An Investigation Into Graph Neural Network Models

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Abstract

Graphs are a powerful representation of data that is ubiquitous and can be flexible in nature. There are many real-time applications where graphs are being used, such as recommending medication, protein interface prediction, handling traffic networks. However, these application areas make use of non-Euclidean graphical data, which involves highly relational or mostly dependent elements. They cannot be processed well by traditional machine learning approaches or deep learning models (e.g., CNN, LSTM, RNN). Most unsupervised learning methods (e.g., network embedding) cannot utilize the inherent logic contained in graph nodes. Inspired from deep learning architectures, graph neural networks (GNNs) are capable of conflating feature information from nodes and graphical structures to learn graph representation via feature propagation and aggregation. In this work, a concise introduction to basic graph concepts, GNN models, and their applications are provided. It starts with the introduction to the basic GNN models. Then several general graph frameworks and some widely used variants of GNN models are explained, such as graph convolutional networks, graph attention networks, graph recurrent networks. Application of GNNs is categorized based on structured and non-structured data, and then GCN models are designed using different graph libraries and trained on some datasets for solving classification tasks. With the analysis of intermediate and final results, it is observed GCN models can successfully process graph data and also outperforms traditional fully connected networks by 4% of classification accuracy. So, it has proven that due to high interpretability, new architectures and libraries, and performance, there is a dramatic increase in applications and research of GNNs as a graphical analysis tool.