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Graph neural network: Current state of Art, challenges and applications

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ABSTRACT

Several areas in science and engineering have the relationships between their underlying data which can be represented as graphs, for example, molecular chemistry, node prediction, link prediction, computer vision, pattern recognition, social networking and more. In this article, an approach to a model which can handle such type of data is elaborated, which is Graph Neural Networks (GNN). GNN encompasses the neural network technique to process the data which is represented as graphs. Due to its massive success, GNN has made its way into many applications and is a popular architecture to work upon. This paper explains the graph neural networks, its area of applications and its day-to-day use in our daily lives. Some of the very common application is a social networking site which is on our hands regularly, and another could be the recommendation system which recommends us friends, or the products of our interest based on our past choices and preferences. This paper also demonstrates the basic challenges encountered while implementing GNN. This paper will be a great help to those researchers who are keen to work in the domain of GNN.

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1. Introduction

Graphs hold an important position in displaying problems since ages due to their capability of denoting the real world in a manner which can be analyzed easily. Graph data are also used because they contain a rich relationship between the data elements. In a broader sense, graph is a data structure which is used to model a set of items(nodes) and the relationship(edges) between them [1]. They can be used to depict a lot of real-world problems such as the social network, geographical maps, linked webpages, structure of molecules and many more. Along with these problems, graph structures can also be imposed on images and text so that graph analysis can be imposed on them. Since graphs are very expressive and can increase the computation power tremendously, a new way of analyzing graphs in machine learning is seen which is graph neural network. Graphs generally are represented as $G(V, E)$ where V is a set of vertices or nodes and E is a set of Edges. Edges may have directions or not depending on the whether there is a directional dependency existing between the nodes.

GNN are studied as the graphs which captures the information by the means of message passing with the neighbors. It varies from the traditional neural networks as it maintains the state information for capturing the properties of the neighborhood node. These captured states can be further used to produce a label as classification of a node or a random function value which is computed by the node. Eventually the network tries to learn the encoding with the help of message passing and mutual data sharing in an iterative manner (Fig. 1 and Fig. 2).

There are two categories of data as we have earlier discussed, the structures one which include the typical graph structure such as the social network, the molecular structure etc. and the second non-structured data which includes the text and images. It should be noted that the non-structures data is also converted to first the graph structures and then the GNN is applied. Another category is convolutional neural networks (CNN) which are the great motivation to use GNN. CNN could operate in the spatial feature data and on the multi-layered environment, which makes machine learning start a new era which was deep learning. CNN key was the local connections, the weights and the layered environment. The other motivation came from the graph embedding where the nodes, the edges and the subgraphs are learnt as low-dimensional vectors.

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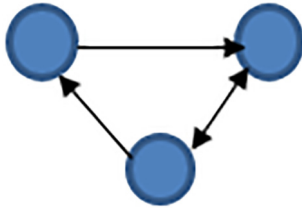


Fig. 1. A Directed Graph.

Many of these architectures are direct analogues of familiar deep neural net counterparts. These include Graph Convolutional Networks, Graph Encoders and Decoders, Graph Attention Networks, and Graph LSTMs. In a Graph Neural Network, a message passing algorithm is executed where the messages and their effect on edge and node states are learned by neural networks.

This paper contains six sections. The very first section is the introduction section, that is followed by the literature review in second section. In third section we discuss the motivation of learning GNN. In the fourth section all the research challenges of GNN are discussed which is followed by the Application of GNN which is the fifth section where we have defined and explained the applications in detail. After the applications we concluded our paper in seventh section with future scope and conclusion.

2. Literature review

GNN is defined as a neural network which can operate on graphical data where most of the convolution operations are implemented as the aggregation of the features of the neighboring nodes of the target node. This increases the representation of the target node although, but it ignores the fact that the neighboring nodes may have possible interactions between them.[2] The article proposes a new model known as Bilinear GNN which is anticipated of perform more comprehensive representation by taking into consideration the local node interaction. For the model, an experiment is performed on citation network dataset where the performance is found to be effective.

Many a times there is a need of considering the heterogeneous graph data to facilitate many applications such as link prediction. This can be challenging because we not only need to incorporate

the heterogeneous data of nodes and edges but also the heterogeneous features of those nodes are to be considered. The article proposes a model which can handle such heterogeneous data to resolve the issue. According to [3], mini-batch gradient descent and graph context loss which can help in modelling the parameter, can be employed for the purpose of training.

