Motif-Aware Graph Embeddings

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Abstract

In this paper, we propose our motif-aware approaches to the unsupervised network embedding and semi-supervised network labeling task. Our first algorithm is an unsupervised network embedding algorithm which uses the most statistically significant network motif as the guiding pattern for random walks to generate network context. We then use a Skipgram neural network to learn the latent network node representations from the generated context via Noise Contrastive Estimation. The second algorithm employs the Graph Convolution Network model on motif Laplacian matrices to inject the higher-order network structure into the neural network. Both of our algorithms utilize the higher-order organization (i.e. motifs organization) of complex networks. We demonstrate the effectiveness of our algorithms in comparison to other state-of-the-art network embedding algorithms.

1 Introduction

1.1 Complex network and machine learning

Network modelings have been an essential tool for a wide range of scientific fields [Newman, 2010; Bader *et al.*, 2003; Tang *et al.*, 2012; Milo *et al.*, 2002; Benson *et al.*, 2016]. The network science view reveals the underlying structure of a complex system. Based on the system's network structure, scientists can make predictions and explanation about the system's behavior. For example, in biology, the study on neuronal systems connectivity indicated that the component arrangement of a neural system is optimized for short processing paths rather than wiring lengths [Kaiser and Hilgetag, 2006]. Similarly, social networks analysis provides communities structures well as social interaction patterns [West *et al.*, 2014; Barabási, 2014]. However, along with the information explosion, analyzing large network-structured datasets poses a great challenge for traditional network analysis methods in term of scalability and complexity. To deal with such challenge, one promising approach is to apply machine learning methods (especially deep learning) to network problems.

Bridging the gap between network-structured data and typical data structure for machine learning is also a challenge.

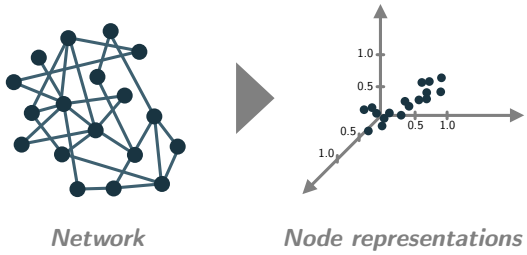

Figure 1: Learning a latent representation of nodes from the network structure. In this figure, the example network is embedded to a 3-dimensional real vector space.

Due to the irregularity in the network-structured data, it is desirable to have a *meaningful* network representation for machine learning applications. Learning network representation in real vector spaces can be viewed as manifold learning (nonlinear dimensionality reduction), and commonly known as *network embedding* in the literature. Traditionally, network embedding can be obtained via graph factorization methods.However, matrix factorization methods such as Spectral Clustering or Non-negative Matrix Factorization are shown to be unscalable due to the complexity of the algorithms [Perozzi *et al.*, 2014; Belkin and Niyogi, 2001]. Recently, several feasible network embedding algorithms have been proposed such as *Deepwalk* [Perozzi *et al.*, 2014] or *GCN* [Kipf and Welling, 2016]. These network embeddings algorithms utilize the state of the art machine learning models like Skipgram [Mikolov and Dean, 2013] and Variational Auto-Encoder [**?**] to achieve high quality node representation. In the context of graph embedding, we justify the *quality* by how well a common machine learning model performs on the learned embeddings.

1.2 Motifs in complex network

There are three scale of network analysis: macroscopic, mesoscopic, and microscopic. In the macroscopic scale, we consider a network as a whole to study its macro-properties such as robustness [Callaway *et al.*, 2000], or dynamics [Barabási, 2014]. In contrast, the microscopic scale studies the pair-wise interactions between nodes in a network which is specific to a given system [Newman, 2010]. In between macroscopic and microscopic, the mesoscopic scale consid-

