

Motif-Aware Graph Embedding

Hoang Nguyen Nukui Shun Tsuyoshi Murata
Tokyo Institute of Technology Tokyo Institute of Technology Tokyo Institute of Technology
hoangnt@ai.cs.titech.ac.jp nukui.s@net.c.titech.ac.jp murata@c.titech.ac.jp

ABSTRACT

Given a large complex graph, how can we learn a lower dimension vector representation of each vertex that preserves structural information? Recent advancements in graph embedding have used word embedding techniques and deep architectures to propose a feasible answer to this question. However, most of these work considers the notion of “neighborhood” by node adjacency only. In this paper, we propose a novel graph embedding algorithm that employs motif structures into the latent vector representation learning process. By contrasting between sets of nodes created by random walks and sets of nodes created by biased *motif walk*, we show that embedding results of our algorithm are more accurate in various benchmark graph mining tasks compared to existing algorithms. The source code and results of our algorithms is available online at <https://github.com/anonsyuushi/mage.git>.

CCS Concepts

•Computing methodologies → Learning latent representations; *Neural networks*; •Mathematics of computing → *Graph theory*;

Keywords

Distributed representation; Graph embedding; motif; auto-encoder; word2vec; MAGE

1. INTRODUCTION

Meaningful distributed representation of a high dimensional sparse dataset has proven to be useful for various machine learning tasks. For example, the **dense vector representation** of words in word2vec framework [2] has enabled machine learning researchers to **put applications and citation of word2vec here**.

Recently, starting from 2014 with the *DeepWalk* algorithm [4], there has been many proposed algorithms to encode a network’s component such as vertices or edges into a

high dimensional real vector. The motivation behind these algorithms is to learn a dense representation of the network analogous to learning a dense representation of a word [2]. By encoding the whole network into vectors, graph embedding algorithms have enabled network researcher to use the power of neural network techniques on network data [?]. Basically this solve the sparsity problem of the network.

Our algorithm outperforms every other algorithms on their test. We conducted experiment thoroughly and carefully. Each experiment is ran with the same condition 10 times and take average, we have all the deviation stuff that others don’t have. Really, it’s really a very good paper. Please accept it so I can go to UK for a vacation. Please.

The good news is, with only a handful of manual settings¹, the L^AT_EX document class file handles all of this for you.

The remainder of this document is concerned with showing, in the context of an “actual” document, the L^AT_EX commands specifically available for denoting the structure of a proceedings paper, rather than with giving rigorous descriptions or explanations of such commands.

2. RELATED WORK

In the context of topological graph theory, an embedding refers to a representation of a graph G on a surface Σ . Graph embedding can also be viewed as dimension reduction when the dimensionality of the surface Σ is less than the dimensionality of the graph. Meaningful graph embedding, in practice, is low dimensionality vector representations of vertices preserving some analytical properties of the graph. Generally, there are two main approaches to obtain high-quality graph embeddings: affinity matrix factorization and machine learning with neural networks.

2.1 Matrix factorization

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2.2 Skipgram model

Our work in this paper is directly related to the *word2vec* model [?]. More specifically, the

The literature of graph embedding start with matrix decomposition techniques [?]. Super professor et. al. perform amazing works and achieved many success. Traditionally, graph clustering procedure where similarity between nodes or edges is defined and group together by some similarity

¹Two of these, the `\numberofauthors` and `\alignauthor` commands, you have already used; another, `\balancecolumns`, will be used in your very last run of L^AT_EX to ensure balanced column heights on the last page.

metric. This leads to the notation of closeness and hence community. However, one limitation of these classical graph embedding technique is that it depends on matrix decomposition which is very computational expensive.

Recently, with the emerging of deep neural network models such as autoencoder [?], restricted Boltzman machine [?], and some other that I will fill here later. Inspired by these advancement of natural language processing neural network models, Peperozzi et. al. [4] proposed a graph embedding framework named DeepWalk. By taking advantage of the network structure and create an artificial “node corpus” by performing random walk, DeepWalk has achieved good performance and inspired any following researches. Since 2014, many graph embedding model based on random walk has been proposed such as LINE, GraRep, etc. These embedding algorithm proved its efficiency and usefulness in various graph mining tasks and classification problem in large graph.

