CAPTURING HIGH-ORDER STRUCTURES ON MOTIF-BASED GRAPH NEURAL NETWORKS

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ABSTRACT

Graph Neural Networks (GNNs) are effective models in graph embedding. It extracts shallow features and neighborhood information by aggregating neighbor information to learn the embedding representation of different nodes. However, the local topology information of many nodes in the network is similar, the network obtained by shallow embedding represents the network that is susceptible to structural noise, and the low-order embedding cannot capture the high-order network structure; on the other hand, the deep embedding undergoes multi-layer convolution. After the filters are stacked, the embedded distribution is destroyed, and graph smoothing occurs. To address these challenges, we propose a new framework that leverages network motifs to learn deep features of the network from low-level embeddings under the assumption of network homogeneity and transitivity, and then combines local neighborhood information with deeper global information fusion results in accurate representation of nodes. On real datasets, our model achieves significant performance improvement in link prediction and node classification.

1 INTRODUCTION

Graphs are a common feature of our world, as they simulate various real-world networks, such as biological networks, social networks, and transactional networks (Borgatti et al., 2009). Due to the ubiquity of graph structures and the powerful representation capabilities of graph neural networks, the transformation of traditional deep learning to the graph domain is becoming a very popular research direction in fields such as computer vision, natural language processing, recommendation systems, and other branches of artificial intelligence (Wu et al., 2020).

In order to reduce the high cost of graph storage and computation, graph embedding algorithms are widely used which aim to map the nodes of the graph into low-dimensional, real-valued, dense vector forms, and to preserve as much structural information as possible. Vector-based machine learning models can use network embeddings to perform downstream graph analysis tasks such as node classification, link prediction, etc. As an example, predicting the interaction between proteins in biology usually requires a lot of experiments to prove (Valencia & Pazos, 2002). Such high experimental costs limit human cognitive capabilities. Using a good network embedding will reduce the experimental cost and improve people’s understanding of these networks. Graph Neural Networks (GNNs) are classic algorithms for network embedding and have demonstrated good performance in a wide variety of fields (Zeng et al., 2019).

However, GNNs face numerous challenges. First, many existing models of networks are limited to low-order connectivity patterns (Chen et al., 2020b), i.e. nodes and edges, limiting the representation of higher-order structure of networks, while building and exploring the network topic of higher-order connectivity patterns (Xia et al., 2019) is very significant in modeling the fundamental structures of many complex systems. Second, multiple nodes in a complex network share the same local information. This indicates that nodes with shallow embeddings sharing the same topological features may be affected by structural noise. On the other hand, the deep graph neural network extracts high-order features by stacking multiple layers of convolutional filters, but the graph signal is
averaged to a vector after multiple Laplace smoothing, and the embedded distribution is destroyed, resulting in the over-smoothing problem (Chen et al., 2020a). Simply put, shallow embeddings are generally concerned with local neighborhood information, but are susceptible to structural noise. Deeper layers are relatively robust to structural noise, but larger receptive fields may cause node representations to converge to indistinguishable vector.

Recently, developments in the field of graph embedding have led to a renewed interest in mining high-order structural information in large-scale complex networks using graph neural networks (Bick et al., 2021). Most of the previous work was mining the average shortest distance, clustering coefficient and other basic network structure information (Zhang et al., 2016), but failed to model and explore higher-order link patterns of the network. Previous research has established that real networks tend to exhibit many statistically significant correlation patterns as network size increases (Yu et al., 2020). Inspired by this, we traverse the basic network blocks, aka motifs, in the graph to explore sub-patterns in the network that appear thousands of times more frequently than in random networks, and use them to better obtain higher-order network structures. For example, patterns commonly detected in DNA or protein sequences may represent genetic sequences, a closed triangle in a social network may represent a circle of friends, etc.

More specifically, by incorporating motif information into GCNs, we propose a novel multilevel graph embedding framework for extracting higher-order network structures, called MD-GCN. As shown in Figure 3, after capturing the node information of the shallow layer, the model extracts the topological information of the deep layer by mining the high-order structure of the network, and use the residual network to fuse the high-order feature with the local information. MD-GCN greatly enhances the expressive power of the network, enabling the network embedding to be integrated into a richer network structure.

