Department of Computer Science
香港城市大學
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COMPUTER SCIENCE COLLOQUIUM

Hypergraph for predicting adverse drug reaction

SPEAKER **Prof. Hiroshi Mamitsuka**

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ABSTRACT

Drug-drug interactions (DDIs), i.e. adverse drug reaction caused by two drugs, are a serious problem in pharmaceutical and medical sciences. Computationally predicting DDIs is so well investigated in not only bio- and chemo-informatics but also machine learning. Existing methods for solving this problem represent DDIs by a graph, with nodes for drugs and an edge (of two drugs) being labeled by a binary vector showing DDI types. The cutting-edge approach for learning the DDI graph is graph neural networks (GNNs), where multiple labels on edges are rather independently used, regardless that relationships among labels would be important for prediction, particularly for minor labels. We thus model DDIs by a hypergraph, where each hyperedge is a triple with two drugs and one DDI type. We then build learning methods of hypergraph neural networks, considering the above problem of GNNs. In this talk, I will describe the motivation and idea behind our hypergraph neural networks and optimization methods. I will further report the performance advantage of our hypergraph neural networks over existing methods through three real benchmark datasets.

BIOGRAPHY

Hiroshi Mamitsuka obtained all degrees (B.S., M.E. and PhD) from University of Tokyo, Japan. After working with industry in business data mining for more than 10 years, he joined academia for doing research on machine learning and scientific data mining. Currently he is a professor of Bioinformatics Center, Institute for Chemical Research, Kyoto University, Japan, being jointly appointed as a faculty of School of Pharmaceutical Sciences of the same university. His current research interests are machine learning, data mining and a wide variety of applications.

All are welcome!

In case of questions, please contact Dr Raymond Wong at cshswong@cityu.edu.hk, or visit the CS Departmental Seminar Web at https://www.cs.cityu.edu.hk/events/cs-seminars/recent-cs-colloquiums.