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Graph neural networks: A review of methods and applications

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ABSTRACT

Lots of learning tasks require dealing with graph data which contains rich relation information among elements. Modeling physics systems, learning molecular fingerprints, predicting protein interface, and classifying diseases demand a model to learn from graph inputs. In other domains such as learning from non-structural data like texts and images, reasoning on extracted structures (like the dependency trees of sentences and the scene graphs of images) is an important research topic which also needs graph reasoning models. Graph neural networks (GNNs) are neural models that capture the dependence of graphs via message passing between the nodes of graphs. In recent years, variants of GNNs such as graph convolutional network (GCN), graph attention network (GAT), graph recurrent network (GRN) have demonstrated ground-breaking performances on many deep learning tasks. In this survey, we propose a general design pipeline for GNN models and discuss the variants of each component, systematically categorize the applications, and propose four open problems for future research.

1. Introduction

Graphs are a kind of data structure which models a set of objects (nodes) and their relationships (edges). Recently, researches on analyzing graphs with machine learning have been receiving more and more attention because of the great expressive power of graphs, i.e. graphs can be used as denotation of a large number of systems across various areas including social science (social networks (Wu et al., 2020), natural science (physical systems (Sanchez et al., 2018; Battaglia et al., 2016) and protein-protein interaction networks (Fout et al., 2017)), neural networks for graphs. In the nineties, Recursive Neural Networks are first utilized on directed acyclic graphs (Sperduti and Starita, 1997; Frasconi et al., 1998). Afterwards, Recurrent Neural Networks and Feedforward Neural Networks are introduced into this literature respectively in (Scarselli et al., 2009) and (Micheli, 2009) to tackle cycles. Although being successful, the universal idea behind these methods is building state transition systems on graphs and iterate until convergence, which constrained the extendability and representation ability. Recent advancement of deep neural networks, especially convolutional neural networks (CNNs) (LeCun et al., 1998) result in the rediscovery of