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Machine Learning Enhanced Optimization of Variational Quantum Eigensolvers

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Variational Quantum Eigensolvers (VQEs) are a powerful class of hybrid quantum-classical algorithms designed to approximate the ground state of a quantum system described by its Hamiltonian. VQEs hold promise for various applications, including lattice field theory and quantum chemistry.
However, the inherent noise present in Noisy Intermediate-Scale Quantum (NISQ) devices poses a significant challenge for running VQEs. These algorithms are particularly susceptible to noise, such as measurement shot noise and hardware noise.
Within this work, we propose to enhance VQEs using Gaussian Processes and Bayesian Optimization. These established machine-learning techniques excel at learning from noisy data, making them ideal candidates for improving VQEs. The contributions of this work are twofold. First, we introduce a "VQE-kernel", a custom kernel function specifically designed to incorporate valuable prior physics information in the Gaussian Process by design. Second, we propose a physics-informed acquisition function for Bayesian Optimization termed "Expected Maximum Improvement over Confident Regions" (EMICoRe). Extensive numerical experiments demonstrate that our approach outperforms state-of-the-art baselines.

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