

The Combinatorial Side of Graph Neural Networks

Dr Sandra Kiefer

University of Oxford

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Abstract:

Graph Neural Networks (GNNs) are a machine learning architecture to learn functions on graphs. For example, since problem instances for combinatorial optimisation tasks are often modelled as graphs, GNNs have recently received much attention as a natural framework for finding good heuristics in neural optimisation approaches.

The question which functions can actually be learnt by message-passing GNNs and which ones exceed their power has been studied extensively. In this talk, I will consider it from a graph-theoretical perspective. I will survey the Weisfeiler-Leman algorithm as a combinatorial procedure to analyse and compare graph structure, and I will discuss some results concerning the power of the algorithm on natural graph classes. The findings directly translate into insights about the power of GNNs and of their extensions to higher-dimensional neural networks.