A Moments Based Estimate of Trial State Fidelity for Variational Quantum Computation

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Techniques to improve variational quantum algorithms (VQA) are extremely important in the noisy intermediate-scale quantum (NISQ) era of quantum computing. The recently introduced Quantum Computed Moments technique [1] based on Lanczos expansion theory [2, 3, 4] has demonstrated increased accuracy in ground state energy estimation and remarkable robustness to noise when applied to quantum magnetism [1] and chemistry [5]. We present a new parameter s_*, determined by Hamiltonian moments $\langle\phi|H^n|\phi\rangle$, as an estimate of the overlap between a trial state $|\phi\rangle$ and energy eigenstates of the problem Hamiltonian. We compute s_* for a range of trial-states on problems including QUBOs, quantum magnetism, and chemistry Hamiltonians. Comprehensive investigations were conducted, by simulation and on real devices, to assess s_* as a consistent estimate of the fidelity of the trial state for a range of instances. The ability to estimate the fidelity of the trial state with respect to eigenvectors of the given Hamiltonian would greatly aid in many VQA applications.

[1] H. J. Vallury, M. A. Jones, C. D. Hill, and L. C. L. Hollenberg, "Quantum computed moments correction to variational estimates" Quantum, vol. 4, p. 373, Dec 2020.

[2] L. C. L Hollenberg, "Plaquette expansion in lattice Hamiltonian models", Phys. Rev. D47 1640 (1993). https://doi.org/10.1103/PhysRevD.47.1640

[3] L. C. L. Hollenberg and N. S. Witte, "General nonperturbative estimate of the energy density of lattice Hamiltonians", Phys. Rev. D50 3382 (1994). https://doi.org/10.1103/PhysRevD.50.3382

[4] L. C. L. Hollenberg and N. S. Witte, "Analytic solution for the ground-state energy of the extensive many-body problem", Phys. Rev. B54 16309 (1996). https://doi.org/10.1103/PhysRevB.54.16309

[5] Jones, M.A., Vallury, H.J., Hill, C.D. et al. "Chemistry beyond the Hartree–Fock energy via quantum computed moments." Sci Rep 12, 8985 (2022). https://doi.org/10.1038/s41598-022-12324-z