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Implementation of Effective Learning convolution Neural Networks For Graphs

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ABSTRACT

For processing graph information, there exists a class of network designs known as Graph Convolutional Networks (GCNs). The complex semantics of the data are typically lost in the existing GCNs' assumption of homogenous graphs, which leads to subpar results. Heterogeneous networks, which intuitively and explicitly express the rich semantical information between nodes, are a more natural way to model several datasets. Minimal effort has been put into developing a GCN for this kind of graph.GRAPH BASED NEURAL NETWORK, or an Attention-Based Heterogeneous Graph Convolutional Network, is what we suggest.GRAPH BASED NEURAL NETWORK is able to obtain more types of links between nodes than any comparable effort has been able to do before because to its effective meta-path generating method. Not only that, but it prioritises values by applying a two-stage convolution based on attention to form node embeddings. An optional pooling layer is included inGraph based neural network to downsample the features while maintaining structural information, making it suitable for graph-level learning problems. Using DBLP and ACM, two transductive graph datasets, and two inductive datasets, we undertake a thorough experimental research (PPI and MUTAG). Classification at the node or graph level shows thatGraph based neural network is far more effective than previous methods.

Keywords: *Text Encapsulation, Text Summarization, Extractive NLP, Text Extraction, Text Rank Algorithm*

1. INTRODUCTION

Convolutional Neural Network (CNN) has been widely used as a machine learning tool

to analyze datasets of regular structure, e.g., 1D sequence such as text, or 2D grid such as image. The regularity in these data structures enables the convolution and pooling layers in CNNs to effectively extract compositional features for purposes such as object detection [22], image classification [13], machine translation [8], etc.

Many real-world datasets are irregular in nature. An example is citation network where each paper is repressented as a node, and a node has different number of neighbors in the graph. While CNN has been proven to be effective for regular data structures, it is not straightforward to extend it into irregular domain while preserving its strong capability of processing compositional structure. Therefore, much effort has been made to process graphs using CNN, the so-called graph convolutional networks (GCNs). In general, GCN approaches can be categorized into two groups, spectral graph convolution and non-spectral counterpart. Spectral graph convolution, first proposed in [3], is to perform convolution in the spectral domain with Fourier basis generated that is, by graph Laplacian matrix eigendata composition. Because the computed basis is tied to the graph structure, spectral methods are only suitable for transductive tasks, where the graph struc- ture is fixed and given in the training phase to computing the basis. Because the process of eigen-decomposition is not efficient and applies only to fixed graph structure, non-spectral approach has been proposed recently to cover dynamic graph as well [1][2][3]. It imitates the convolution by treating the graph as a special form of an image and proposing different sampling policies to collect data from a predetermined subset of a node's neighbours. Because non-spectral methods can extend the learnt knowledge to new structures, it is well suited for inductive learning tasks where the predicted graphs are unseen in the training phase. Moreover, non-spectral methods can be adapted to streaming data whose graph structural information evolves over time [5].

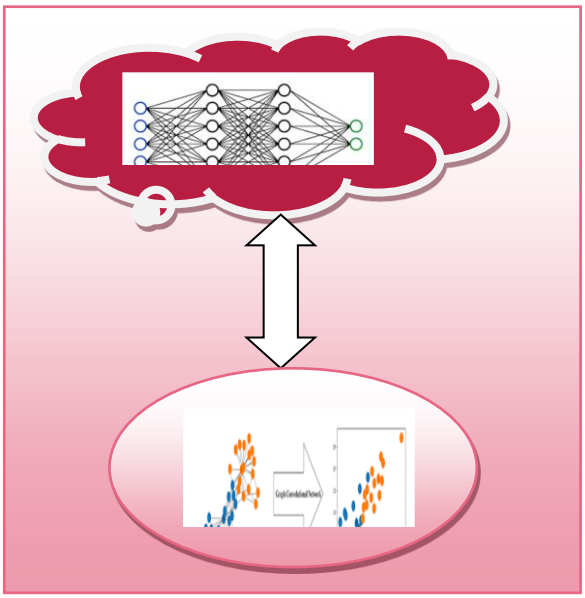

Figure 1. Overview of graph based neural networks

2. RELATED WORKS

Spectral approaches transform fixed graphs to the spectral domain, where convolution operations are conducted. One typical early work, spectral GNN [3], defines convolution in the Fourier domain with the eigenvectors of the graph Laplacian as bases. However, it is computationally intensive for large dataset, mainly due to eigen decomposition operations. It also suffers from the limitation of non-spatially localized filters due to directly defining local filters in spectral domains. Some later works tackle these issues. The work of [5] approximates local filters by Chebyshev expansion of the Graph Laplacian to accelerate computations, and the work of [4] parameterizes the filters with some smooth coefficients to generate spatially localized filters. To further simplify the approach, the recent work of

