$Z = [\sqrt{\sigma_1}\mu_1, ..., \sqrt{\sigma_d}\mu_d],$$
$$Z^c = [\sqrt{\sigma_1}\mu_1^c, ..., \sqrt{\sigma_d}\mu_d^c].$$

Depending on whether the asymmetric property is preserved or not, the embedding of node v_i is either $z_i = Z_i$ or the concatenation, i.e., $z_i = [Z_i, Z_i^c]$.

Insight: To explicitly derive the proximity matrix, the cost and is too expensive for large graphs. In the case in NetMF(13), it typically takes $\Theta(n^2)$.

Recent Works: To avoid the $\Theta(n^2)$ running cost, HOPE(15), AROPE(16), and NRP(17) are proposed to derive the embedding without explicitly computing the proximity matrix.

For instance, instead of computing all-pair proximity scores and then decomposing the proximity matrix, NRP turns to do SVD on the adjacency matrix, which is sparse for most real-life graphs, reducing the embedding computational cost. Another solution to avoid the $\Theta(n^2)$ cost is to calculate a sparsified proximity matrix S. The representative is STRAP(18), which imposes a threshold δ and returns at most $\Theta(\frac{n}{\delta})$ proximity.

Since the second solution explicitly derives the proximity matrix, it allows to take non-linear operations on the proximity matrix, improving the representation powers.

DANE(21) captures the changes of dynamic structures with the adjacency matrix and models the changes of attributes with the attribute matrix, which only considers the first-order proximity. DHPE(22) preserves high-order proximity between nodes

Sum Up: Matrix Factorization method suffers from high computation cost($\Theta(n^2)$). Adjacency matrix-based algorithms only consider pair-wise local relationships, neglecting the global structures. The downstream analysis tasks which are built on Adjacency matrix embedding method usually has overfitting problem.

3.2 Deep Learning Method

So far we have talked about the shallow encoder, which maps a node to a low-dimension vector, but only through one encoding layer. It means that the number of encoding parameters is proportional to the number of nodes. And it's transductive. Graph neural network has allowed the multiple layers of non-linear transformations of graph structure, so called deep encoders. The parameters are shared. Also it's inductive.

Graphs are challenging in deep learning, since it's shape is not fixed and limitless, compared with image input which is a fixed-size matrix and text input which is a line graph with fixed-length sliding window. One way to cope with it is through Graph Convolutional Network(GCN)(23), which aggregate the neighbor nodes information like a convolution kernel, regardless of the shapeless graph structure, as shown in Figure.3. And such multi-layer aggregations contains both local and global propagating information.

Theory: Suppose in initial layer h^0, we have node v features x_v as input, $h_v^0 = x_v$. In last layer, we get node embedding $z_v = h_v^L$. At the middle layer l, the embedding is like,

$$h_v^{l+1} = \sigma(W_l \sum_{\mu \in N(v)} \frac{h_\mu^l}{|N(v)|} + B_l h_v^l), \forall l \in \{0, ..., L-1\}$$

where σ is activation function, usually ReLU, Sigmoid or Parametric ReLU; and inside it, the first part is the aggregation of all neighbors information from last iteration, the second part is the node itself's information from last iteration. W_l and B_l are corresponding trainable weight matrix to learn.

Let matrix A be the adjacency matrix, matrix D be the degrees matrix, and $H^l = [h_1^l, ..., h_{|V|}^l]^T$, the formula can be rewritten as,

$$H^{l+1} = \sigma(\hat{A} H^l W_l^T + H^l B_l^T)$$

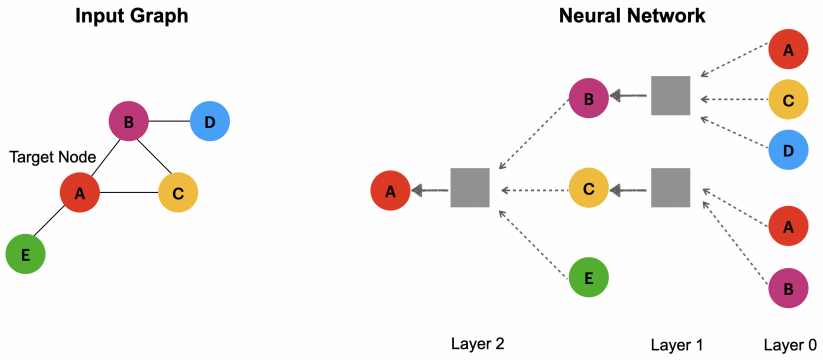

Figure 3: Graph Convolutional Network

where $\hat{A} = D^{-1}A$. Matrix format is computation effective via Gradient Descent. We want to minimize the loss in supervised learning of,

$$\mathcal{L}(y, f(z_v))$$

where $\mathcal{L}$ can be L_2 norm if y is numerical and cross entropy if y is categorical; and in unsupervised learning of,

$$\mathcal{L} = \sum_{z_u, z_v} CE(y_{u,v}, DEC(z_u, z_v))$$

where $y_{u,v} = 1$ if nodes u, v are similar, and CE is the cross entropy, and DEC is the decoder, which can be any embedding vector similarity measurement(see Chapter 2.3 on page 2).

