香港浸會大學
HONG KONG BAPTIST UNIVERSITY

DEPARTMENT OF
COMPUTER SCIENCE
計算機科學系

ONLINE SEMINAR
2023 SERIES

Department of Computer Science

Mr. Tianfan Fu

Department of Computational Science and Engineering
Georgia Institute of Technology

Register Now

Date: 14 February 2023 (Tuesday)
Time: 9:30am – 10:30am
Registration: https://bit.ly/cs-ereg

(*Zoom details will only be provided to registrants)

Deep Learning for Drug Discovery and Development

ABSTRACT

Artificial intelligence (AI) has become woven into therapeutic discovery to accelerate drug discovery and development processes since the emergence of deep learning. For drug discovery, the goal is to identify drug molecules with desirable pharmaceutical properties. I will discuss our deep generative models that relax the discrete molecule space into a differentiable one and reformulate the combinatorial optimization problem into a differentiable optimization problem, which can be solved efficiently. On the other hand, drug development focuses on conducting clinical trials to evaluate the safety and effectiveness of the drug on human bodies. To predict clinical trial outcomes, I design deep representation learning methods to capture the interaction between multi-modal clinical trial features (e.g., drug molecules, patient information, disease information), which achieves 0.847 F1 score in predicting phase III approval. Finally, I will present my future works in geometric deep learning for drug discovery and predictive model for drug development.

BIOGRAPHY

Tianfan Fu is a Ph.D. candidate in the School of Computational Science and Engineering at the Georgia Institute of Technology, advised by Prof. Jimeng Sun. His research interest lies in machine learning for drug discovery and development. Particularly, he is interested in generative models on both small-molecule & macro-molecule drug design and deep representation learning on drug development. The results of his research have been published in leading AI conferences, including AAAI, AISTATS, ICLR, IJCAI, KDD, NeurIPS, UAI, and top domain journals such as Nature, Cell Patterns, Nature Chemical Biology, and Bioinformatics. His work on clinical trial outcome prediction has been selected as the cover paper on Cell Patterns. In addition, Tianfan is an active community builder. He co-organized the first three AI4Science workshop on leading AI conferences (https://ai4sciencecommunity.github.io/); he co-founded Therapeutic Data Commons (TDC) initiative (https://tdcommons.ai/), an ecosystem with AI-solvable tasks, AI-ready datasets, and benchmarks in therapeutic science. Additional information is available at https://futianfan.github.io/.

ENQUIRY

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