The Graph Neural Network Model

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Abstract

Many underlying relationships among data in several areas of science and engineering, e.g. computer vision, molecular chemistry, molecular biology, pattern recognition, data mining, can be represented in terms of graphs. In this paper, we propose a new neural network model, called graph neural network (GNN) model, that extends existing neural network methods for processing the data represented in the graph domain. This GNN model, which can directly process most of the practically useful types of graphs, e.g. acyclic, cyclic, directed, un-directed, implements a transduction function $\tau(\boldsymbol{G}, n) \in I\!R^m$ that maps a graph $\boldsymbol{G}$ and one of its nodes n into an m-dimensional Euclidean space. A supervised learning algorithm is derived to estimate the parameters of the proposed GNN model. Computational cost of the proposed algorithm is also considered. Some experimental results are shown to validate the proposed learning algorithm, and demonstrate its generalization capability.

Index Terms

Graph Neural Networks, Graph Processing, Recursive Neural Networks, Graphical Domains.

I. Introduction

Data can be naturally represented by graph structures in several application areas including proteomics [1], pattern recognition and image analysis [2], scene description [3], [4], software engineering [5], [6] and natural language processing [7]. The simplest kinds of graph structures include single nodes, and sequences. But in several application domains, the information is organized in more complex graph structures such as trees, acyclic graphs, or cyclic graphs. Traditionally, the exploitation of data relationships has been the subject of many studies in the community of inductive logic programming and, recently, this research theme has been evolving in different directions [8], also because of the marriage with statistics and neural networks (see e.g. the recent workshops [9], [10], [11], [12]).

In machine learning, the structured data is often associated with the goal of (supervised or unsupervised) learning from examples a function τ that maps a graph G and one of its nodes n to a vector of reals[1]: $\tau(\boldsymbol{G}, n) \in I\!R^m$.

Applications to a graphical domain can generally be divided into two classes: *graph focused* and *node focused* applications respectively in this paper.

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[1]Note that in most classification problems, the mapping is to a set of integers $I\!N^m$, while in regression problems, the mapping is to a set of reals $I\!R^m$. Here for simplicity of exposition, we will denote only the regression case. The proposed formulation can be trivially re-written for the situation of classification.