

Comparing Constrained and Unconstrained Quantum Approximate Optimization Algorithms (April 2020)

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ABSTRACT We study the differences between constrained and unconstrained combinatorial optimization problems for Quantum Approximate Optimization Algorithms on digital quantum computers. Specifically we analyze the probability distribution of "feasible" states for both types of combinatorial optimization problems and study the dependence on circuit depth and the choice of initial states.

INDEX TERMS Quantum Computing, Quantum Algorithms, Combinatorial Optimization, QAOA.

I. INTRODUCTION

Combinatorial optimization has many applications in engineering and science. Combinatorial optimization problems can be mathematically expressed as follows. Let $C(\mathbf{x}) = \sum_{i=1}^N C_i(\mathbf{x})$ be a function where $\mathbf{x} = [x_1, x_2, \dots, x_N]$ and $C_i(\mathbf{x})$ is the i -th binary clause. The goal of combinatorial optimization is to find a binary vector \mathbf{x}^* that maximizes the number of satisfied clauses $C_i(\mathbf{x})$. Many of these problems are NP-Hard and only approximate solutions are available. Quantum Approximate Optimization Algorithms (QAOA) [1] use quantum mechanics to find these approximate solutions and the hope is that they might be able to do a better job than their classical counterparts. Unconstrained optimization problems are the ones where all the strings \mathbf{x} encode valid or feasible solutions. Examples of these are MaxCut, Max/Min 1-Sat and E3-Lin2 [2]. Constrained optimization problems are those in which not all $\mathbf{x} \in \{0, 1\}^N$ are valid solutions of the problem. The feasible solutions must satisfy hard constraints at all times and the extremization is performed only over the space of feasible solutions. Examples of these are Maximum Independent Set, Maximum Set Packing and MinSet Cover. Our aim in this work will be to study both these types of problems using QAOA and understand their differences.

II. QAOA

To solve a combinatorial optimization problem using QAOA it must be converted into the problem of characterizing a Hamiltonian. The classical objective function C can be con-

verted into a problem Hamiltonian H_C by converting each binary variable $x_i \in \{0, 1\}$ into a spin variable $s_i \in \{-1, +1\}$ ($x_i = \frac{1}{2}(1 + s_i)$) and mapping the spin variables s_i onto the spectrum of the quantum spin operator σ_i^z .

In QAOA, the quantum processor is initialized in some initial state $|s\rangle$ and then the problem Hamiltonian H_C and a mixing Hamiltonian

$$H_M = \sum_{j=1}^N \sigma_j^x \quad (1)$$

are applied alternatively with controlled durations to generate a variational wave function

$$|\psi_p(\boldsymbol{\gamma}, \boldsymbol{\beta})\rangle = e^{-i\beta_p H_M} e^{-i\gamma_p H_C} \dots e^{-i\beta_1 H_M} e^{-i\gamma_1 H_C} |+\rangle^{\otimes N} \quad (2)$$

where $\boldsymbol{\gamma}$ and $\boldsymbol{\beta}$ are $2p$ parameters. The expectation value of H_C in this variational state

$$F_p(\boldsymbol{\gamma}, \boldsymbol{\beta}) = \langle \psi_p(\boldsymbol{\gamma}, \boldsymbol{\beta}) | H_C | \psi_p(\boldsymbol{\gamma}, \boldsymbol{\beta}) \rangle \quad (3)$$

is passed to a classical optimizer to find the optimal parameters that extremize $F_p(\boldsymbol{\gamma}, \boldsymbol{\beta}) = \max_{\boldsymbol{\gamma}, \boldsymbol{\beta}} F_p(\boldsymbol{\gamma}, \boldsymbol{\beta})$. Since the eigenstates of H_C are computational basis states, this maximization is achieved for the states exactly corresponding to the solutions of the original classical problem.

Constrained optimization problems introduce two challenges. First, the initial state must be feasible and moreover must be trivial to implement such that it can be created by a constant depth quantum circuit from the $|0\dots 0\rangle_N$ state.

Second, the mixing unitary $e^{-i\beta_p H_M}$ is required to take feasible states to feasible states for all values of parameters and must provide transitions between all feasible solutions.

III. SIMULATIONS

To understand the differences between the constrained and unconstrained optimization problems we evaluated multiple QAOA problems on the Rigetti Forest and IBM Q simulators. Here we show our results for the MaxCut and Max-independent Set problems on the instance of the graph $K_{2,3}$.

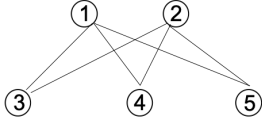


FIGURE 1: $K_{2,3}$ graph.

a: Maxcut

Consider a graph $G = (V, E)$ where $V = \{1, 2, \dots, N\}$ denotes the set of vertices and $E = \{(\langle i, j \rangle)\}$ is the set of edges connecting the vertices i and j . The goal of MaxCut is to divide the graph into two parts so as to maximize the number of edges spanning the two parts.

