Department of Applied and Computational Mathematics and Statistics Colloquium

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Mathematical deep learning for drug design and discovery

Designing efficient drugs for curing diseases is of essential importance for the 21st century's life science. Computer-aided drug design and discovery has obtained a significant recognition recently. However, the geometric complexity of protein-drug complexes remains a grand challenge to conventional computational methods. We assume that the physics of interest of protein-drug complexes lies on low-dimensional manifolds or subspaces embedded in a high-dimensional data space. We devise topological abstraction, manifold reduction, graph simplification, and multiscale modeling to construct low-dimensional representations of biomolecules in massive and diverse datasets. These representations are integrated with various deep learning algorithms for the predictions of protein-ligand binding affinity, drug toxicity, drug solubility, drug partition coefficient and mutation induced protein stability change, and for the discrimination of active ligands from decoys. I will mainly focus on one specific mathematical technique, i.e., persistent homology, to illustrate the working principle of this approach and its performance in D3R Grand Challenges, a worldwide competition series in computer-aided drug design and discovery (http://users.math.msu.edu/users/wei/D3R_GC3.pdf.)

Wed., September 19, 2018
4:15 PM – 5:15 PM
127 Hayes-Healy Center

Colloquium Tea 3:30 PM to 4:15 PM 101A Crowley Commons Room