Customized Graph Embedding: Tailoring the Embedding Vector to a Specific Application

Bitan Hou, Yujing Wang, Ming Zeng, Shan Jiang, Ole J. Mengshoel, Yunhai Tong, Jing Bai

Abstract. The graph is a natural representation of data in a variety of real-world applications, for example as a knowledge graph, a social network, or a biological network. To better leverage the information behind the data, the method of graph embedding is recently proposed and extensively studied. The traditional graph embedding method, while it provides an effective way to understand what is behind the graph data, is unfortunately sub-optimal in many cases. This is because its learning procedure is disconnected from the target application. In this paper, we propose a novel approach, Customized Graph Embedding (CGE), to tackle this problem. The CGE algorithm learns a customized vector representation of the graph by differentiating the varying importance of distinct graph paths. Experiments are carried out on a diverse set of node classification datasets and strong performance is demonstrated.

1 Introduction

Graphs are a natural representation to use in a broad range of real-world applications [10, 9], for example in the context of graph embedding. Graph embedding methods produce dense vector representations of graphs and thus provide information about what is behind the data. Such dense vector representations consequently can benefit a variety of downstream applications such as node classification. Existing graph embedding methods can be categorized into three categories, namely factorization-based [10], random walk-based [20] and deep learning-based [14]. Random walk-based approaches are popular in many real-world problems, because they are efficient and scalable to large graphs. While efficient and effective, the existing random walk methods are often sub-optimal because the path generation procedures are disjoint from the target applications. As a result, these methods do not generate embedding vectors that are customized to the application at hand.

We study in this paper whether the information requirements, as far as the graph is concerned, vary from application to application. A medical Q&A-application provides an example. Suppose that we want to enhance the performance of medical Q&A by exploiting a Wikipedia knowledge graph. Wikipedia is a general knowledge graph which contains knowledge from many domains. Knowledge from non-medical domains may be irrelevant or even distracting for a medical application. It thus makes sense, intuitively, that such non-medical knowledge should be de-emphasized in the embedding learning procedure to obtain more customized embedding. However, it is a non-trivial problem to select the most relevant knowledge automatically from a large graph to provide stronger support to a specific application.

In this paper, we propose Customized Graph Embedding (CGE) to address this problem. With CGE, the path generation procedure is tailored to a specific application. CGE first samples a set of paths randomly from the graph, and then re-weights them through a neural network model before the embedding calculation. CGE’s embedding procedure with path re-weighting is formalized as a bi-level optimization problem [21], which consists of two loops. In the inner loop, we train the embedding vectors and supervised model parameters based on a fixed re-weighting model. In the outer loop, the goal is to optimize the re-weighting model to minimize the semi-supervised loss. We study two neural network architectures for the re-weighting model, i.e., Convolutional Neural Network [13] and Long Short-Term Memory [11]. We also implement a simple re-weighting strategy based on average pooling for comparison. Following Yang et al. [26], we develop both transductive and inductive variants of CGE. The transductive model only learns the embedding for instances observed at the training time, while the inductive model is able to generalize to unobserved instances in the training phase.

We carry out experiments on four open datasets for node classification: CITESEER, CORA, PUBMED and NELL. The experimental results demonstrate the effectiveness and robustness of CGE. On the four datasets, CGE outperforms or performs on par with state-of-the-art methods and establishes the best-ever performance scores when combined with the Graph Convolutional Network (GCN) [14]. The source code is publicly available. To summarize, the contributions of this paper are as follows:

- CGE is, to our best knowledge, the first attempt to customize graph embedding by tailoring the information in the graph to the application at hand.
- CGE achieves state-of-the-art performances on four node classification datasets (CITESEER, CORA, PUBMED and NELL) that are widely used for the empirical evaluation of graph embedding methods.
- We provide deep insights into CGE, to explain the benefits of the path re-weighting. We observe that the method can automatically retrieve task-oriented paths from the graph, and the weighting scores are affected by the lengths and node diversities of the paths, which agrees well with human common-sense.

The code will be open-sourced once the paper is accepted.
In the rest of this paper, we first cover related work in Section 2. We then discuss our novel Customized Graph Embedding (CGE) method in Section 3. Experimental protocols and results for CGE are presented in Section 4, while Section 5 concludes and mentions future research opportunities.

2 Related Work

Graph embedding benefits a wide variety of graph analytic applications. The advantage of graph embedding is that "translates" all kinds of information from graphs into dense vectors. These dense vectors can then be used by downstream applications as advanced feature representation. For example, Zhang et al. [27] propose a deep feature learning paradigm by mining visual-semantic embeddings from noisy, sparse, and diverse social image collections. They demonstrated superior performance of graph embedding in various applications such as content-based retrieval, classification, and image captioning.