- Initial State: $|+\rangle^{\otimes N}$

- Mixing Hamiltonian: $H_M = \sum_{j=1}^N \sigma_j^x$

- Cost Hamiltonian : $H_C = \sum_{\langle i,j \rangle} \frac{1}{2} (1 - \sigma_i^z \sigma_j^z)$

b: Max-Independent Set

Consider a graph $G = (V, E)$, with V the set of nodes of the graph and E the set of edges. Let $\mathcal{N}(i) = \{j \in V : (i, j) \in E\}$ be the neighbors of the i^{th} node in V . Positive weights w_i are associated with each node i . A subset V' of V is represented by a vector $x = (x_i) \in \{0, 1\}^{|V|}$, where $x_i = 1$ means i is in the subset and $x_i = 0$ means i is not in the subset. A subset x is called an independent set if no two nodes in the subset are connected by an edge: $(x_i, x_j) \neq (1, 1)$ for all $(i, j) \in E$. The max independent set is the independent set with the largest number of nodes. We are interested in finding a maximum independent set (MIS) x^* .

- Initial State: The initial state can be the trivial state $|0\rangle^{\otimes N}$ or any state representing the independent set.

- Mixing Hamiltonian: $H_M = \sum_u M_u$ where

$$M_u = \frac{1}{2^l} X_u \prod_{j=1}^l (I + Z_{v_j}). \quad (4)$$

and l are the neighbours of the node u that are not in V' . The above implementation is the simultaneous Hamiltonian based implementation and can be computationally expensive due to non-commuting property of

the terms in the Hamiltonian. We can also implement the above mixing unitary $U_M^H = e^{-i\beta_p H_M}$ sequentially via designed quantum circuits that act on the nodes of the graph sequentially [2], [3].

$$U_M(\beta) = \prod_u U_{M,u}(\beta) \quad (5)$$

where $U_{M,u}(\beta)$ is a quantum circuit with $\mathcal{O}(l)$ depth.

- Cost Hamiltonian: $H_C = \frac{1}{2} \sum_{u \in V} (I - Z_u)$

In Fig 2 we observe that the probability distribution for the MaxCut output states is symmetric whereas the probability distribution is asymmetric for the MIS algorithm, due to the asymmetry of the mixer. The plots for the sequential and simultaneous implementations of the mixer agree with each other as well. Additionally, the output has the tendency to stay in the initial state but as we increase p the output result moves closer and closer to the solution state. For $p = 1$ the solution peaks at the $|00011\rangle$ state, as the value of p increases, the solution begin to peak more at the $|11100\rangle$ state. We also observe that the sequential mixer provides more spread-out distribution for $p=6$, as compared to the single peaks provided by the simultaneous mixer.

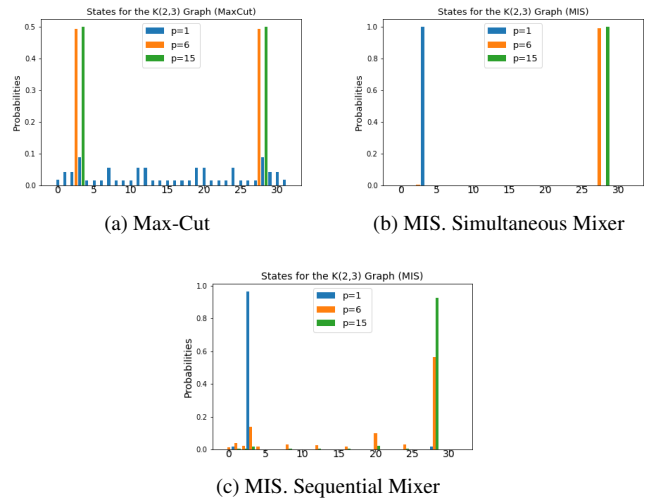


FIGURE 2: Dependence of MIS and MaxCut QAOA on circuit depth. The initial state in the above plots is the $|00000\rangle$ state. The x-axis in the plots lays out the 32 permutations of the possible outcome states ranging from $|00000\rangle$ to $|11111\rangle$.

We also run the MIS QAOA algorithm with different initial states (Fig 3). The dependence of the output clearly depends on which initial states were chosen. The algorithm favors the initial state for low values of p and then slowly moves towards the optimal solution.

IV. CONCLUSION AND FUTURE DIRECTIONS

We have studied the dependence of the algorithm on the circuit depth and initial states, as shown in Figure 3. Our goal is to understand the optimal choice of the number of steps p and the initial states in the algorithm. We are

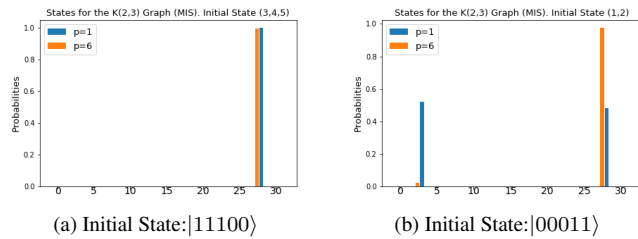


FIGURE 3: Dependence of the MIS QAOA on Initial States

currently investigating other constrained optimization problems such as max-k colorable subgraph, Min graph coloring and travelling salesman problem. Moreover, we also seek to apply the QAOA algorithms to on real world combinatorial optimization problems such as portfolio optimizations [5], computational biology [6] on digital quantum computers and power grid optimization [7].

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