Machine Learning in Condensed Matter Physics

CONTRIBUTED TALKS

GEOMETRY OF LEARNING NEURAL QUANTUM STATES
Chae-Yeun Park (University of Cologne)

Variational quantum Monte Carlo with an Ansatz parameterized by neural networks, which was introduced by Carleo and Troyer, has opened a new possibility in solving quantum many-body problems. However, even for its similarity to the classical machine learning method, first-order optimization algorithms such as Adam, which works incredibly well for modeling real-world data, usually fail to learn quantum states. Instead, the second-order method name stochastic reconfiguration (SR) is widely used for this problem. In this talk, we investigate hidden details of this algorithm to see why this is the case. We study spectra of the quantum Fisher matrix, which encodes local geometry information in the SR, and show that its structure varies greatly depending on the properties of the encoded quantum state. We then explain how this behavior limits the application of the first-order method in learning neural quantum states.

UNSUPERVISED LEARNING UNIVERSAL CRITICAL BEHAVIOR VIA THE INTRINSIC DIMENSION
Tiago Mendes Santos (MPI PKS)

The identification of universal properties from minimally processed data sets is one goal of machine learning techniques applied to statistical physics. Here, we study how the minimum number of variables needed to accurately describe the important features of a data set—the intrinsic dimension (ID) - behaves in the vicinity of (classical and quantum) phase transitions. We employ state-of-the-art nearest-neighbors-based ID estimators to

CONVOLUTIONAL RESTRICTED BOLTZMANN MACHINE AIDED MONTE CARLO: AN APPLICATION TO ISING AND KITAEV MODELS
Daniel Alcalde Puente (Forschungszentrum Jülich)

Machine learning is becoming widely used in analyzing the thermodynamics of many-body condensed matter systems. Restricted Boltzmann machine (RBM) aided Monte Carlo simulations have sparked interest, as they manage to speed up classical Monte Carlo simulations. In the poster/talk, based on my paper (Phys. Rev. B 102, 195148), I will explain how we used the convolutional restricted Boltzmann machine (CRBM) method to reduce the number of parameters to be learned drastically by taking advantage of translation invariance. Furthermore, I will show that it is possible to train the CRBM at smaller lattice sizes, and apply it to larger lattice sizes. To demonstrate the efficiency of CRBM, I show the application to the Ising and honeycomb Kitaev models.

AI-ASSISTED QUANTUM MANY-BODY COMPUTATION BEYOND MARKOV-CHAIN MONTE CARLO
Hongyu Lu (University of Hong Kong)

We find artificial neural networks can constructively help the Monte Carlo computations to provide better sampling and complete absence of autocorrelation between configurations in the study of classical and quantum many-body systems. We design generic generative neural-network architecture for the Ising and Hubbard models on two-dimensional lattices and demonstrate it can overcome the traditional computational complexity as well as the difficulty in generating uncorrelated configurations, irrespective of the system locating at the classical critical point, antiferromagnetic Mott insulator, correlated Dirac semimetal or the Gross-Neveu quantum criticality. Our work therefore paves the avenue for highly efficient AI-assisted quantum many-body computation beyond the Markov-chain Monte Carlo.

LEARNING MANY-BODY HAMILTONIANS FROM DYNAMICAL DATA
Frederik Wilde (FU Berlin)

Hamiltonian learning is the problem of inferring the Hamiltonian of a system from measurement data. In this talk I will introduce the setting where the data consists of measurement outcomes obtained at different points in time and where the system of interest evolves according to the Schrödinger equation. I will introduce a scalable, machine-learning inspired approach to learning many-body Hamiltonians based on efficient quantum state representations in terms of tensor networks. This approach is demonstrated on synthetic data where the parameters of a Heisenberg model are learned successfully.

FROM OBSERVATIONS TO COMPLEXITY OF QUANTUM STATES: AN UNSUPERVISED LEARNING APPROACH
Zala Lenarčič (Jožef Stefan Institute)

The vast complexity is a daunting property of generic quantum states that poses a significant challenge for theoretical treatments, especially in non-equilibrium setups. Therefore, it is vital to recognize states which are locally less complex and thus describable with (classical) effective theories. I will discuss how unsupervised learning can detect the local complexity of states. This approach can be used as a probe of scrambling and thermalization in chaotic quantum systems or to assign the local complexity of density matrices in open setups without knowing the corresponding Hamiltonian or Liouvillian. The analysis actually allows for the reconstruction of Hamiltonian operators or even noise-type that might be contaminating the measurements. Our approach is an ideal diagnostics tool for data obtained from (noisy) quantum simulators because it requires only practically accessible local observations.