Machine Learning Physics Proposal

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Machine learning(ML) techniques are applied to solve quantum many body problems(QMB). In data science, ML techniques aim to find **patterns** in data which is too complex to extract by conventional data analysis approaches.[1] In QMB, complexity is also one of the main difficulty we face since the Hilbert space from which the physical data come is intimidatingly large. We consider applying ML for two **tasks** in QMB. One is classification of quantum phases, and the other is representation of quantum state by artificial neural network(ANN). The purpose of second task is more or less broader than the first one as we'll mention later.

For the first task, depending on which model we're interested in, the pattern we wish machine to learn from data would be different. Those patterns could be local order parameters(may or may not be commonly defined), or non-local ones such as topological order or entanglement entropy. Machine completes learning the pattern as the task is achieved, say 90+ percent accuracy in classification of the quantum phases. Once the pattern is learned, the machine can recognize(generalize) different hard-to-solve system due to the common pattern(say, order parameter) behind them. There has been many works done in this direction. Phases of Ising model are generalized to different shape of lattice. Quantum spin model such as transverse Ising model, XY model are also examined by somehow advanced ANN and the quantum phases within are successfully classified. There are many other exotic quantum systems(eg. quantum spin liquid) going to be investigated and it's believed that some intriguing pattern behind them could be further revealed on the aid of ML.

For the second task, quantum states are parametrized by ANN. It has been shown that representing quantum state by Restricted Boltzmann machine(RBM), Deep Restricted Boltzmann machine(DRBM) for spin, bosonic, fermionic models the capacity of expression could be extended. With the representation, the approximated ground states of several models have been reached better compared to previous methods. Inspired by this, it's plausible to think there are plenty of other exotic states(such as valence bond solids, correlated valence bond states...etc) could be represented by the family of ANN. In representing those by ANN, the ground state(s) of many unsolved models, at some aspect relevant to those exotic states should be further chased.

Bear in mind that interpretability of the learned pattern should be the main concern for physical research, in contrast to the industrial viewpoint whose main concern is the output, leaving the learned pattern as a black box. We specifically describe our strategy below. **For the first task**, we would apply recently mature architecture like CNN to classify quantum phases of our interest. We may also combine it with quantum loop topography(QLT) method. QLT apply some suitably designed operations to the data(physical states) before feeding into machine.[2] This is different from the well-known pre-engineering data of data science in that we are not only to transform data(states) but to encode the operation with data(thus matrix). In this manner, feeding the data into machine is just selecting the correct operator from the operator pool, called quantum loop topography. As an example, in the context of the two original papers on this method, they choose local operators(which is relevant to their problem, and of course physically interpretable) with their MC sampling data and then feed into ANN to learn non-local pattern. Once they classify the phases of their system(in [2] they classified Chern insulator and traditional insulator), they found an correct operator to classify those two phases. Thus, once the phases of our interest are classified, the pattern could be illustrated in a transparent and insightful way in a rather analytically. **For the second task**, we are going to adapt RBM to represent different ansatz of quantum states for variational learning. During the learning process, parametrized ansatz state are updated to lower the energy functional and finally reach a minimum energy. As an example, we could choose the ansatz to be valence bond kind, and we expect to reach a better result of some dimer-inducing Heisenberg models such as J1-J2 model, J-Q model due to the efficiency of variational learning and the structure of RBM for VB trial state.

One additional point to remark is that the two directions we mention above have a common ingredient : Finding or reconstruction of quantum state(mostly ground state). The discussion can be found in [3] and [4] , which conclude the same viewpoint via different routes.

References

[1] Christopher M. Bishop, Pattern Recognition and Machine Learning, 2006 Springer

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[3] J. Carrasquilla, R. G. Melko , Nature Physics, 13, 431(2017)

[4] G. Carleo, M. Troyer, Science 355, 602 (2017)