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For Quantum Algorithm Grand Challenge

Background

Background

1. The current NISQ quantum computer is significantly influenced by noise. Therefore, it is desirable to keep the circuit as shallow as possible to reduce the effects of noise.
2. For a given Hamiltonian, it is currently not obvious what kind of ansatz would be optimal. Therefore, a method for dynamically exploring the structure of the circuit is desired.

Method

Our method is based on the paper "Structure optimization for parameterized quantum circuits", Quantum 5, 391 (2021), (arXiv:1905.09692v3 [quant-ph])

Method

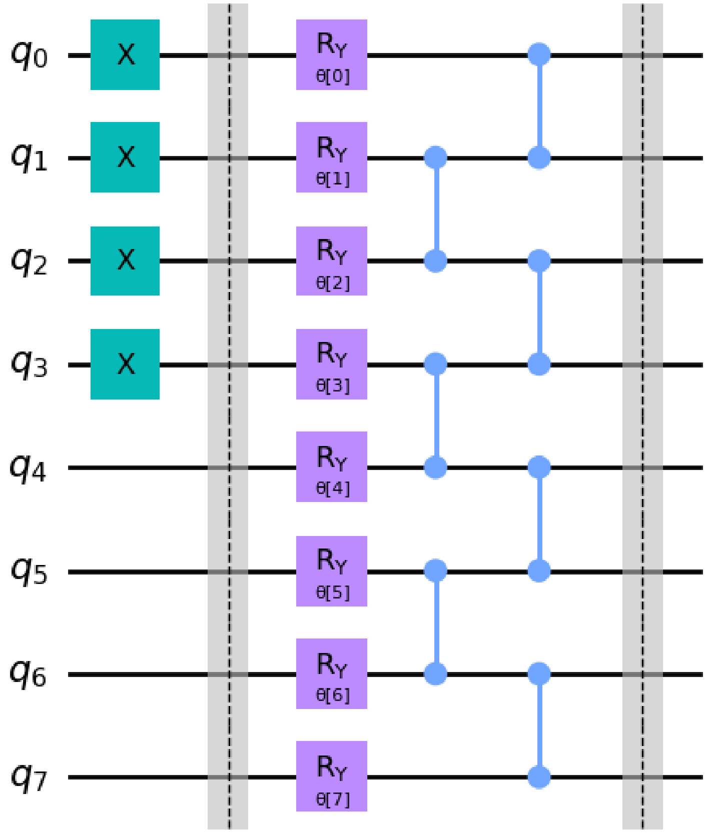
Let $U_1(\theta_1)U_2(\theta_2)...U_D(\theta_D)$ be an ansatz, where $U_d(\theta_d) = e^{-i\frac{\theta_d}{2}P_d}$ and P_d is a Pauli string. We consider determining the set of parameters that minimizes the expectation value of the observable H, $\langle H \rangle$.

When selecting a single parameter θ_d from the set and keeping the others fixed, then the expectation value takes the form of $A\sin(\theta_d + B) + C$. In this case, the value of θ_d that minimizes the expectation value is given as follows:

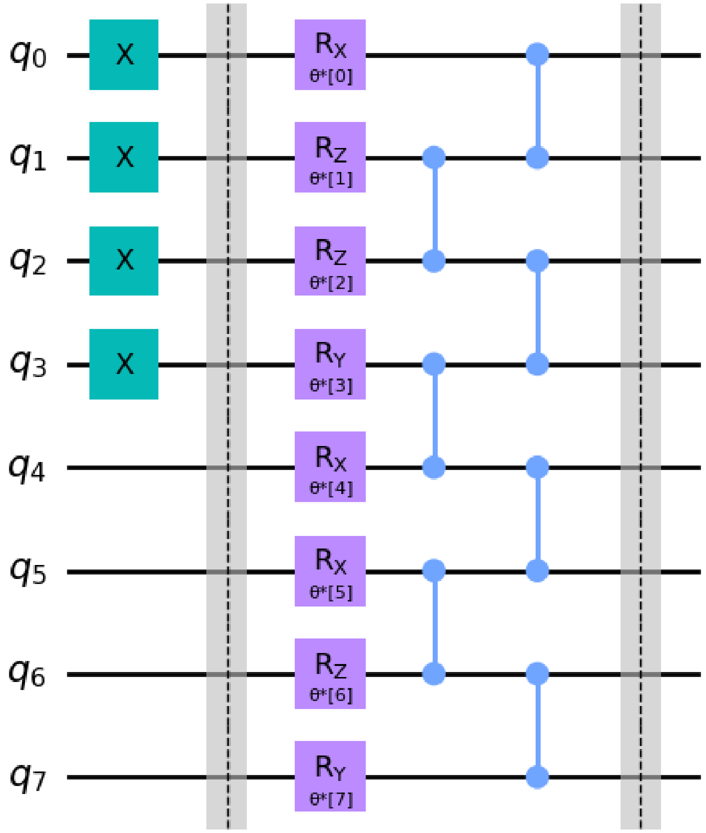
$$\theta_d^* = \arg\min_{\theta_d} \langle H \rangle_{\theta_d} \tag{1}$$

$$= -\frac{\pi}{2} - \arctan\left(\frac{2\langle H \rangle_{\theta_d=0} - \langle H \rangle_{\theta_d=\pi/2} - \langle H \rangle_{\theta_d=-\pi/2}}{\langle H \rangle_{\theta_d=\pi/2} - \langle H \rangle_{\theta_d=-\pi/2}}\right)$$

Focus on each rotation gate, Using Eq.(1), the rotation direction and parameters that minimize the expectation value are determined one by one.



initial



final

The optimization process involves randomly selecting from a list of rotation gates without duplication. Once all rotation gates have been optimized, we consider this as one epoch. This process is then repeated for a given execution time, in this case, 1000 seconds.

Input: Hermitian measurement operator M encoding the objective function, parameterized quantum circuit U, stopping criterion

Initialize $\theta_d \in (-\pi, \pi]$ and $H_d \in \{X, Y, Z\}$ for $d = 1, \ldots, D$ heuristically or at random
repeat
    for $d = 1, \ldots, D$ **do**
        Fix all angles and generators except for the d-th gate
        for $P \in \{X, Y, Z\}$ **do**
            Compute $\theta_d^*(P) = \arg\min_{\theta_d} \langle M \rangle_{\theta_d, P}$ using Eq. (1) with $\phi \leftarrow 0$
            Extrapolate $\langle M \rangle_{\theta_d^*(P), P}$ using the expressions in Appendix A
        $H_d \leftarrow \arg\min_P \langle M \rangle_{\theta_d^*(P), P}$
        $\theta_d \leftarrow \theta_d^*(H_d)$
until stopping criterion is met

algorithm (from the original paper)

Summary

Summary and outlook

1. By fixing the depth of the circuit and dynamically optimizing the circuit, a better ansatz was found with relatively fewer gates.
2. By adopting a method of optimizing one parameter of the ansatz at a time, it provides an approach to analytically find the optimal parameters without using gradient methods. However, it is not necessarily guaranteed to be a global minimum.