The Influence of Network Structural Preference on Node Classification and Link Prediction

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Abstract

Recent advances in complex network analysis opened a wide range of possibilities for applications in diverse fields. For the success of these applications, powerful network analysis techniques that depend on the details of node features are necessary. Topology-based node features are realizations of local and global spatial relations among the nodes. Hence, collecting correct information on the node characteristics and the connectivity structure of the neighboring nodes plays the most prominent role in node classification and link prediction in complex network analysis. In the present work, a new feature abstraction method, namely the Transition Probabilities Matrix (TPM), based on embedding anonymous random walks on feature vectors, is introduced. The node feature vectors consist of transition probabilities extracted from sets of random walks in a predefined radius. Transition probabilities are directly related to the local connectivity structure, hence correctly embedded onto feature vectors. The success of the proposed embedding method is tested on node identification/classification and link prediction on three commonly used real-world networks. In real-world networks, nodes with similar connectivity structures are common; Thus, obtaining information from similar networks for predictions on the new networks is the distinguishing characteristic that makes the proposed algorithm superior to the state-of-the-art algorithms in terms of cross-networks generalization tasks.

Keywords: Graph representation learning, Feature learning, Link prediction, Node classification, Anonymous random walk.

1 Introduction

The network concept is a mathematical model of structures where elements, the nodes, are connected through the edges. Network connections are due to semantic or geometric relations among the nodes. Entities of complex networks, such as individuals, molecules, neurons, and computers, are represented by nodes, while their relations or interactions constitute the edges. These structures, the networks, are observed in diverse areas and they are major mathematical tools to model extremely complex systems [1, 2, 3]. Common properties of complex systems, such as clustering [4], forming communities [5],
and new links [6] are all in the interest of researchers of different disciplines, as the common network structures are observed in diverse areas, such as physical, biological, and social sciences. For this reason, networks have opened new opportunities for a better understanding of the underlying dynamics of diverse problems of ever-growing complexity. Moreover, new challenges appear as the sizes of the networks and the complexity of the problems of interest increase. The challenges are manyfold. Among numerous challenges in the field of data mining, obtaining the correct picture of the relations in extremely large networks profoundly exhibits itself. The problems related to network mining, such as community detection [7], node classification [8], link prediction [9], structural network analysis [10], and network visualization [11], are currently being studied.

Nodes in complex networks carry highly structured information. Considerable effort has been devoted to processing this information over the last few years. The issue is to obtain the correct identification of the nodes and the edges. For that, various graph embedding approaches [12] have been introduced. Graph embedding is a map between high-dimensional, highly-structured data and low-dimensional vector space that preserves the structural information of all nodes in the network. This embedding process gains importance due to the growing number of applications that benefit from network data in a broad range of machine learning domains; such as natural language processing (NLP), bioinformatics [13, 14], social network analysis [15, 16], and recently as building blocks of reinforcement learning algorithms [17, 18, 19].

In-network-related problems, node identification/classification, finding relations, and predicting non-apparent connections among the entities are the crucial steps for approaching the problem. Hence, extraction of implicit information present in the network and identification of the existing links are the base requirements of all network-related problems. The link prediction consists of inferring the existence of connections between network entities. The process of link prediction is based on the properties of the nodes and currently observed links [20]. In this sense, link prediction and node identification/classification are inseparable processes in complex network analysis. The techniques designed to solve node identification/classification and link prediction problems are also used in modeling new networks and predicting network evolution mechanisms [21, 22].

Two main challenges of link prediction are unearthing hidden connections or proposing interaction possibilities between pairs of entities based on their properties. For possible connection predictions, the characteristic features of the nodes must be known and embedded into a low-dimensional, machine-processable form. Hence the success of link prediction lies in node identifications and embedding processes. It is common practice in social networks and recommendation systems that two entities with similar interests are more likely to interact. Hence, commonly shared empirical evidence shows that similar nodes are likely to interact. Palla et al. [23] observed that nodes tend to form connected communities. This observation has led to a commonly accepted similarity definition as the amount of relevant direct or indirect paths between nodes. Therefore the challenge in node identification is to define similarities in-network entities. The nodes carry geometric identities, which are the reflections of network topology. In addition to the
topological characteristics, some networks also provide semantic identities for the nodes. This information has applicability among a wide range of different networks. A better understanding of the domain of the network and the existence of semantic information together with the geometric connectivity helps define the similarity of the nodes and increases the efficiency of the similarity algorithm.

In node identification/classification and link prediction, two main obstacles are the lack of information and the size of the real-world networks. Real-world networks consist of millions of nodes, and the number of links is a large multiple of the number of nodes. For such large structures, only geometric information may not be sufficient for node identification. This is particularly true in very sparse networks. The remedy, found in some algorithms, is to extend the region of the network surrounding the node. By increasing the region to collect information, more sites are included in the information gathering process. Here another bottleneck comes into play. Such algorithms are computationally expensive and can not be applied to very large networks. The amount of information collected from the network, the complexity of the algorithm, and the techniques to collect information must be in good balance.

