The Biological and Biomedical Joint Seminar Series

(Hosted by the departments of Molecular & Cellular Biology, Chemistry & Biochemistry, Cellular & Molecular Medicine, and Plant Sciences)

"Integrating mechanistic modeling and machine learning to understand complex biological systems with 'small data'"

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> Tuesday November 10th, 2020 Zoom Meeting @ IIAM

> Hosted By: Guang Yao (MCB)



At their core, biological systems are information processing systems. For example, in response to numerous environmental cues, the complex molecular interaction networks within human cells integrate these signals and orchestrate a number of intricate cellular behaviors. Verbal argument and intuition alone are insufficient to understand how these complex networks control cellular behaviors or to rationally design treatment, and it is beneficial to translate these molecular networks into realistic and predictive mathematical models. However, the development of such models faces several fundamental challenges: 1) the control network is complex and full of interacting feedbacks, 2) the kinetic constants characterizing the biological reactions are often unavailable, 3) it is often impossible to derive analytical solutions of these models, and 4) once the models become increasingly realistic and complex, they are often as difficult to understand as the original biological system. To address these above mentioned challenges, we have developed an integrated computational pipeline that combines Mechanistic modeling, Bayesian inference, Machine learning and nonlinear dynamical analysis. By integrating different methods with unique strength and limitations, this innovative pipeline can overcome each other's limitations and deliver unprecedented power. This novel, integrated pipeline has been applied to study several different biological systems, and the results have been verified experimentally. Based on our theoretical analysis and experimental confirmation, we propose that his novel pipeline can be generally applied to understand any complex and uncertain biological systems.

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