Maximum weighted independent set and quantum alternating operator ansatz

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We study the maximum weighted independent set problem of graph theory using the quantum alternating operator ansatz. We perform simulations on the Rigetti Forrest simulator and analyze the dependence of the algorithm on the depth of the circuit, initial states and the weights of the vertices. We point out that the probability distribution of observation of the feasible states representing maximum independent sets is asymmetric for the Maximum Independent Set problem unlike the MaxCut problem where the probability distribution of feasible states is symmetric. We also give a numerical comparison of the approximation ratios for the algorithm when we choose different initial states in our graph.

INTRODUCTION

There has been a growing interest in the quantum computation community to develop algorithms that can be implemented on the near term quantum machines [1]. Several hybrid classical-quantum algorithms [2–4] have been proposed that can take advantage of the available quantum resources in the presence of noisy gates and small de-coherence times. The Quantum Approximate Optimization Algorithm (QAOA) [2] and the Variational Quantum Eigensolver (VQE) [3] are such classical-quantum algorithms. The QAOA algorithm has been put forward to tackle combinatorial optimization problems and the VQE algorithm has application in quantum chemistry problems where the ground state of a wave function needs to be determined. The variational quantum eigensolver algorithm can also be used as a subroutine in quantum approximate optimization algorithm.

In most of the hybrid algorithms the quantum part of the algorithm involves preparing a quantum circuit and the classical part involves optimization. In the quantum approximate optimization algorithm a quantum state is created by a p-depth circuit specified by 2p variational parameters. The algorithm is shown to be not efficiently simulatable classically even at the lowest p=1 depth [5]. QAOA is thus a good candidate algorithm to study quantum advantage on near term quantum machines. Although one can theoretically prove the success of QAOA in the \( p \to \infty \) limit as it approximates adiabatic quantum annealing [2] in that limit, little is known about its performance when \( 1 < p \ll \infty \).

There has been a significant amount of work on QAOA in the context of the MaxCut problem. However not much work has been done in the application of the algorithms to other combinatorial optimization problems. In this paper we will study the max weighted independent set (MWIS) problem. The MWIS problem is different than the MaxCut problem "an unconstrained optimization problem" because unlike the MaxCut in which all the \( 2^n \) states are feasible, the feasible states in the MWIS problem consist of a subset of the configuration space. For such "constrained optimization" problems a quantum alternating operator ansatz [6, 7] has been proposed. In this paper we will simulate the quantum alternating operator ansatz on the Rigetti Forrest SDK [15].

MAXIMUM WEIGHTED 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 \( \mathbf{x} = (x_i) \in \{0,1\}^{|V|} \), where \( x_i = 1 \) means \( i \) is in the subset and \( x_i = 0 \) means \( i \) is not in the subset. A subset \( \mathbf{x} \) 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 weighted independent set (MWIS) \( \mathbf{x}^* \).

There is no known polynomial time classical algorithm that solves the Max Independent Set unless \( P=NP \) [8]. The best algorithm known for general graphs give approximations within a polynomial factor. MIS can be approximated to \((D_g+2)/3\) [9] on bounded degree graphs with maximum degree \( D_g \geq 3 \) but it still remains APX-complete [10]. The best known classical algorithm for weighted maximum independent set is the greedy local search algorithm [11] and also gives a polynomial factor approximation.

QUANTUM APPROXIMATE OPTIMIZATION ALGORITHM

QAOA algorithm was proposed for unconstrained discrete optimization problems, such as the MaxSat, Max-
the Hamiltonian with an angle $0 \leq \gamma \leq 2\pi$. The ground state of the driver Hamiltonian is flips algorithm uses an alternating quantum circuit of depth $B$ based on Hamiltonians expected cost function, with $2^n$ qubits independently. The unitary operator for the Hamiltonian with an angle $0 \leq \beta \leq \pi$ is defined as:

$$U(B, \beta) = \exp(-i\beta B) = \prod_{j=1}^{n} e^{-i\beta_j X_j}.$$  \hfill (3)

We also define a driver Hamiltonian $B = \sum_{j=1}^{n} X_j$, which flips $k$-qubits independently. The unitary operator for the Hamiltonian with an angle $0 \leq \beta \leq \pi$ is defined as:

$$U(C, \gamma) = \exp(-i\gamma C) = \prod_{i=1}^{n} e^{-\gamma C_i}. \hfill (2)$$

For the unconstrained combinatorial optimization problems the quantum state is typically initialized to the superposition state $|+\rangle^\otimes n$. For the cost Hamiltonian $C$, let $U(C, \gamma)$ denote a unitary operator with an angle $0 \leq \gamma \leq 2\pi$, defined by

$$|\phi\rangle = |\phi\rangle = \sum_{i=1}^{n} C_i(x), \hfill (1)$$

where $x = [x_1, x_2, \ldots, x_n]$ denotes a binary label and $C_i(x)$ is the $i$th binary clause. The goal in optimization problems is to find a binary vector $x^*$ that maximizes the number of satisfied clauses $C_i(x)$.

