Noise Analysis of Quantum Approximate Optimization Algorithm on Weighted MAX-CUT

by

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Abstract—In this paper, we describe the simulation of Ising minimization on a classical machine by executing variational quantum algorithms on our density-matrix simulator. We outline the Ising formulation of the Graph Partitioning problem and the Hamiltonian Cycle problem, and solve the Max-Cut variant of graph partitioning for a weighted square graph $S_{Q_2}$ using the Quantum Approximate Optimization Algorithm. We finally study the effect of errors present in Noisy Intermediate-Scale Quantum processors on the obtained solutions. This paper illustrates the approach to approximately solving hard combinatorial optimization problems using a hybrid quantum-classical scheme and describes the issues in hardware implementation of such schemes. The simulations of NISQ noise models will be useful in understanding the performance and capabilities of such approaches.

Index Terms—Non-deterministic Polynomial, Ising Model, Combinatorial Optimization, Variational Quantum Algorithms

I. INTRODUCTION

A quantum computational device uses quantum mechanical resources such as superposition, entanglement and tunneling to gain a possible computational advantage over classical processors. The capabilities [1] and limitations [2] of such quantum computational devices are understood. However, fault-tolerant universal quantum computers appear to be more than a decade away. The consistent progress in the field of quantum technologies has lead to the development of Noisy Intermediate-Scale Quantum (NISQ) devices [3]. The computational capabilities of NISQ devices are considerably restricted due to limited connectivity, short coherence time, poor qubit quality and minimal error-correction.

However, there is a growing interest to find the classes of tasks suitable for these current generation devices. A particular class of useful algorithms that can be run with limited circuit depths are variational algorithms which use the following hybrid approach [4]: prepare a highly entangled quantum state using limited depth quantum processor, then apply a classical optimization routine on the gate parameters to converge to that quantum state for which objective function is minimized.

This hybrid classical-quantum approach can be used to solve various kinds of optimization problems. These range from minimizing the energy expectation value for a non-trivial molecular Hamiltonian [5], [6], to solving combinatorial optimization problems mapped to the minimization of an Ising Hamiltonian [7]–[9]. The computational resources required for solving such problems can scale exponentially with respect to the problem size and can even make the problem intractable. The Ising problem, in general, is NP-Hard [10], but various approaches to approximately solve these optimization problems form an important field of research in classical and quantum computation.

II. QUANTUM COMPUTATION

A. Quantum Information

The fundamental unit of information in classical computing is a bit which exists in the equiprobable states: 0 or 1. A bit is deterministic in the sense that a classical register can be read exactly. Analogous to the bit, a qubit is considered to be the fundamental unit of quantum information [11].

A qubit is a normalized vector $|\psi\rangle$ in a two-dimensional Hilbert space $\mathbb{C}^2$ with an orthonormal basis $B = \{|0\rangle, |1\rangle\}$

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle, \quad |\alpha|^2 + |\beta|^2 = 1, \quad \alpha, \beta \in \mathbb{C} \quad (1)$$

Geometrically, a qubit can be represented by a unit-vector in a Bloch sphere with $\hat{\psi} = (\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta)$, where $\theta, \varphi$ are elevation and azimuth angles respectively.

$$|\psi\rangle = \cos \frac{\theta}{2}|0\rangle + e^{i\varphi} \sin \frac{\theta}{2}|1\rangle \quad (2)$$

Figure 1: Representation of Bloch Sphere

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From a quantum mechanical perspective, a qubit describes the state $|\psi\rangle$ of a two-level quantum system, which is a superposition of $|0\rangle$ and $|1\rangle$ in the absence of decoherence and measurement. On measurement, the state $|\psi\rangle$ evolves to either $|0\rangle$ with probability $|\alpha|^2$ or $|1\rangle$ with probability $|\beta|^2$. Hence, a qubit effectively contains one bit of classical information.

B. Density Matrix Representation

The density matrix $\rho$ represents a quantum state as the statistical ensemble of pure states $\{|\psi_1\rangle, |\psi_2\rangle, \ldots |\psi_n\rangle\}$ mapped to a probability distribution $\{p_1, p_2, \ldots, p_n\}$:

$$\rho = \sum_{i}^n p_i |\psi_i\rangle \langle \psi_i|$$

(3)

The density matrix can be represented in the Pauli basis as:

$$\rho = \frac{I + \vec{r} \cdot \vec{\sigma}}{2}$$

(4)

where $\vec{r}$ is known as the Bloch vector, $||\vec{r}|| \leq 1$, and $\sigma$ is the Pauli vector. The equality $||\vec{r}|| = 1$ holds only for pure states.

