Learning Role-based Graph Embeddings

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Abstract

Random walks are at the heart of many existing network embedding methods. However, such algorithms have many limitations that arise from the use of random walks, e.g., the features resulting from these methods are unable to transfer to new nodes and graphs as they are tied to vertex identity. In this work, we introduce the Role2Vec framework which uses the flexible notion of attributed random walks, and serves as a basis for generalizing existing methods such as DeepWalk, node2vec, and many others that leverage random walks. Our proposed framework enables these methods to be more widely applicable for both transductive and inductive learning as well as for use on graphs with attributes (if available). This is achieved by learning functions that generalize to new nodes and graphs. We show that our proposed framework is effective with an average AUC improvement of 16.55% while requiring on average 853x less space than existing methods on a variety of graphs.

1 Introduction

Learning a useful feature representation from graph data lies at the heart and success of many machine learning tasks such as node classification [Neville and Jensen, 2000], anomaly detection [Akoglu et al., 2015], link prediction [Al Hasan and Zaki, 2011], among others [Koyutürk et al., 2006; Ng et al., 2002]. Motivated by the success of word embedding models, such as the skip-gram model [Mikolov et al., 2013], recent works extended word embedding models to learn graph embeddings [Perozzi et al., 2014; Goyal and Ferrara, 2017]. The primary goal of these works is to model the conditional probabilities that relate each input vertex to its context, where the context is a set of other vertices surrounding and/or topologically related to the input vertex. Many variants of graph embedding methods proposed random walks to generate the context vertices [Perozzi et al., 2014; Grover and Leskovec, 2016; Ribeiro et al., 2017; Cavallari et al., 2017]. For instance, DeepWalk [Perozzi et al., 2014] initiates random walks from each vertex to collect sequences of vertices (similar to sentences in language). Then, the skip-gram model is used to fit the embeddings by maximizing the conditional probabilities that relate each input vertex to its surrounding context. In this case, vertex identities are used as words in the skip-gram model, and the embeddings are tied to the vertex ids.

In language, the foundational idea is that words with similar meanings will be surrounded by a similar context [Harris, 1954]. As such, in language models, the context of a word is defined as the surrounding words. However, this foundation does not directly translate to graphs. Since unlike words in languages that are universal with semantics and meaning independent of the corpus of documents, vertex ids obtained by random walks on graphs are not universal and are only meaningful within a particular graph. This key limitation has two main disadvantages. First, these embedding methods are inherently transductive, dealing essentially with isolated graphs, and unable to generalize to unseen nodes. Consequently, they are unsuitable for graph-based transfer learning tasks such as across-network classification [Kuwadekar and Neville, 2011; Getoor and Taskar, 2007], and graph similarity/comparison [Goldsmith and Davenport, 1990; Zager and Verghese, 2008]. Second, by using this traditional definition of random walks, there is no general way to integrate vertex attributes/features to the network representation.

There is no guarantee that similar vertices are surrounded by similar context (obtained using random walks on graphs). Recent empirical analysis shows that using random walks in graph embeddings primarily capture proximity among the vertices (see [Goyal and Ferrara, 2017]), so that vertices that are close to one another in the graph are embedded together, e.g., vertices that belong to the same community are embedded similarly. Although proximity among the vertices does not guarantee their similarity, the idea of a network position or a role [Lorrain and White, 1977; Rossi and Ahmed, 2015a; Henderson et al., 2011] is more suitable to represent the similarity and structural relatedness among vertices. Roles represent vertex connectivity patterns such as hubs, star-centers, star-edge nodes, near-cliques or vertices that act as bridges to different regions of the graph. Intuitively, two vertices belong to the same role if they are structurally similar. Random walks will likely visit nearby vertices first, which makes them suitable for finding communities, rather than roles (structural similarity) (see Sec. 3 for theoretical analysis).

To overcome the above problems, we propose the Role2Vec framework which serves as a basis for generalizing many ex-
isting methods that use traditional random walks. Role2Vec utilizes the flexible notion of attributed random walks that is not tied to vertex identity and is instead based on a function $\Phi : x \to w$ that maps a vertex attribute vector to a type, such that two vertices belong to the same type if they are structurally similar. The proposed framework provides a number of important advantages to any method generalized using it. First, the proposed framework is naturally inductive as the learned features generalize to new nodes and across graphs and therefore can be used for transfer learning tasks. Second, they are able to capture structural similarity (roles) better. Third, the proposed framework is inherently space-efficient since embeddings are learned for types (as opposed to vertices) and therefore requires significantly less space than existing methods. Fourth, the proposed framework naturally supports graphs with attributes (if available/given as input). Furthermore, our approach is shown to be effective with an average improvement of 16.55% in AUC while requiring on average 853x less space than existing methods on a variety of graphs from different application domains.