**QUANTUM ALTERNATE OPERATOR ANSATZ**

A general QAOA circuit is defined by two parameterized families of operators: a family of phase separation operators $U_p(\gamma)$ that depends on the cost function and a family of $U_M(\beta)$ that depends on the domain and its structure. In the earlier implementation of unconstrained QAOA the feasible set of states consisted of all the entire configuration space and therefore the mixing operator in the algorithm was $U_M(\beta) = \exp(-i\beta B)$. The constrained optimization problems however require optimization over feasible solutions which are typically a subset of a configuration space. The feasible solution set is specified by a set of Boolean functions (hard constraints) which are satisfied by the feasible solutions. If the mixing operators preserve feasibility then given a feasible initial state the QAOA algorithm will produce a final state which when measured gives a feasible solution. This is achieved by the quantum alternate operator ansatz. The three main components of the quantum alternate operator ansatz are the initial state, the phase operators, and the mixing operators. 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 $|0\ldots0\rangle_n$ state. The family of mixing unitaries $U_M(\beta)$ are required to take feasible states to feasible states for all values of parameters and must also provide transitions between all feasible solutions. For an objective function $C$ we define $H_C$ to be the Hamiltonian that acts as $C$ on basis states $H_C|x\rangle = C(x)|x\rangle$. The phase separation operators $U_p(\gamma)$ are required to be diagonal in the computational basis and therefore the phase separation unitary is defined as: $U_p(\gamma) = e^{-i\gamma H_C}$ up to trivial global phase terms.

**MWIS AND QAOA**

The qubits represents the nodes in the graph and the configuration space is the $2^n$ states created by the qubits. The domain is the subset of $n$-bit strings corresponding to independent sets of $G$. The three QAOA components for this problem are:

- **Initial State**: The initial state can be the trivial state or any state representing the independent set.
- **Phase separation Hamiltonian**: The objective function $H_C(x) = \sum_{j=1}^{n} x_j$, counts the number of vertices in $V'$, and the Hamiltonian corresponding to the function is

$$H_C = \frac{1}{2} \sum_{w \in V'} w_u (I - Z_u) \hfill (6)$$

- **Mixing Hamiltonian**: When constructing the mixing Hamiltonian there are two points to note: 1)
Given an independent set $V'$, adding a vertex $w \not\in V'$ to $V'$ preserves feasibility only if none of the neighbors of $w'$ are already in $V'$ \footnote{2}) We can always remove any vertex $w \in V'$ and the feasibility of the state doesn’t get affected. The transformation rule that preserves the feasibility is to flip the bit $x_w$ if and only if $\bar{x}_{v_1}\bar{x}_{v_2} \ldots \bar{x}_{v_\ell} = 1$, where $v_1, \ldots, v_\ell$ are the vertices adjacent to $w$. Keeping these observations in mind we can construct the following Hamiltonian:

$$B = \sum_u B_u$$

where,

$$B_u = \frac{1}{2^\ell} X_u \prod_{j=1}^\ell (I + Z_{v_j}).$$

(7)

This is the Hamiltonian based implementation of the mixing unitaries. There is a sequential implementation of the mixing unitaries provided in \cite{6} which has some advantages but we will leave that implementation for later work.

**SIMULATION OF QAOA**

We simulate the quantum alternate operator ansatz on the Rigetti Forrest SDK qvm \cite{15}. We simulate the algorithm without including the noisiness of the gates to study the dependence of the algorithm on various parameters. The variational quantum eigensolver subroutine is used to find the optimized parameters $\beta$ and $\gamma$. Within the VQE we use the classical nelder mead method. We run the algorithm over 50 iterations and present the arithmetic averages of the probabilities of the states over these 50 iterations.

![FIG. 1: Square ring graph (The blue lines represent the two max independent sets)](image)

The graph we use the QAOA algorithm on is the square ring graph $G = [(1, 2), (2, 3), (3, 4), (4, 1)]$. We will need four qubits to execute the algorithm. The independent sets for the graph are $(\phi), (1), (2), (3), (4), (1, 3)$ and $(2, 4)$ corresponding to the states $|0000\rangle, |0001\rangle, |0010\rangle, |0100\rangle, |1000\rangle, |0101\rangle$ and $|1010\rangle$ respectively. There are two maximum independent sets corresponding to $(1, 3)$ and $(2, 4)$. We will study the effects of the circuit depth, initial states and weights on the QAOA. For the circuit depth and initial states we will keep all the weights of the vertices the same and equal to unity.

