

Motif-Aware Network Embeddings

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Abstract

In this paper, we propose a deep convolutional network model for the unsupervised and semi-supervised graph embedding task. Our model employs the higher-order organization (i.e. motifs) of complex networks, and injects the higher-order connectivity patterns into each layer in a deep graph convolutional networks. We demonstrate our results on node labels classification, link prediction, and t-SNE visuallization.

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 skip-gram 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; ?]. 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. ? further improved results from planetoid [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 Motif 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 sub-graphs. 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 $V' \subseteq V$; $E' \subset E$ 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 refered 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.

2 Methods

In this section, we present the detail of our method. Firstly, we propose the use of motif co-occurrence matrix and its Fourier basis. Secondly, we present the graph convolutional architecture. Lastly, the detail of each motif graph convolutional network architecture is presented for each classification task.

2.1 Motif laplacian

Present laplacian and power of laplacian of graph. Present motif types and laplacian for each type. Algorithms and estimation techniques.

2.2 Graph convolutional architecture

Present graph convolutional and estimation technique. Present renormalization trick and GCN. Present using motif types between graph layers.

Graph convolution is computed using the eigenvectors of the graph Laplacian \mathcal{L} . Given two signals x , y , and a filter function $g_{\mathcal{G}}$, the convolution of x and y is defined as:

$$x *_{g_{\mathcal{G}}} =$$

2.3 Unsupervised graph motif auto-encoder

Architecture for auto-encoder.

2.4 Semi-supervised node labeling

Architecture for node labeling.

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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```
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```

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Acknowledgments

The preparation of these instructions and the L_AT_EX and Bib_TE_X files that implement them was supported by Schlumberger Palo Alto Research, AT&T Bell Laboratories, and Morgan Kaufmann Publishers. Preparation of the Microsoft Word file was supported by IJCAI. An early version of this

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document was created by Shirley Jowell and Peter F. Patel-Schneider. It was subsequently modified by Jennifer Balentine and Thomas Dean, Bernhard Nebel, and Daniel Pagenstecher. These instructions are the same as the ones for IJCAI-05, prepared by Kurt Steinkraus, Massachusetts Institute of Technology, Computer Science and Artificial Intelligence Lab.

A \LaTeX and Word Style Files

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