数学与系统科学研究院

计算数学所学术报告

报告人：　Prof. Guo-Wei Wei

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报告题目：

Can AI discover new drugs

邀请人：　卢本卓 研究员

报告时间：2019 年 6 月 12 日（周三）

上午 10:00-11:00

报告地点：　数学院南楼二层

202 教室

Abstract:

The dominant win of Google's Alphafold in the latest Critical Assessment of Structure Prediction (CASP) competition has ushered a new era of scientific discovery. Researchers are excited about what the future may hold for drug design. Artificial intelligence (AI) might make new drug discovery significantly faster and cheaper. This could be particularly beneficial to patients with rare medical ailments, for whom drug discovery is currently not profitable, or for those whose medical ailments currently can't be effectively treated with drugs, such as Alzheimer's disease. However, drug design is much more complex than protein folding prediction. Due to the structural complexity of protein-drug interactions, the high dimensionality of drug candidates' chemical space, and the involved molecular simulation and machine learning, even all the world's computers put together do not have enough power to design drug automatically. In my lab, we tackle these challenges mathematically. Our work focuses on reducing the geometric complexity of protein-drug complexes for computers. We have introduced differential geometry, algebraic topology, and graph theory to obtain high-level abstractions of protein-drug interactions and thus significantly enhance AI's ability to handle excessively large datasets in drug discovery. Our mathematical AI has made us a top competitor in D3R Grand Challenges, a worldwide competition series in computer-aided drug design and discovery in the past three years.

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