In this work, a new scalable unsupervised node embedding algorithm is introduced. The idea is to calculate the transition probabilities between the neighboring sites. The transition probabilities carry the characteristic connectivity structure of the region around the node in concern. The anonymous walks, which preserve the local structural information, are used in calculating the transition probabilities which form a matrix, namely the Transition Probabilities Matrix (TPM), based on embedding anonymous random walks on feature vectors. In the vicinity of any node, the transition probabilities are unique to the node in concern. The efficiency of the new embedding algorithm lies in its local nature of feature extraction scheme and limited computational effort requirement. Despite its being unique to a node in the given network, the topology of the real-world networks allows the node feature vector to be used in different similar networks for prediction. In this sense, the proposed algorithm exhibits possibilities for a wide range of applications. The possibility of obtaining information from a similar network for predictions on the new networks is the most prevalent characteristic that makes the proposed algorithm superior in comparison with random walks or graph convolutional networks-based models for many real datasets.

The rest of the paper is organized as follows: the next section briefly describes the proposed embedding algorithm TPM. In Section 3, we experimentally test TPM on various network analysis tasks over three citation networks and examine the parameter sensitivity of our proposed method. Finally, our conclusions and future works are presented in section 4.

2 Model

Networks are mathematically represented by graphs $G(V,E)$. Graphs consist of a set of nodes ($V$) and edges ($E$) connecting nodes. Assuming no multiple connections exist among the nodes, a network of $N$ nodes can have at most $E_{Max} = N(N-1)/2$ undirected edges. Here, $E_{Max}$ is the maximum number of possible connections. The network
structure with $E_{Max}$ connections is called "fully connected". Apart from the fully connected networks, all network topologies possess a number of connections less than $E_{Max}$. For any specific network, its topology limits the number of edges. Apart from the fully connected networks, each network has a characteristic pattern of connections around the vertices which makes classification of the network topology possible.

The set of known edges $E$ is considered positive (existent), while the set $E_{Max} - E$ edges constitute the set of non-existent edges and are called negative edges. The unique local connectivity structure of the given network plays the most crucial role in node characterization. Node features are representations of relations among the sites in a given neighborhood radius. At this point, there exist different recipes and methods of node feature extraction ([24] for a survey). Different feature extraction algorithms determine the features of a given node with relative success, computational complexity, and computational expense. The success in determining the features of the nodes is important since it is used as an input for more complicated constructions such as the process of link prediction and community detection. The link prediction is an identification process of the possible candidates of positive edge sets in the set of non-existing edges, $E_{Max} - E$. The prediction process proceeds by assigning weights, $w_{i,j}$ to all possible edges between the nodes, labeled $n_i$ and $n_j$. Weights are model-defined similarity relations between the neighboring nodes. The relations are determined by the rules based on the features of the nodes. The prediction of the possible positive edges is made according to their weight values; the higher the score, the more likely that there exists an edge.

The node feature extraction algorithms commonly employ random walks. Particularly, highly cited DeepWalk [25] and node2vec [26] methods base their feature extraction algorithms on creating large sequences of random walks, which are in a similar setting to sentences in natural language processing. Words and sentences correspond to nodes and random walks, respectively. The relational information between the node in concern and neighboring nodes is obtained from random walk sequences. Apart from these two well-established algorithms, a new, random walk-based approach for learning entire network representation has been introduced [27] recently. In this new approach, random walks are converted to anonymous walk sequences by relabeling nodes in accordance with their occurrences in the walk.

In the present work, anonymous walks, a good candidate for extracting topological features of the whole network, are used to extract feature vectors of the nodes. The proposed method showed that learning the node representation is possible by extracting local connectivity information as node features via anonymous walks.

### 2.1 Anonymous Random Walks

An anonymous random walk is a process of relabelling the nodes. In a local random walk sequence, nodes are labeled according to their occurrence to obtain an anonymous walk sequence. A random walk of length $m$ starting from the node $v_i$ is a set of node labels, $R_w = (v_1, \ldots, v_m)$ where $\forall v_i \in V$. The anonymization process is a mapping between the actual node labels and their occurrences in the sequence, $A_w = (f(v_1), \ldots, f(v_m))$. 
This anonymization process provides encapsulated information to reconstruct the local structure of the graph without requiring global node labels. Micali & Zhu [28] have shown that by using anonymous random walks of length, \( m \), starting from a node \( v_i \) are used to reconstruct the immediate neighborhood of the node \( v_i \). Therefore, using anonymous random walks, local topological features of nodes provide consistent information to construct a global structure of the graph.

