Dissertation Defense

Generating Graphs with Deep Learning and Graph Theory

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Abstract: Deep generative models attract lots of attention in recent years. With deep neural networks and specific designs, deep generative models can generate high-quality realistic data. In this dissertation, I focus on combining the deep generative models with the traditional graph theory algorithms to reduce the dependence on the volume of the training data and improve the quality of the generated graphs. I first propose a deep learning method to improve the Havel-Hakimi graph realization algorithm to generate doppelganger graphs from a single graph. Second, I present a few new architectures of normalizing flow models with improved performance and theoretical guarantees. Finally, I develop a permutation invariant method via leveraging graph theory and denoising diffusion models for generating molecular graphs.

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Mathematics and Science Center: MSC E406

Advisor: Yuanzhe Xi

Mathematics
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