2 Framework

We consider an (un)directed input graph $G = (V, E)$, where $N_v = |V|$ is the number of vertices in $G$, and $N_e = |E|$ is the number of edges in $G$. For any vertex $v_i \in V$, let $\Gamma(i)$ be the set of direct neighbors of $v_i$, and $d_i = |\Gamma(i)|$ is the vertex degree. In addition, we consider a matrix $X$ of attributes/features, where each $x_i$ is a $K$-vector for vertex $v_i$. For example, for graphs without attributes, $x_i$ could simply be an indicator vector for vertex $v_i$ and $K$ is equivalent to the number of vertices (i.e., having $x_{ij} = 1$ if $j = i$, and $x_{ij} = 0$ otherwise) [Perozzi et al., 2014; Grover and Leskovec, 2016]. For attributed graphs, $x_i$ may include observed attributes, topological features, and/or node types for heterogeneous graphs. The goal of an embedding method is to derive useful features of particular graph elements (e.g., vertices, edges) by learning a model that maps each graph element to the latent $D$-dimension space. While the approach remains general for any graph element, this paper focuses on vertex embeddings.

To achieve this, an embedding is usually defined with three components: (1) the context function, which specifies a set of other vertices called the context $c_i$ for any given vertex $v_i$, such that the context vertices are surrounding and/or topologically related to the given vertex. Each vertex is associated with two latent vectors, an embedding vector $\alpha_i \in \mathbb{R}^D$ and a context vector $\beta_i \in \mathbb{R}^D$. (2) the conditional distribution, which specifies the statistical distribution used to combine the embedding and context vectors. More specifically, the conditional distribution of a vertex combines its embedding and the context vectors of its surrounding vertices. (3) the model parameters (i.e., embedding and context vectors) and how these are shared across the conditional distributions. Thus, an embedding method models the conditional probability that relate each vertex to its context as follows: $x_{c_i} = x_i \sim \mathbb{P}$, where $c_i$ is the set of context vertices for vertex $v_i$, $x_i$ is its feature/attribute vector, and $\mathbb{P}$ is the conditional distribution.

Our goal is to model $\mathbb{P}(x_{c_i} | x_i) = \prod_{j \in c_i} \mathbb{P}(x_j | x_i)$, assuming the context vertices are conditionally independent. The most commonly used conditional distribution is the categorical distribution (see [Rudolph et al., 2016] for a generalization). In this case, a softmax function parameterized with the two latent vectors (i.e., embedding and context vectors) is used. Thus, for each input-context vertex pair $(v_i, v_j)$,

$$\mathbb{P}(x_j | x_i) = \frac{e^{\alpha_i \cdot \beta_j}}{\sum_{v_k \in V} e^{\alpha_i \cdot \beta_k}}$$

For sparse graphs, the summation in $\sum_{v_k \in V} e^{\alpha_i \cdot \beta_k}$ contains many zero entries, and thus can be approximated by sub-sampling those zero entries (using negative sampling similar to language models [Mikolov et al., 2013]). Finally, the objective function of the embedding method is the sum of the logarithm of likelihood values of each vertex, i.e., $L(\alpha, \beta) = \sum_{v_i=1}^{N_v} \log \mathbb{P}(x_{c_i} | x_i)$.

Clearly, there is a class of possible embedding methods where each of the three components (discussed above) is considered modeling choice with various alternatives. Recent work proposed random walks to sample/collect the context vertices $c_i$ [Perozzi et al., 2014; Grover and Leskovec, 2016].

2.1 Mapping Vertices to Vertex-Types

Given $N_v \times K$ matrix $X$ of attributes and/or structural features, the Role2Vec framework starts by locating sets of vertices, however large or small be the shortest distance between any two in a set, who are placed similarly with respect to all other sets of vertices. Thus, two vertices belong to the same set if they are similar in terms of attributes and/or structural features. We achieve this by learning a function that maps the $N_v$ vertices to a set $W = \{w_1, ..., w_M\}$ of $M$ vertex-types where $M$ is often much smaller than $N_v$, i.e., $M \ll N_v$.

