**RiWalk: Fast Structural Node Embedding via Role Identification**

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**Abstract**—Nodes performing different functions in a network have different roles, and these roles can be gleaned from the structure of the network. Learning latent representations for the roles of nodes helps to understand the network and to transfer knowledge across networks. However, most existing structural embedding approaches suffer from high computation and space cost or rely on heuristic feature engineering.

Here we propose RiWalk, a flexible paradigm for learning structural node representations. It decouples the structural embedding problem into a role identification procedure and a network embedding procedure. Through role identification, rooted kernels with structural dependencies kept are built to better integrate network embedding methods. To demonstrate the effectiveness of RiWalk, we develop two different role identification methods named RiWalk-SP and RiWalk-WL, respectively and employ random walk based network embedding methods.

Experiments on within-network classification tasks show that our proposed algorithms achieve comparable performance with other baselines while being an order of magnitude more efficient. Besides, we also conduct across-network role classification tasks. The results show potential of structural embeddings in transfer learning. RiWalk is also scalable, making it capable of capturing structural roles in massive networks.

**Index Terms**—structural embedding; network embedding; graph kernel; structural role;

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**I. INTRODUCTION**

Nodes in the same network always perform different functions and have different behaviors, leading them to different roles, e.g., leaders of communities or bridges between groups. At the same time, nodes of different networks may share similar roles, e.g., hubs of airline networks and managers of companies. Identifying roles in networks will help researchers to gain a thorough understanding of network evolution and to transfer their knowledge across networks, thus leading to better performances of several real-world tasks, which may include fraud detection [1], network integration [2], protein function prediction of protein interaction networks [3] or individualized recommendation [4].

Intuitively, roles can be reflected in the network topologies, for example, leaders are corresponding to hub nodes of cliques and bridges between groups are corresponding to structural holes. In fact, structural role identification has been studied for decades. However, despite their achievements, most traditional approaches [5]–[7] require computation of multiple complicated graph-metrics, such as PageRank value [8], structural hole value [9] or clustering coefficient [10]. Thus, these approaches are often ad hoc and time-consuming, making them hard to extend to massive networks.

On the other hand, graph representation learning (also known as network embedding), recently shows great potential for capturing neighborhood similarities and community memberships in low-dimensional representations. The learned embeddings can be used as features to boost the results of downstream machine learning tasks. Due to its simplicity, efficiency, and scalability, graph representation learning makes it possible for machine learning on large-scale networks.

However, most state-of-the-art network embedding algorithms [11]–[13] assume that the more two nodes are densely connected, the more similar they are supposed to be. Thus, two nodes residing distantly in a network will be embedded far apart, even if they may share similar roles in the network. Therefore, it is impossible to directly apply typical network embedding methods to learn structural embeddings.

Several approaches [14], [15] have been proposed to fill this gap in recent years. Despite their success, these methods do not make full use of existing network embedding approaches, making them either rely heavily on heuristic feature engineering or suffer from high computation and space cost, thus hard to generalize across graphs and scale to massive networks.

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More details about existing methods will be discussed in Section II.

To overcome the above limitations, we propose RiWalk (Ri as role identification), an algorithmic paradigm that relabels context nodes with their structural roles in the anchor nodes’ local subgraphs (as illustrated in Fig. 1), and thus typical network embedding methods can be directly applied to learn structural embeddings.

The key ideas of RiWalk are as follows:

- RiWalk decouples the structural embedding problem into two procedures: the role identification procedure and the network embedding procedure.
- The role identification procedure takes the idea of substructure and relabeling from graph kernel methods. However, distinct from traditional graph kernels, structural dependencies between substructures are kept after role identification. Through role identification, graph kernel methods and network embedding algorithms are better integrated compared to prior works, thus leading to a lower complexity.
- Since RiWalk is a general meta-strategy, both the role identification procedure and the embedding procedure can be customized for particular purposes. The framework is simple and efficient because of the decoupling, making it easy to apply to different graphs.

To demonstrate the effectiveness of our proposed model, we put forward two different role identification methods named RiWalk-SP and RiWalk-WL, respectively. RiWalk-SP is based on an intuition that two nodes are structurally similar if their neighbor nodes have similar degrees. The identifiers generated by RiWalk-SP are in line with the substructures of the Shortest-Path graph kernel. RiWalk-WL takes the idea of neighborhood aggregation from the Weisfeiler-Lehman graph kernel. It considers permutations of distances to signify the relative positions of context nodes from the anchor node, resulting in an ability to capture more fine-grained connectivity patterns.

We compare our proposed methods with state-of-the-art baselines [11], [14], [15] on several real-world datasets. Firstly, we illustratively demonstrate the difference between typical network embedding and structural embedding on an expressway network. Results show that typical network embedding methods assume the predicted labels to be smoothly distributed over the network. Thus they are not capable of identifying roles of nodes, since roles always distribute non-smoothly over graphs.

