



Graph neural networks: Historical backgrounds, present revolutions, and conventionalization for the future

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Abstract

Graph neural networks (GNNs) have become a powerful framework for analyzing structured data in the form of graphs, with applications spanning diverse fields such as social networks, biology, and recommender systems. This survey explores methodology, development, and advances in GNN architecture. We methodically survey the major classes of GNNs, including convolutional GNNs (ConvGNNs), spatial–temporal graph neural networks (STGNNs), recurrent-based GNNs (RecGNNs), and graph autoencoders (GAEs). Every model is discussed in terms of underlying mathematical formulations, design principles, and practical applications. This survey aims to provide a comprehensive understanding of GNNs for practitioners, students, and researchers alike, highlighting their versatility and potential for future innovations in graph neural networks. This review is broad, addressing the basic ideas behind GNNs, different architectural designs, training and inference methods, common issues and constraints, the variety of datasets used, and real-world applications across numerous fields. We will furthermore discuss applications of graph neural networks across different fields and exemplify open-source codes, benchmark datasets, and model valuation for graph neural networks. In the end, this survey specifies existing challenges in interpretability, generalization, and scalability and proposes possible future research trends to further promote the performance of GNNs across various graph-based learning missions.

Keywords Graph neural networks · Convolutional GNNs (ConvGNNs) · Spatial–temporal graph neural networks (STGNNs) · Recurrent-based GNNs (RecGNNs) · Graph autoencoders (GAEs)

1 Introduction

A graph is a type of data structure that represents a collection of items as vertices (called nodes) and the connections between them (called edges). It can be described mathematically as $G = (A, B)$, where A stands for nodes and B for

edges. Depending on whether there are directional dependencies between nodes, edges in a graph can be either directed or undirected. Since graphs are non-Euclidean spaces, the distance between two nodes in a graph is not always equal to the distance between their coordinates in a Euclidean space. To represent the intricate interactions found in graphs, GNNs employ a message-passing mechanism to collect data from nearby nodes. GNNs perform well in several tasks, such as clustering, link prediction, and node classification. GNNs have garnered significant attention and demonstrated cutting-edge performance in a range of graph analysis tasks by extending models of classical neural networks to graph data [114]. GNNs are specifically made to handle the intricate linkages and patterns seen in graph data, in contrast to classic neural networks, which deal with grid-like structures like pictures or sequences. GNNs are widely used in a wide range of real-world applications, such as knowledge graphs [101, 257], transportation systems [104, 194], chemical structures [61, 102], physical systems [45, 213], social networks [63, 132, 134, 139, 141, 143] as well as several other

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