Learning and Generalization in Graph Neural Networks

Stefanie Jegelka

MIT, Department of Electrical Engineering and Computer Science, Cambridge, USA

Graph Neural Networks (GNNs) have become a popular tool for learning representations of graph-structured inputs, with applications in computational chemistry, recommendation, pharmacy, reasoning, and many other areas. In this talk, I will show some recent results on learning with message-passing GNNs. In particular, GNNs possess important invariances and inductive biases that affect learning and generalization. We relate these properties and the choice of the “aggregation function” to predictions within and outside the training distribution.

This talk is based on joint work with Keyulu Xu, Jingling Li, Mozhi Zhang, Simon S. Du, Ken-ichi Kawarabayashi, Vikas Garg and Tommi Jaakkola.