

Algorithmic graph theory (Graph neural networks)

Topic: Addressing Expressivity and Over-smoothing in Graph Neural Networks

Abstract:

Graph Neural Networks (GNNs) have emerged as powerful deep learning models for analyzing graph-structured data by exploiting relational inductive biases. However, the development of GNNs faces two key challenges: the limited expressive power of deep architectures due to over-smoothing, and the performance degradation of shallow GNNs on heterophilic graphs. This dissertation provides a comprehensive analysis of these obstacles and proposes novel methods to address them. We first define a mathematical framework to characterize the representation space of GNNs, laying the theoretical groundwork for our proposed solutions. We then introduce a new model that utilizes an attention mechanism, allowing the network to selectively attend to different parts of the input graph and mitigating the over-smoothing effect. An application of this architecture to a biomedical graph classification task demonstrates its superior performance, contributing to the advancement of more robust and expressive GNNs.

Thank You

Regards

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