Then we carry out two node classification tasks: a within-network node classification task, where the training data and the testing data come from the same network and an across-network classification task, where classifiers are trained on one network but used to predict the class labels of the nodes in other networks. Besides, an experiment of structural role identification is also conducted. The results of the these experiments prove the effectiveness and efficiency of our proposed model. Specifically, while RiWalk-SP shares similar intuition with our baseline method, by using our proposed paradigm, RiWalk-SP learns more robust node representations. Meanwhile, we show that our proposed algorithms achieve comparable performances with other baselines while being an order of magnitude more efficient.

To summarize, our paper makes the following contributions:
1) We propose the RiWalk, a novel paradigm for learning structural embeddings of nodes. It is based on structural role identifications of subgraphs and can better integrate graph kernels with network embedding methods to leverage recent advancements in network embedding.
2) We put forward two different role identification methods and demonstrate that despite its simplicity, this framework performs surprisingly well on real-world datasets and outperforms state-of-the-art baselines.
3) We discuss the gaps between typical network embedding and structural embedding and give an example to demonstrate the differences.
4) We conduct an across-network node classification task, which proves that structural embeddings can be used for transfer learning.

The rest of this paper is arranged as follows. In Section II, we briefly discuss related works along with their limitations. Section III formally defines the problem of structural role embedding and briefly introduces two related graph kernel methods. We present the RiWalk framework in details in Section IV. In Section V, we empirically evaluate RiWalk on real-world graphs. Finally, we conclude in Section VI.

II. RELATED WORK

Our work is inspired by two lines of research: 1) graph kernels and 2) network embedding.

a) Graph Kernels: Graph kernels are functions that measure similarities between graphs. Most graph kernel methods [16]–[18] can be viewed as R-convolution kernels, which first decompose graphs into substructures and then compute graph similarities based on similarities between these components [19]. With different definition of substructure or different choice of similarity measure, one can define different graph kernels.

b) Network Embedding: Network embedding methods aim to learn distributed representations of nodes in a network. DeepWalk [12] first leverages word2vec [20] to learn a language model for a network by treating truncated random walks as sentences and neighbor nodes as semantically similar words. node2vec [11] generalizes this model by adding flexibility in neighborhood exploring. LINE [13] learns embeddings through optimizing an objective function which preserves both the first- and the second-order proximities. Through these models, distributed representations can successfully capture neighborhood similarities and be directly used as features for machine learning tasks.

Arguably, most presented network embedding approaches learn representations of nodes by minimizing the distance between two distributions. Both the two distributions represent the conditional probabilities of context nodes “generated” by
the anchor nodes but one is specified by the embeddings and the other one is empirical. For example, in DeepWalk and node2vec, context nodes are a set of nodes which appear in the same fixed-sized sliding window with the anchor node in random walks, and in LINE, context nodes are directly linked with the anchor node (first-order proximity) or share the same neighbor node with the anchor node (second-order proximity). Therefore, two nodes will be embedded closely only if they are close and densely connected in the network. When we want two structurally similar nodes which reside distantly (or even in different isolated parts) to be embedded closely, typical network embedding approaches are not suitable.

Considerable effort has been made for learning structural embeddings of nodes recently, for example, struc2vec [15] and GraphWave [14]. struc2vec takes three steps to get structural embeddings. First, it utilizes a simplified graph kernel to measure structural similarities between nodes in different neighborhood sizes. Secondly, it encodes these similarities into weights of edges to construct a hierarchy of complete graphs, such that edges between structurally similar nodes have small weights. Thirdly, a random walk based embedding method is used to learn node embeddings. While this method is effective, it suffers from high time and space cost due to the pair-wise subgraph comparation and complete graph construction.

GraphWave applies graph diffusion kernels [21] and treats these kernels as probability distributions over the embedding. Then embeddings can be obtained by characterizing the distributions using empirical characteristic functions [22]. Since it needs to compute a full eigendecomposition of a large matrix, GraphWave suffers high space cost.

Note that though several approaches [23]–[25] have been proposed to learn representations with structural information, these methods are not designed to learn pure topological embeddings. Since pure topological embeddings can be used for transfer learning (to be shown in V-D), while neighborhood-based embeddings are not, structural representation learning is somewhat orthogonal to typical network embedding.

III. PRELIMINARIES

A. Problem Formulation

Let \( G = (V, E) \) denote an undirected unweighted graph, where \( V \) is the set of \( |V| \) nodes \( \{v_1, v_2, \ldots, v_{|V|}\} \) and \( E \subseteq V \times V \) is the set of \( |E| \) edges. Given only \( G \) itself, we aim to learn a mapping function from nodes to low-dimensional representations \( f: V \rightarrow \mathbb{R}^d \), where \( d \ll |V| \) is the number of dimensions of the learned representations. In the latent space, we hope that structural similar nodes are represented closely and nodes with different local structures are represented far apart.

