Mixed-integer Encoding of Machine Learning Models and its Applications (Two Lectures)

报告人： 张世强　英国帝国理工学院

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地点： **文萃楼G223(12.23)　文萃楼G221(12.24)**

摘要： Mathematical optimization over trained machine learning (ML) models is an area of increasing interest. Relevant applications include verification, minimizing neural acquisition functions, and integrating a trained surrogate into a larger decision-making problem. In this talk, we first introduce optimization and machine learning toolkit (OMLT). We discuss the advances in optimization technology that made OMLT possible, and demonstrate how to use OMLT for solving decision-making problems in both computer science and engineering. The second part is about optimization over trained graph neural networks (GNNs), which is already supported by the latest version of OMLT. Two applications, GNN verification and GNN-based molecular design, will be discussed in detail. Lastly, we will introduce our recent work about global optimization of Gaussian process acquisition functions using a piecewise-linear kernel approximation.

个人简介： 张世强，英国帝国理工学院计算机系博士生，曾于北京理工大学数学与统计学院获学士与硕士学位。研究方向为混合整数规划、贝叶斯优化和机器学习等，相关文章发表在Advances in Neural Information Processing Systems、Machine Learning、Computers & Chemical Engineering等会议或期刊上。