The world's knowledge is represented in different directed graphs which are known as knowledge graphs (KG). Here the entity alignment suffers from the heterogeneous structure [4]. The article proposes a model Multi-channel GNN to know alignment-oriented KG which consumes multiple channels. Multi-channel GNN claims to reconcile the structural differences which occurs between two knowledge-graphs by encoding the graphs from different perspective which are pruning and completion. To test the efficiency of the model, experiment is performed on 5 publicly available datasets which shows a considerable improvement of 5%.

GNN is gaining significance because of it can incorporate the multi-dimensional features on edges and vertices and on graphs to combine them into a joint embedding [5]. The article proposes a model called FeatGraph which requires co-optimizing the traversal of the graph and feature dimension computation to get the desired performance. Alternatively, it can be stated that FeatGraph is a variant of the GNN model which performs by composing coarse-grained designs for sparse graph data which has a smaller number of node connections with fine-grained feature dimension which are applied on edges or vertices in the form of functions which are user defined [6].

The paper proposes a framework theoretically which can analyses the expressive power of Graph Neural Networks. The framework is a study of close connection between the GNN and Weisfeiler-Lehman (WL) graph isomorphism test. In other words, the frameworks in the first step represents the feature vector of the neighboring nodes as a multiset, and in the second step the aggregation function is applied on that multiset. For this reason, GNN must process a strong aggregation in order to perform a high representation. The result which is concluded is: GNN is the most powerful in terms of expressiveness.

To tackle the graph classification Graph Neural Model proved to be the most powerful approach. GNN have proved to be a tool for dissolving the ambiguity raised by the models of Machine Learning [7]. To build the node distribution representation node features and graph topologies are effectively combined. The most common

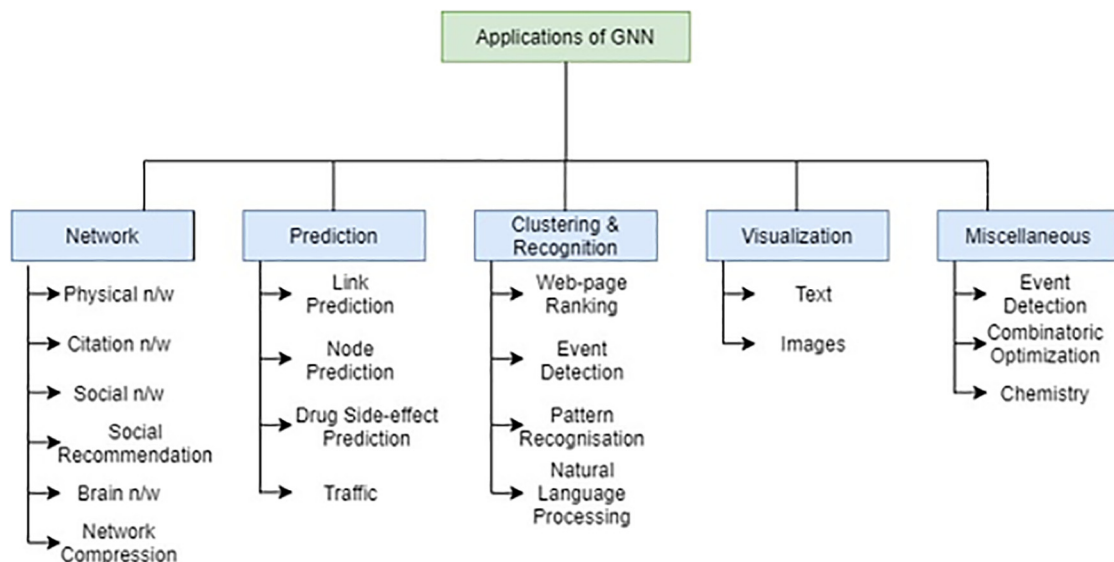


Fig. 2. GNN Applications.

reproducibility problem encountered is the selection of hyperparameters and the correct split of the data for model selection versus model assessment. Also, the fact to be considered is that the evaluation code is sometimes found to be missing or incomplete, and the experiments to be performed are not standardized in terms of nodes and edges. The main purpose of the article is to provide a standard for reproducibility experiments and to investigate that up to what extend the existing GNN can make use of the graph structures. It is proved that providing degree to nodes can prove to be beneficial for the performance of GNN.

GNN have achieved an unparalleled result in the semi-supervised node classification problem which is a fundamental issue in graph mining [8]. When evaluation of a new model is performed, people tend to use the training procedures which are different from the ones used for the baseline which makes it difficult to understand that the improved performance is coming from a greater architecture which is being used, a fine-tuned training method or the hyperparameters which are unfairly benefitting the new model. For such issues a thorough experiment is conducted on four protruding architectures and on four well-known citation network datasets and introduce new datasets for node classification problem. For the results it was found that a simple GCN model can outperform the most complex dataset.