The input types for graph embedding include homogeneous graph, heterogeneous graph, graph with auxiliary information, and graph constructed from non-relational data [3]. The homogeneous graph, such as a Webpage link graph [24], is a primary setting of graph representation. Here, every node and edge in the graph is of the same type. The heterogeneous graph is another standard setting where nodes and edges are of different types. For example, a knowledge graph constructed from Wikipedia consists of three types of nodes (entity e, category c, and word w) and three types of edges (e-e, e-c, and w-w) [28]. One can also build graphs with auxiliary information (e.g., attributes, labels, and text descriptions) on nodes to improve the embedding quality [6]. Besides, the graph can be constructed from non-relational data in order to benefit from graph embedding techniques. For instance, Yan et al. [25] construct an intrinsic graph to capture intra-class compactness, and a penalty graph to characterize inter-class separation. Moreover, there are four major types of graph embedding outputs: node embedding, edge embedding, hybrid embedding, and whole-graph embedding [3]. This paper mainly focuses on node embedding, but the idea of customized graph embedding is not restricted to it and may benefit other types of graph embedding outputs.

The techniques of graph embedding can be categorized into three broad groups, i.e., factorization-based, random walk-based, and deep learning-based approaches [10]. Factorization-based algorithms represent the connection between nodes in the form of a matrix (including an adjacency matrix [1], a Laplacian matrix [2]), or a node transition probability matrix [3]) and calculate the embedding vectors by factorizing the corresponding matrix. The limitation of factorization-based methods is that they are prohibitive on large graphs since the proximity matrix construction or the eigen-decomposition of the matrix is time and space consuming [3]. Random walk-based methods [20] [17] are more efficient and scalable for large graphs and have been extensively studied. Specifically, DeepWalk [20] samples a set of paths by random walks on the graph and leverages SkipGram-based Word2Vec [15] to calculate node representation vectors. However, DeepWalk ignores the label information in embedding learning so that the embedding vectors are not customized for a specific application task. Node2vec [12] offers a way to adapt the sampling strategy to BFS or DFS according to the requirements of different applications, but it is not expressive enough to incorporate all kinds of sampling strategies. Planetoid [25] is a semi-supervised graph embedding framework that jointly optimizes the node label and graph context. Nevertheless, the path sampling strategy is not application task-specific. In addition, deep learning-based approaches utilize auto-encoders [23] or convolutional neural networks [19] on the whole graph directly without a random walk. For example, the Graph Convolutional Network (GCN) [14] is a state-of-the-art semi-supervised graph embedding approach that has obtained a superior result on node classification. It aggregates feature information from local neighborhoods in a graph iteratively using a convolutional neural network.

3 Customized Graph Embedding

The overall pipeline of Customized Graph Embedding (CGE) is illustrated in Figure 1. The inputs to the pipeline include a large graph (with nodes and edges) and a target task with labeled instances (corresponding to graph nodes), and the outputs are embedding vectors (in the transductive setting) or embedding models (in the inductive setting) for each node. Similar to traditional random walk-based approaches, we sample a collection of sub-paths from the input graph, where the start and end nodes in each sub-path formulates a node pair. The most salient procedure proposed in CGE is to re-weight each pair by a neural network model, for instance, LSTM, to reflect its importance for a specific task. Based on the labeled instances, we generate additional node pairs where two nodes within a pair share the same label. As these pairs are well-aligned with the target task, we set the weighting score as 1 and do not apply re-weighting to them during training. The loss function is semi-supervised, where the unsupervised pair can be constructed by the weighted pairs, and the supervised part can be formulated as cross-entropy on labeled instances. Finally, the optimization procedure is conducted on the semi-supervised loss and the embedding vectors or models are generated as outputs.

### 3.1 Path Sampling & Pair Generation

The sampled paths are generated by a random walk on the entire graph. We take each node as a starting point and sample the next node...
uniformly from its neighbors. This sampling process is repeated multiple times until the path is long enough. We then extract sub-paths from each path within a fixed sliding window. For example, if the original path is \( n_1 n_2 n_3 n_4 n_5 \), and the sliding window size is 3, all the sub-path extracted should be \( n_1 n_2 n_3; n_1 n_2 n_4; n_1 n_2 n_5; n_1 n_3 n_2; n_2 n_3 n_1; n_3 n_2 n_1; n_4 n_1 n_5; n_1 n_2 n_3; n_2 n_3 n_4; \) and \( n_3 n_4 n_5 \). The starting and ending node in each sub-path formulates a node pair. To use the labeled instances, following [26], we sample a collection of virtual paths that consist of nodes with the same label. Then, we get additional pairs from these virtual paths because these nodes are highly relevant with each other.