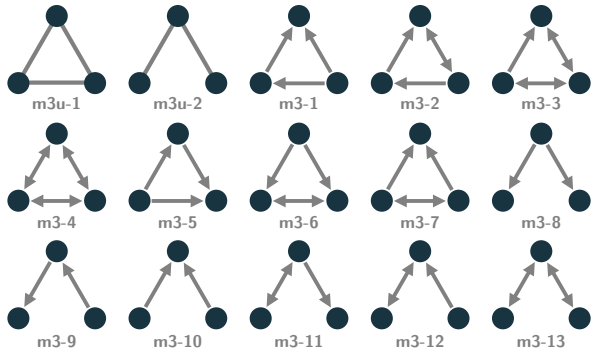

Figure 2: Size-3 motifs

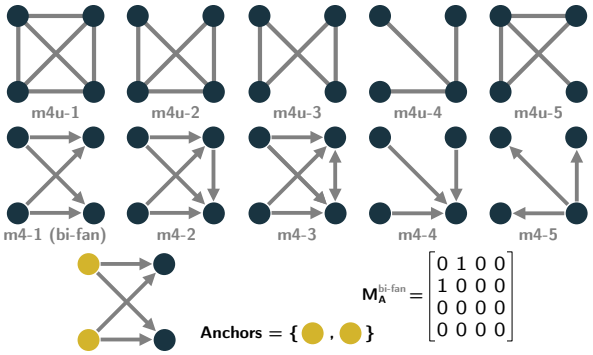

Figure 3: Size-4 motifs and anchor set example

ers the network is a composition of subgraphs. In many research, especially computational biology, the mesoscopic components are called *motifs*, and it is common to think of them as building blocks of a complex system [Milo *et al.*, 2002].

Definition 1.1. *Network motif*: Given a graph $G = (V, E)$, define a subgraph $G' = V', E'$ with $V' \subseteq V$; $E' \subset E$ s.t. $i, j \in V' \forall e_{ij} \in E'$ and $|V'| \ll |V|$. Recurring subgraphs are called *network motif* when they are statistically significant.

Also referred as higher-order organization by Benson *et al.*, network motifs are believed to represent the underlying mechanism of a complex system [Alon, 2007; 2006; Mangan and Alon, 2003]. For instance, the directional bi-fan motif (figure 1.2) and its simplified unidirectional version are crucial in a citation network. Beside having a statistical significance, bi-fan motif is also intuitively sensible in citation network as it represents the citation mechanism. The correlation of recurring subgraphs and system functionality has been studied extensively in biological systems such as transcription networks [Mangan and Alon, 2003] and brain networks [Van Den Heuvel and Pol, 2010; Honey *et al.*, 2007]. As networks motifs have been recognized as the fundamental building block of a complex systems, using them as a structural guidance for machine learning on graph data can yield positive improvements.

Our main idea in this paper is to construct the motif co-occurrence matrix from a given network, and use it as: 1. An adjacency matrix describing a motif network for random walks; 2. A mean to compute motif Laplacian and Fourier basis for the graph convolution operation. Section 2 describes the related work on network motif conductance and network embedding. We give detail of our algorithms in section. The experimental setup and results are given in section 4 and 5 respectively. We discuss the relationship between our two proposed algorithms and their limitations in section 6.

2 Related work

2.1 Unsupervised Network Embedding

Based on the Skipgram model [**?**] in natural language processing, Perozzi *et al.* proposed their scalable graph embedding algorithm named DeepWalk. Their results on node classification proved the effectiveness of *Deepwalk* in learning a lower dimensionality representation of a complex network. Subsequent work to DeepWalk further improved node classification accuracy by modifying graph context generation process [Tang *et al.*, 2015; Cao *et al.*, 2015; Yang *et al.*, 2016; Grover and Leskovec, 2016].

It is worthwhile to mention that *Planetoid*, proposed by Yang *et al.*, works slightly different to other skipgram-based models. Instead of generating graph context only from the network structure, *Planetoid* also samples nodes based on training labels. Furthermore, *Planetoid* injects the network node's feature vectors for better embedding and node labeling results.

2.2 Semi-supervised Network Labeling

Another semi-supervised learning model similar to the aforementioned *Planetoid* is Graph Convolutional Networks (GCN) [Kipf and Welling, 2016]. GCN uses the graph convolutional operation as a transformation for feature vectors on a network. By stacking these convolutional operation into a neural network, the authors of GCN has been able to achieve remarkable accuracy in node classification and link prediction results compared to the previous researches. Moreover, the running time for GCN was superior compared to other algorithms such as *Deepwalk* or *Planetoid*.