C. Evolution

Pure states evolve by unitary transformations $|\psi\rangle \rightarrow U|\psi\rangle$. This evolution is deterministic, continuous and reversible. The unitary evolution of density matrix is described by:

$$\rho = \sum_{i} p_i |\psi_i\rangle \langle \psi_i| \rightarrow \sum_{i} p_i U|\psi_i\rangle \langle \psi_i| U^\dagger = U \rho U^\dagger$$

(5)

The unitary evolution of a quantum state can be represented by the rotation of corresponding Bloch vector. A non-unitary evolution does not preserve the norm of Bloch vector.

D. Measurement

Measurement operator $M_m$ is a projection operator which projects the quantum state to an eigenstate of $M_m$. The post-measurement state is described as:

$$\rho_m = \frac{M_m \rho M_m^\dagger}{\text{tr}(M_m \rho M_m)}$$

(6)

where $m$ refers to the measurement outcome that occurs with the probability $p(m) = \text{tr}(M_m \rho)$, and $\sum_m M_m^\dagger M_m = I$.

III. REDUCABILITY AMONG COMBINATORIAL PROBLEMS

Richard Karp in his 1971 paper [12] showed a polynomial-time reduction from the SAT problem to various graph-theoretic and combinatorial optimization problems. Using the Cook-Levin theorem, it was consequentially proven that these problems were NP-Complete and hence computationally equivalent. These problems include clique, vertex cover, knapsack, graph partitioning, max-cut, and others [8].

These problems have important practical applications in sequencing, packing, covering, assignment and routing tasks. Since these problems are computationally hard to solve exactly, a variety of techniques are used to obtain reasonably satisfactory approximate solutions. A Quantum Approximate Optimization Algorithm proposed by Farhi [13] is an approach to find approximate solutions to such combinatorial optimization problems.

IV. THE ISING MODEL

A. Quantum Adiabatic Optimization

Quantum adiabatic optimization is a meta-heuristic for solving hard combinatorial optimization problems. It is executed by the adiabatic evolution of an N-spin system under a time-dependent Hamiltonian $\hat{H}(t)$ such that

$$\hat{H}(t) = \left(1 - \frac{t}{\tau}\right) \hat{H}_i + \left(\frac{t}{\tau}\right) \hat{H}_p$$

(7)

where $\hat{H}_i$ is the initial Hamiltonian prepared trivially in its ground state, and $\hat{H}_p$ is the target Hamiltonian which encodes the solution to a combinatorial optimization problem. It is necessary that $[\hat{H}_i, \hat{H}_p] \neq 0$. By the adiabatic theorem, the ground state of system is retained if the evolution is sufficiently slow. Hence, the system finally evolves to the ground state of the target Hamiltonian.

B. The Ising Model

The classical version of Ising model can be expressed as a quadratic function of N spins $\sigma \in \{+1, -1\}$

$$H(\sigma) = -\sum_{i<j} J_{ij} \sigma_i \sigma_j - \sum_{i=1}^{N} h_i \sigma_i$$

(8)

where $\sigma_i \in \{+1, -1\}, J_{ij} \in \mathbb{R}, h_i \in \mathbb{R}$ and $(1 \leq i, j \leq N)$. The quantum mechanical description of $H(\sigma)$ is [8]:

$$\hat{H}_i = -h_0 \sum_{i=1}^{N} \sigma_i^z$$

(9)

$$\hat{H}_p = \hat{H}_p (\sigma_1^z, \ldots, \sigma_N^z)$$

(10)

where $\sigma_i^z$ acts on the $i^{th}$ qubit in $\mathbb{C} = \{+1, -1\} \otimes^N$. $\sigma_i^z$ is the Pauli-Z matrix and $\mathbb{C}$ is the Hilbert space of N qubits.

V. ISING FORMULATION OF NP PROBLEMS

The Ising framework can be used to model many different physical systems, and particularly, the systems which describe a set of individual elements (s_i) interacting via pairwise interactions (s_i, s_j). The problem of finding the global ground state of the Ising model can be shown to be NP-Hard by constructing Ising equivalents of the logical operators $\land, \lor, \neg$ of SAT. It follows that many hard combinatorial optimization problems can be mapped to the problem of minimization of an Ising Hamiltonian. The Ising formulation of various NP-Complete problems is outlined by Lucas [8].

