Chapter 2
Graph Neural Network and Its Applications

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ABSTRACT

Graph neural network (GNN) is an emerging field in deep learning. Graphs have more expressive power than any other data structure. Graph neural network is one of the application areas of deep learning, and it has applications in different domains where traditional convolutional neural networks can't give the desired result. Graphs are basically connections of nodes through the edges. In the area of recommendation systems, image processing and fraud detection are some of the few application areas of graph neural networks. As graphs are moveable and mobile in nature, they are more flexible to apply in these domains. GNN deals with these types of problems more effectively than a convolution neural network. To apply GNN to a specific problem domain, data needs to be converted into a graphical format, and then neural network operations can be executed. The main feature of GNN is to inherit information from its neighborhood. This is called graph embedding. This chapter describes basic GNN architecture, GNN advantage over CNN, and its application in different domains.

INTRODUCTION

Graph structure data can be represented in various application fields like natural language processing, image processing, and software engineering. Graphical format data can be processed by Graph Neural Networks (GNNs). Graphs are a fundamental way to represent data that have complex relationships between elements. They are widely used in various domains, such as social network analysis, molecular chemistry, computer vision, and natural language processing. Recently, GNNs have attracted a lot of interest in both the academic and business communities for applying graphs. Classifying nodes, link prediction, and graph clustering are just some of the many downstream tasks and GNN might extract semantic information from these networks. Unlike traditional neural networks that operate on regular grids, such as images and sequences, GNNs operate on irregular graph structures, presenting unique challenges in modeling the relationships between the nodes.

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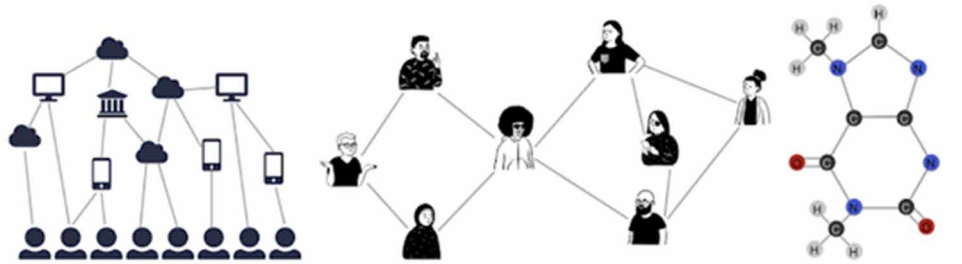
The development of GNNs has been driven by advances in deep learning and graph theory. The first GNN was proposed by (Scarselli et al., 2009), which used a recurrent neural network to propagate information between nodes in a graph. The range of possible uses for GNNs is enormous. Image categorization, object recognition, and semantic segmentation are just some of the computer vision applications that GNNs have been used. For many years, GNNs have been utilized for phrase categorization, entity identification, and relation extraction in the field of natural language processing. GNNs have been implemented for a variety of tasks in social network analysis, including link prediction, node categorization, and community discovery. In the field of molecular chemistry, GNNs have been used for tasks such as drug discovery and molecular property prediction. Single nodes and sequences are the most basic graph structures. Graph data structures are mobile in nature and that's the reason the convolution neural networks cannot process this complicated type of mobile data structure (Scarselli et al., 2009) as it works mainly on static data structure. That is where GNN came into the picture. Nodes and edges make up the data structure known as a graph. Each node in the graph is an entity and the relationship between the entities are defined as edges; these relationships may be established using any suitable similarity metric.

Figure 1. Graph models between different types of data



Graphs have great expressive power and it's the reason GNN (Huang et al., 2019) can be used in many domains such as molecule interaction, natural science, machine learning, and many more research areas. Graph structure can be facile with basic nodes and edge connection, or it may be perplexing in nature like trees, acyclic graphs, or cyclic graphs. In machine learning, problem analysis through graphs acts as a unique non-Euclidian data structure (Shchur et al., 2018) that mainly focuses on node classification, clustering, and connection prediction. Classification is one of the prominent areas where GNN is used. In the classification problem (Fu et al., 2020) each node has a label and without using ground-truth labels the nodes need to be predicted.

BACKGROUND

Because of the ability to process input that is organized as a graph the Graph Neural Network (GNN) has gained lots of popularity in the recent times. In several applications, such as NLP, computer vision, drug discovery and graphical network analysis, GNNs have shown to be effective. The first-time graph neural network was proposed back in 2005 (Scarselli et. al., 2005) to apply the concept of graph data and