### 3.2 Path Re-weighting

In unsupervised graph embedding methods such as DeepWalk [20], paths are usually assumed to be equally weighted in the loss function. However, the embedding vectors learned in this way are not always optimal for an arbitrary application. Take the Wikipedia knowledge graph as an example. Each path in the graph reflects a piece of knowledge in a particular domain, and a random path may be noisy or irrelevant to the target application. Thus, we re-weight the graph paths to indicate their importance scores so that the essential knowledge for a specific task can be emphasized.

Our re-weighting model is based on neural network architecture. We denote the re-weighting model as \( A \), which takes a sequence of nodes in the path as input and outputs an importance weight in the range of \([0, 1]\). The framework is quite general, and a variety of architectures can be leveraged as the re-weighting model. Here we employ two neural network architectures, i.e., Convolutional Neural Network (CNN), and Long Short-Term Memory (LSTM). For comparison, we also implement a baseline re-weighting strategy based on average pooling. The three re-weighting models are described as follows:

- **Average Pooling**: It calculates the average embedding vectors of all nodes in the path. A feed-forward layer is applied before Sigmoid activation.

- **CNN**: Two 1-D convolution layers are stacked on the input vector, as shown in the equations below. In each convolutional layer, the filter size is set to be 3, and the number of filters is 1. The weight of path \( p_k \) is given by:

\[
\begin{align*}
    h_1^k &= \text{Conv1D}(p_k, w^1) \\
    h_2^k &= \text{Conv1D}(h_1^k, w^2) \\
    A(p_k) &= \text{sigmoid}(h_2^k)
\end{align*}
\]

where \( w^1 \) and \( w^2 \) are the parameters in the first and second layers respectively. \( h_1^k \) is a vector, whose dimension equals to the embedding size, and \( h_2^k \) is a scalar.

- **LSTM**: LSTM is a natural choice for modeling sequential input [13]. In our implementation, the hidden state of LSTM is passed to a feed-forward layer and then to a sigmoid output layer. The weight of path \( p_k \) is calculated by:

\[
\begin{align*}
    h_0 &= \text{LSTM}(p_k, w) \\
    v_k &= (w_{linear})^T h_0 \\
    A(p_k) &= \text{sigmoid}(v_k)
\end{align*}
\]

where \( w \) and \( h_0 \) are the parameters and hidden states of LSTM model respectively; \( w_{linear} \) is the vector of parameters for the feed-forward layer.

### 3.3 Loss Function

The loss function is semi-supervised and consists of two parts, i.e., the supervised loss \( L_s \), and unsupervised loss \( L_u \).

The supervised loss optimizes the prediction of the target variables explicitly, while the unsupervised loss is used as regularization. The semi-supervised loss is formulated as:

\[
L(A, e, \theta) = L_s + \lambda L_u, \tag{3}
\]

where \( \lambda \) is a hyper-parameter that controls the trade-off between the \( L_s \) and \( L_u \) and \( \theta \) denotes the set of trainable parameters in the supervised model. \( e \) is the final output embedding vector for the node.

#### 3.3.1 Unsupervised Loss

Given an input graph, our goal is to learn the embedding representation of each node in the graph tailored to the particular task. Learning the embedding vectors of nodes in the graph formalizes an unsupervised graph embedding problem which can be solved by DeepWalk [20], where the loss function is similar to Skip-Gram [18]. We generalize the loss function of previous work by enabling importance weighting on each path, in our revised loss function:

\[
L_u = \sum_k A(p_k) \text{loss}(w_i, e_j) \tag{4}
\]

where \( p_k \) represents a sub-path sampled randomly from the graph; \( A(p_k) \) calculates the importance weight of the sub-path; \( i \) and \( j \) denote the start node and end node of \( p_k \) respectively; \( w_i \) represents the input embedding vector of node \( i \); \( e_j \) is the output vector of node \( j \); and \( \text{loss}(w_i, e_j) \) is the loss of predicting node \( j \) by node \( i \). The loss function is:

\[
\text{loss}(w_i, e_j) = - \log p(e_j | w_i) = - \log \frac{\exp(e_j^T w_i)}{\sum_{k=1}^{K} \exp(e_k^T w_i)} \tag{5}
\]

where \( K \) is the number of all distinct nodes. In practice, if the graph size is too large, we can apply negative sampling [13] to accelerate to training process.