[6] constrains the kernel size within one-step neighboring nodes. Despite these attempts, spectral methods are still highly correlated to the graph structure and cannot be easily ap- plied in inductive learning tasks such as predicting protein labels with different molecular structures.

To operate on multiple graphs for inductive tasks, non-spectral approaches have been proposed, which directly define convolutions on the graph. These methods differ by devising different mechanisms to operate on neighboring blocks with various size and maintain consistent parameter sharing. As for some cases, many weight matrixes are stored for neighbors of different size. The work of [7] utilizes a set of weight matrixes for all the possible node degrees, while diffusion convolutional networks [1] represent filter weights of different input channels and node degrees by the power series of transition matrix. The work of [8] presents a method in a different direction, which samples a fixed number of nodes from each neighborhood and maintains only one weight matrix for all the degrees. Besides, Monti generalizes CNNs to graphs by introducing mixture model CNNs (MoNet) [8], and Hamilton [9] proposes GraphSAGE to perform fixed-size neighbors sampling and aggregations. The latter work has achieved great success over multiple inductive graph datasets. With these well-defined operations, some methods recursively process those operation until getting a stable node representation, while other works [9],[10] stack multiple graph convolution layers.

Some recent works further boost performance by introducing attention mechanisms [2] [3]. The attention mechanism can assign different importance to different input features and concentrate on the most relevant parts, hence achieving better results. The mechanism is most effective when the inputs are extremely large and varied. For instance, significant progresses are made in many sequence-based approaches, including machine reading [4], sentence representations [6], machine translation [8], document classification [5], and in grid-based approaches, such as sailent region detection. Because the input size for graph data can be large and varied, the attention mechanism is well suited for graph neural networks. One recent work named Graph Attention Network (GAT) utilizes the multi-headed attention mechanism to accomplish superior performance.

All the previous works mentioned above fail to consider the heterogeneity of node types and edge types, from which essential semantical information can be retrieved. As far as we know, Heterogeneous Graph Attention Networks (HAN) is the only recent work addressing heterogeneous graph convolution [4]. HAN is a non-spectral method which introduces semantics into the model by defining specific neighbours for each meta-path and assigning corresponding importance with attention mechanisms. It consists of two steps. In the first step, meta-path based node embeddings are calculated, and in the next step,

meta-path specific embeddings for each node are summed with different weights calculated by attention mechanism.

Our Graph based neural network advances from HAN in the following major ways. Firstly, we study how meta-path selection affects model performance and develop an automatic meta-path generation mechanism. Secondly, generalize the meta-path based neighbors to include non-adjacent nodes, which increases the kernel's capability of gathering local information. Lastly, for some inductive machine learning tasks like graph classification, we design

intermediate graph pooling layers to capture multi-scale features while preserving the information of graph structure.

3. METHODOLOGY

Network datasets that contain a wide variety of nodes and edges are known as heterogeneous graphs. In the most general cases, our model applies to graphs contains various node types and edge types. However, to simplify computations, we only focus on heterogeneous graphs with diverse node types.

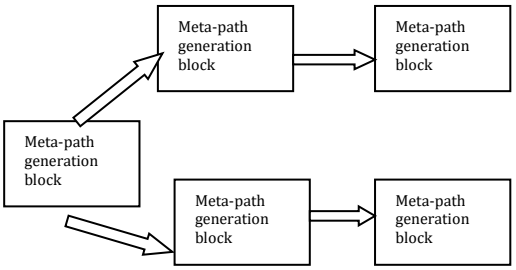

Figure 2: An illustrative overview of graph framework

Heterogeneous Graph [7]. A heterogeneous graph, denoted as G = (V, E), is constructed from a vertex set V and a link set E. There are two functions FV : V → A and FE : E → R, which maps node to node types and link to link types, respectively. Here A denotes pre-defined node type set and R denotes link type set, where |A| + |R| > 2.

