Supervised Machine Learning Optimisation for Variational Quantum Algorithms

Akib Karim[1], Shaobo Zhang[2], Muhammad Usman[1,2]

[1] *Data 61, CSIRO, Research Way Clayton 3168, Victoria, Australia*
[2] *School of Physics, University of Melbourne, Parkville 3010, Victoria, Australia*

Variational Quantum Algorithms (VQA) are quantum-classical hybrid algorithms that use current noisy quantum hardware to calculate computationally difficult problems in fields such as quantum chemistry, quantum system dynamics, and combinatorial optimisation [1]. The classical component minimises across circuit parameters and can compensate for coherent errors that can be corrected with parametrised gates. However, current algorithms require an unknown number of iterations to reach convergence and can be trapped in barren plateaus for arbitrary initial values.

Methods exist to find warm starts that may avoid barren plateaus and typically require pre-calculation of a similar problem and smooth translation of the global minimum or some such mapping [2, 3, 4]. Rather than extra calculation, we aim to use existing calculations from previously useful problems. Specifically, minimisation requires measurements on intermediate parameter values that are discarded once final parameters are found. These intermediate steps across many calculations already contain valuable information about the function between the circuit parameters and resultant measurements. We can use these measurements to create a warm start for future experiments.

In this work, we use supervised machine learning on the parameter and measurement data of VQA runs to create an algorithm to predict optimal parameters from initial measurements. This neural network can be used as a replacement for classical optimisation and can find global minima in one shot in noise free conditions. Furthermore, in noisy conditions, we demonstrate that training data from devices with different gate setting error allows the neural network to learn to compensate for devices with arbitrary gate setting error. We also design the neural network to be used iteratively to confirm convergence as well as be able to compensate for drift in noise over time. We benchmark and demonstrate our method on noisy simulations as well as real data from IBM semiconductor devices for one, two, and three qubit VQE calculations.

This work presents an alternative classical algorithm for VQAs that can find the approximate global minimum with compensation for arbitrary coherent error. This algorithm can be used when quantum shots are limited or expensive for one-shot approximations; or as a warm start. This also demonstrates the utility of retaining a database of intermediate steps across devices, even those with significant noise. We aim to release the neural networks publicly and drive research in generating warm starts from collected quantum data.

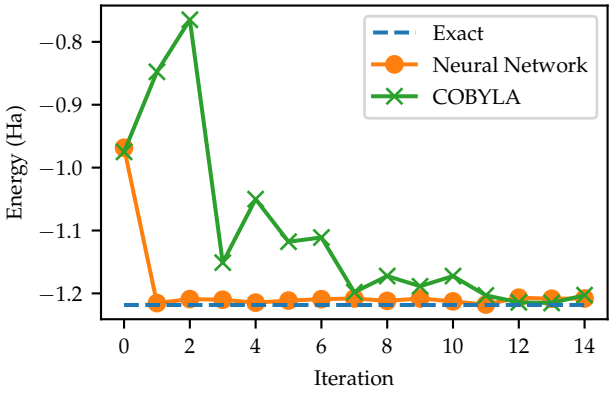

Figure 1: Comparison of Supervised Learning Neural Network minimisation algorithm against COBYLA for ground state variational quantum eigensolver calculation of H_2 with Parity mapping and Z2 symmetry reduction. Our algorithm is able to find the global minimum in one shot and three iterations converge within shot noise. COBYLA requires twelve iterations to find the global minimum but fourteen to confirm convergence.

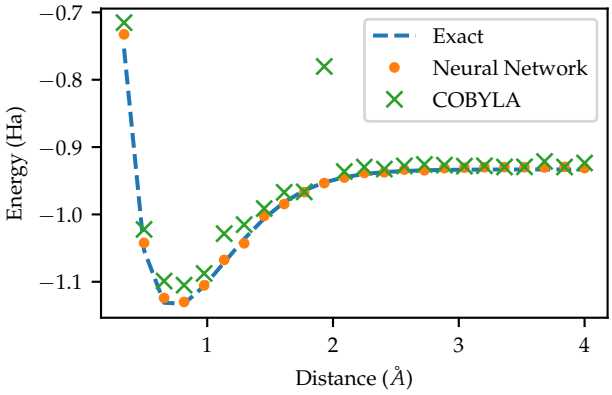

Figure 2: H_2 ground state at different atomic distances found by COBYLA and our Neural Network with simulated noise. Noise model was taken from *ibm_hanoi* with additional gaussian random error with standard deviation of 0.1π radians on circuit parameters. The converged value from COBYLA is reported, whereas the minimum over the same number of iterations is shown from our Neural Network.

References

[1] M. Cerezo et al. "Variational quantum algorithms". In: *Nature Reviews Physics* 3.9 (Sept. 2021), pp. 625–644. ISSN: 2522-5820. DOI: 10.1038/s42254-021-00348-9. URL: https://doi.org/10.1038/s42254-021-00348-9.

[2] James Dborin et al. "Matrix product state pre-training for quantum machine learning". In: *Quantum Science and Technology* 7.3 (May 2022), p. 035014. DOI: 10.1088/2058-9565/ac7073. URL: https://dx.doi.org/10.1088/2058-9565/ac7073.

[3] Antonio A. Mele et al. "Avoiding barren plateaus via transferability of smooth solutions in a Hamiltonian variational ansatz". In: *Phys. Rev. A* 106 (6 Dec. 2022), p. L060401. DOI: 10.1103/PhysRevA.106.L060401. URL: https://link.aps.org/doi/10.1103/PhysRevA.106.L060401.

[4] Manuel S. Rudolph et al. "Synergistic pretraining of parametrized quantum circuits via tensor networks". In: *Nature Communications* 14.1 (Dec. 2023), p. 8367. ISSN: 2041-1723. DOI: 10.1038/s41467-023-43908-6. URL: https://doi.org/10.1038/s41467-023-43908-6.