#### 3.3.2 Supervised Loss

Based on the embedding vectors \( e_i \), supervised loss of node classification can be written as below:

\[
L_s = \sum_i l(y_i, f(x_i, e_i, \theta)), \tag{6}
\]

where \( x_i \) and \( e_i \) represent the feature vector and embedding vector of node \( i \) respectively; \( f \) denotes the supervised model, and \( \theta \) is the parameters of the model. The ground truth label for node \( i \) is \( y_i \), and \( l(\cdot, \cdot) \) denotes the loss function (cross-entropy, mean squared, etc.). In our experiments, we utilize cross-entropy loss in node classification tasks.

We implement two flavors of the supervised loss, namely transductive and inductive [26]. In the transductive setting, the embedding vector \( e_i \) is trained on the training data and retrieved directly when the same node appears in the test phase. The drawback is that the model cannot be generalized to unseen nodes in the training phase. To alleviate this problem, we also implement the inductive setting, where a model is learned to project any feature vector \( x_i \) to the corresponding embedding vector \( e(x_i) \).
Then, keeping the embedding vector $e_i$ serves as additional features to $x_i$ and can be learnt jointly in the semi-supervised model. The transductive semi-supervised loss is:

$$L_s = \sum_i l(y_i, f(x_i, e_i, \theta)),$$

$$f(x_i, e_i, \theta) = \text{softmax}(h^k(x_i), h^l(e_i))$$

where $h^k$ and $h^l$ are single feed-forward layers, taking the feature vectors and embedding vectors as input respectively; $\theta$ represents the learnable parameters of layer $h^k$ and $h^l$. The results of the feed-forward layers are concatenated before calculating the prediction result by softmax.

**Inductive Setting:** the embedding vector $e_i$ is calculated as a function of the input feature vector $x_i$, thus can be generalized to unseen instances. The semi-supervised loss in the inductive flavor is shown below:

$$L_s = \sum_i l(y_i, f(x_i, e(x_i), \theta)),$$

$$f(x_i, e(x_i), \theta) = \text{softmax}(h(x_i), e(x_i))$$

where $h$ is a single feed-forward layer, taking the concatenation of features vector $x_i$ and embedding vector $e(x_i)$ as input; $\theta$ stands for the learnable parameters in layer $h$. In our experiments, the embedding function $e(x_i)$ is implemented as a single feed-forward layer.

### 3.4 Optimization

The goal of customized graph embedding is to automatically find the optimal function $A^*$ that minimizes the validation loss $L(A^*, e^*, \theta^*)$ where the embedding vector $e^*$ and model parameter $\theta^*$ are learned jointly to fit the training data. It can be naturally formulated as a bi-level optimization problem:

$$\min_{A} \quad L_{\text{val}}(A, e^*, \theta^*)$$

s.t. \quad $e^*, \theta^* = \arg\min_{e, \theta} L_{\text{train}}(w_A, e, \theta)$

In this problem, $A$ is constrained to be the solution of a given optimization problem parameterized by $e$ and $\theta$. Let $\alpha = (e, \theta)$ and $w_A$ denotes the parameters in the weighting model $A$. Equation (11) can be rewritten as:

$$\min_{w_A} \quad L_{\text{val}}(w_A, \alpha^*)$$

s.t. \quad $\alpha^* = \arg\min_{\alpha} L_{\text{train}}(w_A, \alpha)$

Solving the bi-level optimization problem in (12) exactly is prohibitive, because of the nested structure: the optimal value of $\alpha^*$ needs to be recomputed whenever $w_A$ has any change. We thus introduce an approximate iterative optimization procedure similar to [16], where $\alpha$ and $w_A$ are updated alternately. First, we update $\alpha = (e, \theta)$ for a single step towards minimizing the training loss $L_{\text{train}}(w_A, \alpha)$. Then, keeping the embedding vector $e$ and supervised model parameter $\theta$ fixed, we update the parameter $w_A$ (which controls the weighting strategy of sampled paths) towards minimizing the validation loss:

$$L_{\text{val}}(w_A, \alpha - \xi \nabla_{\alpha} L_{\text{train}}(w_A, \alpha))$$

where $\xi$ is the learning rate of a virtual gradient step. The idea behind virtual gradient step is to find a weighting strategy $w_A$ which has low validation loss when the supervised parameter $\alpha^*(w_A)$ is optimized. Here the one-step unroll weights serve as a surrogate for the optimal value $\alpha^*(w_A)$.

