How Powerful Do Graph Neural Networks Need to Be?

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Message passing graph neural networks (GNNs) are a powerful, highly expressive class of machine learning models to learn on graphs. Yet, not all graphs are equally effective in facilitating vertex communication, often suffering from challenges like over-squashing and over-smoothing [1, 2]. In this talk, we explore how these issues are intertwined and propose graph rewiring strategies to mitigate their effects [4, 5]. Our analysis further reveals that a critical yet often overlooked factor is the limited trainability of GNNs [1, 2, 3], making them less powerful than theoretically expected. While techniques such as balanced initialization [1], dynamic rescaling [3], and architectural innovations [2, 6] can improve trainability, we show that delaying the learning of specific layers can sometimes enhance generalization, particularly in the context of homophilic tasks [3]. This begs the question whether the trainability issues act as positive implicit regularization and are thus a feature rather than a bug. Motivated by this question, we propose simplifications of GNN architectures that greatly reduce the number of trainable parameters without compromising performance and provide theoretical explanations for their success [6].

Joint work with: Celia Rubio-Madrigal, Adarsh Adarsh Jamadandi, Nimrah Mustafa.

References

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