ADAPT-VQE is insensitive to rough parameter landscapes and barren plateaus

Harper Grimsley Edwin Barnes Samantha Barron
Sophia Economou Nicholas Mayhall

Variational quantum eigensolvers (VQEs) represent a powerful class of hybrid quantum-classical algorithms for computing molecular energies. Various numerical issues exist for these methods, however, including barren plateaus and large numbers of local minima. In this work, we consider Adaptive, Problem-Tailored (ADAPT)-VQE ansätze, and examine how they are impacted by these local minima. We find that while ADAPT-VQE does not remove local minima, the gradient-informed, one-operator-at-a-time circuit construction seems to accomplish two things: First, it provides an initialization strategy that is dramatically better than random initialization, and which is applicable in situations where chemical intuition cannot help with initialization, i.e., when Hartree-Fock is a poor approximation to the ground state. Second, even if an ADAPT-VQE iteration converges to a local trap at one step, it can still "burrow" toward the exact solution by adding more operators, which preferentially deepens the occupied trap. This same mechanism helps highlight a surprising feature of ADAPT-VQE: It should not suffer optimization problems due to "barren plateaus." Even if barren plateaus appear in the parameter landscape, our analysis and simulations reveal that ADAPT-VQE avoids such regions by design.