The optimization procedure updates the following two gradients in equations (14) and (15) alternately:

$$\nabla_{\alpha} L_{\text{train}}(w_A, \alpha) = \nabla_{\alpha} L_{\text{train}}(w_A, \alpha) + \nabla_{\alpha} L_{\text{val}}(w_A, \alpha)$$

$$\nabla_{w_A} L_{\text{val}}(w_A, \alpha - \xi \nabla_{\alpha} L_{\text{train}}(w_A, \alpha))$$

Here $L_{\text{train}}$ represents the supervised loss on the training nodes, $L_{\text{val}}$ is the unsupervised loss on the sampled paths, which do not differentiate for $L_{\text{train}}$ and $L_{\text{val}}$. Note that the supervised loss does not have derivation to $w_A$, so the first item $L_{\text{val}}$ in (15) can be ignored.

Take the transductive setting as an example. The overall procedure of CGE is summarized in Algorithm 1. The inputs include labeled data and unlabeled data, while the outputs are node embedding vectors.

**Algorithm 1:** Transductive algorithm of CGE

**Input:** graph $G$, labeled data $x_{i\in L}$, unlabeled data $x_{i\in L\cup C}$; parameters of weighting model $w_A$; parameters of supervised model $\alpha = (e, \theta)$; hyper-parameter $\lambda$, $\xi$

**Output:** embedding vector $e$, model parameters $w_A$, $\theta$

1. Initialize embedding vector and model parameters
2. Sampling a collection of paths randomly.
3. while not converged do
   4. Update $\alpha$ by descending
   5. Update $w_A$ by descending

4. Experiments

#### 4.1 Datasets

Six datasets generated from four corpora are used for evaluation (Table 1). All datasets reflect graph structures in different learning tasks.

| Corpus    | #Classes | #Nodes | #Edges | #Labeled | #Test&Valid |
|-----------|----------|--------|--------|----------|------------|
| CITESEER  | 6        | 3,327  | 4,732  | 120      | 1,000      |
| CORA      | 7        | 2,708  | 5,429  | 140      | 1,000      |
| PUBMED    | 3        | 19,717 | 44,338 | 60       | 1,000      |
| NELL001   | 210      | 65,755 | 266,14 | 161      | 987        |
| NELL0001  | 210      | 65,755 | 266,14 | 105      | 969        |

**Table 1.** Six datasets used in our experiments: CITESEER, CORA, PUBMED, and three variants of NELL.

In the text classification experiments (CITESEER, CORA, and PUBMED), 20 instances in each class are leveraged for training while 1000 instances are used for validation and test. The NELL (Never-Ending Language Learning) corpus is built on the NELL [7] Datasets are available from [https://linqs.soe.ucsc.edu/data](https://linqs.soe.ucsc.edu/data)
The datasets can be found at http://www.cs.cmu.edu/~zhiliny/data/nell_data.tar.gz.

Table 2. Accuracy of the unsupervised baselines (DeepWalk and node2vec), a state-of-the-art semi-supervised method (PLATOID-T/I), and the Customized Graph Embedding (CGE) models (CGE-Average, CGE-CNN, CGE-LSTM). PLANETOID-T and PLANETOID-I denote transductive and inductive semi-supervised graph embedding respectively. Significance tests show that our CGE-based results are, except for PUBMED, significantly better than the results of PLANETOID-T and PLANETOID-I respectively, with $p < 0.05$ (marked by one star *) and $p < 0.01$ (marked by two stars **).

4.2 Experimental Settings

For all datasets, we follow the original data split [26] and adopt accuracy as the evaluation metric for node classification. We compare CGE with a state-of-the-art semi-supervised graph embedding method, Planetoid [26], in the transductive and inductive settings, respectively [1]. We also adopt two commonly-used unsupervised approaches, DeepWalk [20] and node2vec [12], as baseline methods. Three variants of CGE are evaluated in the experiments, namely CGE-Average (reweighting with average pooling), CGE-CNN (reweighting with CNN), and CGE-LSTM (reweighting with LSTM). In our experiments, the embedding sizes of the CITESEER, CORA, PUBMED, and NELL datasets are set to 50, 135, 128, and 256 respectively. In the path sampling procedure, the max path length is set to 10. Sliding window size is 3 by default, but we change it to 10 when analyzing the correlation between path weights and path lengths. SGD is used for bi-level optimization.

4.3 Results

4.3.1 comparison to baselines

The experimental results are shown in Table 3. On all the six datasets, the transductive CGE methods outperform or perform on par with previous state-of-the-art methods. In particular, comparing to PLANETOID-T, CGE-CNN achieves 2.5% and 4.3% improvements in accuracy on the CITESEER and CORA datasets; CGE-LSTM achieves 1.7% improvement on PUBMED, and 0.2%, 2.6%, and 9% enhancements on the NELL01, NELL001, and NELL0001 datasets respectively. In the inductive setting, CGE-LSTM achieves on par performance with PLANETOID-I on PUBMED and outperforms the best state-of-the-art results by a large margin on the other five datasets. The results suggest that CGE methods effectively learn better embedding representations that significantly improve node classification accuracy. In addition, the LSTM model turns out to be the best re-weighting strategy for CGE.