Example: As shown in Figure 2, part of ACM dataset can be constructed as a simple heterogeneous graph, consisting of three types of nodes (Author (A), Paper (P) and Publication Venue (C). Many semantic information are explicitly demonstrated.

It can be seen from Figure 2 that node entities can be connected via multiple paths. Some paths share the same type of semantical information, while others fall into different categories. We apply meta-path to delineate the semantics into clear and precise sections.

GCN [7]: This network uses spectral approaches and is semi-supervised graph convolutional.As the method is designed for homogeneous graph, in this experiment, we perform it on the modeled heterogeneous graph but neglecting node types.

GAT [8]: It used a self-attention method and is a kind of semi-supervised neural network. Because it is a homogenous graph design method, in this experiment, we perform it on the modeled heterogeneous graph but neglecting node types.

HAN [9]: An artificial neural network for graphs that is semi-supervised and uses attention at both the node and semantic levels concurrently. Aside from GAT, HAN injections are unique.

Table 1: Notation of the contingency table for comparing two clustering results.

Cluster	x1	x2	...	xR	Sum
y1	n11	n12	...	n1R	n1.
y2	n21	n22	...	n2R	n2.

...	...	...	...	...	...
yC	nC1	nC2	...	nCR	nC.
Sum	n.1	n.2	...	n.R	n.. = n

meta-path based graph structure into the node-level attention mechanism. Here we select the all the meta-paths returned by the meta-path generation mechanism ofGraph based neural network.

Besides, when measuring the clustering quality of clustering tasks, we use the following metrics.

Adjusted Rand Index (ARI): The Rand Index is often used in clustering analysis as a measure of the similarity between clusters, and the ARI is the Rand Index adjusted for the chance of elements grouping. Given a set of n objects S = {O1, O2, ..., On}, suppose X = {x1, x2, x3, ..., xR} and Y = {y1, y2, y3, ..., yC} are two different partitions of R and C clusters, we can construct Table 1, where nij is the number of objects that are in both cluster xi and yj. ARI is defined as follows Normalized Mutual Information (NMI): Mutual Information measures the quantity

of information shared by two variables. In cluster analysis, it is used to measure the similarity between two clustering results. However, due to its unbounded range, high values are not intuitive, and hence NMI is introduced. Assume there are two sets of clusters X and Y, NMI is defined as follows,

$$NMI(X, Y) = \frac{2 \times I(X; Y)}{[H(X) + H(Y)]}, \quad (7.2)$$

where I(X, Y) is the mutual information and H(X), H(Y) are the entropy for the set of clusters X and Y

Here we conduct node classification tasks on the two transductive datasets (ACM and DBLP) and two inductive dataset (PPI abd MUTAG). As for ACM and DBLP, whose graph representation are heterogeneous, we set paper as target nodes and study field of the paper as node labels. PPI is modeled as a set of homogeneous graph and we only test the generalizability ofGraph based neural network, and MUTAG is used to test the pooling functionality. All methods exceptGraph based neural network in MUTAG utilize MLP as the last layer to output a graph-level classification result. The detailed classification accuracy is listed in Table 2 .

Table 2: Quantitative results on the node classification task.

Datasets	ACM	DBLP	PPI	MUTAG
DeepWalk	77.3%	73.9%	39.7%	72.1%
metapath2vec	65.1%	77.4%	39.6%	73.6%
GCN	86.8%	81.1%	-	-
GAT	86.2%	81.2%	78.4%	87.9%
HAN	89.4%	83.5%	78.4%	89.3%
GRAPH BASED NEURAL NETWORK	90.1%	87.1%	79.2%	90.7%