The convolution on a graph G of a function of the graph Laplacian g_θ (also called a filter or a kernel) and a signal x is defined as:

$$g_\theta * x = U g_\theta U^\top x,$$

where $L = U \Lambda U^\top$, U is the Fourier basis and Λ is called the frequencies of the graph. Graph convolution has been shown effective in processing graph-structured data, and also argued to be the generalization of convolutional networks [Shuman *et al.*, 2013; Defferrard *et al.*, 2016; Kipf and Welling, 2016]. In practice, given a graph where each node has a feature vector, we can treat the feature vector of the graph as signals. The output y of these "signals" filtered by g_θ on the graph is given by the graph convolution and deconvolution operations:

$$y = g_\theta(U \Lambda U^\top)x = U(g_\theta(\Lambda)U^\top)x \tag{1}$$

Computing equation 1 is computationally expensive due to the matrix multiplication and eigenvector decomposition operations. Therefore, fast estimation methods such as Chebyshev polynomial was suggested in [Hammond *et al.*, 2011].

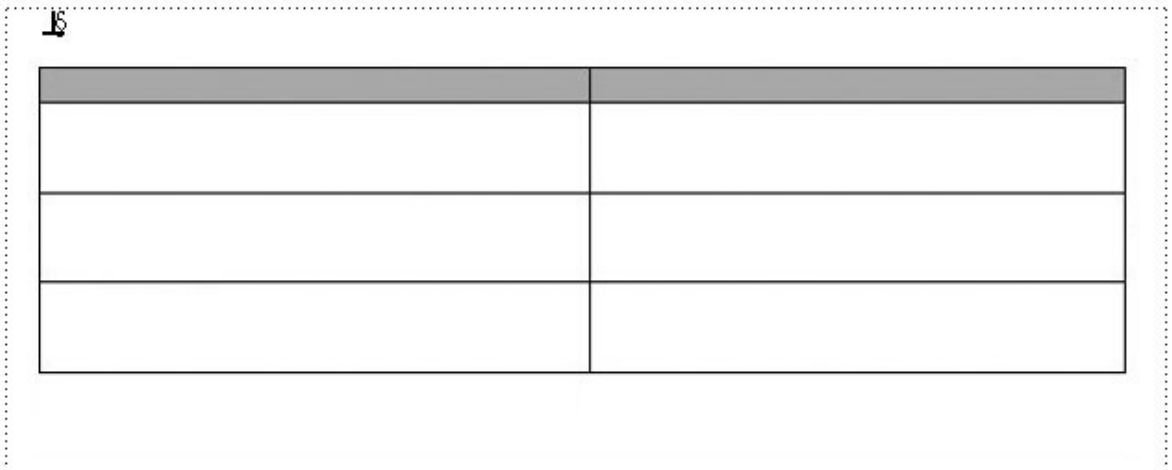

Figure 4: Significant graph for size-3 motifs

These aforementioned approaches to graph embeddings are similar in the sense that they all learn latent representations of a complex network from data, then use this representation to solve a network problem (e.g. link prediction, node labeling, community detection) using various machine learning algorithms.

2.3 Motif Conductance

As an generalization of *network conductance* (also graph conductance or Cheeger constant of a graph), Benson *et al.* proposed the concept of *motif conductance* in [Benson *et al.*, 2016]. Similar to network conductance, motif conductance is a *score* for a cut $(S, \bar{S})$ targeting a motif $\mathbf{m}$:

$$\phi_{\mathbf{m}}(S) = \frac{\text{cut}_{\mathbf{m}}(S, \bar{S})}{\min[\text{vol}_{\mathbf{m}}(S), \text{vol}_{\mathbf{m}}(\bar{S})]},$$

where S is a node set in a network G; $\bar{S}$ is the complement of S; $\text{vol}_{\mathbf{m}(S)}$ is the number of motif instance end points in S. Intuitively, minimizing the motif conductance is equivalent with minimizing the number of motif $\mathbf{m}$ gets *split* by the cut. A motif is split when there is at least one anchor node in S and at least one in $\bar{S}$. Benson *et al.* then perform motif analysis and graph clustering based on this definition of motif conductance. Their result further confirms the structural role of motifs in a complex network.

