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Faster emulation of noisy VQE

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Abstract

Variational quantum eigensolving (VQE) is a much touted application of near-future quantum computers. It involves the minimisation of a highdimensional (but polynomially growing) cost function which is classically intractable to evaluate, but quantumly efficient to explore. Many minimisation strategies have emerged in the literature, from simple quantum gradient descent which involves evaluating cost gradients, to guantum natural gradient which involves the guantum geometric tensor. Classical emulation of VQE is tantamount in its study, but the time to classically compute the aforementioned variational quantities becomes an unignorable bottleneck. Recent works have devised bespoke simulation algorithms to overcome this hurdle in noise-free settings, though they cannot capture realistic noisy behaviours of present day devices. We here present novel algorithms for asymptotically faster classical simulation of quantum gradient descent and the quantum natural gradient, where the latter is generalised for channels and replaces the geometric tensor with an approximate Fisher information matrix. Our work permits the exact numerical investigation of significantly larger variational problems in noisy settings described by arbitrary Kraus channels, which can themselves be parameterised. These schemes have been integrated into QuESTlink, a Mathematica simulator of quantum computers.