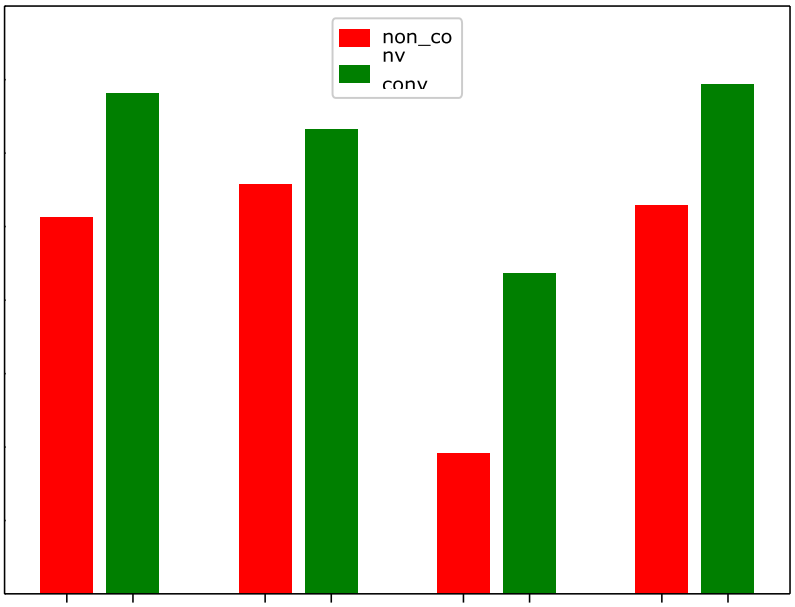

Figure 3: The average classification accuracy between convolution related (GCN, GAT, HAN,Graph based neural network) and non-convolution related groups (DeepWalk, metapath2vec).

The foremost message is thatGraph based neural network outperforms all the comparing approaches. As can be seen from the table 2,Graph based neural network obtains best node classification accuracy in all four datasets. The adoption of convolution operation to graphs and the utilization of semantical information are two major reasons that contribute to this satisfactory result. As can be seen from Figure 3, which demonstrates the average precision between convolution related (GCN, GAT, HAN,Graph based neural network) and non-convolution related groups (DeepWalk, metapath2vec), there is a huge gain by extending convolution to graphs. Besides, when we compare the average precision of meta-path based methods (HAN,Graph based neural network) with non-meta-path based methods (GAT) in Figure 2, the performance improvements is noticeable in the heterogeneous graph Another interesting finding is that the meta-path method can sometimes produce bad accuracy. As can be seen from Figure 2, the performance of metapath2vec is not stable among two different datasets. We believe that is caused by the selection of meta-paths. As we use the default meta-path set defined in the paper of metapath2vec, the set may not cover the dominant semantical information of the classification, and hence produces a inferior result. The performance between HAN and Graph based neural network are more similar in ACM. It is surprising to find that the generated.

meta-path set and the default meta-path set also share more meta-paths. Therefore, the selection of meta-paths is extremely crucial in injecting semantical information for a perfect prediction.

When comparing the precision between transductive dataset and inductive dataset, it is apparent thatGraph based neural network still can not generalize to multiple graphs perfectly. However, comparing with the performance of DeepWalk, metapath2vec,Graph based neural network demonstrates a much better capabilities.

With the above analysis, we portends that the proposedGraph based neural network outperforms[10][11][12] other methods in node classification tasks of heterogeneous graph by the adoption of convolution and utilization of semantic information.

4. CONCLUSION

Previous work on graph graph convolutional network (GCN) predominantly applies to homogeneous graph. We design an attention-based GCN which operates on heterogeneous graph and captures semantical information for both transductive and inductive learning tasks. In contrast to previous work in the area,Graph based neural network does not need domain experts to predefine important meta-paths. Instead, the automatic meta-path generation mechanism can directly detect a set of relevant meta-paths from the training dataset. Furthermore,Graph based neural network adopts a two-stage convolution operation with attention mechanism to retrieve and select hierarchical semantical information.Graph based neural network also has an optional graph pooling layer, which direct downsample the graph while preserving graph structure.

The evaluate Graph based neural network on a wide range of graph data including both transductive and inductive datasets. the study Graph based neural network for both node classification and clustering tasks. Graph based neural network is shown to substantially outperform traditional random walk based methods. Besides, with the attention mechanism and meta-paths, Graph based neural network captures the explicitly displays rich hierarchical information in heterogeneous graph.Graph based neural network accurately retrieve relevant semantics for specific downstream machine learning tasks. The

experimental results in both classification and clustering tasks show thatGraph based neural network benefits from its meta-path generation process, which replaces domain experts in previous works.

In the future, we will study extending Graph based neural network to operate on directed graph, which is universal in smart city projects. Since paths in the directed graph have single direction, we may need to relax the restriction of symmetrical meta-paths.

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