Mathematical AI for drug discovery

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Artificial intelligence (AI) has fundamentally changed the landscape of science, technology, industry, and social media in the past few years. It holds a great future for discovering new drugs significantly faster and cheaper. However, AI-based drug discovery encounters obstacles arising from the structural complexity of protein-drug or protein-protein interactions and the high dimensionality of drug candidates' chemical space. We tackle these challenges mathematically. Our work focuses on reducing the biomolecular complexity and dimensionality in AI. We have introduced evolutionary de Rham-Hodge, multiscale cohomology, and persistent spectral graph to obtain high-level abstractions of protein-drug interactions and thus significantly enhance AI's ability to handle excessively large datasets of complex biomolecules in drug discovery. Using our mathematical AI approach, my team has been a top winner in D3R Grand Challenges, a worldwide annual competition series in computer-aided drug design and discovery in the past three years. I will briefly discuss Math and AI-based drug repositioning and antibody therapies for COVID-19.

Biography: Guowei Wei earned his Ph. D. degree from the University of British Columbia in 1996. He was awarded a postdoctoral fellowship from the NSERC of Canada to pursue his postdoc work at the University of Houston. In 1998, he joined the faculty of the National University of Singapore and was promoted to Associate Professor in 2001. In 2002, he relocated to Michigan State University, where he is an MSU Foundation Professor of Mathematics, Electrical and Computer Engineering, and Biochemistry and Molecular Biology. His current research interests include mathematical molecular bioscience, deep learning, drug discovery, and computational geometry and topology. He has advised over a hundred of students, postdocs, and visiting scientists. Dr. Wei has served extensively in a wide variety of national and international panels, committees, and journal editorships.