A. Graph Partitioning

Consider a graph $G = (V, E)$ such that $V$ is the set of vertices with $|V| = N$, and $E$ is the set of edges. For an integer $k > 1$ and $v \geq 1$, a $(k,v)$ balanced graph partitioning problem aims at partitioning the graph $G$ into $k$ components, each of which has a maximum size of $v(N/k)$, and with the constraint that the capacity of edges between these partitions will be minimum [14]. For $v = 1$, the vertex set $V$ is partitioned into $k$ disjoint subsets $V_1, V_2, \ldots, V_k$ which satisfy the above
constraint. For the case \( k = 2 \) and \( v = 1 \), which is also called the Minimum Bisection problem, the problem is NP-Complete.

The Ising formulation of Minimum Bisection problem is:
To each \( v \in V \), assign an Ising spin \( s_v \in \{+1, -1\} \), such that
\[ s_v = +1 \iff v \in S^+ \quad \text{and} \quad s_v = -1 \iff v \in S^- , \]
where the sets \( S^+ \) and \( S^- \) denote the two partitions of the vertex set.
The energy functional [8] for this problem is:
\[
H = A \left( \sum_{n=1}^{N} s_i \right)^2 + B \sum_{(u,v) \in E} \left( 1 - s_u s_v \right) / 2 \tag{11}
\]
The first term provides a penalty if the two subsets are not cardinally equivalent. The second term provides a penalty for each edge which directly connects vertices from the two subsets. For \( B > 0 \), the objective is to minimize the number of edges between the two partitions. A necessary restriction, where \( \Delta \) denotes the maximal degree of \( G \), is:
\[
\frac{A}{B} \geq \min \left( 2 \Delta, N \right) / 8 \tag{12}
\]
An important variant of the Graph Partitioning problem is Maximum-Cut, which we have discussed in section VIII.

B. Hamiltonian Cycle and Traveling Salesman Problem

Consider a graph \( G = (V, E) \) such that \( V \) is the set of vertices with \( |V| = N \), and \( E \) is the set of edges. The problem is to find a cyclic ordering of \( V \) such that each vertex \( v \in V \) is visited exactly once. This problem is NP-Complete.

Assuming a directed graph and labelling the vertices in \( V \) as \( v_1, \ldots, v_N \), the solution requires \( N^2 \) bits denoted by \( x_{v,i} \), where \( i \) represents the order of vertex \( v \) in an expected cycle. The energy functional [8] for this problem is:
\[
H_S = H_A + H_B + H_C \tag{13}
\]
\[
H_A = A \sum_{i=1}^{N} \left( 1 - \sum_{j=1}^{N} x_{v,j} \right)^2 \tag{14}
\]
\[
H_B = A \sum_{j=1}^{N} \left( 1 - \sum_{v=1}^{N} x_{v,j} \right)^2 \tag{15}
\]
\[
H_C = A \sum_{(u,v) \in E} \sum_{j=1}^{N} x_{u,j} \cdot x_{v,j+1} \tag{16}
\]
\( A > 0 \) is a constant. The terms \( H_A \) and \( H_B \) enforce that a vertex is visited exactly once, and for each \( j \in \{1 \ldots N\} \), the \( j \)th vertex exists in the cycle. The term \( H_C \) imposes a penalty if \((uv) \notin E \) given that \( x_{u,j} \land x_{v,j+1} = 1 \), thus enforcing that adjacent vertices in the cycle are connected in the graph. The ground state \( H_S = 0 \) only if a Hamiltonian cycle exists in \( G \).

In the Traveling Salesman Problem for each edge \( uv \) in the graph \( G \), we assign a weight \( W_{uv} \geq 0 \). Then, we aim to find a Hamiltonian cycle which minimizes the sum of these weights in the cycle. The energy functional for this problem is:
\[
H = H_S + H_D \tag{17}
\]
\[
H_D = B \sum_{(uv) \in E} W_{uv} \sum_{j=1}^{N} x_{u,j} \cdot x_{v,j+1} \tag{18}
\]

VI. VARIATIONAL QUANTUM ALGORITHMS

Many quantum algorithms require computational resources beyond the physical capabilities of currently available quantum processors. Near-term quantum processors are capable of preparing quantum states using shallow quantum circuits. If the fidelity of quantum logic gates is sufficiently high, then the quantum circuit can be executed without the requirement of quantum error correction.