Social Recommendation system is gaining attention in the recent years, it is based on the phenomena that people always want to gather and disseminate the information by the people around them, may it be classmates, friends or relatives which implies that such social relationships can be very helpful in filtering the information [9]. Data for any social system can be represented in the form of two graphs, one graph depicts the relationship between the user and is known as a social graph and the second one depicts user interaction with the item and is called the user-item graph. It is necessary to aggregate the features from the graph to have a better representation. The article proposes a graph for social recommendation GraphRec: a) which provide an approach which can both the interaction and the opinions in the user-item graph, b) can capture the heterogenous interaction mathematically, and c) validate the effectiveness of the proposed frameworks on the different datasets.

[10] The article proposes two constructions for spreading convolution neural network to process graph signal. Firstly, selection GNN are used to replace the convolution operation with filtering graph using the linear shift then pooling is used to aggregate the relevant regional information at the subset node level which is followed by down sampling. The convolution layers can be further computed to deeper layers by keeping a track of the original convolution network with the help of zero padding. Likewise, the selection GNN can reduce the computational complexity at each layer while considering the original topology. The results of the experiment performed on the dataset suggest that the proposed GNN architecture can handle the network data that is represented as signal supported on graph.

According to the findings from literature survey it can be said that there are many types of graphs variants which are now being introduced by the authors. GNN because of its expressive power is a popular field of research. There are mainly three types of Graph Neural Network, a) RNN (Recurrent Neural Network), b) Spatial Convolution Network, c) Spectral Convolution Network. Here the nodes are defined by its neighbors and the connection between the neighbors, if once all the neighbors of a node are deleted, that node will lose all its information. GNN are an instinctive solution to the unstructured form of data having a wide choice of real-world applications. We have also found the challenges of GNN which are still be addressed, the chal-

lenges are discussed in the later section. This purpose of this article is just to give an overview of what GNN is, its applications and research challenges.

3. Motivation

Graph Neural Network proved to be a great tool for applying machine learning on graphs. It works by combining the node features with the graph topology by passing the messages along the edges of the given input graph. It also drives motivations from its area of applications such as link prediction, image classification and more [11,12]. Not everything can be analyzed using a grid like images and text, the real world scenario is changing and we need to model the big picture like the social networking websites, the citation network and the most popular and used by all the social recommendation system. All these things cannot be done using a 2D model, so graphs are important and a way where we can deal with the dynamically changing structure. Graphs are extremely useful and expressive mathematical structure [13]. The applications like recommendation system are a very complex task as it requires us to record and match many features simultaneous in a dynamic environment. The network is growing every second and so as the requirement of the user, we need to recommend the customers according to their preferences. This complex task can be achieved using GNN.

4. Research challenges

Though the Graph Neural Networks have proved to be a very efficient tool for learning graph data, there still exist certain challenges due to the complexity of graphs. Some of the challenges are listed below:

Model Depth: [14] Deep learning model success lies in the architecture of neural networks. But depending on some research, it is found that infinite number of layers converge the representation towards a single point. So, the challenge here is that whether going deep in the neural network layers is still a better option for learning the graph data.

Scalability: Whenever we try to scale or cluster our graph, it is a trivial issue that the completeness of the graph is sacrificed. The model will miss some part of graph information whether we are scaling or clustering. Considering scaling, a node may drop its significant neighbors. Considering clustering, a graph may drop a different structural pattern. Here stands a challenge that how we can manage the scalability without sacrificing the integrity.

Convergence: More and more layers when added to the deep neural networks provide better performance, as it is supposed that it adds more and more levels of estimation to the network. At the same time, it is also found that when the layers are increases to hundreds of layers, then the model starts converging to a similar point. It over-smoothens the results which gives no different results after a certain number of layers.

Dynamics: Graphs are of the changing or dynamic nature in a way that the nodes and edges keep on changing. They may appear at some time and disappear at some other time. Sometimes the nodes change according to the time and the environment. For example, if we take a traffic scenario, it is a very dynamic thing as the nodes keeps changing whether edges do. Every time a new graph convolution is needed to adapt the dynamics of that changing graph. Although the dynamics of the graph is handled by STGNN partially, it is to be taken care that how the changing spatial relationships are to be handled.