Definition 2.1. *Motif co-occurrence matrix*: Given a graph $G = (V, E)$, in which $v \in V$. The motif co-occurrence matrix of a motif $\mathbf{m}$ is given by:

$$M_{i,j}^{\mathbf{m}} = \sum_{(v, \chi_{\mathcal{A}}(v)) \in \mathbf{m}} \mathbf{1}(i, j \subset \chi_{\mathcal{A}}(v))$$

In here, $\mathcal{A}$ represents the anchor set; $(v, \chi_{\mathcal{A}}(v))$ represents pairs of node $v \in V_G$ and the other anchor nodes generated by $\chi_{\mathcal{A}}$. If the anchor node set $\mathcal{A}$ is empty, all motif co-occurrence is counted toward the motif co-occurrence matrix M. Otherwise, only nodes in the anchor set will be counted. Figure 1.2 illustrates the bi-fan motif and its anchor set. Algorithm 1 provides detail for constructing a motif co-occurrence matrix.

Algorithms involving network motifs have high time complexity due to the problem of graph isomorphism. For such reason, in most large graph analysis, only motifs of size 5 or smaller are considered. In our experiments, we only consider motif of size 4 at most. This limitation is due to the large size of networks that we experimented. Although the analysis is limited by the motif size, we have been able to empirically show the effectiveness of the motif-aware methods. Furthermore, as mentioned in [Benson *et al.*, 2016], motif algorithms can be easily parallelized. Therefore, the extension to larger size motifs can be made possible by parallelizing the motif analysis procedures. Further discussion on parallelizing the motif analysis process be provided in later sections.

3 Methods

In this section, we present the detail of our methods. Firstly, we propose the basis for the network motif selection from a network. Secondly, we present two approaches employing motif patterns to learn graph embeddings: *motifwalk* and *mgcn*.

3.1 Motifs Analysis

In the previous section, we have explained the importance of network motifs in network analysis. In this section, we present the metric for measuring network motif significance and the definition of motif Laplacian.

In order to measure the importance of a network motif, we compare the given network against a null model. The null model of an empirical network is an ensemble of randomly generated networks having the same number of nodes and edges as the network. For small networks with less than 10,000 edges, we generated 100 random networks as the ensemble of the null model. On the other hand, we generated 10 random networks for the null model of larger networks. The z-score is given by:

$$z\text{-score} = \frac{N_{\mathbf{m}}(G) - N_{\mathbf{m}}(G_{\text{random}})}{\sigma_{\mathbf{m}}(G_{\text{random}})}$$

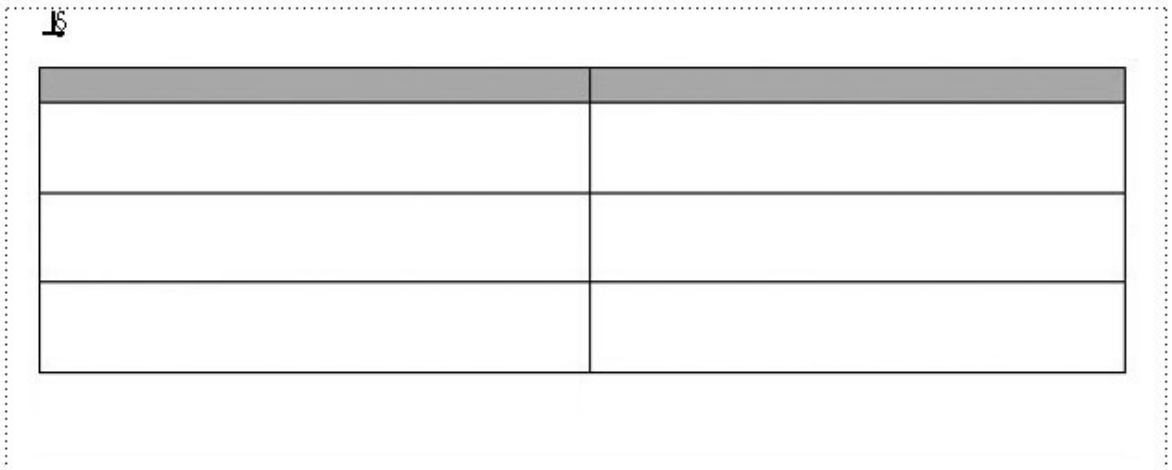

Figure 5: Significant graph for size-4 motifs

where $N_{\mathbf{m}}(G)$ is the count of motif $\mathbf{m}$ in the empirical network; $N_{\mathbf{m}}(G_{\text{random}})$ is the mean of the null model; and $\sigma_{\mathbf{m}}(G_{\text{random}})$ is the variance. The z-score's values can range from $-\infty$ to $+\infty$. In practice, the most simple motifs (figure 1.2-m2,3,4) often have the highest frequencies and negative z-score. We ignored such motifs in our analysis. We select motif which has the highest positive z-score because these motifs highlight the difference between the empirical network and random networks.