$$\Phi : x \to w$$

Thus, $\Phi$ is a function mapping vertices to vertex-types based on the $N_v \times K$ attribute matrix $X$. Clearly, the function $\Phi$ is a modeling choice, which could be learned automatically or defined manually by the user. We explore two general classes of functions for mapping vertices to their types. The first class of functions are simple functions taking the form:

$$\Phi(x) = x_1 \circ x_2 \circ \cdots \circ x_K$$

where $x = [x_1, x_2, \cdots, x_K]$ is an attribute vector and $\circ$ is a binary operator such as concatenation, sum, among others. The second class of functions are learned by solving an objective function. This includes functions based on a low-rank factorization of the $N_v \times K$ matrix $X$ having the form $X \approx f(UV^T)$ with factor matrices $U \in \mathbb{R}^{N_v \times r}$ and $V \in \mathbb{R}^{K \times r}$ where $r > 0$ is the rank and $f$ is a linear or non-linear function. More formally,

$$\arg \min_{U, V \in \mathbb{C}} \frac{1}{2} \left[ D(X, f(UV^T)) + C(U, V) \right]$$

where $D$ is the loss, $C$ is constraints (e.g., non-negativity constraints $U \geq 0, V \geq 0$, and $R(U, V)$ is a regularization penalty. Then, we partition $U \in \mathbb{R}^{N_v \times r}$ into $M$ disjoint sets of nodes (for each of the $M$ vertex-types) $V_1, \ldots, V_M$, where $V_j$ is set of vertices mapped to vertex-type $w_j \in W$, by solving the k-means objective:

$$\min_{\{V_j\}_{j=1}^{M}} \sum_{j=1}^{M} \sum_{u_i \in V_j} ||u_i - c_j||^2$$, where $c_j = \frac{\sum_{u_i \in V_j} u_i}{|V_j|}$
2.2 Attributed Random Walks

Recently, random walks received much attention in learning network embeddings [Perozzi et al., 2014; Grover and Leskovec, 2016], in particular to generate the context vertices. Consider a random walk of length $L$ and starting at a vertex $v_0$ of the input graph $G$, if at time $t$ we are at vertex $v_t$, then at time $t + 1$, we move to a neighbor of $v_t$ with probability $1/d_{v_t}$. Thus, the resulting randomly chosen sequence of vertex indices $(v_t : t = 0, 1, ..., L - 1)$ is a Markov chain. However, a key limitation of these methods is that the embeddings learned based on random walks are fundamentally tied of vertex indices.

The induced vertex-type sequence in the above definition is a function $\Phi(x)$ as discussed in Section 2.1. Then, we pre-compute the random walk transition probabilities $\pi$, which could be uniform or weighted (Line 6). Lines 8-13 initiate random walks from each vertex using the notion of attributed random walks in Lines 17-24. Finally, Role2Vec learns the embeddings using stochastic gradient descent in Line 14.

Recall that $N_v$ is the number of nodes, $M$ is the number of types, and $M \ll N_v$. Role2Vec has the following properties.

Property 2.1 Role2vec is space-efficient with space complexity $O(MD + N_v)$.

Proof. To store the learned embeddings of the vertex-types, Role2vec takes $O(MD)$ space. Also, Role2vec takes $O(N)$ space for a hash table mapping vertices to their corresponding types. Thus, the total space used by Role2vec is $O(MD + N)$, less space compared to baselines that require $O(N_v, D)$. □

As $M \to N_v$, Role2vec converges to the baseline random walk methods [Perozzi et al., 2014; Grover and Leskovec, 2016], since each vertex is mapped to a new type that uniquely identifies it from other vertices, i.e., $\Phi$ is a one-to-one function from $V$ onto itself.

3 Theoretical Analysis

In a graph $G$, the sequence of vertices visited by a random walk of length $L$ is represented by a directed path on the graph. In this section, we analyze the properties and parameters of random walks that affect the embedding methods. Lemmas 1–3 analyze the constraints and bounds on vertex reachability, expected access time, and representation of vertices/edges in random walks respectively.

We consider a random walk of length $L$ and starting at vertex $v_0$ of $G$, if at time $t$ we are at vertex $v_t$, then at time $t + 1$, we move to a neighbor of $v_t$ with probability $1/d_{v_t}$. Clearly,
the randomly chosen sequence of vertex indices \(v_t : t = 0, 1, \ldots, L-1\) is a Markov chain. We denote by \(P_t\) the distribution of \(v_t\), where \(P_t(v_t = i) \) is the probability that the random walk visits vertex \(i\) at time \(t\). Similarly, we denote by \(P_{ij}\) the transition probability from vertex \(i\) to vertex \(j\) in one step, where \(P_{ij} = \Pr(v_{t+1} = j | v_t = i)\). Thus, the Markov property implies that this Markov chain is uniquely defined by its one-step transition matrix \(P = (P_{ij})_{v_i, v_j \in V}\).

