Classically Optimized Variational Quantum Eignensolver for Topological Orderd Systems

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Abstract. We propose a new classical-quantum hybrid algorithm — optimizing parameters of the quantum circuit with a classical computer efficiently and then generating a non-trivial quantum state on an actual quantum computer with the optimized parameters. This can solve the accuracy problem of the existing variational quantum algorithms caused by the operational and statistical errors and make the best use of near-term quantum computing. As an example, we apply the proposed method for quantum machine learning of quantum phase of matter, where the generated quantum states are further used for a clustering algorithm to classify the underlying quantum phase.

Keywords: NISQ, VQE, topological order

Classical-quantum hybrid algorithms using variational quantum circuits [1, 2] repetitively apply the following process: evaluating observables with the parameterized quantum circuit, computing a cost function from them, and updating the parameters with a classical computer (e.g. using gradient methods). While this is one of the most promising applications of NISQ computers [3], there is a severe problem of accuracy. This is because the cost function evaluated by sampling, as mentioned above, suffers from statistical and operational errors.

In this study, we propose a new hybrid classical-quantum algorithm in which the parameter optimization of the quantum circuit is performed solely on a classical computer efficiently and the resultant optimized parameters are further used on an actual quantum computer to generate non-trivial states. Since the expectation values to evaluate the cost function are calculated classically, the proposed algorithm makes the parameter update accurate and feasible. Of course, a classical simulation of quantum computation is inefficient in general. To handle this, we assume the cost function (or Hamiltonian) consists only of local observables and the depth of the parameterized quantum circuits is low (constant or logarithmic in the number of qubits). This allows us to compute the cost functions in polynomial time on classical computers. Due to this strong assumption, one might think that there is no need to use an actual quantum computer. This is true if one is interested in local observables. However, this is not the case, if we are interested non-local information such as non-local observables or sampling on the generated quantum states.

As an example of such a problem, we consider a one-dimensional transverse field cluster model [4]. While this system is exactly solvable, it is known to exhibit a symmetry-protected topological phase transition [5] depending on the strength of the magnetic field and the associated order parameter consists of non-local observables [6]. As a proof of concept, we got the ground state as mentioned above and evaluated a non-local order parameter numerically, while the latter should be done on an actual quantum computer in practice. Furthermore, to learn the quantum phase, we also calculate the inner products of the generated quantum states with different magnetic fields, which can be efficiently done on an actual quantum computer. Thereby, we performed clustering (an unsupervised machine learning) of two phases, which is in good agreement with the behavior of the order parameter and could be applied for the case without the knowledge of the order parameter.

The same method can be applied for genuine topologically ordered systems such as the Kitaev models with perturbations, which would be hard to be simulated classically.

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