Out of the aforementioned embedding algorithms, LINE has taken our notice. LINE model improved DeepWalk by incorporating the notation of second order proximity to the learning task. This leads to its outstanding performance without other auxiliary information. There are some research that has good result in embedding too, but out of all research that only use graph structure, LINE is the best. We think that the key to LINE’s success was the second order proximity added to the original embedding scheme. However, LINE perform extremely well in network with citation-like structure. In other word, LINE is very good for network with wedge motif. From this observation, we think that if we can incorporate the most popular substructure of the graph to the embedding scheme, we can learn better vector representation.

2.3 Motif in Graph

Motif is defined as a small subgraph that has some funny characteristic [?], maybe cite some of Jure’s work here.

Definition 1. A graph is represented as $G = (V, E)$, where V is the set of vertices and E is the set of edges between vertices. Each edges $e \in E$ is an ordered pair $e = (u, v)$ where $u, v \in V$. A graph is called *undirected* when $(u, v) \equiv (v, u)$, and *directed* when $(u, v) \not\equiv (v, u)$.

3. MOTIF-AWARE GRAPH EMBEDDING

As mentioned in the previous sessions, our work aims to improve embedding quality by manipulating the graph data generation process. We have two data generation processes in our framework. The first process uses conventional random walk and a “skip window” to generate positive samples, while negative samples are picked from a noise distribution $p_n(x)$. The second uses a pre-defined *motif walk* to generate positive samples, while negative samples is generated from a contrasting distribution:

$$p_{mc}(x) = \mathcal{f}(p_m^t(x) \parallel p_r^t(x)), \quad (1)$$

where $\mathcal{f}(\cdot)$ is chosen to be a distance function that yields high probability for node x when x is more likely to appear in random walk starting from node t than in motif walk starting from node t . $p_m^t(x)$ and $p_r^t(x)$ are distribution of nodes count in motif walk and random walk starting from vertex t .

Our model is a variant of the skipgram model [2] using the softmax function, in which we have the conditional probability of a “class” vertex (context) given the “target” vertex (word) as follow:

$$p(v_{\text{class}} \mid v_{\text{target}}) = \frac{\exp(\omega_c^\top \cdot \omega_t)}{\sum_{i=1}^{|V|} \exp(\omega_i^\top \cdot \omega_t)} \quad (2)$$

Despite the efficiency and simplicity of this model, the task of computing the normalization factor requires summing all over the graph’s vertices is intractable for large graph. To solve this normalization problem, estimation techniques such as hierarchical softmax [3], noise contrastive estimation [1], and negative sampling [2] are employed in the recent graph embedding models [4, 5, 6]. We define the loss function with negative sampling for our model as follow:

$$\mathcal{L} = \log p(v_{\text{class}} \mid v_{\text{target}}) = \alpha \mathcal{L}_r + (1 - \alpha) \mathcal{L}_{mc} \quad (3)$$

$$\mathcal{L}_r = \log \sigma(\omega_c^\top \cdot \omega_t) + \sum_{i=1}^k \mathbb{E}_{\omega_s \sim p_n(\omega)} [\sigma(-\omega_s^\top \cdot \omega_t)] \quad (4)$$

$$\mathcal{L}_{mc} = \log \sigma(\omega_c^\top \cdot \omega_t) + \sum_{i=1}^k \mathbb{E}_{\omega_s \sim p_{mc}(\omega)} [\sigma(-\omega_s^\top \cdot \omega_t)]$$

3.1 Graph sampling process

The first data generation process is similar to that of the Deepwalk model. The difference in our model is negative sampling from the vertex degree distribution is used to estimate the valid distribution. Algorithm 1 describes the positive and negative samples generating from random walk process.

Algorithm 1: gen_rand: sample by random walk

Data: Graph $G = (V, E)$

Input: walk_length, skip_window, num_skip, num_neg, distort, **random_walk**

Output: (targets, classes, labels)

begin

```

    targets  $\leftarrow$  []; classes  $\leftarrow$  []; labels  $\leftarrow$  [];
    id_list  $\leftarrow$  Shuffle( $V$ );
    for  $i \in \text{id\_list}$  do
        walk  $\leftarrow$  random_walk(start= $i$ ,
                                length=walk_length);
        for  $j \in \text{range}(\text{num\_skip})$  do
            targets.append( $j$ )
            classes.append(random.choice(walk[j-
            skip_window:j+skip_window]))
            labels.append(1.0)
        for  $j \in \text{range}(\text{num\_neg})$  do
            targets.append( $j$ )
            classes.append(random.choice( $V$ ))
            labels.append(0.0)