1. We propose a multi-level network embedding framework based on high-order network structure extraction, extracts deep information by mining network motif information, and integrates the learned embedding into richer graph structure information through residual connections.

2. Taking advantage of the homogeneity and transitivity of the network, we design a novel node representation technology, which facilitates capturing the connection patterns of different nodes by applying motifs to the network, extracting higher-order network structures, and providing deep weighted network embeddings. a paradigm.

3. In this paper, MD-GCN is applied to node classification and link prediction for extensive evaluation. Results indicate that our model is adaptable and advanced.

2 Preliminaries

2.1 Motivation

In this section, we will use a simple figure to explain our motivation. In the figure, there are a total of 14 nodes, in which different nodes only contain different structural information (such as Relationships of nodes in a network: protein interactions, friend relationships, etc.). Figure shows the aggregation of neighbor information for two different nodes during the GCN message passing process. When \( k = 0 \), the convolution filter However, since nodes have exactly the same first-order topological features, they may be affected by structural noise during message passing to obtain similar embeddings (Jin et al., 2021). In experiments conducted in the real network, it has been found that there are many nodes that have similar topological properties, and the similarity between the representations of two nodes that are completely unconnected may be very high. However, the systems for link prediction and recommendation must calculate the similarity according to the similarity. This structure noise a substantial impact on the accuracy (Li & Zhou, 2011).

A solution to the problem of similar local information can be found by increasing the number of layers in the network and the receptive field of the nodes (Li et al., 2019). When \( k > 1 \), the deep convolutional filter aggregates high-order neighbor information to extract a wider range of topological information. But deeper embeddings may destroy the distribution of embeddings. Simply put, node information can be seen as the result of averaging a large number of N-hop neighbor nodes to
a vector, which leads to the convergence of embeddings to indistinguishable vectors due to the law of large numbers.

Figure 1: Aggregation of information about neighbors of different nodes $v_1, v_2$ in the same network.

The observation of the network shows that there are four closed triangles $M_1, M_2, M_3, M_4$. In the receptive field of $V_2$, three triadic closure edges appear, which are included in $M_3$ and $M_4$, due to the homogeneity of the network (ie the connection trend of similar nodes) and the transmission (Milo et al., 2002) (i.e. the tendency to connect when two nodes have common neighbors), triadic closure edges can be used to identify the most plausible mechanism for the existence of each edge in the network, as well as the underlying community structure itself. A triadic closure edge connects nodes with a high degree of similarity. Inspired by this, by assigning weights to triadic closure edges and acting on them in the message passing mechanism, higher-order features can be better captured (Wang et al., 2020).

2.2 Notations

A simple graph can be represented as $G = (V, E)$, where $V$ denotes the set of vertices $v_i, i = 1, 2, ..., n$, $E$ is the set of edges. $E_{i,j} = \{0, 1\}$, i.e., if there is an edge between $V_i$ and $V_j$, then $E(i, j) = m$, $m$ is the weight of the edge, otherwise, $E(i, j) = 0$. We can get the adjacency matrix form of $G A$, define a diagonal matrix $D$, is the degree matrix of the node, where $D_{ii} = \sum_j A_{ij}$.

After motif discovery, the motif-based network can be expressed in terms of a weighted graph $G = (V, E_M)$, and a motif matrix $A_M$ can be obtained as follows: $A_{ij} = m_{ij}$, where $m_{ij}$ represents the frequency of the edge of the motif (the degree of the edge obtained by the motif.) Figure 2 illustrates the M31 and M32 motif topology and the M32 motif detection for a simple network.

Figure 2: The detection of the M32 motif in the graph
3 PROPOSED METHOD

In this section, we will discuss in detail various implementation details of the MG-GCN model, including graph embedding for local structure and high-order feature.

3.1 FRAMEWORK OVERVIEW

In order to accurately learn the embedding of the network, we introduce a deep graph embedding framework MD-GCN for extracting high-order network structure, as shown in Figure 3. It consists of a linear layer, a total of four layers of graph convolution operations in two levels and a fully connected layer. The linear layer embeds the network $G = (V, E)$ into low-dimension, learns a coarse-grained representation, and extracts the local information of the network through the graph convolution operation on the simple graph $G$. The higher-order network structure is obtained using the motif-weighted convolution operation defined by the motif. Finally, according to the idea of residual network, the shallow embedding $H^{(2)}$ is spliced with the deep embedding $H^{(4)}$, and then $H^{(2)}$ is adaptively coordinated through a fully connected layer, $H^{(4)}$ to get the embedded representation of the network.

