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RESEARCH HIGHLIGHT

Speeding up the “quantum” mountain climb

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A central issue in practical quantum computing is how to achieve a desired state or operator efficiently and reliably. An analogy in the classical world can be offered to describe this problem, namely, mountain climbing. Assume a climber would like to reach the top of a mountain from the base as quickly as possible. This is a typical gradient-based optimization task, and the process of finding path could be performed as follows. The climber measures the distance between the mountaintop and his/her current position. If there is a distance, the climber then figures out the gradient direction and keeps climbing along that direction until he/she arrives at the top satisfactorily.

In the quantum world, the mountaintop is the target state or propagator, while the base is the initial state or propagator. This quantum mountain climbing problem plays as a core part in quantum computing, i.e., how to optimize a control pulse to realize high-fidelity state-to-state or unitary evolutions. In 2005, a milestone optimizing algorithm, called the gradient ascent pulse engineering (GRAPE) algorithm, was proposed in the nuclear magnetic resonance (NMR) system to solve this problem [1]. At present, it is not only widely used in NMR, but also in electron spin resonance, nitrogen-vacancy center in diamonds, quantum dots, ion traps, and superconducting circuits. In the GRAPE algorithm, the distance between the top and climber's current position is the fidelity between the desired and current state/operator, and the gradient indicates how to update the control parameters next.

However, the GRAPE algorithm has a fatal drawback. Quantum mountain climbing deals with Hilbert space, whose dimension grows exponentially with the number of qubits. While computing the fidelity and gradient, computation of the evolution of the quantum system is necessary, which involves massive matrix multiplications and exponentiations. This implies an exponential complexity using classical computers. Indeed, practical GRAPE optimizations have only been applied to around 10 qubits to date due to this complexity. Improvements can be obtained by some modified approaches [2, 3]; however, each of them has its pros and cons.

Bhole and Jones proposed a method that can tackle the gradient evaluation without matrix exponentiation [4]. Traditionally, matrix exponentiation occurs when computing the evolution under the system Hamiltonian, as the system Hamiltonian includes two non-commuting terms - the internal Hamiltonian and the control Hamiltonian. The computation of the evolution under either the internal or the control Hamiltonian is trivial, as both can be easily diagonalized in their respective frames. Bhole and Jones' method utilizes the Trotter–Suzuki formula to split the system Hamiltonian into the internal and control component and makes them evolve seperately. As long as the time step of the evolution is small (which holds for most cases), the complex propagation under the total Hamiltonian can be decomposed into sub-propagations in series. Each sub-propagation just undergoes the internal or control Hamiltonian, which is easy to calculate.

Therefore, Bhole and Jones' method avoids the very inefficient calculation of matrix exponentiation during the whole optimization. The tradeoff is the loss of fidelity, because the Trotter–Suzuki formula is an approximation when evaluating quantum evolutions. Fortunately, according to the authors' simulation, this loss is less than 10^{-4} with reasonable settings. It is totally acceptable in quantum optimizations, imagining that one climbs Mount Jolmo Lungma (more than 8000 m high) and reaching a peak merely one meter away from the real peak!

It should be admitted that other obstacles remain while scaling the GRAPE algorithm to large quantum systems. Nevertheless, Bhole and Jones' method provides a decent solution to overcome the matrix exponentiation problem, which lies at the heart of quantum optimization algorithms. The method can also be transferred to other systems, paving the way to the next-round quantum mountain climbing competitions with higher qubits.

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