A new approach that greatly reduces the computational requirements is to divide the problem of interest into classically tractable (classical optimization) and intractable (quantum state preparation) parts. Using a set of variational parameters, a quantum processor prepares a highly entangled quantum state. A classical processor then uses the quantum measurement outputs to optimize the variational parameters, based on some well-defined criteria. The variational parameters are then fed to the quantum processor. This iterative process eventually converges such that energy of quantum state is minimized.

![Figure 2: A schematic of the hybrid quantum-classical algorithm.](image)

The representative algorithms for variational approaches are the Variational Quantum Eigensolver (VQE) [13] and the Quantum Approximate Optimization Algorithm (QAOA) [13]. The VQE is an approach to finding the eigenvalues of operators, while QAOA solves constraint satisfaction problems of binary variables, which is our primary interest.

In QAOA, the adiabatic pathway is discretized in some \( p \) steps, where \( p \) represents precision. This effectively discretizes the time-dependent Hamiltonian \( H(t) \).
\[
H(t) = (1 - t)H_0 + tH_1 \tag{19}
\]
This is done by trotterizing the unitary into $p$ time steps using two parameters $\{\beta, \gamma\}$, over which optimization would be performed based on the energy measurement. Hence, the final split unitary could be realized as

$$U = U(H_0, \beta_0)U(H_1, \gamma_0) \ldots U(H_0, \beta_p)U(H_1, \gamma_p).$$

After sufficient optimization of parameters, this discretized evolution will approximate the adiabatic pathway for going from the ground state of the mixing Hamiltonian $H_0$ to that of the cost Hamiltonian $H_1$. As in the case of quantum annealing, $H_0 = -\sum_i \sigma_i^z$ is the simplest mixing Hamiltonian.

**VII. DENSITY MATRIX SIMULATOR**

We have developed a software library [18] that simulates noisy quantum logic circuits by representing quantum states by their density matrices. We have simulated the Ising formulation of above problems by executing variational quantum algorithms on the density matrix simulator. The simulator is implemented as an extended back-end in the Qiskit platform.

There exist various gate-level quantum software [19], [21]. The density matrix simulator gives us the flexibility to introduce errors which can be used to model noise in the system. It can incorporate possible errors in initialization, logic gates, memory states and measurement operations.

**VIII. SIMULATION ON DM SIMULATOR**

We have executed the Quantum Approximate Optimization Algorithm to solve the weighted MAX-CUT problem on a square graph $S_{q_2}$, which requires four qubits to represent its possible sixteen partitions. The mixing Hamiltonian $H_0$ and cost Hamiltonian $H_1$ for this problem are:

$$H_0 = -\sum_{i=0}^3 \sigma_i^z$$

$$H_1 = w_{01}(\sigma_1^2 \otimes \sigma_3^0) + w_{12}(\sigma_2^2 \otimes \sigma_3^0) + w_{23}(\sigma_3^2 \otimes \sigma_3^0) + w_{30}(\sigma_3^2 \otimes \sigma_3^0)$$

For $p = 2$ and the variational parameters $\{\beta, \gamma\}$, the total unitary $U$ is approximated by two unitary operators as:

$$U = U(H_0, \beta_0) \cdot U(H_1, \gamma_0) \cdot U(H_0, \beta_1) \cdot U(H_1, \gamma_1)$$

where each unitary $U(H_p)$ is approximated by a third order Trotter-Suzuki decomposition with the number of steps $= 1$.

We first prepare a state $|++\rangle$ and then evolve as:

$$|\beta, \gamma\rangle = e^{-iH_0\beta_1}e^{-iH_1\gamma_1}e^{-iH_0\beta_0}e^{-iH_1\gamma_0}|++\rangle$$

The optimal values of $\{\beta, \gamma\}$ is obtained by an iterative classical minimization of the objective function $C$ defined as:

$$C = \langle \beta, \gamma | H | \beta, \gamma\rangle$$

We have plotted the distribution of probabilities corresponding to cuts on a square graph $S_{q_2}$, for the initial and final values of variational parameters. The bit string in each state depicts the node partitioning done by a cut $C$. For example the cut “0001” denotes the vertex set $\{v_0, v_1, v_2\}$, while the cut “1100” denotes the vertex set $\{v_0, v_1, v_2, v_3\}$. As expected, the optimal cut $C_{opt}$ must partition the nodes as denoted by bit string “0011”, or equivalently, “1010”, such
that the cut size is maximum and is equal to 10. We see that probability corresponding to bit string “0101” is maximum in the final state of classical optimization.