2.2 Graph Embedding by Using Anonymous Random Walks

The behavior of the random walks represents the local connectivity structure of any node \( v_i \). The random walk sequences contain new nodes at almost every step if the region is loosely connected, while the probability of returning to the already visited sites increases if the neighborhood is densely connected. This information gives a unique picture of the connectivity structure in the vicinity of the node \( v_i \). Therefore, the transition probabilities are good candidates for the extraction of the topological features of the nodes. The proposed algorithm aims to extract a map of the local topological structure of a given node using the transition probabilities. Hence the connectivity structure, obtained by random walks and converted to anonymous random patterns, is used to extract embedding features of the node. The proposed node embedding is based on the idea of calculating transition probabilities from any node within a certain radius around the node \( v_i \). The probability of reaching a neighboring node is proportional to the degree of the node in concern. In the anonymous random walk sequence, each entity represents either a new node or any already visited node. Hence, from a set of anonymous random walks, all starting from the node \( v_i \), the obtained distribution of reaching a new node or moving back to one of the already visited nodes at the time step \( T_n \) constitute the elements of the transition matrix. Hence, the topological features of a given node are mapped in the transition probabilities matrix. The feature embedding vector of a node \( v_i \) is the transition probabilities matrix obtained from the transition matrix.

2.2.1 Obtaining Transition Matrix-Conceptual Considerations

A set of \( m \) step random walks, starting from the node \( v_i \), are converted to \( m \) step anonymous walks. The initial node, \( v_i \), is considered the zeroth node, \( a_0 \) in the anonymous walk sequence. The first node is one of the nearest neighbors that reached the first step of the random walk. Each neighbor of the node \( v_i \) has the same probability \((1/d_0)\) and if in the sequence, is labeled as the node \( a_1 \). At any step, the node can be any node in the vicinity of the initial node. The underlying topological structure of the neighborhood of the visited nodes is embedded into the details of the next move. In principle, one of the previously visited sites and a new -unvisited- site are reached at any step. The condition to reach any previously visited node is to have a direct link to that node. Hence, the high probability of reaching already visited sites is an indication of the densely connected region. When a node \( v_j \), is reached, there are three possible moves with probabilities:

(i) A new node, \( p_{n\rightarrow m} = \delta_{m,n+1} \frac{d_{m-1}}{d_n} - \sum_k \delta_{k,m} \in A_n \frac{1}{d_n} \)

(ii) Previous node \( p_{n\rightarrow n-1} = \frac{1}{d_n} \)
Table 1: Anonymous random walk probabilities for a set of three-step anonymous walks.

(iii). A node that already visited \( p_{n \rightarrow m} = \sum k \delta_{k, m} \) where \( \sum k \delta_{k, m} \) is the number of edges with the previously visited nodes. The probability of choosing new nodes increases for the nodes with loose connection with the previously visited nodes. If the region is highly connected, the chances of returning to the previously visited nodes will be high.

The calculated probabilities for a three-step anonymous random walk are presented in table 1 to exemplify the idea. From the transitions between the neighboring nodes, the probability matrix with rows (walk steps) and columns (node labels) indicates the transition probabilities during the anonymous random walk 1. From the first neighbour, \( a_1 \) a randomly chosen neighbour \( a_2 \) (with probability \( p_{1 \rightarrow 2} = (d_1 - 1)/d_1 \)) can either be a new entity or the previous node (with probability \( p_{1 \rightarrow 0} = 1/d_1 \)).

Hence a transition probabilities matrix TPM:

\[
TPM = \begin{bmatrix}
0 & P^{(1)}_{1,0} & 0 & 0 \\
0 & 0 & P^{(2)}_{2,1} & 0 \\
P^{(3)}_{2,0} & P^{(3)}_{0,1} + P^{(3)}_{2,1} & P^{(3)}_{0,2} & P^{(3)}_{0,3} + P^{(3)}_{2,3}
\end{bmatrix}
\] (1)

Elements of the transition matrix contain local connectivity information of the nodes; therefore, TPM has practical importance as a node feature for any complex network applications.

2.2.2 Obtaining Transition Matrix - Implementation

In practice, the above transition probabilities matrices 1 are obtained from a given graph by creating a set of random walks starting from each node of the network. The elements of the probability matrix are obtained by counting the number of anonymous random walk sequences.

\[
d_{i, j} = \sum k \delta(A_{i,j}^{(k)}, j)
\] (2)
This process provides a distribution matrix for each node. The obtained distributions are normalized to obtain transition probabilities matrices. The algorithm 1 illustrates the process of creating a set of anonymous random walks and obtaining the transition probabilities matrix.