\[
P_{ij} = \begin{cases} 
1/d_i, & \text{if } (i, j) \in E \\
0, & \text{otherwise}
\end{cases}
\]  

(8)

Let \(P^m\) be the transition matrix whose entries are the \(m\)-step transition probabilities, such that

\[
P^m_{ij} = \Pr(v_{t+m} = j | v_t = i)
\]

(9)

is the probability that the walk moves from vertex \(i\) to vertex \(j\) exactly \(m\) steps. Finally, we denote by \(r^t_{ij}\) the probability that starting at vertex \(i\), the first transition to vertex \(j\) occurs at time \(t\).

\[
r^t_{ij} = \Pr(v_t = j, \forall 1 \leq t \leq t-1, v_t \neq j | v_0 = i)
\]

(10)

**Lemma 1** If \(u\) and \(v\) are two non-adjacent vertices in a connected graph \(G\), then there is at least one neighbor \(j \in \Gamma(u)\) where \(r^1_{uv} \leq r^t_{ij}\) for all \(t > 1\).

**Proof.** Let \(d_u = |\Gamma(u)|\) be the degree of vertex \(u\), and denote by \([d_u]\) the set of neighbors of \(u\). For each neighbor \(j \in [d_u]\), start a random walk at \(j\), and let \(r^t_{ij}\) be the probability that the first transition from \(j\) to \(v\) occurs at time \(t\). Now begin a random walk at \(u\) and let \(r^1_{uv}\) be the probability that the first transition from \(u\) to \(v\) occurs at time \(t\). By conditioning on the first transition, we have

\[
r^1_{uv} = \sum_{j=1}^{d_u} P_{uj} \cdot r^0_{jv} = \frac{1}{d_u} \sum_{j=1}^{d_u} r^0_{jv} = \frac{1}{d_u} \sum_{j=1}^{d_u} r^0_{jv}
\]

Set \(t_1 = t - 1\), thus the probability \(r^t_{uv}\) is the mean of the probabilities of \(u\’s\) neighbors, \(r^t_{ij}\) for \(j \in [d_u]\) and \(t_1 < t\). This implies that there is at least one neighbor \(j\) where \(r^t_{uv} \leq r^t_{ij}\) for \(t_1 < t\), and Property 1 is proved.

**Lemma 2** If \(u\) and \(v\) are two non-adjacent vertices in a connected graph \(G\), with \(h_{uv}\) the expected access time from \(u\) to \(v\), and \(\tilde{h}_{vy}\) the average neighbor access time for \(u\), then with probability less than \(\frac{1}{2}\), a random walk starting at \(u\) takes at least \(L = 2 h_{uv} > 2 \tilde{h}_{vy}\) time to reach \(v\).

**Proof.** Recall that \(r^t_{uv}\) is the probability that starting at \(u\), the random walk first visits \(v\) at time \(t\), then the expected access time from \(u\) to \(v\) is \(E[t] = h_{uv} = \sum_{t \geq 1} t \cdot r^t_{uv}\). By conditioning on the first transition, we have

\[
h_{uv} = \sum_{t \geq 1} t \cdot \sum_{j=1}^{d_u} P_{uj} \cdot r^t_{jv} = \sum_{j=1}^{d_u} P_{uj} + \sum_{t \geq 1} t \cdot \sum_{j=1}^{d_u} P_{uj} \cdot r^t_{jv} = 1 + \frac{1}{d_u} \sum_{j=1}^{d_u} h_{jv}.
\]

where \(d_u\) is the degree of \(u\), and \(h_{jv}\) is the expected access time for some neighbor vertex \(j \in [d_u]\). Since \(t \geq 0\) for any vertex in \(G\), then by Markov’s inequality, for any \(L > 0\),

\[
\Pr(t \geq L) \leq \frac{E[t]}{L} = \frac{h_{uv}}{L}
\]

Let \(\tilde{h}_{jv} = \frac{1}{d_u} \sum_{j=1}^{d_u} h_{jv}\) be the average neighbor access time for vertex \(u\). Then, with \(\Pr(t \geq L) \leq \frac{1}{2}\), a random walk starting at \(u\) takes at least \(L = 2 h_{uv} > 2 \tilde{h}_{jv}\) to reach \(v\).