4.3.2 Combination with GCN

The Graph Convolutional Network (GCN) is a relatively recent state-of-the-art method for semi-supervised node classification for graphs [14]. GCN encodes the graph structure using a neural network and trains the supervised target on all labeled nodes. As this method does not calculate node embedding vectors, it is not directly comparable to other graph embedding approaches. Instead, we combine GCN and CGE, in a GCN + CGE hybrid, for the purpose of node classification. Specifically, the softmax output from CGE is used as an additional feature for each node in the GCN model.

Strong results for our GCN + CGE hybrid relative to the GCN baseline are summarized in Table 3. These results suggest that the output of CGE provides extra information to the original GCN model, achieving new state-of-art performances on the CITESEER, CORA, and PUBMED datasets.

4.4 Analysis of Re-weighting

The weighting scores learned in the CGE model are distinctive, a distribution of which is illustrated in Figure 2. To better understand how path re-weighting benefits the graph embedding results, we further analyze the correlation of different graph paths and their weighting scores. We adopt the CGE-LSTM-inductive algorithm in these empirical studies. To summarize, these studies suggest the following observations: (1) CGE automatically retrieves very relevant paths from knowledge base [5] and a hierarchical entity classification dataset [7]. The entities and relations in the graph are extracted from the NELL knowledge base [25]. The goal is to classify the entities in the knowledge base into one of the 210 classes given the features of graph nodes. Following Yang et al. [26], we use three datasets (NELL01, NELL001, NELL0001) generated from the NELL corpus, with different labeled data ratios.

Dataset statistics are shown in Table 1. The original datasets do not distinguish between validation and test, so we randomly select 50% for test and 50% for validation. The same data split is used for the different algorithms.
the graph. (2) The re-weighting scores are highly related to some key attributes of the graph paths. Details underlying these two observations are provided below in Section 4.4.1 and Section 4.4.2 respectively.

\[ \text{Set contain target labels} \]

\[ \text{Contain target labels} \]

\[ \text{Not contain target labels} \]

\[ \text{Path Relevance} \]

\[ \text{Weight} \]

\[ \text{Not contain target labels} \]

\[ \text{Contain target labels} \]

\[ \text{Figure 2. Weighting score distribution of CGE-LSTM-Transductive method on CITESEER dataset} \]

\[ \text{Figure 3. Comparison of average weighting score of graph paths with (light blue) and without (dark blue) target labels in CGE-LSTM.} \]

\[ \text{Class Label} \]

\[ \text{Number} \]

| Class Label               | Number |
|---------------------------|--------|
| Communications of ACM     | 817    |
| Computer                  | 254    |
| IEEE Transactions on Computer | 776   |
| Discrete Mathematics      | 10     |
| Theoretical Computer Science | 114   |
| Computational and Applied Mathematics | 36 |

\[ \text{Table 4. Summary of paper citation graph} \]

To examine if our method can select highly (and perhaps even the most) relevant paths automatically, we randomly sample half of the paths to create a target supervision task. Other labels are masked in the training phase so that they can be leveraged only in an unsupervised manner. We train the CGE model and compare the average weighting scores of the paths. If our hypothesis holds, the most relevant paths (with target labels) should be emphasized by larger weights than other paths that do not contain the target labels. As shown in Figure 3, the results agree well with our intuition that the weighting scores of relevant paths are consistently larger than the remaining paths, at least in this case.

Since we do not know the semantic meaning of the labels, we need another graph to analyze path relevance and hopefully provide more profound insights. We build a sub-graph from a paper citation network extracted from DBLP, ACM, MAG (Microsoft Academic Graph), and other sources. The dataset contains 629,814 papers and 632,752 citations in total. Each paper is associated with the title, authors, abstract, venue, and published year. We exclude the nodes with incomplete information and choose the nodes with a high number of edges (to make the graph denser than the original dataset). Eventually, we obtain a sub-graph with 2,007 nodes and 2,721 edges. Each node belongs to one of 6 classes (venues), as summarized in Table 4. In the experiments, we use each class as the target task, respectively. Taking class Discrete Mathematics as an example, the target task is boiled down to a binary classification problem: identify if an arbitrary node belongs to this class or not. We classify the sampled path into different categories and compare the average re-weighting score of each category. Specifically, if a path contains a node that belongs to class \( y \), the path is classified into this category. Note that a path may contain nodes with different labels so that the categories can overlap. Although the categorization rule is somewhat crude, it does not prevent us from obtaining valid insights into the operation of the CGE algorithm.