![Figure 3: the diagram of MD-GCN](image)

3.2 GRAPH EMBEDDING FOR LOCAL STRUCTURE

In the case of a simple graph $G = (V, E)$, we construct a linear layer to determine a coarse-grained low-dimensional representation of each node, where $X \in \mathbb{R}^{|v| \times d}, H^{(0)} \in \mathbb{R}^{|v| \times d}$.

$$H^{(0)} = AX + b \quad (1)$$

Following this, the shallow information of the network is extracted by performing graph convolution on a simple graph. The graph convolution utilizes the Laplace smoothing property of the symmetric normalized Laplace matrix to aggregate the low-order neighbor information of the nodes, where the hidden layer of the $l$th layer is hidden. These hidden features are aggregated from adjacent nodes in the $(l-1)$ layer, denoted by $H \ast (l)/inR \ast v/timesd$, where $d$ is the dimension of each embedding vector.

$$H^{(l)} = \sigma(D^{-\frac{1}{2}} \hat{A} D^{-\frac{1}{2}} W^{(l)}) \quad (2)$$

where $W^{(l)}$ represents the trainable weights in the $l$-layer convolution, $\sigma(\cdot)$ is a nonlinear activation function, and $Relu(\cdot)$ is usually selected according to the downstream tasks. $\text{tanh}(\cdot)$, $\hat{A} = A + I$, which can better extract negative edge features. $A$ represents the adjacency matrix of the graph, $A$ is adding self-loop to the network. Afterwards, all eigenvalues caused by the graph filter are shrunk to achieve the low-pass filtering effect required by the graph convolution.
3.3 Graph Embedding for High-order Structure

Weight-tying is a powerful tool for improving the parameter efficiency of deep learning models (Diaconu & Worrall, 2019). After the motif traversal of the network $G = (V, E)$, all Motif $M \subseteq E$ and edge-based The Motif represents $E_M$ to get Motif-based network $G = (V, E_M)$, and its adjacency matrix is represented as $A_M$

$$A_M(ij) = \begin{cases} m, & E_{(i,j)} \subseteq \{E_M\} \\ 0, & otherwise \end{cases}$$ (3)

where $m$ represent how many motifs are made by $E_{(i,j)}$. Proving the parameter efficiency of language models. In terms of the homogeneity and transitivity of the network, the motif can be used to identify the probability that each edge exists in the network, i.e., the edges connecting nodes with more motifs will have a higher level of similarity.

In terms of GCN aggregation, we want to aggregate points with high similarity into neighbouring nodes. We propose a motif-weighted propagation mechanism for GCN embeddings, which favors the influence of more stable nodes, and vice versa:

$$AGG_W H^{(l)}(v) = g(v) \sum_{v_i \in N(v)} m(v, v_i)g(v_i)H^{(l-1)}(v_i)W^{(l)}$$ (4)

Where $g(v) = \text{deg}(v)^{-0.5}$, $N(v)$ means all neighbor nodes of $v$, $m(v_i, v_j)$ is the motif-weight factor between node $v_i$ and $v_j$, representing the two node The strength of node similarity.

$$m(v_i, v_j) = E_{(i,j)} + A_M(ij)$$ (5)

In order to prevent the loss of low-order neighbor information in the network, the edges in the original graph are preserved. According to its definition Motif-based graph convolution:

$$H^{(l)} = \sigma(\hat{D}_M^{-\frac{1}{2}} \hat{A}_M \hat{D}_M^{-\frac{1}{2}} W^{(l)})$$ (6)

where $\hat{A}_M = A + \lambda I$, $\hat{D}_M = \sum_{j} \hat{A}_M(ij)$, $\lambda$ is the Laplace matrix of the weighted network. Therefore, the corresponding convolution filter for the motif is still the low-pass filter we hope. After the edges are weighted and the message is passed through graph convolution, the node captures the high-order features of the network.