**Lemma 3** Suppose we start \(d_u\) random walks of length \(L\) from any vertex \(u \in V\) in \(G\). For a given edge \(e = (u, v)\), let \(I_e\) denote the total number of random walks containing \(e\). Then, the expectation of the random variable \(I_e\) is upper bounded by \(L\), i.e., \(\mathbb{E}[I_e] \leq L\).

**Proof.** Recall that the probability of a random walk starting at \(u\) visits \(v\) at time \(t\) is \(P_{uv}^t = \lambda_u \mathbf{P}^t \mathbf{X}_v\), where \(\lambda_u\) is the indicator vector for vertex \(u\), which equals 1 in coordinate \(u\) and 0 otherwise. Then, for a given edge \(e = (v', v)\), the probability that the random walk visits \(v\) at time \(t\) and \(v'\) at time \(t+1\) is \(\lambda_v \mathbf{P}^t \mathbf{X}_v / d_v\) (since the transition probability from \(v\) to \(v'\) is \(1/d_v\)). Suppose we start \(d_u\) random walks of length \(L\) from \(u\), let \(I_e\) denote the total number of random walks containing \(e\), then the expectation of \(I_e\) is the sum of the probabilities that there exists a random walk visiting \(e = (v, v')\) as follows

\[
\mathbb{E}[I_e] = \sum_{t=1}^L \sum_{d_u} \lambda_u \mathbf{P}^t \mathbf{X}_v / d_v = \sum_{t=1}^L \mathbf{1} \mathbf{D} \mathbf{P}^t \mathbf{X}_v / d_v = \sum_{t=1}^L \mathbf{1} \mathbf{D} \mathbf{P}^t = \sum_{t=1}^L = 1 = L
\]

where \(\mathbf{D}\) is the degree matrix with the \(i\)th diagonal entry is the vertex degree \(d_i\), \(\mathbf{1}\) is the unit vector with all entries equal to 1, and \((\mathbf{1} \mathbf{D} \mathbf{P}^t = \mathbf{1})\).

**4 Experiments**

In this section, we investigate the effectiveness of the proposed framework using a variety of graphs. Unless otherwise mentioned, all experiments use logarithmic binning\(^1\) and the bin size \(\delta\) is chosen by searching over \(\delta \in \{0.01, 0.1, 0.5, 0.9, 0.99\}\). In these experiments, we use a simple function \(\Phi(x)\) that represents a concatenation of the attribute values in the node attribute vector \(x\). We searched over 10 subsets of the 9 motif features of size 2-4 nodes shown in Figure 1. We evaluate the role2vec approach presented in Section 2.3 that leverages the attributed random walk framework (Section 2) against a number of popular

\(^1\)Logarithmic binning assigns the first \(\delta N_u\) nodes with smallest attribute value to 0 (where \(0 < \delta < 1\), then assigns the \(\delta\) fraction of remaining unassigned nodes with smallest value to 1, and so on.
methods including: node2vec [Grover and Leskovec, 2016],
DeepWalk [Perozzi et al., 2014], struc2vec [Ribeiro et al.,
2017], and LINE [Tang et al., 2015]. For our approach and
node2vec, we use the same hyperparameters (D = 128, R =
10, L = 80) and grid search over p, q ∈ {0.25, 0.50, 1, 2, 4}
as mentioned in [Grover and Leskovec, 2016]. We use lo-
gistic regression (LR) with an L2 penalty. The model is se-
lected using 10-fold cross-validation on 10% of the labeled
data. Experiments are repeated for 10 random seed initial-
izations. All results are statistically significant with p-value
< 0.01. We use AUC to evaluate the models. Data was ob-
tained from NetworkRepository [Rossi and Ahmed, 2015b].

Figure 1: Summary of the 9 motifs and 15 orbits with 2-4 nodes.

4.1 Comparison
This section compares the proposed approach to other embed-
ning methods for link prediction. Given a partially observed
graph \( G \) with a fraction of missing edges, the link predic-
tion task is to predict these missing edges. We generate a
labeled dataset of edges as done in [Grover and Leskovec,
2016]. Positive examples are obtained by removing 50% of
edges randomly, whereas negative examples are generated by
randomly sampling an equal number of node pairs that are
not connected with an edge, i.e., each node pair \((i, j) \notin E\).
For each method, we learn features using the remaining graph
that consists of only positive examples. Using the learned
embeddings from each method, we then learn a model to pre-
dict whether a given edge in the test set exists in \( E \) or not.
Notice that node embedding methods such as DeepWalk and
node2vec require that each node in \( G \) appear in at least one
erge in the training graph (i.e., the graph remains connected),
otherwise these methods are unable to derive features for such
nodes. This is a significant limitation that prohibits their use
in many real-world applications.

