Quantum and classical methods for ground state optimisation in quantum many-body problems

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Ground state optimisation

Many characteristics of a quantum state are embodied by the wavefunction, ψ. One can model a wavefunction by introducing an ansatz for computing the amplitude of each eigenstate.

In this work we will compare two approaches for modelling the ground state wavefunction of the transverse field Ising model (TFIM): variational quantum eigensolver (VQE) and variational Monte Carlo (VMC) using a restricted Boltzmann machine (RBM) anstaz.

The TFIM Hamiltonian, with a variable strength transverse field, h, is

$$H = \sum_i \sigma_i^z \sigma_{i+1}^z + h \sum_i \sigma_i^x \tag{1}$$

We will also raise the question of **whether the ground state energy alone is a sufficient loss function** and offer up *non-stabiliserness* (a metric of quantum complexity) as a second quantity to keep in mind.

Non-stabiliserness as a metric of quantum complexity

In the fight for supremacy between quantum and classical computing, various metrics of quantum complexity were conceived to try and estimate a task's ability to be classically simulated; it assumed that highly quantum complex problems would require quantum solutions. Non-stabiliserness, often known as *magic*, is one such measure.

The Gottesman-Knill theorem states that any stabiliser operation acting on a stabiliser state can be efficiently simulated by a classical computer [1]. **Therefore, the distance between the state in question and a purely stabiliser state is the non-stabiliserness of the system: the measure of how 'quantum' the state is.**

We can compute the non-stabiliserness using the stabiliser Renyi-2 entropy (SRE), $M_2(|\psi\rangle)$, defined as [2]

$$M_2(|\psi\rangle) = -\log \sum_{P \in \mathcal{P}_N} \frac{\langle\psi| P |\psi\rangle^4}{2^N}. \tag{2}$$

Here, $\mathcal{P}_N$ is the complete set of Pauli strings of length N.

We are interested in how the SRE of the solutions from the quantum and classical algorithms compare.

Variational quantum eigensolver

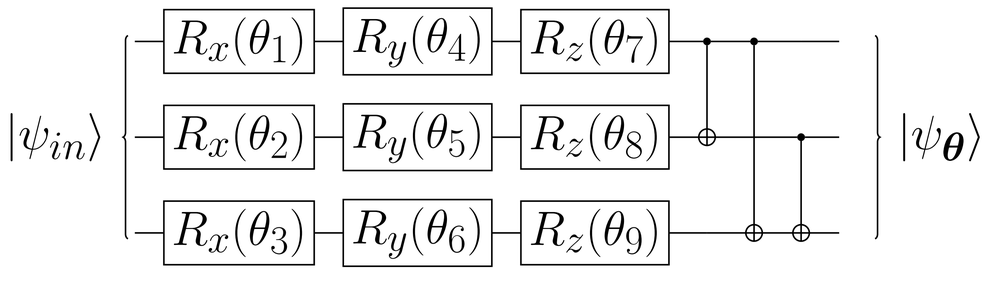

Figure 1. An example circuit that acts as the ansatz for the variational quantum eigensolver. $R_i(\theta_j)$ is a rotation gate in the i axis by angle θ_j.

In the VQE algorithm, proposed in [3], the costly task of preparing a high-dimensional, parameterised wavefunction, ψ_θ, is handled by a parameterised quantum circuit. Figure 1 is one such example; an easily prepared input state is fed into the circuit, the output is a trial wavefunction. One can compute the expectation of the Hamiltonian with respect to this wavefunction and estimate its energy. **Therefore, the ground state energy is treated as the loss function, and minimised by varying θ.** The optimisation procedure is ceased when one is in some optimisation minima.

Phrased like this, it begs the question as to whether this loss function alone, paired with this stopping criterion, is enough.

Restricted Boltzmann machine

Similarly, one can represent the wavefunction as the output of a neural network, in this case, an RBM as depicted in Figure 2.

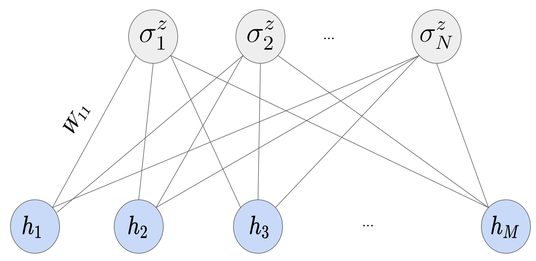

Figure 2. An example of a restricted Boltzmann machine, a function approximator, that we are using as an ansatz for the wavefunction.