Convolution operations on a network can be viewed as a method to incorporate the nodes' information (e.g. feature vectors) and the network structure. The Fourier basis and network frequencies of a motif co-occurrence matrix is obtained through the eigenvalue decomposition of the motif Laplacian matrix $\mathcal{L}_{\mathbf{m}}$:

$$\mathcal{L}_{\mathbf{m}} = U_{\mathbf{m}} \Lambda_{\mathbf{m}} U_{\mathbf{m}}^{\top} \tag{2}$$

In here, $\Lambda_{\mathbf{m}} = diag(\lambda_{\mathbf{m}})$ is called the frequencies of the motif network; $\mathcal{L}_{\mathbf{m}}$ is the normalized motif Laplacian given by:

$$\begin{aligned} \mathcal{L}_{\mathbf{m}} &= D_{\mathbf{m}}^{-1/2} L_{\mathbf{m}} D_{\mathbf{m}}^{-1/2} \\ &= I - D_{\mathbf{m}}^{-1/2} M^{\mathbf{m}} D_{\mathbf{m}}^{-1/2} \end{aligned} \tag{3}$$

where $L_{\mathbf{m}} = D_{\mathbf{m}} - M^{\mathbf{m}}$; $M^{\mathbf{m}}$ is the motif co-occurrence matrix; and $D_{\mathbf{m}} = \text{diag}(\sum_j M_{i,j}^{\mathbf{m}})$.

$U_{\mathbf{m}}$ from equation 3 is the Fourier basis of the network motif structure which is used for motif convolution. Given signal $x \in \mathbb{R}^n$ on a network, the motif Fourier transform is defined as $\hat{x} = U_{\mathbf{m}}^{\top} x$, and its inverse as $x = U_{\mathbf{m}} \hat{x}$. It follows that the output of signal x filtered by a function of graph Laplacian $g_\theta(L)$ parameterized by a set of coefficient θ is given by:

$$\begin{aligned} y = g_\theta * x &= g_\theta(U_{\mathbf{m}} \Lambda_{\mathbf{m}} U_{\mathbf{m}}^{\top}) x \\ &= U_{\mathbf{m}}(g_\theta(\Lambda_{\mathbf{m}}) U_{\mathbf{m}}^{\top}) x \end{aligned} \tag{4}$$

Due to the complexity of eigenvector decomposition and matrix multiplication, we use the linear formulation suggested in [Kipf and Welling, 2016] to estimate the costly convolution operation:

$$\begin{aligned} y = g_{\theta'} * x &\approx \sum_{k=0}^{K} \theta'_k T_k(\tilde{L}) x \\ &\approx \theta'_0 x + \theta_1 (L - I) = \theta'_0 x - \theta'_1 D_{\mathbf{m}}^{-1/2} M^{\mathbf{m}} D_{\mathbf{m}}^{-1/2} \\ &\approx \theta \left(I + D_{\mathbf{m}}^{-1/2} M^{\mathbf{m}} D_{\mathbf{m}}^{-1/2} \right) \end{aligned} \tag{5}$$

The motif Laplacian is a positive semi-definite matrix similar to the matrices used in previous graph convolution researches [Hammond *et al.*, 2011; Defferrard *et al.*, 2016; Kipf and Welling, 2016]. However, the difference is that motif Laplacian

Algorithm 1: Motif co-occurrence matrix generation

Data: Graph $G = (V, E)$
Input: isBinary, $\mathbf{m}$, $\mathcal{A}$
Output: $M^{\mathbf{m}}$
begin
  diam ← Diameter($\mathbf{m}$, $\mathcal{A}$);
  $V \leftarrow G$.nodes();
  for $i \in$ *nodes* **do**
    $G' \leftarrow$ induced graph from BFS(node, diam);
    for $j \in G'$*.nodes()* **do**
      if *(i,j) satisfies* $\mathcal{A}$ **then**
        $c \leftarrow$ count $\mathbf{m}$ in G';
        if *isBinary* **then**
          $M_{i,j}^{\mathbf{m}} \leftarrow 1$ if $c > 0$ else 0
        else
          $M_{i,j}^{\mathbf{m}} \leftarrow c$
      else
        $M_{i,j}^{\mathbf{m}} \leftarrow 0$
  return $M^{\mathbf{m}}$