**Algorithm 1:** Methodology of Creating Transition Probabilities Matrix

**Input:**
- Graph \( G(V; E) \)
- Walks per node \( \eta \)
- Walk length \( m \)

**Output:** Node representation \( X(v) \) for each node \( v \in V \)

1. for each \( v \in V \) do
   2. Initialize \( \text{walks}_v \) to Empty \hspace{1cm} // Random walks set
   3. Initialize \( \text{anons}_v \) to Empty \hspace{1cm} // Anonymous random walks set
   4. Initialize \( \text{tpm}_v = [t]_{(m+1)\times(m+1)} \) \hspace{1cm} // Transition probabilities matrix
   5. for \( i = 0 \) to \( \eta \) do
      6. \( w = \text{UniformlyRandomWalk}(G, v, m) \)
      7. Append a walk \( w \) to \( \text{walks}_v \)
      8. \( \text{anons}_v = \text{AnonymousRandomWalk}(\text{walks}_v, v, m) \)
      9. \( k = 0 \)
   10. for step in \( \text{anons}_v \) do
       11. Update \( \text{tpm}_v[k, \text{step}] += 1 \)
       12. Update \( k += 1 \)
   13. \( X(v) = \text{tpm}_v \)
   14. Return \( X \)

Once the transition probabilities matrix is obtained for each node, the unique features matrix, the transition probabilities matrix, may be used in various ways for calculating the network properties. In this work, the aim is to show how well the local characteristics of a given node are preserved in the definition of the transition probabilities matrix. To this end, it is used as node features in node classification, link prediction, visualization, and cross-networks generalization tasks.
The implementation of the embedding process consists of four steps (Please see, Figure 1):

(i). Creation of a set of random walks, starting from each network node. For each node, \( \eta \) random walks of \( m \) steps.

(ii). For each node, the local connectivity structure is stored as a set of random walk sequences. The information stored in each set of random walks is mapped onto a set of anonymous random walks.

(iii). For each node, the sets of anonymous walks are used to construct the Transition Probabilities Matrix (TPM, \(|m+1| \times |m+1|\) matrix).

(iv). The flattened transition probabilities matrices are used as embedding vectors of each node.

3 Experiments

The proposed method (TPM) is compared against numerous state-of-the-art baseline embedding techniques on four downstream tasks: node classification, link prediction, network visualization, and cross-networks generalization. In addition, parameter sensitivity is conducted. The results demonstrate that our method considerably outperforms the baseline embedding techniques in all the network analysis tasks.

3.1 Datasets

Three different citation networks are employed to test the quality of the proposed embedding method (TPM). Table 2 shows the network statistics of Cora [29], Citeseer [30], and Pubmed [31] networks which are commonly used for testing algorithms and predicting network properties in a considerable number of publications [32, 33, 34, 35, 36]. All of the datasets are open to the public.

Table 2: Overview of three citation networks datasets.

|          | Cora   | CiteSeer | Pubmed |
|----------|--------|----------|--------|
| Nodes    | 2,708  | 3,327    | 19,717 |
| Edges    | 5,429  | 4,732    | 44,338 |
| Classes  | 7      | 6        | 3      |

3.2 Baselines

We compare the performance of our proposed TPM model with six well-established feature extraction algorithms (DeepWalk [25], node2vec [26], LINE [37], GCN-Graph Convolutional Network [38], GraphSAGE [39], and GAT [40]). According to the relevant literature, these baselines have exhibited state-of-the-art embedding performances on the datasets used in our tests. As for parameter settings, the number of walks per node,

\(^1\)https://linqs.soe.ucsc.edu/data [Accessed date: 12 March 2022]
length of walks, window size, and the number of negative sampling are set to 10, 80, 30, and 10 for both DeepWalk and node2vec, respectively. We observed experimentally that setting $p = 2$ and $q = 1$ in node2vec produces superior results across all datasets. We used the recommended hyperparameters and default architectures for the rest baseline methods based on the corresponding original papers. We set the number of walks per node $\eta = 20$ and the length of walks $m = 10$ for our proposed (TPM) model. For the sake of fair comparison, the representational dimension ($d$) for all baselines has been fixed to 128.

### 3.3 Node Classification

Node classification is the process of classifying unlabeled nodes based on their proximity to nodes whose classes are already known (called labeled nodes). The node features embedding data are divided into test and training data sets. Two different train and test sets consist of 80% for training data and 20% for the test data for each of the three networks. To solve the problem of imbalanced target classes, 10-fold cross-validation is performed, and the experiment results are a 10-run average. As the classification method, Logistic Regression, Support Vector Machine (SVM), Decision Tree, and Multi-Layer Perceptron (MLP) algorithms have been used for testing and comparison purposes using the default settings for the scikit-learn Python package [41]. The results of the above-mentioned classification algorithms are within the error limits.