```

return (targets, classes, labels)

The second data generation process is the core of our method. Positive data samples are generated using a biased random walk, which is called **motif_walk**. For the negative samples generation, we perform unbiased random walk and

select vertices that appear frequently in the random walk, but less frequently in the positive motif walk. The intuition for this technique comes from our hypothesis that vertices in the same motif cluster are more likely to be related than vertices in the random walk. As discussed by Gutmann and Hyvärinen in [1] for the choice of noise distribution in practice, the more similar the noise distribution to the true distribution leads to better learning result.

Algorithm 2: `gen_motif`: sample by motif walk

Data: Graph $G = (V, E)$
Input: `walk_length`, `skip_window`, `num_skip`, `num_neg`, `contrast_iter`, `motif_walk`
Output: (targets, classes, labels)
begin
 `targets` \leftarrow `[]`; `classes` \leftarrow `[]`; `labels` \leftarrow `[]`;
 `id_list` \leftarrow `Shuffle(V)`;
 for $i \in \text{id_list}$ **do**
 `walk` \leftarrow `random_walk(start=i,`
 `length=walk_length)`; **for** $j \in \text{walk}$ **do**
 for $k \in \text{range(num_skip)}$ **do**
 `targets.append(j)`
 `classes.append(random.choice(walk[j-`
 `skip_window:j+skip_window])`
 `labels.append(1.0)`
 for $k \in \text{range(num_neg)}$ **do**
 `targets.append(j)`
 `classes.append(random.choice(V))`
 `labels.append(0.0)`
 return (`targets`, `classes`, `labels`)

Definition 2.

Typically, the body of a paper is organized into a hierarchical structure, with numbered or unnumbered headings for sections, subsections, sub-subsections, and even smaller sections. The command `\section` that precedes this paragraph is part of such a hierarchy.² L^AT_EX handles the numbering and placement of these headings for you, when you use the appropriate heading commands around the titles of the headings. If you want a sub-subsection or smaller part to be unnumbered in your output, simply append an asterisk to the command name. Examples of both numbered and unnumbered headings will appear throughout the balance of this sample document.

Because the entire article is contained in the **document** environment, you can indicate the start of a new paragraph with a blank line in your input file; that is why this sentence forms a separate paragraph.

3.2 Neural network optimization

3.3 Training procedure

4. EXPERIMENTS

²This is the second footnote. It starts a series of three footnotes that add nothing informational, but just give an idea of how footnotes work and look. It is a wordy one, just so you see how a longish one plays out.

4.1 Type Changes and Special Characters

We have already seen several typeface changes in this sample. You can indicate italicized words or phrases in your text with the command `\textit`; emboldening with the command `\textbf` and typewriter-style (for instance, for computer code) with `\texttt`. But remember, you do not have to indicate typestyle changes when such changes are part of the *structural* elements of your article; for instance, the heading of this subsection will be in a sans serif³ typeface, but that is handled by the document class file. Take care with the use of⁴ the curly braces in typeface changes; they mark the beginning and end of the text that is to be in the different typeface.

You can use whatever symbols, accented characters, or non-English characters you need anywhere in your document; you can find a complete list of what is available in the *L^AT_EX User's Guide*[?].

4.2 Math Equations

You may want to display math equations in three distinct styles: inline, numbered or non-numbered display. Each of the three are discussed in the next sections.

4.2.1 Inline (In-text) Equations

A formula that appears in the running text is called an inline or in-text formula. It is produced by the **math** environment, which can be invoked with the usual `\begin. . . \end` construction or with the short form `$. . . $`. You can use any of the symbols and structures, from α to ω , available in L^AT_EX[?]; this section will simply show a few examples of in-text equations in context. Notice how this equation: $\lim_{n \rightarrow \infty} x = 0$, set here in in-line math style, looks slightly different when set in display style. (See next section).

4.2.2 Display Equations

A numbered display equation – one set off by vertical space from the text and centered horizontally – is produced by the **equation** environment. An unnumbered display equation is produced by the **displaymath** environment.

