Dual-VQE: A Quantum Algorithm to Lower Bound the Ground-State Energy

Hanna Westerheim [1,2] Jingxuan Chen [3,2] Zoë Holmes [4] Ivy Luo [2] Theshani Nuradha [2] Dhrumil Patel [3] Soorya Rethinasamy [1] Kathie Wang [2] Mark M. Wilde [2]

[1]School of Applied and Engineering Physics, [2]School of Electrical and Computer Engineering, [3]Department of Computer Science, Cornell University, Ithaca, New York 14850, USA
[4]Institute of Physics, Ecole Polytechnique Fédérale de Lausanne (EFPL), CH-1015 Lausanne, Switzerland

Variational Quantum Eigensolver

- The variational quantum eigensolver (VQE) produces an upper bound on the ground-state energy of a Hamiltonian.
- A semi-definite program (SDP) can output precise estimates for sufficiently small system sizes.
- However, an SDP approach is not viable for large sizes.

Key Question

How can we assess the quality of VQE's upper-bound estimate of $\lambda_{\min}(H)$ without access to a reliable classical algorithm for estimating $\lambda_{\min}(H)$?

Dual-VQE Approach

Dual-VQE estimates a lower bound on the ground-state energy, which can be compared to the upper-bound estimate obtained from VQE.

1. Use SDP duality theory to reformulate $\lambda_{\min}(H)$ as a maximization problem.
2. Further reformulate this maximization problem such that it can be estimated by means of a VQA:

$$\begin{aligned}\sup_{\eta\in\mathbb{R}}\{\eta : \eta I \le H\} &= \sup_{\eta\in\mathbb{R},W\ge 0}\{\eta : H-\eta I = W\}\\ &= \sup_{\substack{\eta\in\mathbb{R},\nu\ge 0,\\ \omega\in\mathcal{D}}}\{\eta : H-\eta I = \nu\omega\}\\ &= \lim_{c\to\infty}\sup_{\substack{\eta\in\mathbb{R},\nu\ge 0,\\ \omega\in\mathcal{D}}}\left\{\eta - c\left\|H-\eta I-\nu\omega\right\|_2^2\right\}\\ &\ge \sup_{\substack{\eta\in\mathbb{R},\nu\ge 0,\\ \theta\in\Theta}}\left\{\eta - c\left\|H-\eta I-\nu\omega(\theta)\right\|_2^2\right\}. \quad (1)\end{aligned}$$

From (1), our main objective is to find the supremum of the following function:

$$f(\eta,\nu,\theta,c) := \eta - c\big(\operatorname{Tr}[H^2] + \eta^2 2^n + \nu^2\operatorname{Tr}[\omega(\theta)^2] - 2\eta\operatorname{Tr}[H] - 2\nu\operatorname{Tr}[H\omega(\theta)] + 2\eta\nu\big).$$

Dual-VQE on Transverse-Field Ising Model

- The Transverse-Field Ising model simulates spin interactions in a ferromagnetic substance, with Hamiltonian

$$\sum_{i=1}^{n-1} J_i \sigma_Z^i \otimes \sigma_Z^{i+1} + \sum_{i=1}^{n} g_i \sigma_X^i.$$

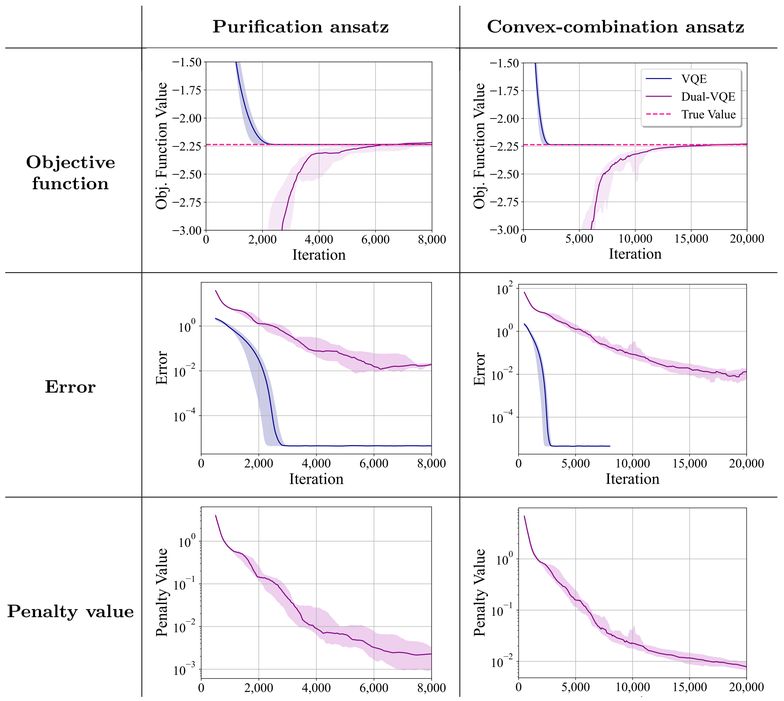


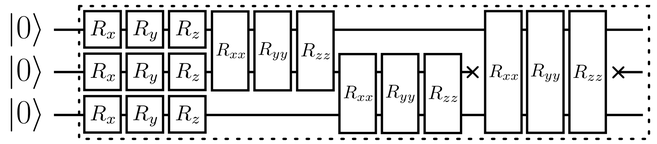
Figure 1. Convergence of dual-VQE and comparison to standard VQE for a two-qubit example problem instance. Solid lines show the median value of the estimate, shaded regions represent the interquartile range, and ground truths are marked by dashed lines.

- Simulations used either a three-layer purification ansatz or a convex-combination ansatz with a two-layer quantum circuit Born machine and a two-layer unitary.
- Obtained an error of 10^{-2} after $20,000$ iterations of training. Training speed was improved by using the SPSA algorithm.
- Penalty terms were also very close to 0, indicating that the constraints were satisfied.

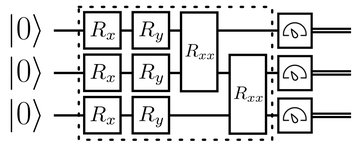
Preparing Mixed States

Prepared state $\omega(\theta)$ using two methods and then performed destructive SWAP test to estimate objective function terms.

- Purification Ansatz:



- Convex Combination Ansatz:



Discussion

- Dual-VQE approach on a two-qubit example takes more iterations to converge than a standard VQE optimization.
- Objective function values across training are noisier for dual-VQE; we expect this behavior due to the increase in the number of terms and parameters.
- It is of interest to scale up dual-VQE to larger systems beyond the reach of brute-force classical simulation.

Conclusion

- Used SDP duality to rewrite the ground-state optimization problem as a constrained maximization problem, which is then rewritten as an unconstrained optimization problem to be solved by a variational quantum algorithm.
- For the example considered, our simulations give evidence that VQE and dual-VQE do indeed bound the optimal ground-state energy from above and below.

AFRL
AIR FORCE RESEARCH LABORATORY

arXiv:2312.03083

kw684@cornell.edu