Recent Works: GraphSage(24), rather than sum the node vector with neighbors' inside the activation function, it concatenates them. Also, for the aggregation of all neighbors' information, it offers choices of mean, pool, even LSTM. Note that LSTM is not order invariant, a random selection of neighbors has been applied.

Graph Attention Network(GAT)(25) introduced the attention mechanism. It assigned the different weighs of different neighbors. Multi-head attention(26) further replicates the attention operations at a given layer for R times, and output the concatenating or adding result, which stabilize the learning process. TemporalGAT(31) has applied attention algorithm on dynamic graphs.

Other than homogeneous graph algorithms, some deep learning methods(e.g., HNE(28) TransE(29), ProxEmbed(30)) are applied in heterogeneous graphs as well.

3.3 Random Walk Method

The general concept of Random Walk Method is that, starting from a node v_i, as shown in Figure.4, within a k-step random walk, the sum of the probability $p(v_j|v_i)$ of co-occurring nodes, should be maximized.

Random Walk Method is efficient, because it only considers the nodes that show up in walk paths, drastically reducing the computation cost in traditional deep learning embedding method.

Theory: Now let u be the starting point, and $N_R(u)$ notates the multiset of nodes visited on random walks. Then the loss function is,

$$\mathcal{L} = \sum_{\mu \in V} \sum_{v \in N_R(\mu)} -log(P(v|z_u))$$

where

$$P(v|z_u) = \frac{exp(z_u^T z_v)}{\sum_{n \in V} exp(z_u^T z_n)}$$

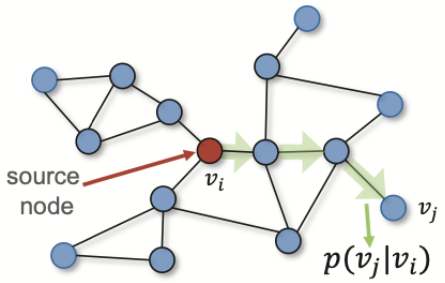

Figure 4: Graph Random Walk

It means that, iterate all starting points u; for each given u, maximize the log co-occuring possibility of visited nodes. And the probability could be nearly represented as their embedding vectors' doc product $z_u \cdot z_v^T$, normalized by the Softmax function.

But in order to simplify the normalization and summing less nodes, two methods are introduced to approximate the problem. First is the Negative Sampling method,

$$log(\frac{exp(z_u^T z_v)}{\sum_{n \in V} exp(z_u^T z_n)}) \approx log(\sigma(z_u^T z_v)) - \sum_{i=1}^{k} log(\sigma(z_u^T z_{n_i})), n_i \sim P_v$$

where k negative samples are selected from a noise distribution P_v. And parameter k is usually set in range 15 to 20 rather than whole vertex set, reducing the computation cost from $\Theta(|V|^2)$ to $\Theta(k|V|)$.

Second way is the Hierarchical Softmax. A binary tree is constructed, and only the path from the root to the corresponding leaf needs to be evaluated,reducing the computation cost from $\Theta(|V|^2)$ to $\Theta(|V|log(|V|)$.

Recent Works: DeepWalk(31) applies the above algorithm via deep learning encoding model SkipGram. But its random walk path is fixed-length and unbiased. Node2vec(32) enables biased parameters to explore either breath-first or depth-first random walks to bias towards local or global view, as shown in Figure.5.

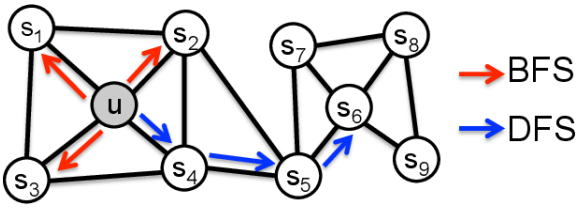

Figure 5: Node2vec

The choices over encoders can vary from SkipGram with hierarchical softmax(e.g., DeepWalk), to SkipGram with negative sampling(e.g., Node2vec), to LSTM(e.g., ProxEmbed(30) HSNL(33), RMNL(34)), and to GRU(e.g., DeepCas(35)).