Here we introduce the basic notations and terminologies which will be used throughout this paper. Given a graph \( G \) defined as above, we use \( s_{ij} \) to denote the distance (i.e., the length of the shortest path) between two nodes \( v_i \) and \( v_j \). Then we let \( k^* \) to denote the diameter (i.e., the length of the longest shortest path between any pairs of nodes) of \( G \). Given a specific node \( v_i \), the set of neighbor nodes within radius \( k \) of \( v_i \) is defined as \( N_i^k = \{v_j \in V \mid s_{ij} \leq k\} \). Thus for each \( v_i \in V, V = N_i^\infty \). Letting \( N_i = N_i^1 \) denote the set of direct neighbor nodes of \( v_i \), we use \( d_i = |N_i| \) to denote its degree.

Given a set of nodes \( S \subseteq V \), we use \( G(S) \) to denote the subgraph induced by \( S \).

B. Graph Kernels

Firstly, we summarize the core concepts of graph kernels and introduce the two of them that are related to our work. Given a set of graphs \( \mathcal{G} \), R-convolution kernels first decompose each graph into atomic substructures. Then for each two graphs \( G, G' \in \mathcal{G} \), a kernel function \( K \) is defined as

\[
K(G, G') = \langle \phi(G), \phi(G') \rangle,
\]

where \( \phi(G) \) denotes a vector of counts of substructures in \( G \) and \( \langle \cdot, \cdot \rangle \) denotes an inner product in a reproducing kernel Hilbert space (RKHS).

The two graph kernels to be introduced are both defined on labeled graphs. A graph is labeled if there is a mapping \( l: V \rightarrow \Sigma \) where \( \Sigma \) is a discrete set of labels.

1) Shortest-path graph kernel: The Shortest-Path graph kernel [16] decomposes each graph \( G \in \mathcal{G} \) into shortest paths. Specifically, let \((l(v_a), l(v_b), s_{ab})\) denote a triplet where \( s_{ab} \) signifies the length of the shortest path between two node \( v_a, v_b \) and \( (l(v_a), (l(v_b)) \) are the labels of them, respectively. By collecting all the triplets in \( G \), one can get a list of unique triplets \( T_G \) and the Shortest-Path kernel can be defined as:

\[
K_{SP}(G, G') = \langle \phi_{T_G}(G), \phi_{T_G}(G') \rangle,
\]

where \( \phi_{T_G}(G) \) denotes a vector and the \( i \)-th element of it is the count of the \( i \)-th triplet \( T_G^{(i)} \) occurring in \( G \).

2) Weisfeiler-Lehman graph kernel: The Weisfeiler-Lehman kernel [17] decomposes each graph \( G \in \mathcal{G} \) into subtree patterns. Specifically, it replaces the label of each node in a graph with a compressed multiset label. The multiset label consists of the original label of the node and the sorted labels of its neighbors. This relabeling procedure is repeated for multiple times. By collecting all labels that occur at least once in one relabeling iteration of one graph of \( \mathcal{G} \) as a list \( L_G \). The Weisfeiler-Lehman kernel can be defined as:

\[
K_{WL}(G, G') = \langle \phi_{L_G}(G), \phi_{L_G}(G') \rangle,
\]

where \( \phi_{L_G}(G) \) denotes a vector and the \( i \)-th element of it is the count of the \( i \)-th label \( L_G^{(i)} \) occurring in the relabeling iterations of \( G \).

IV. RIVALK

As stated above, there are gaps between structural embedding and typical network embedding. We further summarize them as follows:

- Existing network embedding methods treat nodes in anchor nodes’ local neighborhoods as contexts. Thus two anchor nodes residing far apart can hardly be related.
- To identify structural roles, one should focus on how an anchor node connects with its context nodes, rather
than which nodes it links to. However, typical network embedding methods focus on the latter.  
- Typical network embedding methods require some measure of smoothness (e.g., community memberships) over the network [14] while roles are not (to be shown in V-B).

To fill these gaps, existing structural embedding methods take a simple intuition: treating each node’s local topology as a subgraph of the original graph, two nodes have similar roles if their local subgraphs are similar. One can come up with a naive solution based on this intuition: first use graph kernels to compute similarities between subgraphs, then construct a complete graph in which edge weights are proportional to subgraph similarities, finally employ network embedding methods on this weighted complete graph to learn node representations.

However, since typical graph kernels are built on graph level, subgraphs seen from perspectives of different nodes are not distinguished. struc2vec corrected this by building a hierarchy based on a simplified rooted kernel. Despite its success, struc2vec still suffers time and space cost due to the pair-wise subgraph comparison and complete graph construction.

