Optimized Gradient and Hessian Estimators for Scalable Variational Quantum Algorithms

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With current noisy intermediate-scale quantum (NISQ) devices, circuit sampling is a fundamental step that converts coherent quantum-circuit outputs to measurement data for running variational quantum algorithms that utilize gradient and Hessian methods in cost-function optimization tasks. This step, however, incurs sampling errors in the resulting gradient or Hessian computations. A thorough understanding of the inherent sampling errors is therefore vital to ensure the reliability of NISQ computation.

To minimize these errors, based on rigorous analyses of sampling errors in gradient and Hessian computation, we introduce tunable finite-difference estimators (and their generalized versions) and provide analytically operational recipes to optimize these estimators. These optimally-tuned estimators not only offer significantly low sampling errors but are also compatible with the barren-plateau phenomenon; that is, given a fixed number of sampling copies, the average sampling errors based on these optimized estimators scale with the corresponding root-mean-squares of circuit-function gradient and Hessian components, both of which drop exponentially with the number of qubits employed. This desirable feature prevents all gradient and Hessian computation from turning into random guesses.

As a benchmark, we show that, below a critical sampling-copy number, such an optimized estimator incurs a smaller average sampling error in contrast to the corresponding estimator obtained from the so-called parameter-shift rule that has recently been regarded as a standard for gradient estimation. Furthermore, this critical number grows exponentially with the number of qubits employed by the NISQ device, and the fundamental reason is that the parameter-shift-rule sampling errors are asymptotically independent of the circuit dimension and therefore do not scale closely with the gradient- and Hessian-component magnitudes unless exponentially many sampling copies are measured. These results demonstrate the superior statistical performance of optimally-tuned estimators for scalable quantum computing.