Hence, only the results obtained by using Multi-Layer Perceptron are presented in this section. Table 3 shows classification results of all seven embedding algorithms obtained by using a three-layer neuron network. The Multi-Layer Perceptron model consists of three dense layers of 128, 64 neurons with ReLU activation, while in the final layer number of neurons is chosen according to the number of classes of the given network with softmax activation. Adam optimizer [42] and the categorical_crossentropy loss function employed in the Multi-Layer Perceptron. Micro-F1 and Macro-F1 [43] were used as the accuracy measure. Table 3 exhibits comparative results obtained by using six well-tested node feature extraction methods and the proposed transition probabilities matrix, TPM, based feature extraction algorithm. TPM-based feature vectors performed better in classifying the nodes for all three networks in terms of both Micro-F1 and Macro-F1.

**Table 3: Summary of node classification results. Bold values mean the best results.**

|          | CORA  | CiteSeer | Pubmed |
|----------|-------|----------|--------|
|          | Micro-F1 | Macro-F1 | Micro-F1 | Macro-F1 | Micro-F1 | Macro-F1 |
| DeepWalk | 0.715  | 0.692    | 0.560    | 0.521    | 0.659    | 0.652    |
| node2vec | 0.846  | 0.838    | 0.751    | 0.703    | 0.722    | 0.717    |
| LINE     | 0.797  | 0.793    | 0.582    | 0.536    | 0.728    | 0.723    |
| GCN      | 0.819  | 0.807    | 0.714    | 0.680    | 0.788    | 0.781    |
| GSAGE    | 0.829  | 0.813    | 0.684    | 0.661    | 0.760    | 0.754    |
| GAT      | 0.834  | 0.830    | 0.729    | 0.688    | 0.795    | 0.789    |
| TPM      | **0.858** | **0.849** | **0.781** | **0.743** | **0.821** | **0.818** |
3.4 Link Prediction

Once the success of the proposed embedding methodology has proved to be successful for node classification, it also has been used for link prediction. In the present work, the embedding vectors are used together with four amalgamation operators introduced in the literature [26]. The operators, Average, Hadamard, Weighted-L1, and Weighted-L2 have been tested for the best result. The use of the Hadamard operator has given the best predictions. In this part, we perform binary classification on three citation networks, i.e., Cora, Citeseer, and Pubmed. As the prediction method, Multi-Layer Perceptron (MLP) algorithm has been used for testing and comparison purposes. The Multi-Layer Perceptron model consists of three dense layers of 128, 64 neurons with ReLU activation, while in the final layer sigmoid activation function is employed. All experiments are performed 10 times, and the average AUC is reported. For link prediction at each batch,

(i). 10% of the positive links randomly selected as the test set, the same number of negative links chosen from the original graph.

(ii). The remaining positive and negative links are used as the training set.

Table 4: Summary of link prediction results measured by AUC. Bold values mean the best results.

| Method   | CORA   | CiteSeer | Pubmed  |
|----------|--------|----------|---------|
| DeepWalk | 0.851  | 0.824    | 0.864   |
| node2vec | 0.927  | 0.941    | 0.912   |
| LINE     | 0.856  | 0.803    | 0.833   |
| GCN      | 0.918  | 0.889    | 0.957   |
| GSAGE    | 0.910  | 0.877    | 0.931   |
| GAT      | 0.908  | 0.914    | 0.924   |
| TPM      | **0.959** | **0.962** | **0.969** |

Table 4 gives the comparisons of the link prediction results. Transition probabilities matrix-based feature vectors, TPM exhibits comparatively good results.

![Visualization of 2D representations for LFR network.](image)

Figure 2: Visualization of 2D representations for LFR network.
3.5 Visualization

Visualization is one of the best methods for testing the success of embedding algorithms. Using a controlled experiment approach, objective discrimination between the algorithms can be realized. To start the experiment, a common approach is to use well-known networks, such as Zachary Karate Club [44], or Cora [29] for comparison purposes. Despite the common usage of these networks, real-world networks exhibit very different characteristic heterogeneous distributions of community sizes and node degrees. For this reason, instead of using any one of the commonly used networks, a network creation algorithm Lancichinetti–Fortunato-Radicchi [45] (LFR algorithm), which is particularly designed for testing embedding algorithms is used. The TPM algorithm was applied to a network of 3 communities, 600 nodes, and 1334 edges. LFR algorithm has an extra parameter $\mu$ that controls the "noise". "Noise" parameter, which takes values between 0 and 1, is an indicator of the heterogeneity of the network. In this work, the heterogeneity parameter is taken as $\mu = 0.2$. The visualization results of two well-established embedding algorithms, DeepWalk, and GCN, are compared for visual inspection with the proposed algorithm (TPM). For dimensional reduction t-Distributed Stochastic Neighbor Embedding (t-SNE) visualization tool [46] is used. Figure 2 shows that our model is capable of producing more compact and distinct clusters than the other two methods. From Figure 2, we observe that the representations generated by the DeepWalk method have multiple clusters that overlap with each other. The GCN model provides a little more coherent representation because it transfers the attributes of the neighboring nodes through the connectivity structure to capture additional global structural data. The visual inspection of Figure 2c indicates that the proposed embedding algorithm (TPM) has distinct separation among three classes of the created network.