To tackle the above problems, we take the idea of relabeling and substructures from graph kernels and introduce a role identification procedure to better integrate the network embedding process. Role identification traverses the subgraphs to capture the connecting patterns of the context nodes in their relation with the anchor node (i.e., roles of the context nodes in the subgraphs), and encode these patterns into new identifiers to get relabeled subgraphs. Thus a bridge from “how” to “which” is built.

In the relabeled subgraphs, context nodes which connect with their anchor nodes in the same manner will be treated as the same node even if they belong to different subgraphs. At the same time, structurally similar anchor nodes tend to have similar connecting patterns with their context nodes, and thus they share many context nodes in their relabeled subgraphs. Therefore, they are indirectly densely connected, and thus typical network embedding methods can be directly applied to learn structural embeddings.

Given a specific anchor node $v_i$ and a radius $k \leq k^*$, the role identification for a local subgraph $G(N_i^k)$ is a mapping function $\psi_i : N_i^k \setminus \{v_i\} \to I_i^k$, where $I_i^k$ is a set of new identifiers.

In the following subsections, we will propose two different role identification methods.

### A. RiWalk-SP

Firstly, we take similar intuition with struc2vec and develop a role identification method named RiWalk-SP. We assume that two nodes are structurally similar if degrees of their neighbor nodes exhibit similar distribution. Similar to struc2vec, which measures similarities for different neighborhood sizes, we take distances between context nodes and anchor nodes into account. Given a specific anchor node $v_i$ and a radius $k \leq k^*$, for a subgraph $G(N_i^k)$, we define the following role identification function:

$$\psi_i(v_j) = h(\delta_i) \oplus h(\delta_j) \oplus s_{ij}, \quad \text{for each } v_j \in N_i^k \setminus \{v_i\},$$  \hspace{1cm} (4)

where $\oplus$ is the concatenation operator. To avoid the exponential growth in the number of new identifiers, we employ a discount function, which is defined as:

$$h(x) = [\log_2(x+1)].$$ \hspace{1cm} (5)

Both $\delta_i, \delta_j$ and $s_{ij}$ are simple to measure, requiring no more than traversing (e.g., breadth-first searching) each member of $G(N_i^k)$.

**Relation with the Shortest-path kernel:** It can be observed that the new identifiers generated by RiWalk-SP are in line with the triplets in the Shortest-Path kernel. The difference between them is that RiWalk-SP is rooted and it can be viewed as having a labelling mapping defined as:

$$l(v_j) = h(\delta_j), \quad \text{for each } v_j \in N_i^k.$$ \hspace{1cm} (6)

### B. RiWalk-WL

Since degree is an ambiguous measure of structural connectivities. struc2vec and RiWalk-SP lack the ability to distinguish between context nodes that are at the same distance from $v_i$ and have the same degrees. Fig. 1 gives an illustrative example. As we can see, since node $b$ and $d$ have the same degree of 3 and are both at distance of 1 from the anchor node $a$, they cannot be distinguished by struc2vec and RiWalk-SP, even though $d$ is more densely connected with $a$ than $b$. Therefore, we develop the RiWalk-WL based on permutations of distances to capture fine-grained connectivity patterns.

Basically, there will always be multiple paths from the anchor node to each context node in its local subgraph, and permutations of these paths constitute the local topology. Thus, topological information (e.g., motifs) will be implied in the permutation of lengths of these paths.

For each context node, its relative position to the anchor node can be precisely revealed in the enumeration of all possible paths from the anchor node to it. However, enumerating all possible paths between two nodes is time consuming. On the other hand, the simplest definition of relative position is the length of the shortest path but the definition is too broad. We trade off between the above two definitions and develop a neighborhood aggregation process to get the relative positions of the context nodes.

Given a specific anchor node $v_i$ and a radius $k \leq k^*$, for a subgraph $G(N_i^k)$, we let each context node $v_j \in N_i^k$ correspond to a vector $x_{ij}$ of length $k + 1$. Using $x^{(n)}$ to denote the $n$-th element of $x$, we set

$$x_{ij}^{(n)} = |\{v \in N_j \mid s_{il} = n\}|, \quad \text{for } n \in \{0, 1, \ldots, k\}.$$ \hspace{1cm} (7)

In other words, the $n$-th element of $x_{ij}$ denotes the number of neighbor nodes of $v_j$ whose distance from $v_i$ is exactly $n$.