Heterogeneity: It is widely seen that majority of GNN deals with the homogenous graphs. The current given GNN are may does

not handle the heterogenous graph data, as it may contain different types of nodes and edges or it may contain different features, for example text and images. So, an approach must be developed to handle such heterogenous data.

Narrow Structure: The neural networks traditionally used to stack hundreds of layers in its model to get better performance as deep networks give better performance as it has more parameters. But GNN are shallow structure as the maximum layers it has is three layers. Several experiments show that adding more layer's results in over-smoothing of results which may also be said to convergence at the same point. To tackle this challenge there is a need for designing a real deep neural network.

Non-Structural Scenarios: We have seen the various applications of GNN in different scenarios, then also there do not exist a proper method to generate graphs from raw data. For example, when talking about image data, some research utilizes the CNN to obtain the features and then decode them to form super pixel as nodes, whereas some research directly leverages the object for detection of nodes. And on the cases like text data, some work uses syntactic trees for using syntactic graphs while others can adapt fully connected graphs.

4.1. Other challenges

Missing Edge Label: The model proposed can only handle the graphs with node labelling but cannot handle the edge features. In some area like chemistry it is required to include the edge labelling feature [15].

Memory Requirement: With a setup of full batch gradient decent, the memory requirements grow with the size of dataset linearly. It is shown that the datasets which cannot perform on GPU memory can still run on the CPU memory. This issue will be more severe with the mini-batch gradient decent. For creating the mini batches, the number of layers of the GCN model should be taken into consideration as the Kth order neighbors with a total of K layers must be stored on the exact memory location. So, for a very large graph which is densely populated graphs, exact calculations might be necessary [16].

Higher-order Motif: In the recent studies, several works are done towards developing an encoding algorithm for node embedding, many still rely on the decoders which are pairwise, which only consider the pair-wise relation between the nodes and ignores the higher order relations which involves more than two nodes. It is known that in order to handle the complex structure and function of graph data it is necessary to involve the higher order relations so it is a challenge to develop a decoding algorithm which can handle the higher-order motif.

Interpretability Problem: Representation learning, the representation of problem as graphs discharges the pressure of hand designing the features. Due to this we are unaware of the underlying limitations or you can say the biases. Further, it should be taken care of that while developing the new techniques this issue of interoperability should be considered outside the benchmarking and visualization [17].

5. Applications of GNN

Typical neural networks work with an array whereas GNN works with graphs.

Graphs have gained popularity in the recent years due to their ability to represent the real-world problem in a way which can be analyzed. They are having applications in the field of social networks, molecular structures, web link data etc. which are a structured form of data, and on the other hand they can be used in the non-structured form of data such as text and images which can be modelled as graph to perform analysis.

Every node in a GNN operated on a single recurrent unit, where with recurrent unit we mean that the nodes get the inputs from the data as well as the previous output. It takes the input from all the neighbors' nodes and then computes the output.

GNN are an extension to neural networks to capture the information, which is represented as graphs and also, they maintain state information to capture the neighborhood properties. The structural is the one which has a structure explicitly like social network whereas with the non-structured data such as text and images the approach is to transform the data in the structured format and then apply GNN to it.

Some of the applications are:

5.1. Network

1. **Social Networks:** The main application of social media is to connect the people. For this there is something called feed which is decided based on the connections of that user. Here, each user will aggregate the data from all the adjacent users to decide what should be shown on the feed. There are some other criteria such as the friend connections or the recommendations.[18]
2. **Physical Networks:** Human brain generates its process with the help of creation of graphs which is learned by daily experience from the real world. We are trying to achieve human like artificial intelligence by converting the real-world scenarios in the form of nodes and edges and can analyse them. Used in interaction network and visualization network.
3. **Network Compression:** For a Graph G , G^* is defined with contains a smaller number of edges. This is done so that the graph can be stored efficiently, and the algorithms can be run faster. The maximum layers we have the better the neural network is supposed to be. But this is not true and efficient for mobile devices or the devices which have less memory and energy consumption. So, for these reasons network should be compressed which also leads to less network bandwidth consumption and fast processing.

