



The Hong Kong University of Science and Technology

Department of Mathematics

PhD THESIS EXAMINATION

***Studies on Biomolecular Structure Learning
and Federated Privacy Protection***

By

Mr. Hanlin GU

ABSTRACT

In this thesis, I developed algorithms in two aspects: 1) Elucidating the structure and dynamics of biological macromolecules 2) Privacy-protecting of federated deep learning.

Understanding the structure and dynamics of biological molecules is a central pillar of molecular biology. We develop a series of machine learning tools in experiment and computation through simulation or experimental data. In particular, one part of the work involves better utilization of Cryo-EM images obtained experimentally. A robust denoising approach is proposed in Cryo-EM images to help structure reconstruction and conformations distinguish. Then a two-stage classification scheme is presented that could accurately classify the denoised Cryo-EM images from multiple conformations, which helps to infer the underlying free energy landscape. In addition, a kinetic algorithm based on projection operator framework via deep learning is designed to assign numerous microstates into a handful of metastable states (macrostates). It is helpful to understand the conformational dynamics of complex biomolecules from the simulation perspective.

Another important work focus on federated privacy protection. Federated deep learning aims to preserve users' data privacy by decentralizing data from the central server to end-devices. However, an adversary may still infer the private training data from the released model and updated gradients. A privacy-preserving Federated Deep Learning with Private Passport framework is proposed without sacrificing the model performance and computation efficiency.

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| External Examiner | : | Prof. Jimin XIAO, Department of intelligent science
Xi'an Jiaotong-Liverpool University |

(Open to all faculty and students)

The student's thesis is now being displayed on the reception counter in the General Administration Office (Room 3461).