Then we define a role identification function as follows:

$$\psi_i(v_j) = h(x_{ii}) \oplus h(x_{ij}) \oplus s_{ij}, \quad \text{for each } v_j \in N_i^k \setminus \{v_i\},$$ \hspace{1cm} (8)

where $h$ is the same discount function as in IV-A.
Algorithm 1 RiWalk \((G, k, d, \gamma, \lambda, \omega)\)

**Input:** Graph \(G = (V, E)\), Neighborhood size \(k\), Dimensions \(d\), Walks per node \(\gamma\), Walk length \(\lambda\), Window size \(\omega\)

1. Initialize walks \(W\) to \(\emptyset\)
2. for \(i = 1, 2, \ldots, |V|\) do // parallel walks per node
3. \(\tilde{G}(N^k_i) = \text{RoleIdentificationSubgraph}(G(N^k_i))\)
4. \(W_i = \text{RandomWalkOnSubgraph}(\tilde{G}(N^k_i), \gamma, \lambda)\)
5. Add \(W_i\) to \(W\)
6. end for
7. \(f = \text{SkipGram}(W, d, \omega)\) // parallel
8. return the learned node embeddings \(f\)

Relation with the Weisfeiler-Lehman kernel: RiWalk-WL takes the idea of neighborhood aggregation from the Weisfeiler-Lehman kernel. The differences between them are 1) RiWalk-WL is rooted, 2) RiWalk-WL takes a labelling mapping defined as:

\[ l(v_j) = s_{ij}, \text{ for each } v_j \in N^k_i, \]  

3) RiWalk-WL counts the labels of the neighbors instead of sorting them, 4) RiWalk-WL takes discount on the counts when compressing the multiset label, 5) RiWalk-WL takes only one iteration.

C. Random-walk-based Embedding

Given a role identification method defined as above, we are able to get a relabeled subgraph \(\tilde{G}(N^k_i)\) for each anchor node \(v_i\). In this newly generated graph, only the anchor node \(v_i\) keeps its original identifier, while the other context nodes get new ones.

For parallelizability and simplicity, we adopt random-walk-based network embedding approaches to learn representations. Specifically, for each subgraph \(\tilde{G}(N^k_i)\), we perform fixed-length random walks starting from the anchor node \(v_i\) for a certain number of times. Note that random walk on each subgraph can be performed in parallel.

Through random walk simulating, the structural dependencies between substructures (i.e., new identifiers) are kept in random walks. By merging all random walks together as a corpus, we can train a language model to learn node embeddings by treating node sequences as sentences. For this work, we use the Skip-Gram model with negative sampling [20], [26].

D. The RiWalk Algorithm

The pseudocode of RiWalk is present in Algorithm 1. RiWalk takes a graph as input, and outputs low-dimensional representation for each node in the graph. Nodes with similar roles will have similar representations. For each node, RiWalk generates a relabeled subgraph for it and simulates random walks on the generated subgraph. By putting all random walks together and learning a language model, the embeddings can be obtained. It is worth noting that both the role identification procedure (line 2) and the network embedding procedure (line 7) are parallelizable, making RiWalk suitable for large networks.

E. Complexity Analysis

1) Time complexity: Given a subgraph \(G(N^k_i)\) rooted at an anchor node \(v_i\), computation of \(s_{ij}\) for each context node \(v_j\) needs to traverse each edge in the subgraph. Suppose \(k = k^*\), which means there is \(G(N^k_i) \equiv G\) for each anchor node \(v_i\). Thus traversing all subgraphs takes a complexity of \(O(|V| \cdot |E|) = O(\delta |V|^2)\), where \(\delta\) is the average degree of the nodes in the graph. Then the final complexity of RiWalk-SP in the worst case is \(O(\delta^2 |V|^2)\). Since RiWalk-WL needs to traverse each neighbor of the context node to get the vector \(x\), the complexity of RiWalk-WL in the worst case is \(O(|V|)\).

2) Space complexity: RiWalk-SP needs to store the mapping \(\phi\) and RiWalk-WL needs to store the vectors \(x\), both of which require space proportional to \(N^k_i\). Suppose \(k = k^*\), which means there is \(G(N^k_i) \equiv G\) for each anchor node \(v_i\). Since the role identification procedure is performed parallelizably on subgraphs, the final space complexity of RiWalk-SP and RiWalk-WL in the worst case is \(O(|V|)\).

V. EXPERIMENTS

We conduct extensive experiments to prove the effectiveness and efficiency of RiWalk. The experiments are carried out on a single machine with 32GB RAM, 16 CPU cores at 3.4GHz using 10 threads (without GPU support). The source code of RiWalk is available online\(^1\).

A. COMPARED ALGORITHMS

We compare our algorithm with the following state-of-the-art embedding methods.

- **node2vec**: A typical network embedding method which adopts biased random walks and language models to learn node representations. The biased random walk introduces flexibility in neighborhood exploring to learn richer embeddings. Default parameter settings for this approach are in line with the typical values described in the paper, i.e., dimensions of embedding \(d = 128\), number of walks per node \(\gamma = 10\), walk length \(\lambda = 80\), window size \(\omega = 10\). The hyper-parameter \(p, q\) are fine-tuned in all our following experiments.