3.2 Biased Random Walk

Previous Skipgram-based graph embedding models employ random walks for graph context generation. To improve

the embedding results, structure-aware context generation methods were proposed in [Tang *et al.*, 2015; Grover and Leskovec, 2016]. However, the limitation of *LINE* lies at the fact that it only consider the second-order proximity (bi-fan motif), *node2vec* requires the costly cross-validation search for its hyper- parameters p and q. To solve the above mentioned problems, we propose a biased random walk algorithm for graph context generation which can be considered the generalization of *LINE* and *deepwalk*. Since our algorithm decides the walk pattern supported by the most significant network motif before performing context generation, we achieve the simplicity of *deepwalk* while having the structure-aware context as of *LINE* and *node2vec*.

Our *motifwalk* algorithm has two steps: motif adjacency matrix construction and context generation. Firstly, we construct a binary motif co-occurrence matrix from the given network. We select the motif pattern as described in the previous section. Since the constructed matrix accounts the co-occurrence of network node pairs in a motif, it is a symmetric matrix. Secondly, after having the motif adjacency matrix, we run random walks on this new network induced by the adjacency matrix for motif context generation. The obtained motif context is used jointly with random walks context generated with the original network to train an embedding skip-gram model. Algorithm 1 and algorithm 2 describe the *motifwalk* algorithm.

Algorithm 2: Motif-aware graph context generation

Data: Graph $G = (V, E)$, Motif Graph $G_{\mathbf{m}} = (V, E)$
Input: length, nwalk, nmwalk
Output: context
begin
  context ← [ ];
  V ← G.nodes();
  nodes ← Shuffle(V);
  for *node* ∈ *nodes* **do**
    walks ← [ ];
    for *i=0; i* < *nwalk; ++i* **do**
      walks += RandomWalk(graph=G,start=node, len=length)
    for *i=0; i¡nwalk; ++i* **do**
      walks += RandomWalk(graph=$G_{\mathbf{m}}$start=node, len=length)
    context += walks
  return *context*

Similar to Skipgram-based models, *motifwalk* is an unsupervised algorithm which learns graph embedding through an optimization process. Since there is two network contexts generated in our algorithm, the objective function is given by:

$$\mathcal{O} = \arg\max_{W^{\text{emb}}} \left(\gamma \ell_{\text{random walk}} + (1-\gamma)\ell_{\text{motif walk}}\right) \tag{6}$$

where $\ell_{\text{random walk}}$ and $\ell_{\text{motif walk}}$ are the log-likelihoods of the network contexts generated by random walk and motif walk respectively; γ is a hyper-parameter controlling the ratio between random walk. γ is selected empirically based on the z-score of the targeted motif. The likelihood of a *context* vertex v_c, given a *target* vertex v_t is:

$$\Pr(v_c|v_t) = \frac{\exp\left(\langle \omega_{v_c}, \omega_{v_t} \rangle\right)}{\sum_{k \in V} \exp\left(\langle \omega_{v_k}, \omega_{v_t} \rangle\right)}, \tag{7}$$

here, $\langle \cdot, \cdot \rangle$ denotes the inner product; and ω_v denotes the real vector representation of node v. Although the log-likehood given by equation 7 is straight forward, the normalization factor will be a computational bottle neck in large graphs. Therefore, we use noise contrastive estimation as suggested in [**?**; Grover and Leskovec, 2016] for estimating the normalization factor of our model. The final output of *motifwalk* is a set of real vectors representing each node in the given network. These vectors encode the underlying structural relationship between network nodes and can be used as feature vectors for link prediction and node classification.

3.3 Motif Convolutional Architecture

In this section we propose our motif convolutional deep neural network architecture for semi-supervised graph labeling tasks. As mentioned above, graph convolution is a signal processing technique in which a network of signals reside on nodes (e.g. sensor network) is processed in the graph spectral domain defined on the graph structure.

