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 explaination 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 challendges, 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.* propsed 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 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 $V' \subseteq V$; $E' \subset E$ 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 strucutural guidance for machine learning on graph data can yield possitive improvements.

2 Methods

In this section, we present our general approach to inject network motif patterns into a deep neural network, and propose specific architecture for each of the pattern recognition 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.

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 worldnetworks.

Limitation:

6.1 Layout

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Acknowledgments

The preparation of these instructions and the LaTeX and BibTeX 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 document was created by Shirley Jowell and Peter F. Patel-Schneider. It was subsequently modified by Jennifer Ballentine 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.

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References

[Alon, 2006] Uri Alon. *An introduction to systems biology: design principles of biological circuits*. CRC press, 2006.

[Alon, 2007] Uri Alon. Network motifs: theory and experimental approaches. *Nature Reviews Genetics*, 8(6):450–461, 2007.

[Bader *et al.*, 2003] Gary D Bader, Doron Betel, and Christopher WV Hogue. Bind: the biomolecular interaction network database. *Nucleic acids research*, 31(1):248–250, 2003.

[Barabási, 2014] Albert-László Barabási. Network science book. *Network Science*, 2014.

[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.

[Callaway *et al.*, 2000] Duncan S Callaway, Mark EJ Newman, Steven H Strogatz, and Duncan J Watts. Network robustness and fragility: Percolation on random graphs. *Physical review letters*, 85(25):5468, 2000.

[Cao *et al.*, 2015] Shaosheng Cao, Wei Lu, and Qiongkai Xu. Grarep: Learning graph representations with global structural information. In *Proceedings of the 24th ACM International on Conference on Information and Knowledge Management*, pages 891–900. ACM, 2015.

[Grover and Leskovec, 2016] Aditya Grover and Jure Leskovec. node2vec: Scalable feature learning for networks. In *Proceedings of the 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, 2016.

[Honey *et al.*, 2007] Christopher J Honey, Rolf Kötter, Michael Breakspear, and Olaf Sporns. Network structure of cerebral cortex shapes functional connectivity on multiple time scales. *Proceedings of the National Academy of Sciences*, 104(24):10240–10245, 2007.

[Kaiser and Hilgetag, 2006] Marcus Kaiser and Claus C Hilgetag. Nonoptimal component placement, but short processing paths, due to long-distance projections in neural systems. *PLoS Comput Biol*, 2(7):e95, 2006.

[Mangan and Alon, 2003] Shmoolik Mangan and Uri Alon. Structure and function of the feed-forward loop network motif. *Proceedings of the National Academy of Sciences*, 100(21):11980–11985, 2003.

[Mikolov and Dean, 2013] T Mikolov and J Dean. Distributed representations of words and phrases and their compositionality. *Advances in neural information processing systems*, 2013.

[Milo *et al.*, 2002] Ron Milo, Shai Shen-Orr, Shalev Itzkovitz, Nadav Kashtan, Dmitri Chklovskii, and Uri Alon. Network motifs: simple building blocks of complex networks. *Science*, 298(5594):824–827, 2002.

[Newman, 2010] Mark Newman. *Networks: an introduction*. Oxford university press, 2010.

[Perozzi *et al.*, 2014] Bryan Perozzi, Rami Al-Rfou, and Steven Skiena. Deepwalk: Online learning of social representations. In *Proceedings of the 20th ACM SIGKDD international conference on Knowledge discovery and data mining*, pages 701–710. ACM, 2014.

[Tang *et al.*, 2012] Lei Tang, Xufei Wang, and Huan Liu. Scalable learning of collective behavior. *IEEE Transactions on Knowledge and Data Engineering*, 24(6):1080–1091, 2012.

[Tang *et al.*, 2015] Jian Tang, Meng Qu, Mingzhe Wang, Ming Zhang, Jun Yan, and Qiaozhu Mei. Line: Large-scale information network embedding. In *Proceedings of the 24th International Conference on World Wide Web*, pages 1067–1077, 2015.

[Van Den Heuvel and Pol, 2010] Martijn P Van Den Heuvel and Hilleke E Hulshoff Pol. Exploring the brain network: a review on resting-state fmri functional connectivity. *European Neuropsychopharmacology*, 20(8):519–534, 2010.

[West *et al.*, 2014] Robert West, Hristo S Paskov, Jure Leskovec, and Christopher Potts. Exploiting social network structure for person-to-person sentiment analysis. *arXiv preprint arXiv:1409.2450*, 2014.

[Yang *et al.*, 2016] Zhilin Yang, William W. Cohen, and Ruslan Salakhutdinov. Revisiting semi-supervised learning with graph embeddings. In *Proceedings of the 33rd International Conference on Machine Learning*. ICML, 2016.