Data Science and Machine Learning Seminar Series

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Virtual Presentation: https://purdue.webex.com/meet/aselvite

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Deep learning for determining 3D structures of biomolecules

Proteins are working molecules in the cells in our body. In principle, in any cellular activities and functions that involves motions, chemical reactions, and molecular transfer in living cells, there are various kinds of proteins in action involved in carrying out the functions. Since functions are carried out by specific physical interactions of proteins and other molecules, determining the 3D structure of proteins is crucial for understanding the mechanisms of their functions and diseases. Protein 3D structure information is also very important for drug discovery, since a drug is usually a chemical molecule that fits to a target protein and alter the protein's function. To compensate experimental approaches for determining protein 3D structures, computational methods have been developed for modeling protein structures. Recently, deep learning has been successfully applied for many unsolved problems in structural biology. In this talk, we will discuss our recent developments that use deep learning, including tools for protein 3D structure prediction, protein 3D structure modeling for low-resolution cryo-electron microscopy images, and protein-protein docking. These methods use 2D or 3D convolutional neural network to capture 3D image and atom position patterns of protein structures.