Figure 2: AUC gain of Role2Vec (R2V) over the other methods for
link prediction bootstrapped using Hadamard \( \alpha_i \odot \alpha_j \).

For comparison, we use the same set of binary opera-
tors [Grover and Leskovec, 2016] to construct features for the
dges by combining the learned embeddings of its endpoints.
The AUC results are provided in Table 1 and 2. Moreover, the
AUC scores from our method are all significantly better
than the other methods at \( p < 0.01 \). Note that we also used
the role2vec framework to generalize DeepWalk (DW) by us-
ing the notion of attributed random walk, we call this R2V-
DW. We summarize the gain/loss in predictive performance
over the other methods in Figure 2. In all cases, our method
achieves better predictive performance over the other meth-
ods across a wide variety of graphs with different character-
istics. Overall, the mean and product binary operators give
an average gain in predictive performance (over all graphs)
of 11.1% and 22%, respectively.

We also investigated learning types using low-rank matrix
factorization (Eq. 4) with squared loss. No regularization or
constraints were used. Eq. 5 was used to partition nodes into
\( M \) types. Results are provided in Table 3 and are comparable
to previous results that use concatenation to derive types. Due
to space, we report results for only a few graphs using the
mean operator.

4.2 Space-efficient Embeddings
We now investigate the space-efficiency of the learned em-
beddings from the proposed framework and intermediate rep-
sentation. Observe that any embedding method that imple-
ments the proposed attributed random walk framework (and
intermediate representation) learns an embedding for each of
the \( N_e \) vertices in the graph and we recover the baseline meth-
ods across a wide variety of graphs with different character-
istics. In general, the best embedding most often lies
between such extremes and therefore the embedding learned
from a method implementing Role2Vec is often orders of
magnitude smaller in size, since \( M \ll N_e \).

Given an attribute vector \( \mathbf{x} \) of motif counts (Figure 1) for
an arbitrary node in \( G \), we derive embeddings using each of
the following:

\[
\Phi(x_i = [x_2 x_3], \text{ for } i = 1, \ldots, N_e) \quad (11)
\]

\[
\Phi(x_i = [x_2 x_3 x_4 x_5 x_9], \text{ for } i = 1, \ldots, N_e) \quad (12)
\]

\[
\Phi(x_i = [x_2 x_3 x_4 x_5 \cdots x_9], \text{ for } i = 1, \ldots, N_e) \quad (13)
\]

\[
\Phi(x_i = [x_1 x_2 x_3 x_4 x_5 \cdots x_9], \text{ for } i = 1, \ldots, N_e) \quad (14)
\]

where \( \Phi(\cdot) \) is a function that maps \( x_i \) to a type \( w \in W \).
In these experiments, we use logarithmic binning (applied to
each \( N_e \)-dimensional motif feature) with \( \delta = 0.5 \) and use
\( \Phi \) defined as the concatenation of the logarithmically binned
attribute values. Embeddings are learned using the different

| GRAPH | R2V | R2V-DW | N2V | DW | LINE | S2V |
|-------|-----|--------|-----|----|------|-----|
| bn-cat | 0.710 | 0.688 | 0.627 | 0.627 | 0.672 | 0.669 |
| bn-rat-brain | 0.748 | 0.731 | 0.716 | 0.716 | 0.691 | 0.729 |
| bn-rat-cerebral | 0.867 | 0.846 | 0.813 | 0.811 | 0.709 | 0.858 |
| ca-Csphd | 0.858 | 0.858 | 0.768 | 0.735 | 0.620 | 0.791 |
| ecc-fweb-baydpy | 0.681 | 0.656 | 0.655 | 0.627 | 0.660 | 0.623 |
| ia-radoslav-email | 0.867 | 0.847 | 0.756 | 0.745 | 0.769 | 0.857 |
| soc-anymail | 0.961 | 0.960 | 0.854 | 0.848 | 0.850 | 0.883 |
| soc-dolphins | 0.656 | 0.597 | 0.580 | 0.498 | 0.551 | 0.590 |
| fb-Yale | 0.793 | 0.793 | 0.742 | 0.728 | 0.763 | 0.758 |
| web-EPA | 0.926 | 0.925 | 0.804 | 0.738 | 0.768 | 0.861 |
subsets of attributes in Eq. (11)-(14). For instance, Eq. (11) indicates that vertex types are derived using the (logarithmic binned) number of 2-stars $x_2$ and triangles $x_3$ incident to the given vertex (Figure 1). We measure the space (in bytes) required to store the embedding learned by each method. In Figure 3, we summarize the reduction in space from our approach compared to the other methods. In all cases, the embeddings learned from our approach require significantly less space and thus more space-efficient. Specifically, the embeddings from our approach require on average 853 times less space than the best method averaged across all graphs.

