Motif-Aware Network Embeddings

Anonymous authors

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 machine learning tasks.

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 Style and Format

LaTeX and Word style files that implement these instructions can be retrieved electronically. (See Appendix A for instructions on how to obtain these files.)

2.1 Layout

Print manuscripts two columns to a page, in the manner in which these instructions are printed. The exact dimensions for pages are:

- left and right margins: .75″
- column width: 3.375″
- gap between columns: .25″
- top margin—first page: 1.375″
- top margin—other pages: .75″
- bottom margin: 1.25″
- column height—first page: 6.625″
- column height—other pages: 9″

All measurements assume an 8-1/2″ × 11″ page size. For A4-size paper, use the given top and left margins, column width, height, and gap, and modify the bottom and right margins as necessary.

2.2 Format of Electronic Manuscript

For the production of the electronic manuscript, you must use Adobe's *Portable Document Format* (PDF). A PDF file can be generated, for instance, on Unix systems using `ps2pdf` or on Windows systems using Adobe's Distiller. There is also a website with free software and conversion services: `http://www.ps2pdf.com/`. For reasons of uniformity, use of Adobe's *Times Roman* font is strongly suggested. In LaTeX2e, this is accomplished by putting

```
\usepackage{times}
```

in the preamble.[1]

Additionally, it is of utmost importance to specify the American **letter** format (corresponding to 8-1/2″ × 11″) when formatting the paper. When working with `dvips`, for instance, one should specify `-t letter`.

[1]You may want also to use the package `latexsym`, which defines all symbols known from the old LaTeX version.

2.3 Title and Author Information

Center the title on the entire width of the page in a 14-point bold font. Below it, center the author name(s) in a 12-point bold font, and then center the address(es) in a 12-point regular font. Credit to a sponsoring agency can appear on the first page as a footnote.

Blind Review

In order to make blind reviewing possible, authors must omit their names and affiliations when submitting the paper for review. In place of names and affiliations, provide a list of content areas. When referring to one's own work, use the third person rather than the first person. For example, say, "Previously, Gottlob [**?**] has shown that…", rather than, "In our previous work [**?**], we have shown that…" Try to avoid including any information in the body of the paper or references that would identify the authors or their institutions. Such information can be added to the final camera-ready version for publication.

2.4 Abstract

Place the abstract at the beginning of the first column 3″ from the top of the page, unless that does not leave enough room for the title and author information. Use a slightly smaller width than in the body of the paper. Head the abstract with "Abstract" centered above the body of the abstract in a 12-point bold font. The body of the abstract should be in the same font as the body of the paper.

The abstract should be a concise, one-paragraph summary describing the general thesis and conclusion of your paper. A reader should be able to learn the purpose of the paper and the reason for its importance from the abstract. The abstract should be no more than 200 words long.

2.5 Text

The main body of the text immediately follows the abstract. Use 10-point type in a clear, readable font with 1-point leading (10 on 11).

Indent when starting a new paragraph, except after major headings.

2.6 Headings and Sections

When necessary, headings should be used to separate major sections of your paper. (These instructions use many headings to demonstrate their appearance; your paper should have fewer headings.)

Section Headings

Print section headings in 12-point bold type in the style shown in these instructions. Leave a blank space of approximately 10 points above and 4 points below section headings. Number sections with arabic numerals.

Subsection Headings

Print subsection headings in 11-point bold type. Leave a blank space of approximately 8 points above and 3 points below subsection headings. Number subsections with the section number and the subsection number (in arabic numerals) separated by a period.

Subsubsection Headings

Print subsubsection headings in 10-point bold type. Leave a blank space of approximately 6 points above subsubsection headings. Do not number subsubsections.

Special Sections

You may include an unnumbered acknowledgments section, including acknowledgments of help from colleagues, financial support, and permission to publish.

Any appendices directly follow the text and look like sections, except that they are numbered with capital letters instead of arabic numerals.

The references section is headed "References," printed in the same style as a section heading but without a number. A sample list of references is given at the end of these instructions. Use a consistent format for references, such as that provided by BibTEX. The reference list should not include unpublished work.

2.7 Citations

Citations within the text should include the author's last name and the year of publication, for example [**?**]. Append lowercase letters to the year in cases of ambiguity. Treat multiple authors as in the following examples: [**?**] or [**?**] (for more than two authors) and [**?**] (for two authors). If the author portion of a citation is obvious, omit it, e.g., Nebel [**?**]. Collapse multiple citations as follows: [**?**; **?**].

2.8 Footnotes

Place footnotes at the bottom of the page in a 9-point font. Refer to them with superscript numbers.[2] Separate them from the text by a short line.[3] Avoid footnotes as much as possible; they interrupt the flow of the text.

3 Illustrations

Place all illustrations (figures, drawings, tables, and photographs) throughout the paper at the places where they are first discussed, rather than at the end of the paper. If placed at the bottom or top of a page, illustrations may run across both columns.

Illustrations must be rendered electronically or scanned and placed directly in your document. All illustrations should be in black and white, as color illustrations may cause problems. Line weights should be 1/2-point or thicker. Avoid screens and superimposing type on patterns as these effects may not reproduce well.

Number illustrations sequentially. Use references of the following form: Figure 1, Table 2, etc. Place illustration numbers and captions under illustrations. Leave a margin of 1/4-inch around the area covered by the illustration and caption. Use 9-point type for captions, labels, and other text in illustrations.

[2]This is how your footnotes should appear.

[3]Note the line separating these footnotes from the text.

Acknowledgments

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A LATEX and Word Style Files

The LATEX and Word style files are available on the IJCAI–17 website, `http://www.ijcai-17.org/`. These style files implement the formatting instructions in this document.

The LATEX files are `ijcai17.sty` and `ijcai17.tex`, and the BibTEX files are `named.bst` and `ijcai17.bib`. The LATEX style file is for version 2e of LATEX, and the BibTEX style file is for version 0.99c of BibTEX (*not* version 0.98i). The `ijcai17.sty` file is the same as the `ijcai07.sty` file used for IJCAI–07.

The Microsoft Word style file consists of a single file, `ijcai17.doc`. This template is the same as the one used for IJCAI–07.

These Microsoft Word and LATEX files contain the source of the present document and may serve as a formatting sample.

Further information on using these styles for the preparation of papers for IJCAI–17 can be obtained by contacting `pcchair@ijcai-17.org`.

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