3.6 Cross-networks generalization: Scale-free networks

Scale-free networks have a unique position since they constitute most real-world networks [47, 48]. Nodes with similar connectivity structures are ubiquitous in scale-free networks due to their heavy-tailed character, which means they exhibit power-law degree distributions. Therefore, we perform the task of cross-networks generalization, which is learning information from networks of similar connectivity structures to make predictions on new networks. In this experiment, we conduct a link prediction task on networks previously unseen during training. We generate 12 Barabási-Albert networks (BA) with the following parameters: $n = \{1000, 10000\}$ (number of nodes) and $\alpha = 6$ (how many existing nodes may be attached to a new one). We train each embedding method on ten networks and then calculate the average AUC score on two test networks. We compare the performance of our proposed TPM model with four feature extraction algorithms (DeepWalk, node2vec, GCN, and GraphSAGE), and the experimental results are shown in Table 5. For all random walk-based models (TPM, DeepWalk, and node2vec), we run a total of 50 random walks of 10 steps for each node (5 random walks from each generated training Barabási-Albert network). For all graph convolutional networks-based models (GCN and GraphSAGE), we perform information aggregation per node evenly from ten generated training Barabási-Albert networks. Moreover, in the generated Barabási-Albert networks, nodes lack features. For features, we use node degrees and an embedding weight that is updated for each node during training. Table 5
shows that TPM significantly outperforms all four feature extraction algorithms. These results demonstrate that our TPM model well captures the local structural patterns of nodes, even in different networks having similar topologies.

Table 5: Summary of results in terms of cross-networks generalization for two scale-free networks. Bold values mean the best results.

| Scale-free networks (n = 1,000) | DeepWalk | node2vec | GCN   | GSAGE | TPM   |
|-------------------------------|----------|----------|-------|-------|-------|
| 0.611                         | 0.664    | 0.702    | 0.713 | **0.746** |
| Scale-free networks (n = 10,000) | 0.620    | 0.659    | 0.719 | 0.717 | **0.751** |

3.7 Parameter Sensitivity

The proposed embedding algorithm, TPM, includes two essential hyper-parameters, $\eta$, and $m$, the number of walks per node and the length of walks. The Micro-F1 score of node classification over Cora, Citeseer, and Pubmed with various $\eta$ and $m$ demonstrate the impact of the hyper-parameters in TPM. The number of walks per node $\eta$ and length of walks $m$ were set to $\{5, 10, 15, 20, 25, 30\}$ and $\{5, 8, 10, 15, 20, 30, 50\}$. The training ratio was set to 80%, and the results can be seen in Figure 3. As shown in Figure 3a, the performance of the proposed model is relatively steady over the three citation networks when $\eta$ varies from 20 to 30. Hence, the larger the number of walks, the better the model’s performance since the characteristic connectivity structure of the region around the given node is captured more thoroughly. In Figure 3b, the proposed embedding algorithm TPM achieves the best Micro-F1 score over the three citation networks when $m$ equals 10. The score gradually decreases with increasing walk length because the walker may move away from the node’s neighborhood when the walk length $m$ is too large, thereby failing to incorporate local structural patterns properly into the walk statistics. Consequently, the parameters $\eta$ and $m$ must be tuned appropriately for various applications.

![Figure 3](image.png)

Figure 3: Results of parameter experiment. (a) Influence of the number of walks $\eta$ on three citation networks. (b) Influence of the length of walks $m$ on three citation networks.
Conclusions

The traditional machine learning frameworks can only be applied to networks, by mapping high dimensional information contained in the network, to low dimensional vector spaces. Hence, a vector representation of each node, which is called node embedding, is an essential initial step for processing the data obtained from networks. The embedding algorithm must represent the graph’s connectivity structure, which requires mixing properties of nodes and edges. Most of the existing representation learning techniques concentrate only on the local structure of nodes, hence lacking representation of local structural patterns in downstream network analysis tasks.

The present study introduces a new, scalable unsupervised node embedding algorithm that inherently contains the local connectivity structure of the nodes. Moreover, since the node embeddings overlap, node similarities are also part of the embedding representation. The proposed algorithm uses anonymous walks for structural node embeddings. Each walk, starting from a given node, collects local structural information in a predetermined neighborhood radius. Each node in the network is represented by a unique transition probabilities matrix. Elements of each transition probabilities matrix consist of the probability of reaching the neighboring nodes starting from the original. Hence the transition probabilities matrices of neighboring nodes overlap. The overlapping transition probabilities matrices ensure the correct similarity measures between the neighboring nodes. Moreover, the transition probabilities matrix method has superior prediction potential in the identification of similar connectivity structures in remote parts of the network. This possibility extends the use of the proposed embedding vectors, created using the information of a given network, onto unstudied networks. In the present work, the flattened transition probabilities matrix elements are used as node feature vectors. Experiments on three commonly used real-world networks and synthetic networks, presented in the experiments section, demonstrated the effectiveness of the proposed method (TPM). For future work, the extensibility of TPM on attributed networks and temporal dynamic networks will be considered.

