THE UNIVERSITY OF HONG KONG

Faculty of Science

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Project Title: Quantum-Inspired explainable-AI

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Abstract:

For the method of Monte Carlo (MC) simulations, previously researchers including the PI have designed the self-learning Monte Carlo scheme which improves the simulation of quantum many-body model and material systems and inspired many extensions. However, this method is still technically limited as it may be not applicable to all systems, and it has not enjoyed the development and neural networks. On the other hand, there have been various applications of (generative) neural networks to the research of physics and quantum materials.

In this project, we design a generic parallel-chain Monte Carlo (PCMC) scheme with the assistance of some generative neural networks. Our method generates Monte Carlo configurations with complete absence of autocorrelation and from which direct measurements of physical observables can be employed, irrespective of the system locating at the classical critical point, fermionic Mott insulator, Dirac semimetal and quantum critical point. We further propose a generic parallel-chain Monte Carlo scheme based on such neural networks, which provides independent samplings and accelerates the Monte Carlo simulations by reducing the thermalization process. We demonstrate the performance of our approach on the two-dimensional Ising and fermion Hubbard models.

Reference: https://arxiv.org/abs/2106.00712