Expressibility of Quantum Circuits for Chemistry Applications

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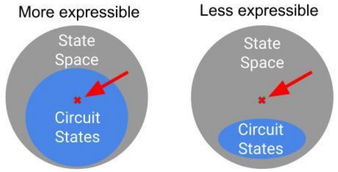
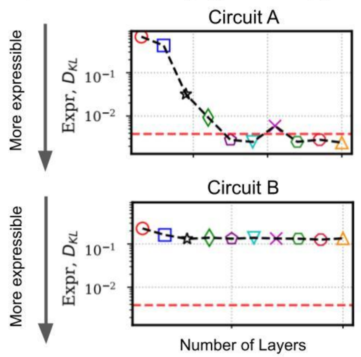
Motivation

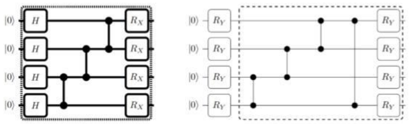
In Variational Quantum Algorithms (VQAs), the choice of the parameterized quantum circuit (PQC) is crucial. It is proposed that PQCs must span a majority of the Hilbert space of quantum states, which is quantified in a descriptor known as *expressibility* [1]. In our work, we propose a new descriptor of expressibility that is better suited for chemistry applications.

$$\mathrm{Expr} = D_{\mathrm{KL}}(\hat{P}_{\mathrm{PQC}}(F;\boldsymbol{\theta}) \parallel P_{\mathrm{Haar}}(F))$$



As noted in [1], increasing the layers of a PQC will typically improve the expressibility until $P_{PQC}(F;\ \theta)$ matches $P_{Haar}(F)$, e.g. Circuit A. However, in some PQCs, e.g. Circuit B, increasing the layers does little to improve the expressibility. This is inconsistent with the observation that Circuit B is proposed to be competent for chemistry applications [2].

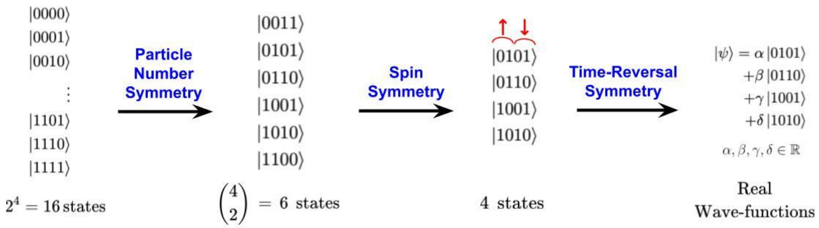




Circuit A Circuit B

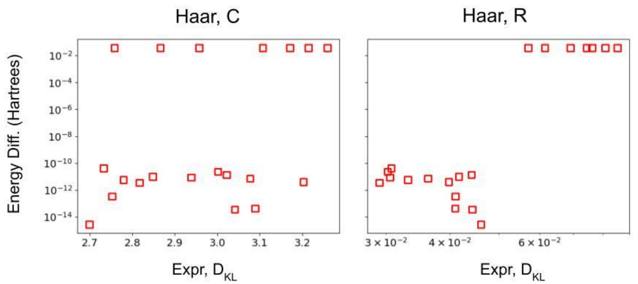
Methodology

Complex State Space	Real State Space
$x\|0\rangle + y\|1\rangle,\quad x, y \in C$	$x\|0\rangle + y\|1\rangle,\quad x, y \in R$
$P_{Haar,\,C} = (d-1)(1-F)^{d-2}$	$P_{Haar,\,R} = \pi^{-\frac{1}{2}} \frac{\Gamma\left(\frac{d}{2}\right)}{\Gamma\left(\frac{d-1}{2}\right)} F^{-\frac{1}{2}}(1-F)^{\frac{d-3}{2}}$



PQCs often represent the quantum state of a given molecule in chemistry applications. Thus, certain rules must be obeyed in order to be a valid quantum state. Particle number symmetry mandates that the number of particles must be the same, spin symmetry restricts the possible spin configurations of the particles, and time-reversal symmetry implies that the wavefunction should be real. Conventional expressibility ignores these symmetries and considers complex wavefunctions on 2^n possible basis states, however only a fraction of these should be considered. We propose a new descriptor of expressibility that takes into consideration these symmetries and account for real wavefunctions.

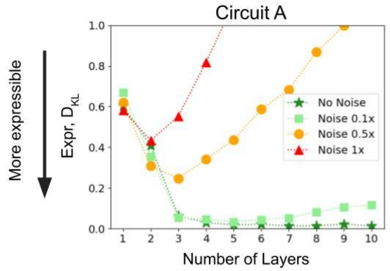
Results



The Variational Quantum Eigensolver (VQE) [2] was simulated to solve for the ground state energy of H_2(bond length 1.05 Angstroms) using 15 chemistry-inspired PQCs. Each point represents a different PQC used in the VQE. The vertical axis shows the difference between the ground state energy computed using VQE and the exact ground state energy. The horizontal axis sorts the points by expressibility. The plot on the left sorts the points according to the conventional expressibility, computed using $P_{Haar,\ C}$, while the plot on the right sorts the points according to the proposed expressibility, computed using $P_{Haar,\ R}$. The proposed expressibility is able to differentiate between PQCs that yield accurate results and those that do not, while the conventional expressibility is unable to differentiate them. The circuits used are ASWAP-type [3], UCCS, and UCCSD, up to 5 layers each.

Impact of Noise

While increasing the layers of a PQC tends to improve the expressibility, one concern is that increasing the number of gates will lead to more gate-based errors, which may have a detrimental effect on the expressibility. We discovered that PQCs have a balance point where additional layers improves the expressibility before incurred noise errors affect it. We computed the (conventional) expressibility using 1x, 0.5x, and 0.1x the error-rate of IBM Kyiv.



Conclusion

Conventional methods of evaluating the expressibility of PQCs fail to capture the symmetries that a quantum state must obey. We presented an alternative approach that obeys these symmetries, and demonstrated that this method can result in a stronger correlation to VQE accuracy, which is indicative of performance in chemistry applications. The proposed expressibility can be an indicator of whether a PQC is suitable for chemistry applications. Finally, we note that increasing circuit layers must be moderate to avoid the negative effects of hardware noise.

References

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