3.4 Representation Learning

For MD-GCN, the loss function is designed by maximizing the co-occurrence probability of two direct neighbour nodes for positive edges and minimizing the probability of negative sampling edges:

$$L = \sum_{(v_i, v_j) \in E} \log(\eta(X_i, X_j)) + \sum_{k=1}^{K} (\log(1 - \eta(X_i, X_k^{neg})))$$ (7)

where $\eta$ is the sigmoid function and $X_i, X_j$ are the corresponding embeddings of $v_i, v_j$, the second term is to minimize the likelihood of a node and $K$ negative sampling nodes.

4 EXPERIMENTS

In this section, we evaluate the performance of MD-GCN by performing link prediction and node classification tasks on various complex network datasets such as biological networks, social networks, and citation networks.

4.1 Data Description

we only discuss the problem of link prediction and node classification in undirected networks. We used 7 real-world datasets from different domains, as follows: CE-LC(Rossi & Ahmed, 2015a), Power-Bus(Rossi & Ahmed, 2015b), PPI, BlogCatalog, Pubmed, Cora, (Kunegis, 2013) Facebook(McAuley & Leskovec, 2012).
Table 1: Real Dataset Description

| Network Dataset     | Struct Information | Network Dataset     | Struct Information |
|---------------------|--------------------|---------------------|--------------------|
|                     | Nodes | Edges | Ave.Deg | Nodes | Edges | Ave.Deg |
| CE-LC (Biological)  | 1.4K  | 1.6K  | 2.0     | PPI (Protein)     | 2.4K  | 11.7K  | 28.8   |
| Power-Bus           | 685   | 2.0K  | 5.74    | Cora (Cite)       | 2.7K  | 5.2K   | 3.9    |
| Facebook (Social)   | 4.0K  | 88K   | 46.9    | Pubmed (Cite)     | 19.7K | 47.3K  | 4.8    |
| BlogCatalog (Cite)  | 5.2K  | 131.4K| 63.3    |                   |       |        |        |

4.2 Metric

4.2.1 Link Prediction

In order to evaluate the accuracy of link prediction, we divide $E$ into $E^T$ and $E^P$, where $E^T \cup E^P = E$, $E^T \cap E^P = \emptyset$, the ratio of training set to test set is 9:1. The link prediction algorithm gives matching scores $S_{ij}$ for all possible links, and calculates the accuracy of link prediction by calculating AUC and precision.

AUC The area under the receiver operating characteristic Curve is that the matching score of the existing link is higher than the matching score of the randomly selected non-existing connection. In the experiment, we compare the edge in the test set with the randomly selected non-existing connection score, and the comparison is n times. where $n'$ represents the number of missing edge score higher than noexitent link, and $n''$ denotes the same score times.

$$AUC = \frac{n' + 0.5n''}{n} \quad (8)$$

Precision Presion in link prediction represents the ratio of edge predicted correctly in top-L links. (i.e. the top L links with score ranks). If m edges appear in the top-L candidates in the test set, define Precision:

$$Precision = \frac{m}{L} \quad (9)$$

4.2.2 Node Classification

For node classification tasks, the performance is directly measured using the correct ratio of classification:

Accuracy degree of conformity of a measure to true value.

$$Acc = \frac{\#\{Predicted\ Correctly\}}{|V|} \quad (10)$$

4.3 Related Work

For non-spectral embedding method to obtain high-order information of network, including convolutional and random walk domain. The random walk algorithm uses random walks to sample nodes in the graph, and uses the co-occurrence relationship between nodes in the graph to learn the vector representation of nodes. The graph convolutional neural network applies the deep learning neural network to the graph data, and obtains the node representation of the network by aggregating the neighbor information. The current research focus of mining high-order structural information in complex networks focuses on deep random walks and network embedding. In order to extract high-order network features, algorithms and applications for network Motif discovery have been greatly developed.

For random walk embeddings, (Yang et al., 2017) present an algorithm to improve the performance of any given network embeddings by implicitly approximating higher order proximity matrix. (Zhu et al., 2018) adopt the generalized SVD to preserve the high-order proximity and incorporate the changes of dynamic networks. However, This method has two serious shortcomings. The first
is that the weights in the node encoding are not shared, resulting in a linear increase in the number of weights as the number of nodes increases, and the direct embedding method lacks generalization ability.