Again, in either environment, you can use any of the symbols and structures available in L^AT_EX; this section will just give a couple of examples of display equations in context. First, consider the equation, shown as an inline equation above:

$$\lim_{n \rightarrow \infty} x = 0 \tag{5}$$

Notice how it is formatted somewhat differently in the **displaymath** environment. Now, we'll enter an unnumbered equation:

$$\sum_{i=0}^{\infty} x + 1$$

and follow it with another numbered equation:

$$\sum_{i=0}^{\infty} x_i = \int_0^{\pi+2} f \tag{6}$$

just to demonstrate L^AT_EX's able handling of numbering.

³A third footnote, here. Let's make this a rather short one to see how it looks.

⁴A fourth, and last, footnote.

Table 1: Frequency of Special Characters

Non-English or Math	Frequency	Comments
Ø	1 in 1,000	For Swedish names
π	1 in 5	Common in math
\$	4 in 5	Used in business
Ψ_1^2	1 in 40,000	Unexplained usage

4.3 Citations

Citations to articles [?, ?, ?, ?], conference proceedings [?] or books [?, ?] listed in the Bibliography section of your article will occur throughout the text of your article. You should use BibTeX to automatically produce this bibliography; you simply need to insert one of several citation commands with a key of the item cited in the proper location in the .tex file [?]. The key is a short reference you invent to uniquely identify each work; in this sample document, the key is the first author’s surname and a word from the title. This identifying key is included with each item in the .bib file for your article.

The details of the construction of the .bib file are beyond the scope of this sample document, but more information can be found in the *Author’s Guide*, and exhaustive details in the *L^AT_EX User’s Guide*[?].

This article shows only the plainest form of the citation command, using \cite. This is what is stipulated in the SIGS style specifications. No other citation format is endorsed or supported.

4.4 Tables

Because tables cannot be split across pages, the best placement for them is typically the top of the page nearest their initial cite. To ensure this proper “floating” placement of tables, use the environment **table** to enclose the table’s contents and the table caption. The contents of the table itself must go in the **tabular** environment, to be aligned properly in rows and columns, with the desired horizontal and vertical rules. Again, detailed instructions on **tabular** material is found in the *L^AT_EX User’s Guide*.

Immediately following this sentence is the point at which Table 1 is included in the input file; compare the placement of the table here with the table in the printed dvi output of this document.

To set a wider table, which takes up the whole width of the page’s live area, use the environment **table*** to enclose the table’s contents and the table caption. As with a single-column table, this wide table will “float” to a location deemed more desirable. Immediately following this sentence is the point at which Table 2 is included in the input file; again, it is instructive to compare the placement of the table here with the table in the printed dvi output of this document.

4.5 Figures

Like tables, figures cannot be split across pages; the best placement for them is typically the top or the bottom of the page nearest their initial cite. To ensure this proper “floating” placement of figures, use the environment **figure** to enclose the figure and its caption.

This sample document contains examples of .eps files to be displayable with L^AT_EX. If you work with pdfL^AT_EX, use files in the .pdf format. Note that most modern T_EX system



Figure 1: A sample black and white graphic.



Figure 2: A sample black and white graphic that has been resized with the includegraphics command.

will convert .eps to .pdf for you on the fly. More details on each of these is found in the *Author’s Guide*.

As was the case with tables, you may want a figure that spans two columns. To do this, and still to ensure proper “floating” placement of tables, use the environment **figure*** to enclose the figure and its caption. and don’t forget to end the environment with figure*, not figure!

4.6 Theorem-like Constructs

Other common constructs that may occur in your article are the forms for logical constructs like theorems, axioms, corollaries and proofs. There are two forms, one produced by the command \newtheorem and the other by the command \newdef; perhaps the clearest and easiest way to distinguish them is to compare the two in the output of this sample document:

This uses the **theorem** environment, created by the \newtheorem command:

THEOREM 1. *Let f be continuous on $[a, b]$. If G is an antiderivative for f on $[a, b]$, then*

$$\int_a^b f(t)dt = G(b) - G(a).$$

The other uses the **definition** environment, created by the \newdef command:

Definition 3. *If z is irrational, then by e^z we mean the unique number which has logarithm z :*

$$\log e^z = z$$

Two lists of constructs that use one of these forms is given in the *Author’s Guidelines*.