References

[1] Réka Albert and Albert-László Barabási. Statistical mechanics of complex networks. Reviews of modern physics, 74(1):47, 2002.

[2] Albert-László Barabási. Network science. Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences, 371(1987):20120375, 2013.

[3] Mark Newman. Networks. Oxford university press, 2018.

[4] Xiaohui Han, Lianhai Wang, Chaoran Cui, Jun Ma, and Shuhui Zhang. Linking multiple online identities in criminal investigations: A spectral co-clustering framework. IEEE Transactions on information forensics and security, 12(9):2242–2255, 2017.

[5] Hocine Cherifi, Gergely Palla, Boleslaw K Szymanski, and Xiaoyan Lu. On community structure in complex networks: challenges and opportunities. Applied Network Science, 4(1):1–35, 2019.
[6] Kuo Chi, Guisheng Yin, Yuxin Dong, and Hongbin Dong. Link prediction in dynamic networks based on the attraction force between nodes. *Knowledge-Based Systems*, 181:104792, 2019.

[7] Santo Fortunato. Community detection in graphs. *Physics reports*, 486(3-5):75–174, 2010.

[8] Smriti Bhagat, Graham Cormode, and S Muthukrishnan. Node classification in social networks. In *Social network data analytics*, pages 115–148. Springer, 2011.

[9] Víctor Martínez, Fernando Berzal, and Juan-Carlos Cubero. A survey of link prediction in complex networks. *ACM computing surveys (CSUR)*, 49(4):1–33, 2016.

[10] Gueorgi Kossinets and Duncan J Watts. Empirical analysis of an evolving social network. *science*, 311(5757):88–90, 2006.

[11] Roberto Tamassia. *Handbook of graph drawing and visualization*. CRC press, 2013.

[12] Ke Sun, Lei Wang, Bo Xu, Wenhong Zhao, Shyh Wei Teng, and Feng Xia. Network representation learning: From traditional feature learning to deep learning. *IEEE Access*, 8:205600–205617, 2020.

[13] Chensi Cao, Feng Liu, Hai Tan, Deshou Song, Wenjie Shu, Weizhong Li, Yiming Zhou, Xiao Chen Bo, and Zhi Xie. Deep learning and its applications in biomedicine. *Genomics, proteomics & bioinformatics*, 16(1):17–32, 2018.

[14] Xiao-Meng Zhang, Li Liang, Lin Liu, and Ming-Jing Tang. Graph neural networks and their current applications in bioinformatics. *Frontiers in genetics*, 12, 2021.

[15] Mark S Handcock, Adrian E Raftery, and Jeremy M Tantrum. Model-based clustering for social networks. *Journal of the Royal Statistical Society: Series A (Statistics in Society)*, 170(2):301–354, 2007.

[16] Angelo Mele. A structural model of homophily and clustering in social networks. *Journal of Business & Economic Statistics*, pages 1–13, 2021.

[17] Peter W Battaglia, Jessica B Hamrick, Victor Bapst, Alvaro Sanchez-Gonzalez, Vinicius Zambaldi, Mateusz Malinowski, Andrea Tacchetti, David Raposo, Adam Santoro, Ryan Faulkner, et al. Relational inductive biases, deep learning, and graph networks. *arXiv preprint arXiv:1806.01261*, 2018.

[18] Alvaro Sanchez-Gonzalez, Nicolas Heess, Jost Tobias Springenberg, Josh Merel, Martin Riedmiller, Raia Hadsell, and Peter Battaglia. Graph networks as learnable physics engines for inference and control. In *International Conference on Machine Learning*, pages 4470–4479. PMLR, 2018.

[19] Ziwei Zhang, Peng Cui, and Wenwu Zhu. Deep learning on graphs: A survey. *IEEE Transactions on Knowledge and Data Engineering*, 2020.

[20] David Liben-Nowell and Jon Kleinberg. The link-prediction problem for social networks. *Journal of the American society for information science and technology*, 58(7):1019–1031, 2007.
[21] Maria Evangelia G Pavlopoulou, Grigoris Tzortzis, Dimitrios Vogiatzis, and George Paliouras. Predicting the evolution of communities in social networks using structural and temporal features. In 2017 12th International Workshop on Semantic and Social Media Adaptation and Personalization (SMAP), pages 40–45. IEEE, 2017.

[22] Taleb Khafaei, Alireza Tavakoli Taraghi, Mehdi Hosseinzadeh, and Ali Rezaee. Tracing temporal communities and event prediction in dynamic social networks. Social Network Analysis and Mining, 9(1):1–11, 2019.