**Dependence on circuit depth:** The initial state we use to study the dependence of the performance of QAOA on circuit depth corresponds to the empty set $|0000\rangle$. We perform the experiment for $p = 1, 6, 15$. The results are summarized in the figures below:

![FIG. 2: $p=1$, Initial State=$|0000\rangle$, Weights=$[1,1,1,1]$](image)

In Fig. 2 we see that the maximum probability is for the state $|0101\rangle$ corresponding to the max independent set $(1, 3)$. Its interesting to see that the probability distribution of states is asymmetric unlike the MaxCut case \cite{14} where the probability distribution of the feasible states is symmetric. but when we increase the circuit depth like in Fig. 2 we notice that the probability of finding the state $|1010\rangle$ or the max independent set $(2, 4)$ increases too. This is an indication that increasing the circuit depth increases the exploration of the domain of feasible states.

![FIG. 3: $p=6$, Initial State=$|0000\rangle$, Weights=$[1,1,1,1]$](image)
The graph we are considering has two independent set of maximum same size (1,3) and (2,4). At around the circuit depth of p=15 we see that there is an equal probability of finding both the sets.

**FIG. 4:** p=15, Initial State=|0000⟩, Weights=[1,1,1,1]

**Dependence on initial States:** We also check the dependence of the outcome of our QAOA algorithm on the choice of initial states. In the experiments that tested the dependence on the circuit depth we were using the zero state as our initial state which corresponds to an empty set. We saw that for large p we get an equal probability of finding both the maximum independent sets of our problem. We set the circuit depth therefore to the large value p=15 and then see the dependence of the outcome on the choice of our initial state. When we set the initial state to be |0001⟩ we see that the probability of seeing the outcome of the (1,3) state increases and the probability distribution for the maximum independent states is again not symmetric anymore.

**FIG. 5:** p=15, Initial States= |0001⟩, weights=[1,1,1,1]

When we set our initial state to be |1000⟩ the probability of seeing the (2,4) as the outcome increases.

**FIG. 6:** p=15, Initial States= |1000⟩, weights=[1,1,1,1]

**Dependence on weights:** Lastly we checked the dependence of our algorithm on the weights. When we increase the weights of the vertices 2,4 from one to two the probability of seeing the state (2,4) becomes almost equal to one. This is in line with our expectations of the algorithm.

**FIG. 7:** p=15, Initial States= |0000⟩, weights=[1,2,1,2]

**INITIAL STATES AND ⟨γ, β|C|γ, β⟩**

The analytical calculation of ⟨C⟩ = ⟨γ, β|C|γ, β⟩ is tricky for the maximum independent set problem even on bounded degree graphs because the mixing Hamiltonian contains the exponential of non-commuting pauli matrices. We therefore calculate numerically the expectation of the cost function ⟨C⟩ for the above given square ring graph. Let us define \( A = e^{-iβH_M} e^{-iγH_C} \). For p = 1 the we have to calculate \( \langle s | A_1^T C A_1 | s \rangle \) where |s⟩ is the initial state. We perform the numerical calculation for different choices of initial states. The expectation value for the independent sets (IS’s) |1000⟩, |0100⟩, |0010⟩ and |0001⟩ are the same and the expectation value for the maximal independent sets (MIS’s) |0101⟩ and |1010⟩ are the same.
For the minimum depth QAOA circuit and $C_{max} = 2$ we plot $\langle C_1 \rangle vs \beta_1$ as $\gamma_1$ cancels out of the expectation value.

$$\langle C_1 \rangle = \frac{\langle s|A_1^T CA_1|s \rangle}{C_{max}}$$

(8)

The maximum value for the expectation $\max_{\gamma_1, \beta_1} \langle C_1 \rangle = 1.0, 0.89$ and $0.68$ for the MIS’s, empty set and IS’s respectively. It is interesting to see that the approximation ratio is better for the empty set compared to the Independent set states.

CONCLUSION

We have studied the maximum weighted independent set problem using the quantum alternating operator ansatz. We noticed that the probability distribution of observance of the maximum independent states is asymmetric unlike the MaxCut problem where the probability distribution of MaxCut states is symmetrically distributed. We also calculated the approximation ratios for our graph for the different initial states. In this paper we have considered a very simple graph and seen the differences with the unconstrained problem. There is much progress to be made to understand our results analytically. In the future we intend to run the experiments on larger graphs with larger circuit depths and as the parameter space increases it would be useful to understand improvements that can be made in the classical parameter optimization algorithms. It will also be interesting to execute the algorithm on a quantum computer and see how far we can push it on a noisy intermediate scale quantum device (NISQ).

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