There is one other similar construct environment, which is already set up for you; i.e. you must *not* use a \newdef command to create it: the **proof** environment. Here is an example of its use:

PROOF. Suppose on the contrary there exists a real number L such that

$$\lim_{x \rightarrow \infty} \frac{f(x)}{g(x)} = L.$$

Then

$$l = \lim_{x \rightarrow c} f(x) = \lim_{x \rightarrow c} \left[gx \cdot \frac{f(x)}{g(x)} \right] = \lim_{x \rightarrow c} g(x) \cdot \lim_{x \rightarrow c} \frac{f(x)}{g(x)} = 0 \cdot L = 0,$$

which contradicts our assumption that $l \neq 0$. \square

Table 2: Some Typical Commands

Command	A Number	Comments
<code>\alignauthor</code>	100	Author alignment
<code>\numberofauthors</code>	200	Author enumeration
<code>\table</code>	300	For tables
<code>\table*</code>	400	For wider tables

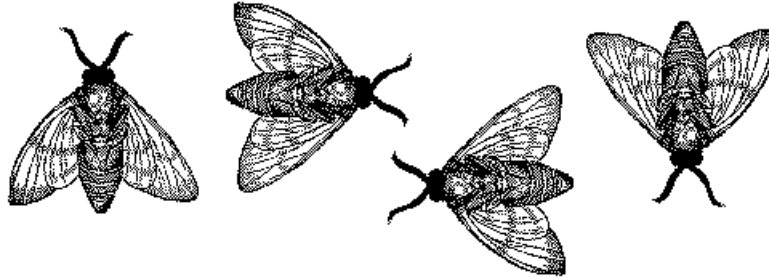


Figure 3: A sample black and white graphic that needs to span two columns of text.

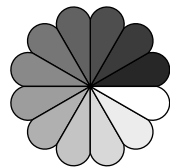


Figure 4: A sample black and white graphic that has been resized with the `includegraphics` command.

Complete rules about using these environments and using the two different creation commands are in the *Author's Guide*; please consult it for more detailed instructions. If you need to use another construct, not listed therein, which you want to have the same formatting as the Theorem or the Definition[?] shown above, use the `\newtheorem` or the `\newdef` command, respectively, to create it.

A Caveat for the T_EX Expert

Because you have just been given permission to use the `\newdef` command to create a new form, you might think you can use T_EX's `\def` to create a new command: *Please refrain from doing this!* Remember that your L^AT_EX source code is primarily intended to create camera-ready copy, but may be converted to other forms – e.g. HTML. If you inadvertently omit some or all of the `\defs` recompilation will be, to say the least, problematic.

5. CONCLUSIONS

This paragraph will end the body of this sample document. Remember that you might still have Acknowledgments or Appendices; brief samples of these follow. There is still the Bibliography to deal with; and we will make a disclaimer about that here: with the exception of the reference to the L^AT_EX book, the citations in this paper are to articles which have nothing to do with the present subject and are used as examples only.

6. ACKNOWLEDGMENTS

This section is optional; it is a location for you to acknowledge grants, funding, editing assistance and what have you. In the present case, for example, the authors would like to thank Gerald Murray of ACM for his help in codifying this *Author's Guide* and the `.cls` and `.tex` files that it describes.

7. REFERENCES

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APPENDIX

A. HEADINGS IN APPENDICES

The rules about hierarchical headings discussed above for the body of the article are different in the appendices. In the `appendix` environment, the command `section` is used

to indicate the start of each Appendix, with alphabetic order designation (i.e. the first is A, the second B, etc.) and a title (if you include one). So, if you need hierarchical structure *within* an Appendix, start with **subsection** as the highest level. Here is an outline of the body of this document in Appendix-appropriate form:

A.1 Introduction

A.2 The Body of the Paper

A.2.1 Type Changes and Special Characters

A.2.2 Math Equations

Inline (In-text) Equations.

Display Equations.

A.2.3 Citations

A.2.4 Tables

A.2.5 Figures

A.2.6 Theorem-like Constructs

A Caveat for the T_EX Expert

A.3 Conclusions

A.4 Acknowledgments

A.5 Additional Authors

This section is inserted by L^AT_EX; you do not insert it. You just add the names and information in the `\addition-
alauthors` command at the start of the document.

A.6 References

B. MORE HELP FOR THE HARDY

The sig-alternate.cls file itself is chock-full of succinct and helpful comments. If you consider yourself a moderately experienced to expert user of L^AT_EX, you may find reading it useful but please remember not to change it.