On the other hand, capturing high-order information based on graph neural networks have led to a renewed interest, of which research on motifs and hypergraphs is particularly important. (Sankar et al., 2020) learns statistical dependencies between structurally similar nodes with co-varying attributes and independent of network proximity, it maximizes motif-based mutual information, and dynamically prioritizes the significance of different motifs to learn network embedding. (Chen et al., 2021) proposed redundancy minimization among motifs which compares the motifs with each other and distills the features unique to each motif. However, these methods either rely heavily on node attributes, or cannot distinguish isomorphic low-order graph structures, and their direct use of motif matrix for motif convolution will also cause certain structural losses.

4.4 BASELINE

We compared the performance of MD-GCN with seven representative network embedding methods: Second-order random walks based graph embedding Node2Vec (Grover & Leskovec, 2016), Second-order structure preserved proximity embedding LINE (Tang et al., 2015), multilayer perceptron MLP (Serpen & Gao, 2014), graph attention networks GAT (Veličković et al., 2017), plain GCN (Kipf & Welling, 2016), multiple forms of ablation experiment. Comparing different baseline methods depending on the task.

4.5 RESULTS

Table 2 shows an node link prediction comparison of our proposed model with the baseline techniques and ablation model.

Figure 4: Performance comparison with baselines of Precision@k, k = 1, 5, 10, 20, 30, 40, 100 for link prediction on Power-Bus and CE-LC datasets.

Firstly, our model outperforms all the baselines in terms of the quality of embedding. Our model achieves superior results for the important metrics of AUC and precision on all real network datasets. On the one hand, by defining motif convolution, the higher-order pattern characteristics of the network are accurately captured; on the other hand, the traditional network embedding method can’t provide any flexibility for the sampling process and often performs unstable on the real data set (e.g., Node2Vec and LINE).

Secondly, MD-GCN shows stronger performance than GCN and GAT on all datasets. This is because our model can capture the shallow topological features of the network and the characteristics of the higher-order pattern. Compared GCN and GAT that only consider aggregating neighbor information, MD_GCN maintains high-level performance by learning high-order and global feature.
Table 2: Link Prediction Result

| Dataset | Metric | MD-GCN | Node2Vec | LINE | GAT | GCN |
|---------|--------|--------|----------|------|-----|-----|
| PPI     | AUC    | 0.9688 | 0.7981   | 0.9411 | 0.9392 |
|         | Precision | 0.3529 | 0.212   | 0.1540 | 0.3246 | 0.3246 |
| Facebook| AUC    | 0.9791 | 0.7972   | 0.5363 | 0.9552 | 0.9134 |
|         | Precision | 0.1343 | 0.1249  | 0.0679 | 0.1077 | 0.09646 |
| CE-LC   | AUC    | 0.7164 | 0.6737   | 0.5761 | 0.6703 | 0.5836 |
|         | Precision | 0.3279 | 0.2500  | 0.1646 | 0.3140 | 0.2938 |
| Cora    | AUC    | 0.9736 | 0.9744   | 0.6553 | 0.9715 | 0.9157 |
|         | Precision | 0.6919 | 0.6619  | 0.1866 | 0.6525 | 0.6184 |
| Power-Bus| AUC  | 0.9608 | 0.8012   | 0.8432 | 0.9278 | 0.9153 |
|         | Precision | 0.7547 | 0.3820  | 0.4720 | 0.7360 | 0.7143 |

4.6 Ablation Test

In this section, by comparing our model and its variants (Table 3) in some datasets, we also explain how does each component of our model matter:

**GCN-1** No weighted layers and get embedding only by stacking multiple layers of simple convolutional filters with residual step.

**GCN-2** Replace the simple convolution kernel that extracts shallow features with motif-weighted convolution kernel.

**GCN-3** The convolution is divided into two steps, embedding is learned by the simple convolution and the motif-weighted convolution respectively, final embedding is obtained by coordinating them (Four weighted convolutional layers).

Table 3 shows that our original model outperformed the other variants, thus proving the importance of getting high-order network information by our motif-based weighted convolution process and residual link.

