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Perspective

Using Machine Learning Algorithms to Compute Electronic Structure

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DESCRIPTION

Machine learning algorithms are clearly effective tools that successfully compress high dimensional data. These techniques have been used in a wide range of scientific and engineering fields, including the simulation of both classical and complex quantum systems as well as the computation of excitonic dynamics, energy transfer in light-harvesting systems, molecular electronic properties, surface reaction networks, and molecular electronic properties. Due to their capacity to evaluate and decipher exponentially enormous data sets and to expedite the search for new energy generation/storage materials, contemporary machine learning techniques have been applied to the state space of complicated condensed-matter systems.

A potent method for permitting quantum speedups and enhancing conventional machine learning algorithms is emerging as quantum machine learning, which combines classical machine learning approaches with quantum computation. A Restricted Boltzmann Machine (RBM) can be trained faster thanks to quantum computing, which also offers a deeper framework for deep learning than its conventional counterpart. The conventional RBM uses the Gibbs distribution to represent probability for a particular configuration of visible and hidden units, with interactions between layers limited. Here, we concentrate on an RBM whose visible and hidden units have the forms +1, -1.

In the fields of chemistry and material science, accurate electronic structure computations for large systems continue to be a difficult problem. In order to do this, simulations based on quantum computing have been investigated in addition to the amazing advancements in the creation of classical algorithms based on ab initio and density functional approaches. Electronic structure Hamiltonians with linear depth and connectivity can be simulated using a certain set of gates (a fermionic swap network). The cost of quantum simulation for both variational and phase estimation-based quantum chemical simulation approaches has been decreased as a result of these studies.

A constrained Boltzmann machine has recently been presented as a method for solving quantum many-body issues, including those involving stationary states and time evolution of the quantum Ising and Heisenberg models. However, when the wave function's phase is necessary for precise computations, this straightforward method must be altered.

Here, we suggest a three-layered RBM structure that consists of the visible and hidden layers as well as a new layer adjustment for the coefficients' signs for the basis functions of the wave function. We will demonstrate that, when compared to the outcomes estimated by a limited minimal basis set, STO-3G, this model has the capacity to resolve intricate quantum many-body issues and produce remarkably precise answers for straightforward molecules. As an additional tool for training method optimization, we used a quantum algorithm.

CONCLUSION

Hybridizing quantum computing with machine learning for the purpose of performing electronic structure calculations is a logical progression in light of recent developments and successes in the development of effective quantum algorithms for those calculations as well as impressive results using machine learning techniques for computation. Here, we present a hybrid quantum approach for obtaining precise molecule potential energy surfaces using a constrained Boltzmann machine. We achieved an effective method for computing the electronic ground state energy for a small molecule system by utilizing a quantum algorithm to assist in optimizing the underlying goal function. With a finite basis set, our method provides excellent accuracy for the ground state energy for H_2, LiH, and H_2O at a specified place on its potential energy surface. Quantum machine learning approaches are expected to develop into potent instruments for obtaining precise values for electronic structures when larger-scale quantum computers become more accessible in the future.

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