Figure 4 shows the average weighting score of paths containing each target when taking another category as the classification target. This figure is similar to the visualization of pairwise attention, where a larger weighting score indicates higher relevance between the corresponding classes. For example, when the supervision target is Discrete Mathematics, the paths related to Discrete Mathematics and Computational and Applied Mathematics are emphasized by larger weighting scores due to the topic relevance. The results suggest that the CGE algorithm underlines the more relevant paths automatically based on the graph structures, although it does not have the exact semantics of each label. Another finding in Figure 4 is that each node has the strongest relevance to itself. Moreover, the average weights of categories Communications of ACM, Computer and IEEE Transactions on Computer are lower. It is reasonable because the three categories contain papers from broader areas and have a larger amount of nodes. Therefore, the CGE algorithm puts more emphasis on the rare paths so that the specialized information can be fully captured.

To demonstrate the benefit of reweighting, Figure 2 shows weight distribution of CITESEER dataset in CGE-LSTM-Transductive, which means the learned weights do have considerable variance, and our re-weighting scheme indeed benefits the target application. Moreover, our algorithm is a general framework which adapts to each dataset automatically. If some paths conform to the labels more naturally, the algorithm will set large weighting score to them, otherwise the weight score should be small. Thus, the variance of weighting scores reflects how much the algorithm benefits from re-weighting. For example, using CGE-LSTM-Transductive algorithm, CITESEER dataset has lower weight variance 0.0272, and PUBMED dataset has higher weight variance 0.0467, which means PUBMED dataset benefits more from path reweighting.

\[ \text{4.4.2 Weight Correlation} \]

We also visualize the correlation between weighting scores and two major properties of the graph path, i.e., length and diversity. Given a path \( (n_i, n_{i+1}, ..., n_j) \), the length is \( j - i + 1 \) and the diversity is the number of distinct nodes in the path. The correlation between path weight and path length is visualized in Figure 4. The x-axis
Figure 4. Correlation coefficient $r$ between path weight and node distance for three different datasets from left to right: (a) CITESEER ($r = -0.82$) (b) CORA ($r = -0.97$) (c) PUBMED ($r = -0.62$).

Figure 5. Correlation coefficient $r$ between path weight and path diversity for three different datasets from left to right: (a) CITESEER ($r = 0.98$) (b) CORA ($r = 0.92$) (c) PUBMED ($r = 0.84$).

Figure 6. Visualization of relevance between different categories.

denotes the path length, and the $y$-axis shows the average weighting score of the corresponding path. Figure 4 shows that the path weight decreases when the length becomes larger. This suggests that FILL IN SOME MORE DETAIL HERE.

Figure 5 shows the impact of node diversity on path weights, visualizing the results of the CGE-LSTM algorithm on the CITESEER, CORA, and PUBMED datasets, respectively. The $x$-axis indicates node diversity, while the $y$-axis shows the average weight of the corresponding path. We observe that the path weight increases with the enlargement of node diversity. The visualization results indicate that the path containing more distinct nodes is much informative, so it receives a higher path weight.

5 Conclusion and Future Work

In this paper, we introduce a new method for semi-supervised graph embedding, namely Customized Graph Embedding (CGE). In contrast to previous semi-supervised graph embedding approaches, our method is capable of capturing the varying importance of different graph paths when learning node embedding vectors. The experimental results demonstrate significant improvements over state-of-the-art methods. Further analysis shows that the CGE algorithm automatically distinguishes highly relevant paths in the graph. In addition, there are strong correlations between the weighting scores and specific properties of graph paths, which agree well with human intuition. One direction of future work is to extend our customized node embedding framework to support the embedding of edges and subgraphs. We also hope to apply this method to other applications, such as search relevance and recommendation systems.

