Variational Quantum Algorithms in the era of NISQ devices

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Variational Quantum Algorithms (VQA) have become a de-facto model of quantum computation for today's Noisy Intermediate Scale Quantum (NISQ) devices. In this approach a short depth parameterized quantum circuit is tuned using a classical co-processor, in an attempt to minimize a given cost function, encoded as a problem Hamiltonian. While these variational algorithm can alleviate certain limitations of NISQ devises, they are still prone to stochastic noise and gate errors.

In the present work we propose hardware inspired strategies and modifications to the existing variational algorithms, thus ensuring efficient implementation on NISQ devices. First, we propose [1] a modification of the so called Quantum Approximate Optimization Algorithm (QAOA)—a type of VQA designed to solve combinatorial problems—tailored to ion based quantum computers. In our implementation we employ native multiqubit interaction in order to minimize certain problem Hamiltonians, not native to the hardware considered. We simplify algorithm execution by avoiding the gate based approach, and demonstrate performance improvement in terms of lower resources (circuit depth) required to minimize the instances. Second, motivated by inhomogeneities in the errors of entangling gates between different pairs of qubits in NISQ devices, we propose a hardware inspired Zero Noise Extrapolation (ZNE) technique [2]. By considering different abstract-to-physical qubit mappings, this approach allows to approximate noiseless expectation values, using energies measured from noisy circuits. We demonstrate that the ZNE recovered energy can be orders of magnitude closer to the noiseless expectation value, than energies measured from any of the noisy circuits.

Traditional QAOA ansatz. Traditional QAOA makes use of an ansatz state

$$|\Psi_p(\boldsymbol{\beta},\boldsymbol{\gamma})\rangle = \left(\prod_{k=1}^p e^{-i\beta_k H_x} e^{-i\gamma_k H_P}\right)|+\rangle^{\otimes n},\tag{1}$$

where $H_x = \sum_{k=1}^n X_k$. The ground state of H_P is then prepared by tuning 2p parameters β, γ variationally following the minimization $\min_{\beta,\gamma} \langle \Psi_p(\beta,\gamma | H_P | \Psi_p(\beta,\gamma) \rangle$. An evident problem of traditional gate based implementation of (1) is that propagator $e^{-i\gamma_k H_P}$, which typically has no efficient implementation, has to be decomposed into a sequence of single and two qubit gates. This, together with potentially large depth of the circuit p, required to minimize H_P , can translate into large gate counts, which can fall out of the capabilities of NISQ devices.

Ion native QAOA ansatz. To circumvent the realization of propagator $e^{-i\gamma_k H_P}$ in (1), we replace it with a propagator of the tunable Hamiltonian

$$H_I = \frac{1}{2} \sum_{j \neq k} J_{jk} X_j X_k, \quad J_{jk} \approx \frac{J_{\max} A_j A_k}{|j - k|^{\alpha}}, \tag{2}$$

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which can natively be realized in an ion based quantum computer. Here j and k indicate positions of ions in a chain and A_j are proportional to Rabi frequencies of oscillations induced for jth ion. Thus, we develop an ansatz

$$|\Psi_p(\boldsymbol{\beta},\boldsymbol{\gamma}\rangle) = \prod_{k=1}^p \exp(-i\beta_k \mathcal{H}_x) \mathbf{H}_+ \Big(\exp(-i\gamma_k \mathcal{H}_I)\Big) \mathbf{H}_+^{\dagger} |+\rangle^{\otimes n}, \qquad (3)$$

where $H_+ = (|+\rangle \langle 0| + |-\rangle \langle 1|)^{\otimes n}$, and use it to minimize a problem H_P . We benchmark this algorithm by minimizing instances of n = 6 qubit Sherrington-Kirkpatrick (SK) Hamiltonian

$$H_P = \frac{1}{2} \sum_{j \neq k} K_{jk} Z_j Z_k, \quad K_{jk} \in \{1, -1\}$$
(4)

with respect to the ansatz (3). We exhaustively solve all SK instances and study the fraction of instances that got solved at each respective depth for various configurations of A_j . The results are demonstrated in figure 1. Here the orange curve shows the results for the symmetric configuration



FIG. 1. Fraction of n = 6 qubit SK instances that could be minimized by the proposed QAOA ansatz.

 $A_j = 1$ in (2) for all ions. The fraction of instances solved saturates due to symmetry protection, induced by symmetric configuration. The blue curve shows a typical result for a specific fixed nonsymmetric configuration. It is seen that the fraction of instances solved slowly increases and reaches 100% at depth p = 20. Moreover, if we do not keep the same values of A_j for all the instances, but take a best possible configuration (out of 50 random ones) for each instance, already by depth p = 6 all the instances can get solved (green curve). This result even exceeds the performance of standard QAOA, which requires depth up to p = 10 to solve all the instances (red curve).

Zero noise extrapolation. In alternative scenarios, where the gate based approach is unavoidable, certain error mitigating techniques become necessary. Here we propose a hardware inspired ZNE technique, which allows to reconstruct noiseless VQE energy from noisy expectation values.

To simulate a noisy circuit, we assume that every two-qubit gate is followed by a noisy channel of strength q_{ij} , which transforms quantum state as $\rho \to (1 - q_{ij})\rho + q_{ij}\mathcal{E}(\rho)$. Here noise strength q_{ij} depends on the pair of physical qubits (i, j), to which the gate is applied. In that case the energy of the state, prepared by noisy circuit can be written as

$$E = E_{noiseless} + \sum_{gates} q_{ij} E_{ij} + O(q^2) = E_{noiseless} + \langle E \rangle \sum_{gates} q_{ij} + \sum_{gates} q_{ij} (E_{ij} - \langle E \rangle) + O(q^2), \quad (5)$$

where energies E_{ij} are expectations of the problem Hamiltonian in the state, where only one gate gets perturbed. Importantly, in practical realities the errors q_{ij} depend on the pair of physical qubits the gate is applied to. Therefore, the sum over gates $\sum_{gates} q_{ij}$ depends on the abstract to physical qubit mapping. Thus, by changing this mapping, one can control this error sum of the circuit, allowing to perform ZNE. To test this proposal in our work we perform VQE for different types of Hamiltonians, introduce noise to the gates, calculate energy for different qubit permutations and perform linear extrapolation of data. The results are summarized in figure 2. It can be seen that the proposed ZNE protocol indeed allows to recover noiseless VQE energy with a good precision, surpassing energies even of the least noisy circuits. The similar results were obtained for various noise channels \mathcal{E} , error distributions $\{q_{ij}\}$ and problem sizes, demonstrating potential of the proposed technique.



FIG. 2. Zero noise extrapolation performed over all permutations for n = 6 qubit transverse field Ising Hamiltonian (a) and water molecule Hamiltonian (b). Blue dots represent energy E as per (5) for different qubit permutations and the red line is a linear fit taken over energies corresponding to all possible permutations. The blue horizontal lines show the noiseless VQE energy.

Conclusion. Variational quantum algorithms, while being promising for NISQ devises, still suffer from hardware imperfections. Nevertheless, in certain algorithms the effect of noise can be reduced by employing the system's native Hamiltonian and bypassing the gate model completely. Moreover, even when gate errors are unavoidable, their inhomogeneity can be used to foster the algorithm performance by performing Zero Noise Extrapolation over different abstract to physical qubit mappings. Both proposed strategies can assist quantum algorithms, promising performance improvement even in the era of NISQ devices.

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