Exploring the Role of Hamiltonian Expressibility in Ansatz Selection for Variational Quantum Algorithms

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Abstract

A key challenge in Variational Quantum Algorithms (VQAs) consists in designing effective parametric quantum circuits, or ansatzes, that account for both the specific problem and the limitations of quantum hardware. While Machine Learning-based methods for circuit construction have been developed, selecting the appropriate metrics to include in the cost function to ensure the circuit has the desired properties remains a non-trivial task. Hamiltonian expressibility has been proposed as a metric to quantify a circuit ability to explore the problem energy landscape. However, its potential to enhance the likelihood of obtaining high-quality solutions remains underexplored. In this work, we investigate the correlation between an ansatz Hamiltonian expressibility and the quality of solutions found using the Variational Quantum Eigensolver (VQE), aiming to determine whether such metric could enhance Machine Learning methods for ansatz design. Specifically, we propose a protocol to estimate the Hamiltonian expressibility of a given ansatz and Hamiltonian, and employ VQE to solve the associated optimization problem. By conducting a correlation analysis, we assess the relationship between Hamiltonian expressibility and solution quality. Our results suggest that Hamiltonian expressibility could serve as a valuable metric to enhance Machine Learning techniques used for ansatz design.

Keywords

Variational Quantum Algorithms, Expressibility, Ansatz, Correlation Analysis

1. Introduction

Variational Quantum Algorithms (VQAs) are a class of hybrid quantum-classical algorithms that use a parametric quantum circuit, or ansatz, and a classical optimizer which tunes the circuit parameters with the goal of minimizing a cost function. Among the most widely used VQAs is the Variational Quantum Eigensolver (VQE), specifically designed to find the ground state of a Hamiltonian operator by minimizing its expectation value on the final state of the circuit. VQAs have recently gained significant attention due to their resilience to noise and decoherence of the qubits, making them particularly suitable for the currently available noisy intermediate-scale quantum (NISQ) devices. However, a significant challenge in their application lies in the selection of an effective ansatz tailored to the specific problem being addressed. This task is not straightforward, as it requires balancing solution accuracy, computational time, and resource usage. To address this, researchers are exploring methods based on adaptive algorithms and Reinforcement Learning [1]. However, these approaches come with high computational costs and require further investigation.

In this context, *expressibility* has been proposed as a metric to quantify the ansatz ability to explore the quantum state space or the problem energy space. Several definitions of expressibility exist in the literature, including the problem-oriented *Hamiltonian expressibility*, which evaluates how effectively a quantum circuit approximates the Haar uniform distribution in generating the final energies [2].

Formally, given a parametric circuit $U(\vartheta)$ acting on n qubits and a problem Hamiltonian H, the Hamiltonian expressibility of the ansatz with respect to H is defined as:

$$\varepsilon^{\mathcal{H}}(U,H) := \left\| \int_{Haar} V^{\otimes 2} H^{\otimes 2} (V^{\dagger})^{\otimes 2} d\mu(V) - \int_{\Theta} U^{\otimes 2}(\vartheta) H^{\otimes 2} (U^{\dagger})^{\otimes 2}(\vartheta) d\vartheta \right\|_2, \tag{1}$$

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where the first integral is computed over the Haar measure, V is a generic unitary operator, $d\mu(V)$ is the volume element of the Haar measure, and the second integral is over the parameter space Θ.

While higher Hamiltonian expressibility allows the circuit to explore a broader range of quantum states, it has been shown that high expressibility favours the occurrence of barren plateaus - regions where the gradient of the cost function vanishes - making it difficult to train the ansatz as the system size increases [2]. Therefore, a trade-off between exploration capability and trainability is crucial.

In this work, we propose a method to evaluate Hamiltonian expressibility and investigate whether this metric can guide the selection of a suitable ansatz within the VQE framework.

2. Experimental Protocol

We propose a procedure to estimate the Hamiltonian expressibility of a circuit, taking inspiration from the protocol in [3]. Specifically, we compute the contribution from the Haar measure in (1) by using a closed-form expression and adopt a Monte Carlo approach to estimate the ansatz contribution, drawing 500,000 random parameters for each estimate.

Our experimental dataset includes Hamiltonians from six specific problem classes: Maximum Cut, Minimum Vertex Cover, Maximum Clique, Heisenberg XXZ, Transverse Ising Field, and Adiabatic. Additionally, we include two random classes: Random Diagonal (diagonal matrix with random real values) and Random Non-diagonal (non-diagonal matrix constructed as a linear combination of Pauli string matrices with random real coefficients). These problem instances are generated for both 4 and 8-qubit systems. We evaluate the same ansatzes analyzed in [3] by computing their Hamiltonian expressibility for each of the defined Hamiltonians. Each circuit is then trained using the VQE protocol in a noiseless setting. We run VQE on each problem instance 10 times and use the average normalized approximation ratio for evaluating the quality of the solutions found.

Finally, we compute Pearson and Spearman correlation coefficients between Hamiltonian expressibility and approximation ratio to assess the relationship between expressibility and VQE effectiveness.

3. Results

Our results show that circuits with high Hamiltonian expressibility tend to perform better on problems with non-diagonal Hamiltonians and superposition state solutions. In contrast, low Hamiltonian expressibility circuits are more effective for diagonal Hamiltonians or problems with basis state solutions. This trend is particularly evident in the Heisenberg XXZ problem, which contains both basis and superposition state solutions, allowing us to directly observe this behavior.

Moreover, the correlation between Hamiltonian expressibility and VQE effectiveness is stronger in small problem instances (4 qubits), while, as the problem size increases (8 qubits), such correlation diminishes, likely due to the increased occurrence of barren plateaus in highly expressive circuits.

In conclusion, Hamiltonian expressibility can provide valuable insights for selecting ansatzes in VQE protocols, particularly for small-scale systems. Therefore, it holds potential for guiding researchers in choosing a suitable ansatz, for instance, by incorporating Hamiltonian expressibility as a penalty term in the cost function of Machine Learning-based methods for ansatz design. However, further research is needed to fully harness the power of this metric and explore its broader applications.

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