4 Applications

Graph embedding is beneficial for various graph analysis applications because it can handle vector representations efficiently in both time and space. This section classifies applications that support graph embeddings into node related, edge related and graph related.

4.1 Node Related Applications

4.1.1 Node Classification

Node classification is the assignment of class labels to each node in the graph based on the rules learned from the labeled nodes. Intuitively, "similar" nodes have the same label. This is one of the most common applications described in the Graph Embedding literature. Generally, each node is embedded as a low-dimensional vector. Node classification is performed by applying a classifier to a set of labeled node embeddings for training.Examples of classifiers include SVM logistic regression and k-nearest neighbor classification. Second, if an unlabeled node is embedded, the trained classifier can predict its class label. Relative to the above sequential processing of node embedding and then node classification, some other works have designed a unified framework that jointly optimizes graph embedding and node classification, classifies each node, and learns a classification-specific expression.

4.1.2 Node Clustering

Node clustering aims to group similar nodes together, so that nodes in the same group are more similar than nodes in other groups. It can be used as an unsupervised algorithm when node labels are not available. After representing nodes as vectors, traditional clustering algorithms can be applied to node embeddings.

4.1.3 Node Recommendation

The task of node recommendation is to recommend the top K nodes of interest to a specific node according to certain criteria such as similarity. In real-world scenarios, recommendation nodes are of different types, such as research topics, items for customers, curated images of web users, friends of social network users, and queried documents. It is also popular in community-based QA. Given a question, it predicts the relative ranking of users or answers. Proximity search sorts certain types of nodes (e.g., "users") into specific query nodes (e.g., "bob") and proximity categories (e.g., "graduate"). For example, the ranking of graduate users. Bob's. Some works focus on cross-modal search, such as keyword-based image/video search.

4.2 Edge Related Applications

The following is an edge-related application that contains edges or pairs of nodes.

4.2.1 Link Prediction

Graph embeddings are designed to represent graphs with low-dimensional vectors, but interestingly, their output vectors are also useful for inferring the graph structure. In practice, graphs are often incomplete. For example, a social network may lack a friendship link between two users who actually know each other. In graph embedding, low-dimensional vectors are expected to maintain network proximity in different orders (e.g., DeepWalk, LINE, etc.) and structural similarity at different scales (e.g., GCN, struc2vec, etc.). Therefore, these vectors can be used to encode a wealth of information about the network structure and predict missing links in incomplete graphs. Most attempts at graph-embedded link prediction are made with homogeneous graphs. For example, to predict friendship between two users. Relatively little work has been done on graph embeddings dealing with heterogeneous graph link prediction. For example, in a heterogeneous social graph, ProxEmbed attempts to predict missing links for a specific semantic type (e.g. schoolmate) between two users based on embedding connection paths into the graph. D2AGE solves the same problem by embedding two users connected by a directed acyclic graph structure.

4.2.2 Triple Classification

Triplet classification is a specific application of the knowledge graph. This is intended to classify whether the invisible triple <h, r, t> is correct, that is, whether the relationship between h and t is r.

4.3 Graph Related Applications

4.3.1 Graph Classification

Graph classification assigns a class label to the entire graph. This is important when the graph is a unit of data. For example, each diagram is a chemical compound, organic molecule, or protein structure. In most cases, the whole graph embedding is used to compute graph-level similarity. Recently, some work has started to match node embeddings for the similarity of graphs. Each graph is represented as a set of nodes with embedded vectors. Graphs are compared based on two sets of node embeddings, decompose the graph into a set of substructures, then embed each substructure as a vector, and compare the graphs by substructure similarity.

4.3.2 Visualization

Graph visualization produces graph visualization in low-dimensional space. Usually for visualization purposes, all nodes are embedded as 2D vectors and then different graphs are drawn in 2D space. The color indicates the node category. It clearly shows whether nodes belonging to the same category are embedded close to each other.

5 Summary and Discussion

This study provides a comprehensive review of the graph embedding literature. We formally define the problem of embedding graphs and introduce some basic concepts. More importantly, we propose two taxonomies for graph embeddings, each of which classifies existing work based on the problem setting and embedding method. Regarding the taxonomy of problem settings, we introduce four embedded inputs and four embedded outputs, and summarize the challenges faced by each setting. As for the taxonomy of embedding methods, we will introduce the work of each category and compare them from the perspective of advantages and disadvantages. Finally, we summarize the applications that enable graph embedding.

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