This algorithm uses Monte Carlo sampling to estimate the expectation value of the Hamiltonian with respect to a set of RBM parameters. Thus, similar to in the VQE regime, **we can tune the parameters of the RBM such that the wavefunction it represents minimises the ground state energy.** For more details see [4].

Results

Figure 3 shows the non-stabiliserness and energies of the estimations of the ground state from the VQE and RBM approaches.

Despite the VQE algorithm being executed at least partially on a quantum device, both methods perform similarly when it comes to arriving at a ground state that has the correct energy and quantum complexity.

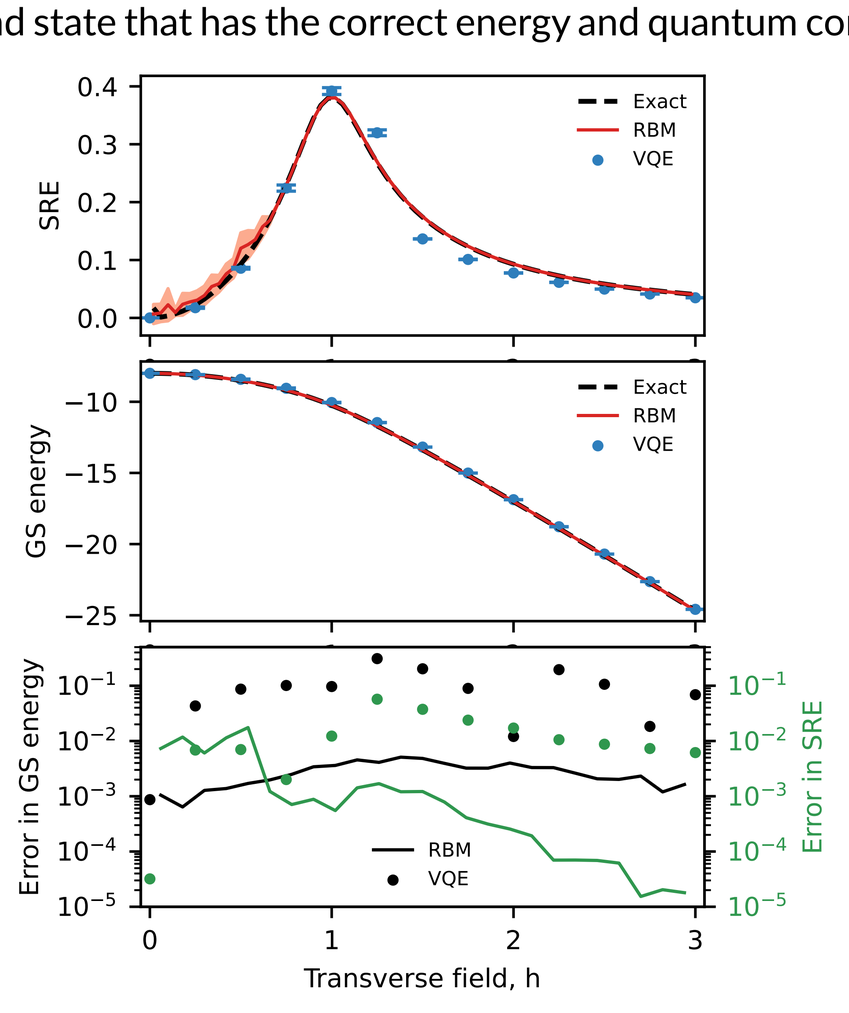

Figure 3. Comparison between: the VQE algorithm and VMC using an RBM ansatz, applied to finding the ground state of the TFIM with 8 qubits. Shown are the SRE (top) and ground state energy (middle) of the ground states found by each model. The differences between these approximate ground states and the exact solution (found through exact diagonalisation) are shown in the bottom pane.

References

[1] E. Chitambar and G. Gour, "Quantum resource theories," *Reviews of Modern Physics*, vol. 91, Apr. 2019.

[2] T. Haug and L. Piroli, "Stabilizer entropies and nonstabilizerness monotones," *Quantum*, vol. 7, p. 1092, Aug. 2023.

[3] A. Peruzzo, J. McClean, P. Shadbolt, M.-H. Yung, X.-Q. Zhou, P. J. Love, A. Aspuru-Guzik, and J. L. O'Brien, "A variational eigenvalue solver on a photonic quantum processor," *Nature Communications*, vol. 5, July 2014.

[4] G. Carleo and M. Troyer, "Solving the quantum many-body problem with artificial neural networks," *Science*, vol. 355, p. 602–606, Feb. 2017.

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