

THE UNIVERSITY OF HONG KONG

Faculty of Science

HKU-TCL Joint Research Centre for Artificial Intelligence

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Project Title: Solving multi-particle Schrödinger equations using deep learning methods

Abstract:

Accurate numerical solutions for multi-particle Schrödinger equations are of utmost importance in physics, chemistry, and materials science. However, the computational cost of current high-accuracy methods scales poorly with the number of interacting particles. Inspired by the recent successful applications of deep learning methods in machine learning and computer vision tasks, we aim to combine Monte Carlo methods with artificial neural networks-based deep learning methods to solve multi-particle Schrödinger equations.

The objective of the project is threefold.

- (1) To develop efficient deep learning methods for solving multi-particle Schrödinger equations for molecules with up to dozens of electrons.
- (2) To analyze the accuracy, convergence, and stability of the proposed numerical algorithms, which aims to gain insight into the expressibility of deep neural networks and the performance of the optimization methods (e.g., stochastic gradient descent method) in the deep learning methods.
- (3) To implement our deep learning methods to solve application problems, for instance, computing the ground state of individual atoms and molecules, and the transition state that occurs during chemical reactions, which can promote the development of quantum chemistry.

It is expected that the new methods can alleviate the curse of dimensionality and obtain accurate wavefunctions for the multi-particle Schrödinger equations. Moreover, the new methods developed in this project will have many applications in quantum physics, quantum chemistry, and material science, and thus generate a broad impact on the science and engineering community.