SFU Data Science Research Group presents

Seminar Series on Trustworthy Data Science and AI

SFU SIMON FRASER UNIVERSITY

Jian Tang

Assistant professor at Mila-Quebec AI Institute
and HEC Montreal, Canada CIFAR AI Research Chair

Graph Representation Learning for Drug Discovery

Wednesday, December 16, 2020
4:30 - 6:00 pm Pacific time

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Abstract

Drug discovery is a very long and expensive process, taking on average more than 10 years and costing $2.5B to develop a new drug. Artificial intelligence has the potential to significantly accelerate the process of drug discovery by extracting evidence from a huge amount of biomedical data and hence revolutionizes the entire pharmaceutical industry. In particular, graph representation learning techniques---a fast growing topic in the machine learning and data mining community focusing on deep learning for graph-structured data---has seen great opportunities for drug discovery as many data in the domain are graph-structured such as molecules and biomedical knowledge graphs. In this talk, I will introduce our recent progress on graph representation learning for drug discovery including: (1) molecule properties prediction; (2) de novo molecular design and optimization; and (3) retrosynthesis prediction.

Biography

Jian Tang is currently an assistant professor at Mila-Quebec AI Institute and HEC Montreal (business school of University of Montreal), and also a Canada CIFAR AI Research Chair. His main research interests are graph representation learning, graph neural networks, deep generative models, knowledge graphs and drug discovery. He obtained his PhD from School of EECS, Peking University in 2014, was an associate researcher at Microsoft Research Asia in 2014-2016, and was a joint postdoc fellow at University of Michigan and Carnegie Mellon University. During his PhD, he was awarded with the best paper in one of the top three machine learning conferences—ICML2014; in 2016, he was nominated for the best paper award in the top data mining conference World Wide Web (WWW); in 2020, he is awarded with Amazon and Tencent Faculty Research Award. He is one of the most representative researchers in the growing field of graph representation learning and has published a set of representative works in this field such as LINE, LargeVis, and RotatE. His work LINE on node representation learning has been widely recognized and is the most cited paper at the WWW conference between 2015 and 2019. He is the program committee and area chair of many prestige conferences in machine learning and data mining including NeurIPS, ICML, ICLR, KDD, WWW, AAAI, IJCAI, etc.

All are welcome.
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