- **struc2vec**: A structural embedding approach which learns structural node representations based on degree distributions in the neighborhoods. Default parameter settings for this approach are in line with node2vec for fair comparison, i.e., dimensions of embedding \(d = 128\), number of walks per node \(\gamma = 10\), walk length \(\lambda = 80\), window size \(\omega = 10\). It is worth noting that all the three optimizations of struc2vec described in the paper are used in our following experiments. As a result, the number of layers of the hierarchy \(k\) in struc2vec becomes a hyper-parameter to be tuned. We set \(k = 4\) as default.

- **GraphWave**: A structural embedding method which treats diffusion kernels as probability distributions over the

\(^1\)https://github.com/maxuewei2/RiWalk
B. Case Study: Expressway Network

As stated in Section IV, typical network embedding methods require some measure of smoothness over the network. Here we empirically demonstrate the fact by giving an illustrative example.

1) Data and setup: We collect data from Wikipedia pages under the category “Chinese national-level expressways”\(^2\) to construct an undirected, unweighted expressway network (shown in Fig. 2(a)). Nodes in the network are cities and edges indicate the existence of expressways between the cities. The network has 348 nodes and 675 edges. It is worth noting that the diameter of this network is 24.

We assign class labels to the nodes in three different ways to get three datasets:

- Expressway geo. region (Fig. 2(b)): The cities are split into four classes based on their geographical regions. Thus the class labels indicate community memberships.
- Expressway status (Fig. 2(c)): The cities are split into two classes based on their statuses: 1) municipalities, special administrative regions or provincial capitals, 2) neither of the former three. Thus the class labels are related to the roles (i.e., administrative levels) of the cities.
- Expressway Starbucks (Fig. 2(d)): Class labels are assigned based on the number of stores of Starbucks in the cities. Specifically, for the cities which have Starbucks stores, we use the median number to divide them into two groups: cities with more Starbucks and cities with less Starbucks. Then the third group is formed by the cities with no Starbucks.

Since this is a road network, it is flat and we can visually see the distributions of the class labels over the network. Imagine that different colors denoting different heights. As we can see, labels corresponding to geographical regions are smoothly distributed over the network while labels corresponding to statuses are completely not. Besides, labels based on numbers of Starbucks stores are semi-smoothly distributed. For example, cities with most Starbucks (the red ones in Fig. 2(d)) are either southeastern coastal cities or capitals of provinces, and the coastal cities are distributed smoothly while the provincial capitals are not.

For each of the three datasets, we perform a multi-class node classification task on the network w.r.t. the corresponding assigned labels. Specifically, for each dataset, we learn latent representations of nodes of the network using different embedding approaches. Then for each approach, a portion (\(70\%\)) of node embeddings along with their labels are randomly chosen to be training data. The rest node embeddings and their labels are used as test. We feed the training data to a one-vs-rest logistic regression classifier with L2 regularization (implemented by LibLinear [28]). Then the trained classifier is used to predict the labels of the test feature embeddings. We take the F1 score as the performance metric since the classes of the three datasets are both imbalanced. Note that each individual embedding is evaluated 10 times to reduce the noise introduced by classifier. This embedding process is repeated for 10 times and the average performance is reported. The parameter settings for each approach on each dataset are tuned to be optimal by using grid search. We report the Macro-F1 scores in Table I. The results of Micro-F1 scores are omitted since they follow a similar trend.

2) Results: As we can see, the classification accuracy is highly related to the smoothness of the label distribution. In particular, when class labels distribute smoothly over the network (i.e., the Expressway geo. region dataset), the typical network embedding method (i.e., \(\text{node2vec}\)) gives the best performance. When such a kind of smoothness does not exist (i.e., the Expressway status dataset), typical network embedding method performs the worst. And in this case, since the class labels are related to the roles of the nodes, all the structural embedding methods perform better than \(\text{node2vec}\). In the third

\(^2\)https://wikipedia.org/wiki/Category:Chinese_national-level_expressways
case, node2vec and RiWalk-SP achieve 107.9% and 76.19% gain over the Majority method, respectively. We argue that this is a consequence of the semi-smooth distribution of the class labels over the network. node2vec leverages the smooth part of it and structural embedding methods leverage the non-smooth part. This case also shows potential of combining both typical network embedding and structural embedding, where the former one captures community memberships and the latter one captures structural roles.

C. Within-Network Role Classification

We conduct the node classification task on the following datasets.

- European air-traffic network (shortly Europe) and American air-traffic network (shortly USA) [15]: Both the two networks are air-traffic networks, with nodes indicating airports and edges representing commercial flights between airports. Class labels indicate the levels of activity (e.g., the total number of landings plus takeoffs in a corresponding period) of the airports, thus the labels are related to the roles of the nodes.
- English-language film network (shortly Film) [29]: This is a film-director-actor-writer network, with each node assigned a label indicating it belonging to one of the four roles. The edges between nodes denote co-occurrences on the same Wikipedia page.
- Actor co-occurrence network (shortly Actor) [29]: This is the actor only subgraph of the Film network. We sort the nodes based on the number of words of their Wikipedia pages, and then use quartiles to split the nodes into four groups. Thus the group labels can be seen as a measure of the influences of the nodes.

