Chapter 4
Graph Classification of Graph Neural Networks

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ABSTRACT

Graph neural networks have recently come to the fore as the top machine learning architecture for supervised learning using graph and relational data. An overview of GNNs for graph classification (i.e., GNNs that learn a graph level output) is provided in this chapter as pooling layers, or layers that learn graph-level representations from node-level representations, are essential elements for successful graph classification because GNNs compute node-level representations. Hence, the authors give a thorough overview of pooling layers. The constraints of GNNs for graph categorization are further discussed, along with developments made in overcoming them. Finally, they review some GNN applications for graph classification and give an overview of benchmark datasets for empirical analysis.

INTRODUCTION

In mathematics and computer science, a graph is a collection of vertices (also known as nodes) and edges that connect pairs of vertices. Graphs are widely used to model and represent relationships and connections between different entities, such as people in a social network, web pages on the internet, or molecules in a chemical compound (Trudeau, 2013). Graph classification is the task of predicting a single label for an entire graph. In recent years, Graph Neural Networks (GNNs) have emerged as a powerful approach

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for graph classification. A graph is typically represented visually as a set of points (vertices) and lines (edges) connecting them (Kumar & Thakur, 2017). Each edge represents a relationship between two vertices, and may have a direction or be undirected. A directed edge connects two vertices in a specific direction, while an undirected edge connects two vertices in both directions. There are many different types of graphs, including directed graphs, undirected graphs, weighted graphs, and bipartite graphs. Directed graphs have edges with a direction, while undirected graphs have edges without a direction. Weighted graphs have a value assigned to each edge, which can represent attributes such as distance, cost, or strength. Bipartite graphs are a type of graph where the vertices can be divided into two disjoint sets, and all edges connect vertices from one set to the other.

Graphs have a wide range of applications in various fields, including computer science, mathematics, physics, and biology. They are used in algorithms for shortest path problems, network flow, and clustering. Graph databases are used to store and analyze large-scale data, while graph theory is used to study properties of graphs and their applications.

GNNs are deep learning models that operate directly on graphs, and they can learn to extract features and make predictions for graphs of varying sizes and shapes. Since data from real-world applications have very diverse forms, from matrix and tensor to sequence and time series, a natural question that arises is why we attempt to represent data as graphs (Hamilton, 2020). Graphs, which describe pairwise relations between entities, are essential representations for real-world data from many different domains, including social science, linguistics, chemistry, biology, and physics. Graphs are widely utilized in social science to indicate the relations between individuals. In chemistry, chemical compounds are denoted as graphs with atoms as nodes and chemical bonds as edges (Bonchev, 1991). The basic idea behind GNNs is to propagate information between neighboring nodes in the graph. This is done by defining a neural network that takes as input the features of a node and its neighboring nodes, and produces an output that represents the updated features of the node. The updated features can then be propagated to its neighbors, and the process is repeated for several layers of the network. In this way, the GNN can learn to encode information about the local structure of the graph, as well as global information about the graph as a whole. In linguistics, graphs are utilized to capture the syntax and compositional structures of sentences. For example, parsing trees are leveraged to represent the syntactic structure of a sentence according to some context-free grammar, while Abstract Meaning Representation (AMR) encodes the meaning of a sentence as a rooted and directed graph (Banarescu et al., 2013). Hence, research on graphs has attracted immense attention from multiple disciplines.

Graph classification is a task in which a machine learning model is trained to predict the class labels of graphs. Graph neural networks (GNNs) are a popular class of models used for graph classification tasks. GNNs extend traditional neural networks to operate on graph-structured data, which makes them well-suited for tasks involving graphs, such as graph classification.

The basic idea behind GNNs is to learn node embeddings (i.e., low-dimensional representations of each node in the graph) that capture both local and global structural information of the graph. The node embeddings are updated iteratively by aggregating the embeddings of neighboring nodes and applying a neural network (Ziwei Zhang et al., 2015). There are many variations of GNNs, such as Graph Convolutional Networks (GCNs), Graph Attention Networks (GATs), and GraphSAGE, among others (Zhang et al., 2019). These models differ in how they update node embeddings and aggregate information across the graph (Lalotra et al., 2022). The classification of Graph Neural Networks (GNNs) is important because it allows researchers and practitioners to select the most appropriate GNN architecture and message-passing mechanism for a given task and graph data. Different types of graphs have unique characteristics and

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