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HYPERGRAPH FOR PREDICTING ADVERSE DRUG REACTION

PROFESSOR HIROSHI MAMITSUKA
Bioinformatics Center, Institute for Chemical Research, Kyoto University, Japan

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🕐 3:00-4:00 PM (Malaysia time)

📍 Meeting Room, School of Mathematical Sciences, Universiti Sains Malaysia

Abstract. Drug-drug interactions (DDIs), i.e., adverse drug reactions caused by two drugs, is a serious problem in pharmaceutical and medical sciences. Computationally predicting DDIs is 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. In the DDI graph, 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. In general, a fundamental assumption behind a graph (or a hypergraph) is nodes in an edge (or a hyperedge) should share similar features, while this assumption is not mandatory for DDIs. Instead, we focus on the similarity between hyperedges to build our original model for learning hypergraph neural networks. 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 hyper graph neural networks over existing methods through three real benchmark datasets.