All these networks are undirected and unweighted. The detailed statistics of these datasets are summarized in Table II.

As the name suggests, in the within-network classification task setting, the training and the testing data are from the same network. In fact, all the node classification task carried out in V-B are within-network classification tasks. Here we follow the same experimental procedure as in V-B except that we range the training ratio ($T_R$) from 10% to 90%. The parameter settings used for the USA network are tuned to be optimal by using grid search. And the parameters used for the Film and the Actor network are default settings. The average Micro-$F_1$ scores are reported.

We summarize the results of within-network node classification in Table III. Highest performances are shown in bold. As we can see, RiWalk-SP and RiWalk-WL outperform the other approaches on the USA dataset when the training ratio $T_R \geq 40\%$. On the Film and the Actor network, GraphWave runs out of memory when running the algorithm and the other three structural embedding methods outperform node2vec. This indicates that typical network embedding methods are not capable of identifying structural roles of nodes. When comparing between structural embedding methods, on the Film network, RiWalk-SP and RiWalk-WL perform the best and give us 9% and 8% gain over struc2vec, respectively. On the Actor network, RiWalk-SP and RiWalk-WL achieve comparable performance with struc2vec.

Besides, we also notice that struc2vec performs inferior to all the other structural embedding methods when $T_R$ is small. For example, on the USA dataset, even though struc2vec achieves comparable performance with the other approaches when $T_R \geq 70\%$, it performs worst when $T_R = 10\%$. And on the Actor network, even if struc2vec gives the best performance when $T_R \geq 20\%$, it performs worse than RiWalk-SP when $T_R \leq 10\%$. Since RiWalk-SP shares similar intuition with struc2vec, this phenomenon demonstrates the effectiveness of our framework, which provides robust performance on sparsely labeled graphs.

1) Time and space usage analysis: We record the running time and the memory usage of each approach in the within-network classification tasks. Since all algorithms were implemented using Python, we are able to make more fair comparisons on algorithm level. The results are listed on the right side of Table III (Real refers to actual elapsed time; User refers to CPU time used only by the process). Since node2vec is a typical network embedding algorithm, it is omitted when comparing.

As shown in the table, GraphWave uses 10x more memory than RiWalk-SP and this memory usage prevents it from running on the two larger networks. Besides, on the Film network, struc2vec also uses 10x more memory than RiWalk-SP and RiWalk-WL.

On the Film network, RiWalk-SP and RiWalk-WL use 11x and 3x less time than struc2vec w.r.t. real time usage, respectively. On the Actor network, RiWalk-SP and RiWalk-WL use 20x and 6x less time than struc2vec w.r.t. user time usage, respectively.

The above results demonstrate the efficiency of our proposed framework, which achieves comparable performances while
Table III: Micro-F1(%) scores of within-network role classification.

| Dataset | Method          | Labeled Nodes (%) | Time and Memory Usage |
|---------|----------------|-------------------|-----------------------|
|         |                | 10    20  30  40  50  60  70  80  90 | Mem (M) Real (s) User (s) |
| USA     | node2vec       | 54.86 58.84 61.03 61.78 62.79 63.44 63.74 63.86 64.18 | 82       94       863    |
|         | struc2vec      | 54.39 58.06 60.23 60.93 61.86 62.73 63.17 64.38 65.75 | 127      6        74     |
|         | GraphWave      | **60.30** **61.30** **62.45** **62.90** **63.28** **62.98** **63.26** **63.25** **64.67** | 13       4        19     |
|         | RiWalk-SP      | 58.62 60.35 61.21 63.03 63.69 63.58 64.47 65.83 64.60 | 42       17       146    |
|         | RiWalk-WL      | 58.25 60.82 62.39 **63.04** **64.34** **64.38** **65.92** **66.17** **66.25** |           |

Table IV: Macro-F1(%) scores of across-network role classification.

| Algorithm          | Dataset          | USA:Europe | Europe:USA | Actor:USA | USA:Actor |
|--------------------|------------------|------------|------------|-----------|-----------|
| node2vec           |                  | 42.92      | 45.99      | 46.91     | 42.88     |
| struc2vec          |                  | 78.87      | 79.74      | **80.13** | 57.48     |
| GraphWave          |                  | 86.17      | 73.98      |           |           |
| RiWalk-SP          |                  | **81.98**  | **80.07**  | 78.95     | **73.97** |
| RiWalk-WL          |                  | 81.95      | 78.99      | **80.90** | **67.34** |
| Majority           |                  | 42.91      | 42.87      | 42.87     | 42.86     |

Fig. 3. Performance w.r.t. neighborhood size k.