[23] Gergely Palla, Imre Derényi, Illes Farkas, and Tamás Vicsek. Uncovering the overlapping community structure of complex networks in nature and society. nature, 435(7043):814–818, 2005.

[24] Mengjia Xu. Understanding graph embedding methods and their applications. SIAM Review, 63(4):825–853, 2021.

[25] Bryan Perozzi, Rami Al-Rfou, and Steven Skiena. Deepwalk: Online learning of social representations. In Proceedings of the 20th ACM SIGKDD international conference on Knowledge discovery and data mining, pages 701–710, 2014.

[26] 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, pages 855–864, 2016.

[27] Sergey Ivanov and Evgeny Burnaev. Anonymous walk embeddings. In International conference on machine learning, pages 2186–2195. PMLR, 2018.

[28] Silvio Micali and Zeyuan Allen Zhu. Reconstructing markov processes from independent and anonymous experiments. Discrete Applied Mathematics, 200:108–122, 2016.

[29] Andrew Kachites McCallum, Kamal Nigam, Jason Rennie, and Kristie Seymore. Automating the construction of internet portals with machine learning. Information Retrieval, 3(2):127–163, 2000.

[30] C Lee Giles, Kurt D Bollacker, and Steve Lawrence. Citeseer: An automatic citation indexing system. In Proceedings of the third ACM conference on Digital libraries, pages 89–98, 1998.

[31] Prithviraj Sen, Galileo Namata, Mustafa Bilgic, Lise Getoor, Brian Galligher, and Tina Eliassi-Rad. Collective classification in network data. AI magazine, 29(3):93–93, 2008.

[32] Hongchang Gao and Heng Huang. Deep attributed network embedding. In Twenty-Seventh International Joint Conference on Artificial Intelligence (IJCAI), 2018.

[33] Bonaventure Molokwu, Shao Bhatta Shuvo, Narayan C Kar, and Ziad Kobti. Node classification and link prediction in social graphs using rlvecn. In 32nd International Conference on Scientific and Statistical Database Management, pages 1–10, 2020.
[34] Yu Xie, Peixuan Jin, Maoguo Gong, Chen Zhang, and Bin Yu. Multi-task network representation learning. *Frontiers in Neuroscience*, 14:1, 2020.

[35] Sarmad N Mohammed and Semra Gündüç. Degree-based random walk approach for graph embedding. *Turkish Journal of Electrical Engineering and Computer Sciences*, 30(5):1868–1881, 2022.

[36] Davide Buffelli and Fabio Vandin. The impact of global structural information in graph neural networks applications. *Data*, 7(1):10, 2022.

[37] Jian Tang, Meng Qu, Mingzhe Wang, Ming Zhang, Jun Yan, and Qiaozhu Mei. Line: Large-scale information network embedding. In *Proceedings of the 24th international conference on world wide web*, pages 1067–1077, 2015.

[38] Max Welling and Thomas N Kipf. Semi-supervised classification with graph convolutional networks. In *J. International Conference on Learning Representations (ICLR 2017)*, 2016.

[39] Will Hamilton, Zhitao Ying, and Jure Leskovec. Inductive representation learning on large graphs. *Advances in neural information processing systems*, 30, 2017.

[40] Petar Velickovic, Guillem Cucurull, Arantxa Casanova, Adriana Romero, Pietro Lio, and Yoshua Bengio. Graph attention networks. *stat*, 1050:20, 2017.

[41] Fabian Pedregosa, Gaël Varoquaux, Alexandre Gramfort, Vincent Michel, Bertrand Thirion, Olivier Grisel, Mathieu Blondel, Peter Prettenhofer, Ron Weiss, Vincent Dubourg, et al. Scikit-learn: Machine learning in python. *the Journal of machine Learning research*, 12:2825–2830, 2011.

[42] Diederik P Kingma and Jimmy Ba. Adam: A method for stochastic optimization. *arXiv preprint arXiv:1412.6980*, 2014.

[43] Mohammed J Zaki, Wagner Meira Jr, and Wagner Meira. *Data mining and analysis: fundamental concepts and algorithms*. Cambridge University Press, 2014.

[44] Michelle Girvan and Mark EJ Newman. Community structure in social and biological networks. *Proceedings of the national academy of sciences*, 99(12):7821–7826, 2002.

[45] Andrea Lancichinetti, Santo Fortunato, and Filippo Radicchi. Benchmark graphs for testing community detection algorithms. *Physical review E*, 78(4):046110, 2008.

[46] Laurens Van der Maaten and Geoffrey Hinton. Visualizing data using t-sne. *Journal of machine learning research*, 9(11), 2008.

[47] Albert-László Barabási and Réka Albert. Emergence of scaling in random networks. *science*, 286(5439):509–512, 1999.

[48] Albert-László Barabási and Eric Bonabeau. Scale-free networks. *Scientific american*, 288(5):60–69, 2003.