IX. Noise Characterization

Next, we try to characterize the effects of noise on the performance of QAOA by introducing the following errors in our quantum routine: thermal and depolarization error, rotation gates error, decoherence error and amplitude decay, using our quantum simulator [18]. Since, these noise models are a characteristic property of current generation NISQ systems, we proceed to see how success of QAOA would be affected on these current generation systems.

In order to study the fidelity (or the overlap) of quantum states, $\rho$ and $\rho_0$, prepared by the quantum routine in the presence and absence of errors, we use the following metric:

$$Tr(\rho_0 \rho)$$

(26)

Clearly, the fidelity of states (Fig. 6) prepared by the quantum routine and consequently the success probability of QAOA is affected by memory errors: thermalization, decoherence and amplitude decay. The off-diagonal coefficients are contracted by decoherence factor $f \in [0, 1]$ and by $\sqrt{g}$, where $g \in [0, 1]$ is the decay factor. The diagonal coefficients decay with rate $g$ towards the thermal state specified by thermal factor $p$.

In our implementation the circuit used for discretizing the evolution along the adiabatic pathway had 2479 gates and depth of 1576. With over 800 entangling gates present in the circuit we see that decoherence and thermalization have a far more significant effect on the success probability, in comparison to the amplitude decay. This is certainly due its lower contribution in the variation of the off-diagonal elements of the quantum state prepared by our QAOA routine.

We have also modeled the rotation gate imprecision in our simulation by introducing error parameters $r$ and $\overline{\alpha}$:

$$\cos \theta \rightarrow r \cos(\theta + \overline{\alpha}), \quad \sin \theta \rightarrow r \sin(\theta + \overline{\alpha})$$

(27)

where $\overline{\alpha}$ is mean rotation error and $r$ is radius obtained after averaging over fluctuations observed in $\alpha$. Error in $R_z(\theta)$ affects state fidelity relatively more than error in $R_y(\theta)$ because of Euler decomposition, $R_z(\phi)R_y(\theta)R_z(\lambda)$, implemented in our density matrix simulator for the single unitary gates, $U_3(\theta, \phi, \lambda)$, [18].

Finally, we have modeled the errors encountered during the measurement of expectation value for Hamiltonian $\hat{H}$, by
considering the effect of depolarization during single qubit measurement operations. In the case of binary measurement, this kind of error is equivalent to the bit flip error. We have used a depolarization factor, $d \in [0, 1]$ to characterize the extent of its effect during measurement. We see an exponential decay in the value of $\langle H \rangle$ with respect to parameter update iteration.

This information about the effect of errors on fidelity of state prepared by a quantum routine, and the minimized expectation value is essential in the design exploration of near-term quantum devices dedicated to run approximate optimization algorithms like QAOA and VQE. In a typical hardware development life-cycle, the error that affects the success probability the most, should be mitigated first. It is necessary for the scalability of the hardware.

X. CONCLUSION

Near-term quantum processors provide methods to approximately solve optimization problems through a hybrid quantum-classical approach, but these methods are highly dependent on the robustness and capabilities of concerned quantum computational device. The quantum hardware determines the size of the problem by restricting the number of qubits and also imposes a restriction on quantum state preparation depending on the possible quantum logic gates.

Since these devices require extreme execution environments and are prone to noise, it becomes crucial to characterize the behaviour of quantum hardware on the particular problem, in the presence of noise. As the variational algorithms require precise estimates of quantum state measurement, it is necessary to develop techniques which minimize the effect of noise.

Simulation is an effective tool to characterize such systems and model the behaviour of hardware in the presence of noise. Our simulation of QAOA provides insightful data about the effect of amplitude decay, decoherence, thermalization, and logic gate imprecision, which will help in designing specific quantum hardware for variational quantum algorithms that will allow us to approximately solve NP problems more efficiently. In future, we aim to demonstrate the simultaneous effect of different kinds of errors on the results.

CODE AVAILABILITY

The code for the density matrix simulator is open-sourced [22]. The code implemented to run these simulations and related supplementary data could be made available to any reader upon reasonable request.

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