D. Across-Network Role Classification

To test the potential of RiWalk in transfer learning, we study the problem of role classification across networks. In the across-network classification setting, one network along with all the class labels of its nodes are treated as training data, and the task is to predict the class labels of the nodes in another network. Obviously, the key problem of this task is to capture the features that transfer across networks.

Here we consider the problem of identifying hub nodes in different networks. That is, given a network whose nodes are already classified as hub nodes or non-hub nodes, we aim to leverage this knowledge to determine if one node in another network is a hub.

We use the Europe, USA and Actor network to create four merged-network datasets: First, for each network, we treat the nodes of the first group (e.g., hub airports, famous actors) as hub nodes and the other three groups as non-hub nodes. We treat these binary class labels as ground-truth facts. Then, given two networks $G_a$ and $G_b$, we construct a network $G_{a,b}$ composed of the two networks. The merged network then is fed to different embedding approaches to learn node embeddings. Treating embeddings of nodes in $G_a$ along with their class labels as training data, we train a logistic regression classifier to predict the labels of all nodes in $G_b$. The parameter settings for different approaches are tuned to be optimal. The experiments are repeated for 10 times and we report the average Macro-F1 score among the runs.

As shown in Table IV, node2vec gives close performance with the Majority method. This indicates that typical network embeddings are not able to transfer across networks. At the same time, all the structural embedding methods show much better performances, which demonstrates the potential of structural embeddings in transfer learning.

As we can see, RiWalk-SP and RiWalk-WL give the...
Table 1: Performance of structural hole identification.

| Dataset       | RiWalk-SP | RiWalk-WL | GraphWave | struc2vec |
|---------------|-----------|-----------|-----------|-----------|
| Europe:USA    | 32.7%     | 15.2%     | 13.5%     | 10.4%     |
| USA:Actor     | 30.8%     | 14.1%     | 12.3%     | 9.6%      |
| Europe:Actor  | 31.9%     | 14.5%     | 12.7%     | 9.9%      |

*Note: The performances are in terms of % gain over the baselines.*

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**E. Structural Hole Identification**

Structural holes [9] play an important role in the information exchange process over the network. Identifying structural holes in networks would help researchers to gain a thorough understanding of network evolution and information cascades.

Here we take the Europe, USA and Actor network as our datasets. Given a network, we first compute the constraint on all nodes in the network. We take the constraint values as ground-truth measurements of nodes bridging structural holes. That is, the lower constraint value one node has, the more opportunities it has for bridging structural holes. Then the first 300 nodes with smallest constraint values are chosen to be positive instances. We then learn node embeddings on the network with different approaches. Denoting the node with the smallest constraint value as $v_{ab}$, for each approach, we compute cosine similarities between $v_{ab}$ and all nodes in the network using their embeddings. The first 300 nodes that have most similar embeddings with $v_{ab}$ are treated as predicted positive instances. The number of correctly predicted instances are reported in Fig. 4. The parameter settings for each approach are tuned to be optimal.

As we can see, thanks to the flexibility of neighborhood exploring introduced by biased random walk, node2vec can capture structural equivalence in small networks (i.e., the Europe network). However, when it comes to larger networks, the performance of node2vec drops significantly. Similar performance drops are also observed on the four structural embedding methods. struc2vec drops the most, and as a result, RiWalk-SP and RiWalk-WL give us 145% and 127% performance gains over struc2vec on the Actor network, respectively. This experiment once again shows the robustness of our proposed algorithms.

**F. Scalability**

To evaluate the scalability of our proposed methods, we learn node representations on the Erdos-Renyi graphs using RiWalk-SP (default parameter settings, 10 thread). The graphs are generated with constant degree of 10 and sizes ranging from 100 to 1,000,000. We plot the running time w.r.t. the sizes of the graphs in Fig. 5 (in log-log scale). The sampling procedure comprises of the role identification procedure and the random walk simulating procedure. The optimization procedure is the language model training with negative sampling. From the figure, we can observe that RiWalk-WL scales super-linearly with the complexity of about $O(n^{1.2})$, which indicates that RiWalk is capable for massive networks.

**VI. Conclusions**

We propose a new paradigm RiWalk for learning structural representations. RiWalk generates relabeled subgraphs by relabeling context nodes with their structural roles in the anchor node’s local topologies, and then apply typical network embedding methods to learn structural embeddings. We develop two different relabeling methods. Comprehensive
experiments prove the effectiveness and efficiency of our proposed methods. The results of the experiments show that the learned structural embeddings are robust and can transfer across networks. Our experiments also show differences between typical network embedding and structural embedding.

In the future, we plan to investigate a good way to combine typical network embeddings and structural embeddings, such that we can capture both community memberships and structural roles. Besides, we are also interested in investigating the potentials of structural embeddings in transfer learning tasks.

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