**Table 2: AUC scores comparing types derived using concatenation vs. factorization.**

| GRAPH | R2V | R2V-DW | N2V | DW | LINE | S2V |
|-------|-----|--------|-----|----|------|-----|
| bn-cat | 0.694 | 0.681 | 0.621 | 0.621 | 0.494 | 0.662 |
| bn-rat-brain | 0.775 | 0.775 | 0.715 | 0.715 | 0.562 | 0.736 |
| bn-rat-cerebral | 0.867 | 0.838 | 0.796 | 0.793 | 0.498 | 0.834 |
| ca-CSphd | 0.758 | 0.738 | 0.678 | 0.660 | 0.533 | 0.699 |
| eco-fweb-baydry | 0.684 | 0.644 | 0.673 | 0.631 | 0.516 | 0.599 |
| ia-radoslaw-email | 0.852 | 0.821 | 0.746 | 0.731 | 0.471 | 0.843 |
| soc-anybeat | 0.945 | 0.945 | 0.730 | 0.728 | 0.618 | 0.798 |
| soc-dolphins | 0.787 | 0.787 | 0.593 | 0.508 | 0.549 | 0.553 |
| fb-Yale4 | 0.940 | 0.906 | 0.912 | 0.904 | 0.784 | 0.905 |
| web-EPA | 0.907 | 0.885 | 0.808 | 0.797 | 0.650 | 0.841 |

**Table 3: AUC scores for various methods using $\alpha_i \odot \alpha_j$. Note $N2V=node2vec$, $DW=DeepWalk$ and $S2V=struc2vec$.**

| GRAPH | R2V | R2V-DW | N2V | DW | LINE | S2V |
|-------|-----|--------|-----|----|------|-----|
| bn-cat | 0.710 | 0.748 | 0.867 | 0.926 |
| bn-rat-brain | 0.707 | 0.761 | 0.848 | 0.905 |

**Figure 3: Evaluating the space savings of Role2Vec.** Space savings is defined as the reduction in embedding size (bytes) relative to the smallest embedding size among the baseline methods. Let $\sigma$ denote the size (bytes) of a Role2Vec embedding and $\sigma_b$ be the smallest embedding size from the baseline methods, then space savings is defined as $1 - \frac{\sigma}{\sigma_b}$. Hence, larger values indicate a larger space savings (reduction in size). Notably, the Role2Vec variants require significantly less space than existing methods as shown above. Note $[x_2 \ x_3], \ldots, [x_1 \ \ldots \ x_0]$ is the attribute sets in Eq. (11)-(14) used as input to $\Phi$ for mapping nodes to types.

**5 Related Work**

Recent embedding methods for graphs have largely been based on the popular skip-gram model [Mikolov et al., 2013; Cheng et al., 2006] originally introduced for learning vector representations of words in text. In particular, DeepWalk [Perozzi et al., 2014] used this approach to embed the nodes such that the co-occurrence frequencies of pairs in short random walks are preserved. Node2vec [Grover and Leskovec, 2016] introduced hyperparameters to DeepWalk that tune the depth and breadth of the random walks. These approaches are becoming increasingly popular and have been shown to outperform a number of existing methods. These methods (and many others) are all based on simple random walks and thus are well-suited for generalization using the attributed random walk framework. While most network representation learning methods use only the graph [Perozzi et al., 2014; Tang et al., 2015; Cao et al., 2015; Grover and Leskovec, 2016], our framework exploits both the graph and structural features (e.g., motifs).

While most work has focused on transductive (within-network) learning, there has been some recent work on graph-based inductive approaches. Yang et al. [2016] proposed an inductive approach called Planetoid. While Planetoid is an embedding-based approach for semi-supervised learning and does not use any structural features, Rossi et al. [2017] proposed an inductive approach for (attributed) networks called DeepGL that learns (inductive) relational functions representing compositions of one or more operators applied to an initial set of graph features. Recently, Hamilton et al. [2017] proposed a similar approach that also aggregates features from node neighborhoods. However, these approaches are not based on random-walks. Heterogeneous networks [Shi et al., 2014] have also been recently considered [Chang et al., 2015; Dong et al., 2017] as well as attributed networks [Huang et al., 2017b; 2017a]. Huang et al. [2017b] proposed an approach for attributed networks with labels whereas Yang et al. [2015] used text features to learn node representations. Liang et al. [2017] proposed a semi-supervised approach for networks with outliers. Bojchevski et al. [2017] proposed an unsupervised rank-based approach. Coley et al. [2017] introduced a convolutional approach for attributed molecular graphs that learns graph embeddings as opposed to node embeddings. Duran et al. [Duran and Niepert, 2017] proposed an embedding Propagation method to learn node representations. However, most of these approaches are neither inductive nor space-efficient.