5.2. Prediction

1. **Link Prediction:** [17] Link prediction means to predict that whether there exist a link between the two nodes or nodes. Link prediction has several applications such as friend recommendation, knowledge graph representation, movie recommendation and metabolic network construction. One of the common and effective approach is heuristic method to compute heuristic nodes similarity for link prediction.
2. **Node Prediction:** Node Classification is the most common benchmark which is used for evaluation the node embedding. Node prediction is a form of semi-supervised approach where the labels are only available for a small number of nodes where the goal is to label the full graph based on those labels which are initially available to us. Common applications includes, classifying document, videos, web pages into different categories and classifying protein based on their biological functions [19].
3. **Predict side-effect due to Drug Interaction:** By applying a type of GNN called a Graph Convolutional Network (GCN), a team at Stanford has been able to produce a model that can predict specific drug-drug interaction effects due to the interaction of more than 2 drugs.
4. **Traffic:** Accurately forecasting traffic speed, volume or the density of roads in traffic networks is fundamentally important in a smart transportation system. The traffic prediction problem is addressed using STGNNs. They consider the traffic network as a spatial-temporal graph where the nodes are sensors installed on roads, the edges are measured by the distance between pairs

of nodes, and each node has the average traffic speed within a window as dynamic input feature.

5. **E-Commerce:** A graph-based learning system can explore the relation and interaction between a user and a product to make the highly accurate recommendation to that user. Recommender system measures the user's preferences by utilizing their interest and the item properties [20].

5.3. Clustering & prediction

Ranking Web Pages: GNNs can learn a ranking function by examples and they can generalize over unseen data. GNN can use a generic model and can encompass various types of page ranking algorithms which are numeric. The graphs output is computed based on the information about the nodes and the links. Once we have a trained GNN model, it can fetch the output for unknown or unseen data [21].

Clustering: Clustering is an application which is applied on the graph network when we want to group the homogenous nodes. The clusters then can be used when we need to apply certain algorithm or model on the cluster. GNN and the unsupervised learning approaches are applied to determine the clusters sharing the strong relations which can be consumed in better understanding of the graph structure of the network and use this extra information for effective discoveries [22].

Pattern Recognition: Pattern recognition is a technique which takes raw data as input and acts depending on the category of that pattern. It extracts the patterns based on certain conditions and separates one class from another [23].

Natural Language Processing: Text classification is one of the common applications of GNN in NLP. It utilizes the interconnection between the documents or words to infer the label of the document. Some of the NLP tasks such as reading comprehension and fact verification requires reasoning over multi-hop sentences or paragraphs. Using GNN can improve the performance of such task magnificently [24].

5.4. Visualization

1. **Visualization:** Visualization is a very helpful application as when there is a question of clarity, visualizing the different features of neural networks is unmatched. And especially when we are dealing with thousands and millions of images, this has more weightage. Visualization is used when we need to classify the images using some features of those images. It helps us know what are those features which is guiding a models' decision for classification of those images [25].
2. **Image classification:** It derives numerous solutions using machine learning mechanism with the most popular CNN (Convolution neural networks). GNN is an extension to CNN which derives appropriate results, and the focus has now shifted to zero-shot and a few-shot learning mechanisms. GNN can help in achieving the zero-shot task as the graph may be based on the similarities between the images or the objects in the images which are taken out using the object detection [26].
3. **Text:** Like images, text does not have an implicit relationship, the data is not structured. So, we need to first structure the data so that GNN can be applied. We have ways to structure the data as we can convert the words or sentences into graph, or we also have a different approach where the sentences can be thought of as a node and the words inside it can be a sub-graph. The most interesting area where it is applied is reading comprehension. Reading comprehension is the most complex

task which human brain performs as it does not have the answers at any particular location [27].

5.5. Miscellaneous

1. **Chemistry:** The molecular structure is already defined in the graph like structures where the atoms are the nodes and the bond between them are the edges. The structure is taken to be analyzed or a new structure can be discovered.
2. **Combinatorial Optimization:** GNN can be applied to a number of optimization problem such as minimum vertex cover problem or the travelling salesman problem.
3. **Others:** Applications of GNN is not limited to these areas, there have been explorations of applying GNN in problems such as program reasoning, brain networks, social influencer prediction, event detection, combinatorial optimization, adversarial attacks prevention, and electrical health records modelling.

6. Future scope and conclusion

In this research paper, we have explained what is a GNN, and how powerful it has proved to be based on its area of applications and expressiveness. We further explained the fields where GNN is being currently deployed to get the best results and where it can be further applied. With the great power that GNN possesses, it also has some challenges like scalability which means with many nodes and edges it becomes quite difficult to scale the graph when some new information is added, heterogeneity which means that the current graphs are designed to handle the similar type of data and when the data is not of same type there is a challenge. The major challenge is to construct a graph that accurately describe the data. For the future direction, the challenges like the heterogeneous data can be explored to utilize the power of GNN. There are still many problems where GNN can be applied and many challenges which are yet to be explored. To complete, it would be interesting to understand GNNs optimized landscape.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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