Table 3: Ablation Test For Link Prediction

| Dataset | Metric | MD-GCN | GCN-1 | GCN-2 | GCN-3 |
|---------|--------|--------|-------|-------|-------|
| PPI     | AUC    | 0.9688 | 0.9392 | 0.9248 | 0.9435 |
|         | Precision | 0.3529 | 0.3225 | 0.3045 | 0.3392 |
| Facebook| AUC    | 0.9791 | 0.9208 | 0.9635 | 0.9778 |
|         | Precision | 0.1343 | 0.0855 | 0.1134 | 0.1136 |
| Power-Bus| AUC  | 0.9608 | 0.9244 | 0.9361 | 0.9316 |
|         | Precision | 0.7547 | 0.7248 | 0.7181 | 0.7422 |

In more details, our model performs significantly better than GCN-1, even GCN shows high quality than it, which prove that the multilayer graph convolutional extraction features will cause the problem of graph smoothing, and the necessity of motif-deep convolution is confirmed.

On the other hand, our model has 2%-11% of precision better than GCN-2 for all datasets, which confirms simply performing high-order feature extraction on the model will cause precision decrease. This is because multilayer convolutional filters based on motif damage the local information. This illustrates the need to extract deep features from local information. In GCN-3, we divided the model into two parallel steps: simple convolution and motif convolution, causes the degradation of 1%-8% of Precision. This highlights the superior of original model mechanism in the network embedding, which incorporates node information extracted from local neighbourhood.

4.7 Scalability Analysis

In this section, we investigate the scalability of the techniques by applying our model to node classification tasks and extracting local information (replace GCN layer) using other graph neural network models.
Table 4 shows that our model is still ahead of other baseline approaches in terms of node classification.

| Training Size | 20% | 10% | 5% |
|---------------|-----|-----|----|
|               | Citeeseer | Pubmed | Blog | Citeeseer | Pubmed | Blog | Citeeseer | Pubmed | Blog |
| GCN           | 0.5687 | 0.7913 | 0.7173 | 0.5219 | 0.7761 | 0.6968 | 0.4755 | 0.7656 | 0.6595 |
| GAT           | 0.5447 | 0.7680 | 0.4948 | 0.5142 | 0.7758 | 0.4738 | 0.4717 | 0.7198 | 0.4422 |
| MLP           | 0.4827 | 0.7304 | 0.6637 | 0.4177 | 0.6696 | 0.6299 | 0.3477 | 0.6313 | 0.5939 |
| MD-GCN        | 0.5735 | 0.7950 | 0.7211 | 0.5122 | 0.7790 | 0.7028 | 0.4707 | 0.7693 | 0.6727 |

Furthermore, in order to extract more accurate shallow features while verifying the scalability of the model, we employ GAT and SAGE [Hamilton et al., 2017] convolution layer to extract local network information, Table 5 shows the result that our model has scalability.

| Method | Metric | PPI | Facebook | CE-LC | Cora | Power-Bus |
|--------|--------|-----|----------|-------|------|-----------|
| GCN    | AUC    | 0.9688 | 0.9791 | 0.7164 | 0.9376 | 0.9608 |
|        | Precision | 0.3529 | 0.1343 | 0.3279 | 0.6919 | 0.7545 |
| SAGE   | AUC    | 0.9501 | 0.9834 | 0.7409 | 0.9668 | 0.9503 |
|        | Precision | 0.3469 | 0.1437 | 0.3720 | 0.6553 | 0.7640 |
| GAT    | AUC    | 0.9529 | 0.9744 | 0.6628 | 0.9774 | 0.9379 |
|        | Precision | 0.3469 | 0.1375 | 0.3012 | 0.6591 | 0.7484 |

5 CONCLUSION

The original GNNs transmits node information by aggregating the information of direct neighbors, but cannot learn high-order network features through multi-layer convolution filters; when the number of layers in the network increases, graph smoothing may occur. We present a novel network embedding framework that utilizes frequently occurring sub-pattern motifs in the network to define a convolutional filter that extracts high-order features from the network, and is able to fuse local information of the network with high-order representations to create a more accurate representation of each node in the network. Our method is a general framework that is highly extensible and suitable for improving various embedding methods and downstream tasks associated with representation learning. Results based on multiple domain datasets show that our method achieves significant performance improvement.

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