**6 Conclusion**

This work proposed a flexible framework based on the notion of attributed random walks. The framework serves as a basis for generalizing existing techniques (that are based on random walks) for use with attributed graphs, unseen nodes, graph-based transfer learning tasks, and allowing significantly larger graphs due to the inherent space-efficiency of the framework. Instead of learning individual embeddings for each node, our approach learns embeddings for each type based on functions that map feature vectors to types. This allows for both inductive and transductive learning.
References

[Ahmed et al., 2015] Nesreen K. Ahmed, Jennifer Neville, Ryan A. Rossi, and Nick Duffield. Efficient graphlet counting for large networks. In ICDM, page 10, 2015.

[Ahmed et al., 2016] Nesreen K. Ahmed, Jennifer Neville, Ryan A. Rossi, Nick Duffield, and Theodore L. Willike. Graphlet decomposition: Framework, algorithms, and applications. KAIS, pages 1–32, 2016.

[Akoglu et al., 2015] Leman Akoglu, Hanghang Tong, and Danai Koutra. Graph based anomaly detection and description: a survey. DMKD, 29(3):626–688, 2015.

[Al Hasan and Zaki, 2011] Mohammad Al Hasan and Mohammad J Zaki. A survey of link prediction in social networks. In Social Network Data Analytics, pages 243–275, 2011.

[Benson et al., 2016] Austin R Benson, David F Gleich, and Jure Leskovec. Higher-order organization of complex networks. Science, 353(6295):163–166, 2016.

[Bojchevski and Günnemann, 2017] Aleksandar Bojchevski and Stephan Günnemann. Deep gaussian embedding of attributed graphs: Unsupervised inductive learning via ranking. arXiv:1707.03815, 2017.

[Cao et al., 2015] Shaosheng Cao, Wei Lu, and Qiongkai Xu. GraRep: Learning graph representations with global structural information. In CIKM, pages 891–900. ACM, 2015.

[Cavallari et al., 2017] Sandro Cavallari, Vincent W Zheng, Hongyun Cai, Kevin Chen-Chuan Chang, and Erik Cambria. Learning community embedding with community detection and node embedding on graphs. In CIKM, pages 377–386, 2017.

[Chang et al., 2015] Shiyu Chang, Wei Han, Jiliang Tang, Guo-Jun Qi, Charu C Aggarwal, and Thomas S Huang. Heterogeneous network embedding via deep architectures. In SIGKDD, pages 119–128, 2015.

[Cheng et al., 2006] Winnie Cheng, Chris Greaves, and Martin Warren. From n-gram to skipgram to concgram. Int. J. of Corp. Linguistics, 11(4):411–433, 2006.

[Coley et al., 2017] Connor W Coley, Regina Barzilay, William H Green, Tommi S Jaakkola, and Klaas F Jensen. Convolutional embedding of attributed molecular graphs for physical property prediction. J. Chem. Info. & Mod., 2017.

[Dong et al., 2017] Yuxiao Dong, Nitesh V Chawla, and Ananth Grama. Pairwise alignment of protein interaction networks. JCB, 13(2):182–199, 2006.

[Du et al., 2017] Jian Tang, Meng Qu, Mingzhe Wang, Ming Zhang, Jun Yan, and Qiaozhu Mei. LINE: Large-scale Information Network Embedding. In WWW, pages 1067–1077, 2015.
[Yang et al., 2015] Cheng Yang, Zhiyuan Liu, Deli Zhao, Maosong Sun, and Edward Y Chang. Network representation learning with rich text information. In IJCAI, pages 2111–2117, 2015.

[Yang et al., 2016] Zhilin Yang, William W Cohen, and Ruslan Salakhutdinov. Revisiting semi-supervised learning with graph embeddings. arXiv:1603.08861, 2016.

[Zager and Verghese, 2008] Laura A Zager and George C Verghese. Graph similarity scoring and matching. Applied mathematics letters, 21(1):86–94, 2008.