How to Encode Quantum Many-body Physics into Neural Networks

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Achieving both quantitative description and qualitative understanding on quantum matters has long remained as one of the most intriguing yet challenging problems in quantum science. One of the most intensively studied regime is the physical properties of quantum many-body systems in equilibrium. Although empirical/deductive approaches based on physical insights of scientists have been very successful, it has been nontrivial how to obtain quantitive description of strongly correlated materials, interfacial chemical reactions, and so on. As for non-equilibrium properties, theoretical approaches are even more limited than those for equilibrium physics; even the limitations of perturbation theory methods still remain unclear for many-body systems. Such situations strongly motivate us to construct bias-free and systematically improvable methodology to hunt down the unexplored regime.

Machine learning is a research field that has been attempting to construct such powerful nonlinear functions that can inductively/unbiasedly cover vast data space. The success of deep learning, in particular, has ignited surging number of attempts to overcome computational difficulties by using neural networks (NNs), which is well-known in the machine learning community to be capable of approximate arbitrary probability distributions (the universal approximation theorem). Surprisingly, Carleo and Troyer numerically showed that, quantum many-body wave functions of strongly correlated spins systems can also be accurately represented using NNs [1]. This work inspired applications to ground states and excited states of fermionic and bosonic systems [2,3,4], their thermodynamic properties [5], non-equilibrium properties [6], and so on. There are also directions that seek to compare and connect the novel representation formalism and other variational forms, which further inspired machine learning community to use quantum many-body tools to learn real-world data [7].

In this talk, I aim to walk through the field of the neural-network representation of quantum many-body wave functions, and overview its application in condensed matter physics, statistical physics, quantum chemistry, and quantum information. We first introduce the variational wave function form based on (restricted) Boltzmann machine, and explain its characteristics and optimization. Then, we further explore the frontier of wider network structures including convolutional neural networks, autoregressive models, and more generalized ones. After overviewing the state-of-the-art achievement by neural quantum states, we also discuss the application of neural networks for quantum state tomography, quantum control, etc. Finally, we discuss the future direction of the entire research field.

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