

Motif-Aware Graph Embeddings

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Abstract

In this paper, we propose two motif-aware approaches for the unsupervised and semi-supervised graph embedding task. Our first model applies the most significant motif pattern on a graph as a guiding pattern for random walks. We then use a skipgram model with noise contrastive estimation to learn the graph embedding from generated random walk context. The second model employs the higher-order organization (i.e. motifs organization) of complex networks, and injects the higher-order connectivity patterns into each layer in a deep graph convolutional networks. We demonstrate the effectiveness of our motif-aware approaches on node labels classification, link prediction, and t-SNE visualization.

1 Introduction

1.1 Complex network and machine learning

Network modeling 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 usually 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 as well as social interaction patterns [West *et al.*, 2014; Barabási, 2014]. However, along with the information explosion, the large graph-structured data poses a great challenge for traditional network analysis methods in term of scalability and complexity. To deal with such challenges, one promising approach is to apply machine learning methods (especially deep learning) methods to network problems.

Bridging the gap between network science and machine learning is also a challenging task. Due to the irregularity in network and graph-structured data, it is desirable to have a *meaningful* and structural network representation for machine learning application. Traditionally, vector representation can

be obtained via graph spectral methods. However, spectral methods are shown to be unscalable without estimation methods TODO: find theoretical citation [Perozzi *et al.*, 2014; Grover and Leskovec, 2016]. Recently, inspired by the skipgram model in natural language processing [Mikolov and Dean, 2013], Perozzi *et al.* proposed their scalable graph embedding algorithm named DeepWalk. Their results node classification proved the effectiveness of their algorithm in learning a lower dimensionality representation of a complex network. Subsequence works to DeepWalk further improved node classification accuracy by modifying graph context generation process [Tang *et al.*, 2015; Cao *et al.*, 2015; Grover and Leskovec, 2016]. On the other hand, more direct (and more effective) approaches were proposed in [Yang *et al.*, 2016; Kipf and Welling, 2016]. Instead of learning the network representation using only network structure (e.g. adjacency matrix), Yang *et al.* proposed to injects the known labeling and node feature into the representation learning process. Kipf and Welling further improved results from plane-toid [Yang *et al.*, 2016] by applying graph convolution technique in their deep network model. These aforementioned approaches are similar in the sense that they all learn a latent representation of a complex network from data, then use this representation to solve a network problem using various machine learning tools.

1.2 Motifs in complex network

There are three scale of network analysis: macroscopic, mesoscopic, and microscopic. The macroscopic scale displays a network as a whole to study its robustness [Callaway *et al.*, 2000] or dynamics TODO: find citation [Barabási, 2014]. In contrast, the microscopic scale studies the pair-wise interactions between nodes in a network which is specific to the given system TODO: find citation [Newman, 2010]. On the other hand, the mesoscopic scale is an intermediate in which we consider 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 for 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 $V' \subseteq V$; $E' \subseteq E$ 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 TODO: figure and its simplified undirectional version TODO: figure 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 as an activity in a subgraph. 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.

Generally, algorithms involving network motifs have to deal with the problem of graph isomorphism. For such reason, in most analysis, only motifs of size 5 or smaller are considered. In this paper, we only consider motif of size 4 at most. This limitation is due to the large size of networks that we experimented. Although limited by the motif size, we have been able to practically show the effectiveness of the motif-aware methods. On the other hand, 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 parallelize the motif analysis procedures. Further discussion will be provided in later sections.

2 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 *m-cn*.

2.1 Network Motifs

In the previous section, we have introduced 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:

$$z\text{-score} = \frac{N_{\mathbf{m}}(G) - N_{\mathbf{m}}(G_{\text{random}})}{\sigma_{\mathbf{m}}(G_{\text{random}})} \quad (1)$$

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 formal definition of the motif co-occurrence matrix for a motif \mathbf{m} on an unweighted, directed graph G is given by:

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

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 ?? illustrates the bi-fan motif and an anchor set.

TODO: Present laplacian and power of laplacian of graph. Present motif types and laplacian for each type. Algorithms and estimation techniques. Discuss about the change in maximum eigenvalue due to the weighted motif laplacian.

2.2 Biased Random Walk

Present the original motifwalk model.

2.3 Motif Convolutional Architecture

In this section we propose our motif convolutional deep neural network architecture for semi-supervised graph labeling tasks. 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. 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:

$$y = g_{\theta}(U \Lambda U^{\top}) x = U(g_{\theta}(\Lambda) U^{\top}) x \quad (2)$$

Computing equation 2 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]. Based on the further linear approximation proposed by Kipf and Welling, we propose our two layers motif convolutional network model as:

$$\begin{aligned} Z_{\text{forward}} &= f(X, A, M) \\ &= \text{softmax}(\hat{M} \text{ReLU}(\hat{A} X W^{(0)}) W^{(1)}), \end{aligned} \quad (3)$$

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, the weight of layer k is updated as follow:

$$\frac{\partial E}{\partial W_{i,j}^{(k)}} = \sum_{s=1}^S [x]^\top \frac{\partial E}{\partial y_{k,j}} \quad (4)$$

3 Experiments

3.1 Datasets and observations

3.2 Motif significance

3.3 Architectures

4 Results

4.1 Unsupervised

Traditional task on blogcatalog and others. Link prediction. t-SNE.

4.2 Semi-supervised

Task on featured networks.

5 Related work

5.1 Spectral approaches

5.2 Skipgram-based approaches

5.3 Deep neural network approaches

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:

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