

Project Summary/Abstract

Neurological and psychiatric disorders affect millions globally and include a wide variety of brain diseases and disorders while our understanding on the exact neuropathological mechanism of many of such diseases is still unclear. The objectives of this project are to develop high-expressive-power methods working for general hypergraphs that are essential for understanding the pathological basis of brain diseases and to improve the explainability of deep hypergraph neural networks (HGNNs) in brain network analysis. The PI has been working in hypergraph and graph theory since 2011 and using theory, principles, and methods in graph algorithm design to solve problems in machine learning, AI healthcare, drug discovery and development. In the past three years, the laboratory focused on developing novel graph machine learning techniques such as HGNNs, hypergraph representation learning, hypergraph clusterings and their applications in the biomedical field. Existing HGNNs posed strong assumptions that the number of interactions is the same as the number of brain regions of interest or all possible interactions involve the same number of brain regions, and thus have limited power in expressing diverse higher-order interactions between brain regions. Despite HGNNs have achieved state-of-the-art performance across a wide range of application domains, their applications are still limited by our inability to explain their behavior. In particular, without being able to explain the patterns HGNNs rely on to make predictions, it is impossible to justify their use in brain disease diagnosis where trust and safety are critically needed. The explanations of HGNNs have received very few studies, although the counterpart in graph neural networks (GNNs) have attracted intensive studies recently. As far as our knowledge, it is still unknown how these methods designed for GNNs can be generalized to HGNNs and whether we can design HGNN explanation methods directly. This project envisions to carry out investigations on this critical research in the application domains of brain network analysis and disease diagnosis, which will also stimulate the explainability of deep HGNN models in other biomedical problems. The research findings will be instigated and used in at least two upper-level and graduate courses, exposing students to the latest development of AI and neuroscience. We will make all the data, models, and programs produced during the project publicly available.