REFERENCES

[1] Amr Ahmed, Nino Shervashidze, Shravan Narayanamurthy, Vanja Josifovski, and Alexander J Smola, 'Distributed large-scale natural graph factorization', in Proceedings of the 22nd international conference on World Wide Web, pp. 37–48. ACM, (2013).
[2] Mikhail Belkin and Partha Niyogi, 'Laplacian eigenmaps and spectral techniques for embedding and clustering', in Advances in neural information processing systems, pp. 585–591, (2002).
[3] Hongyun Cai, Vincent W. Zheng, and Kevin Chang, 'A comprehensive survey of graph embedding: problems, techniques and applications', in IEEE Transactions on Knowledge and Data Engineering, IEEE, (2018).
[4] Shaosheng Cao, Wei Lu, and Qiongkai Xu, ‘Grarep: Learning graph representations with global structural information’, in Proceedings of the 24th ACM international conference on information and knowledge management, pp. 891–900. ACM, (2015).
[5] Andrew Carlson, Justin Betteridge, Bryan Kisiel, Burr Settles, Estevam R Hruschka Jr, and Tom M Mitchell, ‘Toward an architecture for never-ending language learning.’, in AAAI, volume 5, p. 3. Atlanta, (2010).
[6] Hanjun Dai, Bo Dai, and Le Song, ‘Discriminative latent variable models for structured data’, in International Conference on Machine Learning, pp. 2702–2711, (2016).
[7] Bhavana Dalvi, Aditya Mishra, and William W Cohen, ‘Hierarchical semi-supervised classification with incomplete class hierarchies’, in Proceedings of the Ninth ACM International Conference on Web Search and Data Mining, pp. 193–202. ACM, (2016).
[8] James Demmel, Ioana Dumitriu, and Olga Holtz, ‘Fast linear algebra is stable’, Numerische Mathematik, 108(1), 59–91, (2007).
[9] Xiaoyi Fu, Xinqi Ren, Ole J Mengshoel, and Xindong Wu, ‘Stochastic optimization for market return prediction using financial knowledge graph’, in 2018 IEEE International Conference on Big Knowledge (ICBK), pp. 25–32. IEEE, (2018).
[10] Palash Goyal and Emilio Ferrara, ‘Graph embedding techniques, applications, and performance: A survey’, in Knowledge-Based Systems, volume 151, 78–94, Elsevier, (2018).
[11] Alex Graves and Jürgen Schmidhuber, ‘Frame-wise phoneme classification with bidirectional lstm and other neural network architectures’, Neural Networks, 18(5-6), 602–610, (2005).
[12] Aditya Grover and Jure Leskovec, ‘node2vec: Scalable feature learning for networks’, in Proceedings of the 22nd ACM SIGKDD international conference on Knowledge discovery and data mining, pp. 855–864. ACM, (2016).
[13] Sepp Hochreiter and Jürgen Schmidhuber, ‘Long short-term memory’, Neural computation, 9(8), 1735–1780, (1997).
[14] Thomas N Kipf and Max Welling, ‘Semi-supervised classification with graph convolutional networks’, arXiv preprint arXiv:1609.02907, (2016).
[15] Alex Krizhevsky, Ilya Sutskever, and Geoffrey E Hinton, ‘Imagenet classification with deep convolutional neural networks’, in Advances in neural information processing systems, pp. 1097–1105, (2012).
[16] Hanxiao Liu, Karen Simonyan, and Yiming Yang, ‘Darts: Differentiable architecture search’, in arXiv preprint arXiv:1806.09055, (2018).
[17] Mathias Niepert, Mohamed Ahmed, and Konstantin Kutzkov, ‘Learning convolutional neural networks for graphs’, in International conference on machine learning, pp. 2014–2023, (2016).
[18] Ankur Sinha, Pekka Malo, and Kalyanmoy Deb, ‘A review on bilevel optimization: from classical to evolutionary approaches and applications’, IEEE Transactions on Evolutionary Computation, 22(2), 276–295, (2018).
[19] Yao Tang, Jing Zhang, Limin Yao, Juanzi Li, Li Zhang, and Zhong Su, ‘Arnetminer: Extraction and mining of academic social networks’, in Proceedings of the 14th ACM SIGKDD international conference on Knowledge discovery and data mining, pp. 990–998, (2008).
[20] Daixin Wang, Peng Cui, and Wenwu Zhu, ‘Structural deep network embedding’, in Proceedings of the 22nd ACM SIGKDD international conference on Knowledge discovery and data mining, pp. 1225–1234. ACM, (2016).
[21] Xiao Wang, Peng Cui, Jing Wang, Jian Pei, Wenwu Zhu, and Shiqiang Yang, ‘Community preserving network embedding’, in AAAI, pp. 203–209, (2017).
[22] Shuicheng Yan, Dong Xu, Benyu Zhang, Hong-Jiang Zhang, Qiang Yang, and Stephen Lin, ‘Graph embedding and extensions: A general framework for dimensionality reduction’, IEEE transactions on pattern analysis and machine intelligence, 29(1), 40–51, (2007).
[23] Yu Zhao, Zhiyuan Liu, and Maosong Sun, ‘Representation learning for measuring entity relatedness with rich information’, in IJCAI, pp. 1412–1418, (2015).