

Deep Learning in a Human-in-the-Loop Setting

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Abstract

In this talk, we will be concerned with techniques for achieving deep learning in a human-in-the-loop setting. We will be focusing on deep neural networks (DNNs) suitable for real-world scientific problems with the following characteristics: (a) Data are naturally graph-structured (relational); (b) The amount of data available is typically small; and (c) There is significant domain-knowledge available from human experts, usually expressed in some logical form (rules, taxonomies, constraints and the like). Recently, the obvious choice of tools for learning from graph-structured data has been graph neural networks (GNNs), primarily due to their tremendous success in this area. However, the machine learning community has focused mainly on (a), and less has been done to deal with (b) and (c). In this talk, we would be interested in graph representation learning in the mentioned problem setting. We will explore some recent techniques for the inclusion of relational information into GNNs when learning from graph-structured data. We will see how this allows us to combine deep learning with logical representation and achieve better predictive models. In applications, we will see some recent empirical results obtained for problems arising in drug discovery.

Keywords Graph Representation Learning, Neuro-Symbolic Learning, Inductive Logic Programming, Drug discovery