Chapter 3
Introduction to Graph Neural Network:
Types and Applications

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ABSTRACT

Deep learning on graphs is an upcoming area of study. This chapter provides an introduction to graph neural networks (GNNs), a type of neural network that is designed to process data represented in the form of graphs. First, it summarizes the explanation of deep learning on graphs. The fundamental concepts of graph neural networks, as well as GNN theories, are then explained. In this chapter, different types of graph neural network (GNN) are also explained. At the end, the applications of graph neural network where GNN is used and for what purpose it is going to be used are explained. This also explores the various applications of GNNs in fields such as social network analysis, recommendation systems, drug discovery, computer vision, and natural language processing. With the increasing prevalence of graph data, GNNs are becoming increasingly important and will likely continue to play a significant role in many fields in the future.

INTRODUCTION

A concise and interesting lesson on the key ideas and building blocks involved in neural networks for graphs is provided by researchers from the University of Pisa in Italy. Graph networks (Gori et al., 2005) are frequently used in the social sciences to describe the connections between individuals. For instance, they are used to represent the molecular structure of a drug, protein interaction networks, as well as biological and biochemical relationships in chemistry and material sciences. Graphs, in general, are an effective representational tool for rich and complicated data generated by a range of artificial and natural processes. A graph can be thought of as a structured datatype with nodes and edges that is relational and compositional in nature. Recent interest in deep learning models that can handle graphs in an adaptable

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way is increased due to the amount of information carried by such data and the growing accessibility of enormous repositories. The field of deep learning for graphs has its roots in early 1990s research on recursive neural networks (RecNN) for tree-structured data and neural networks for graphs. Later, the RecNN method was rediscovered in relation to applications for natural language processing. It was first applied to directed acyclic graphs and has since been generalized to more intricate and varied forms. Similar to the RecNN, the GNN model is based on a state transition system but allows for cycles in state computation. Therefore, the development of deep learning models that automatically extract the necessary features from a graph can be the focus of research. Deep Graph Networks are the name given to these models (DGNs). The authors classify deep graph networks (DGNs) into three main groups: deep neural graph networks (DNGNs) which include models based on neural architectures; deep Bayesian graph networks (DBGNs) whose representatives are probabilistic models of graphs and deep generative graph networks (DGGNs) which include generative approaches to graphs that may include both neural and probabilistic models.

Graph Neural Network (GNN)

Data structures called graphs are used to simulate difficult real-world issues. Learning chemical fingerprints, simulating physical systems, managing traffic networks and friend recommendations on social media are few examples. While classic deep learning models such as Convolutional Neural Networks (CNNs) or Recurrent Neural Networks (RNNs) are not well suited to handle these tasks, they do require dealing with non-Euclidean graph data that contains rich relational information between nodes. The graph neural network is useful in this situation.

A deep learning neural network that is graph-structured is called a "graph neural network." It can be compared to a graph where the nodes represent the data to be analyzed and the edges represent the connections between them. Conceptually, GNNs are built on deep learning and graph theory. A group of models has known as graph neural networks use graph representations to learn data structures and graph-related tasks (Kumar & Thakur, 2017). In order to acquire better representations on graphs via feature propagation and aggregation, graph neural networks (GNNs) are offered as a way to merge feature information and the graph structure.

Bronstein et al. (2017) provide an overview of deep learning techniques for non-Euclidean domains, such as graphs and manifolds, under the title geometric deep learning. Despite being the initial review of GNNs, this article focuses mostly on convolutional GNNs. A small selection of GNNs are covered by Hamilton et al. (2017) who concentrate on finding a solution to the network embedding issue. In comprehensive analysis of GNNs, Battaglia et al. (2018) place graph networks as the fundamental components for learning from relational data, reviewing part of GNNs under a unified framework. A partial survey of GNNs using various attention mechanisms is carried out by Lee et al. (2019).

Advantages

Graph Neural Networks have a number of advantages over regular neural networks:

- GNNs may be trained on any dataset that has both input data and pairwise relationships between items. An important advantage graph neural networks have over regular deep learning is that graph neural networks are able to capture the graph structure of data – which is often very rich.