In the previous section, we have defined the graph convolution operation on motif co-occurrence matrix. We use the motif convolution as the second layer in our motif convolutional network (m-gcn). Based on the linear approximation proposed by Kipf and Welling, we define the forward computation of our model as:

$$\begin{aligned} Z_{\text{forward}} &= f(X, A, M) \\ &= \text{softmax}(\hat{M}\text{ReLU}(\hat{A}XW^{(0)})W^{(1)}), \end{aligned} \tag{8}$$

where A and M is a binary adjacency matrix and motif co-occurrence matrix respectively; $\hat{A}$ and $\hat{M}$ are constructed by the *renormalization trick* as suggested in [Kipf and Welling, 2016]; X contains the feature vectors for each graph node; $W^{(0)}$ and $W^{(1)}$ are learnable variables. With the backpropagation learning algorithm and the softmax cross entropy loss, the weight of layer k is updated as follow:

$$\frac{\partial E}{\partial W_{i,j}^{(k)}} = \sum_{s=1}^{S} [x]^{\top} \frac{\partial E}{\partial y_{k,j}} \tag{9}$$

4 Experiments

4.1 Datasets

To compare *motifwalk* performance with other unsupervised graph embedding models, we have chosen the node labeling task on various type of networks (with ground-truth node labels). In this paper, we compare the performance of *motifwalk* to *Spectral Clustering*, *deepwalk* [Perozzi *et al.*, 2014], *node2vec* [Grover and Leskovec, 2016]. Table 2 gives the networks' statistics. The second model *m-gcn* is a semi-supervised model for node labeling task. We present the comparison of our model to *planetoid* and *gcn* under the same

METHOD	CITESEER	CORA	PUBMED	NELL
Deepwalk	43.2	67.2	65.3	58.1
motifwalk	45.7	68.0	64.9	58.8
Planetoid	64.7	75.7	77.2	61.9
GCN	70.3	81.5	79.0	66.0
m-GCN	**71.2**	**82.1**	**79.5**	**66.1**
m-GCN (rand. splits)	70.2 ± 0.5	81.1 ± 0.5	79.3 ± 0.7	62.0 ± 1.4

Table 1: Accuracy score for multi-class labeling

DATASET	#CLASSES	#NODES	#EDGES	#FEATURES
CITESEER	39	10,312	333,983	3,703
CORA	6	2,708	4,732	1,433
PUBMED	3	19,717	44,338	76,584
NELL	210	65,755	266,144	5,414

Table 3: Datasets for semi-supervised embeddings

experimental setting in [Kipf and Welling, 2016]. Table **??** shows details of each dataset.

Blogcatalog3 [Tang and Liu, 2009] is a blogger social network. Each node in the network represents an user. The node labels represent a blogger's interests and each node has at least one label. Since Blogcatalog is a social network, the results obtained from motif analysis agrees with the term "friends of friend are friends".

PPI [**?**] is a protein transcription network.

Citeseer, Cora, Pubmed [**?**; **?**; **?**] are citation networks consist of scientific papers and their citations represented by directed edges.

NELL [**?**] is a knowledge network with triplet description.

DATASET	#CLASSES	#NODES	#EDGES	TRAINING RATIO
BLOGCATALOG	39	10,312	333,983	0.5
CITESEER	6	3,327	4,732	0.5
PPI	50	3,890	76,584	0.5

Table 2: Datasets for unsupervised embeddings

4.2 Motif significance

For each of the networks in experiment, we computes the z-scores for size-3 and size-4 directed motifs and report the motif significance in figure 2.2 and 3.1. Based on these results, we select the most significant motif of each network for our algorithms.

5 Results

We report the performance of each algorithm on graph node labeling task.

DATASET	MOTIF
BLOGCATALOG	Figure 1.2-m2
PPI	Figure 1.2-m4
CITESEER	Figure 1.2-m7
CORA	Figure 1.2-m7
PUBMED	Figure 1.2-m7
NELL	Figure 1.2-m4

Table 4: Target motifs for each network

5.1 Unsupervised node labeling

METHOD	BLOGCATALOG	CITESEER	PPI
Spectral clustering	0.23	0.30	0.14
Deepwalk	0.22	0.65	0.18
Node2Vec	0.22	0.66	**0.18**
motifwalk	**0.24**	**0.68**	0.17

Table 5: F1-macro score for multiclass labeling

5.2 Semi-supervised node labeling

6 Discussion

Our paper's contributions are proposing an extension to the graph convolutional architecture; proposing the uses and demonstrate the importance of motifs in real world networks.

Limitation:

Acknowledgments

I would like to thank.

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