ELECTRICAL & COMPUTER ENGINEERING BIO-SEMINAR Fall 2017

When: **Friday 13:50 – 14:50**
Where: **ETB 1035**

Speaker: **Prof. Yang Shen**

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Title: **Optimization and Learning for Protein Docking**

Date: **11-17-2017**

Abstract: Living cells can be viewed as systems of interacting biomolecules including DNA, RNA, proteins, and so on. Being the second most abundant molecule of cells (next to waters), proteins are the "workhorse" molecules that participate in and enable virtually every cellular process. In recent years, high-throughput biotechnologies are generating quickly growing data about the identities of the nodes and the vertices of biomolecular systems: what proteins are there and which pairs of proteins are interacting. However, it remains a technology bottleneck to determine how proteins interact, which prevents us from more insights into life and better development of therapeutics. Protein docking aims at addressing this challenge by computationally predicting how proteins interact in the 3D space given their individual 1D sequences or 3D structures.

In this talk, I will present algorithmic challenges and progresses in protein docking, including principle-driven, data-driven, and combined approaches. Following the energy minimum principle, protein docking can be formulated as optimizing an expensive yet inaccurate nonconvex objective function in an extremely high dimensional space of rigid and flexible motions. From a data perspective, protein docking can be viewed as learning from known 1D sequence or 3D structure data to predict unknown 3D structures of a protein pair. I will introduce ongoing progresses in optimization and learning to these ends, including (1) dimensionality reduction, range reduction and diffeomorphism for the search space; (2) machine learning for the objective function; (3) nonconvex optimization for the search; and (4) statistical inference for additional constraints (or restraints).

Biography: Dr. Yang Shen received his Ph.D. in Systems Engineering from Boston University and postdoctoral training in the Departments of Biological Engineering and Electrical Engineering & Computer Science at the Massachusetts Institute of Technology. He was a Research Assistant Professor at the Toyota Technological Institute at Chicago. He is currently an Assistant Professor in the Department of Electrical and Computer Engineering and the Center for Bioinformatics and Genomic Systems Engineering at the Texas A&M University. His research interests are in developing algorithms including optimization and learning for modeling biological molecules, systems, and data. Applications include protein docking, protein and drug design, systems and synthetic biology, and omics.