The QAOA with Slow Measurements

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The Quantum Approximate Optimization Algorithm (QAOA) was originally developed to solve combinatorial optimization problems, but has become a standard for assessing the performance of quantum computers. Fully descriptive benchmarking techniques are often prohibitively expensive for large numbers of qubits (\(n \gtrsim 10\)), so the QAOA often serves in practice as a computational benchmark. The QAOA involves a classical optimization subroutine that attempts to find optimal parameters for a quantum subroutine. Unfortunately, many optimizers used for the QAOA require many shots (\(N \gtrsim 1000\)) per point in parameter space to get a reliable estimate of the energy being minimized. However, some experimental quantum computing platforms such as neutral atom quantum computers have slow repetition rates, placing unique requirements on the classical optimization subroutine used in the QAOA in these systems. In this paper we investigate the performance of a gradient free classical optimizer for the QAOA - dual annealing - and demonstrate that optimization is possible even with \(N = 1\) and \(n = 16\).

I. INTRODUCTION

The Quantum Approximate Optimization Algorithm (QAOA) is a hybrid quantum-classical algorithm that uses a subroutine run on a quantum computer together with a classical optimizer to find approximate solutions to combinatorial optimization problems \([1, 2]\). While many results have demonstrated that the QAOA faces substantial challenges if it is to outperform classical algorithms \([3, 11]\), it has nevertheless become a standard technique for benchmarking quantum computers \([12, 14]\), serving as a holistic test.

The classical optimization routine in the QAOA is used to select a collection of angles that parameterize a quantum circuit. While \([11]\) discusses the feasibility of an open-loop grid search for the QAOA, in practice classical optimizers are closed-loop and require accurate estimates of the energy expectation value for any choice of angles. Previous work \([13, 15, 16]\) has often chosen classical optimizers that require a large number of measurement repetition rates \([1, 12, 17, 20]\). Furthermore, theoretical works also often assume that the optimizer has access to the expectation value at each point in parameter space \([21, 22]\).

However, this assumption is not always justified - some quantum computing platforms, such as neutral atoms, have substantially slower circuit repetition rates. In the case of neutral atoms, this is due in part to atom reloading \([23, 24]\). Modern neutral atom quantum computers use lossy measurements which remove atoms from the trap, requiring atoms to be reloaded between measurements. Moreover modern systems such as \([14]\), can have measurement durations as long as 30mns. These facts together can give total shot-to-shot measurement rates of around 5Hz \([25]\).

This places substantial difficulties on the classical optimizer used in the QAOA. While noise is commonly modeled as coming from decoherence and miscalibration, it can also be a result of shot noise in sampling from the quantum computer a limited number of times. This noise can cause unreliable estimates of quantities such as the gradient and the energy.

In this paper we explore a classical optimization routine for circumventing these difficulties - dual annealing. Dual annealing is a form of simulated annealing, which explores the search space while annealing a “temperature” that parameterizes how likely the algorithm is to jump to higher energy configurations. This can be useful for avoiding local minima. We first discuss modifications that can be made to the algorithm to accommodate the error from taking a limited number of shots. Next, we find empirically that this optimizer performs well even without modification. In particular, we find that dual annealing can find global maxima with a single shot at each point in parameter space that it evaluates.

To assess the efficacy of this optimization technique, we propose a family of graphs and use the QAOA to find the maximum cut of a member of this family. We provide complexity theoretic arguments that suggest these graphs have maximum cuts that may be hard for classical computers to approximate. While several families of graphs are known to be poor choices for showing quantum advantage \([1, 3, 6, 26]\), it is an open problem to find families of graphs on which the QAOA can be shown to outperform classical algorithms.

II. THEORY

The quantum circuit used by the QAOA is described by 2\(p\) parameters, in a layered ansatz. Specifically, the unitary evolution of the quantum computer has input angles \(\vec{\gamma}, \vec{\beta}\) and is given as

\[
U(\vec{\gamma}, \vec{\beta}) = \prod_{j=1}^{p} e^{(-i\beta_j X^\otimes n)} e^{(-i\gamma_j H)},
\]

(1)
where $H$ is called the driver and $\gamma^n$ is called the mixer. An example of this circuit is shown in Fig. 1 and the details of $H$ for the problem considered in this paper are given in Eq. 2. $H$ is a Hamiltonian whose ground state encodes the solution to an optimization problem. In this paper, we consider the MAX-CUT problem, with associated Hamiltonian

$$H = \sum_{(i,j) \in E} \frac{1}{2} \omega_{ij}(1 + \hat{Z}_i \hat{Z}_j).$$

(2)

Here $E$ is the set of edges in a graph, and $\omega_{ij}$ are the weights for the associated edges.

The goal of the QAOA is to find optimal values of $\gamma$ and $\beta$ that minimize

$$C(\gamma, \beta) = \left< + \left| U(\gamma, \beta)^\dagger H U(\gamma, \beta) \right| + \right>.$$  

(3)

In this paper, instead of minimizing $C(\gamma, \beta)$, we equivalently maximize $-C(\gamma, \beta)$. We will only consider the $p = 1$ QAOA, and therefore only have $\gamma_1$ and $\beta_1$. Because there is only one of each angle in the examples we consider, we will refer to them as $\gamma$ and $\beta$ for the rest of the paper. Numerous descriptions of the QAOA and MAX-CUT exist in the literature (11), and further discussion is omitted here. MAX-CUT is a common problem to consider for demonstrations of QAOA due to the locality of the Hamiltonian, requiring only two-body terms. This makes it attractive for early demonstrations of hardware such as that in (14).

To find the optimal angles, $\gamma$ and $\beta$, we consider simulated annealing algorithms. Simulated annealing is traditionally introduced in analogy to the metallurgical process, wherein the optimizer has a temperature which controls random fluctuations and an energy function that is used for preferentially exploring certain configurations. The system has “thermal kinetic energy”, with a visiting temperature which allows it to probabilistically explore the search space while avoiding local minima. The transition between any two points has an associated hopping probability that characterizes how likely a transition between the two states is. As the temperature is lowered, exploration becomes more difficult in the presence of energy barriers.

Simulated annealing over a discrete set (such as that achieved by discretizing $\gamma$ and $\beta$) can be shown to converge to the set of global minima (27). For each temperature, the hopping probabilities form a Markov chain, whose stationary distribution is given by

$$\pi_T(i) = \frac{1}{Z_T} \exp \left( - \frac{J(i)}{T} \right) \quad (4)$$

where $Z_T$ is a normalizing constant. In the limit that $T \to 0$, we see that this distribution concentrates around the collection of minima of $J$.

We further note that if the energy estimate is noisy, this convergence is not guaranteed. This can easily be seen by considering the space with two elements, $i_1$ and $i_2$, and function $K$ such that $K(i_1) = 0$ and

$$K(i_2) = \begin{cases} 2, & \text{with probability } 1/2 \\ -1, & \text{otherwise} \end{cases}.$$  

(5)

Taking $J = \langle K \rangle$ to be the energy function, we see that minimum is $i_1$, however the stationary point of the Markov chain will be the uniform distribution over $i_1, i_2$.

The algorithm can, however, be modified to maintain its convergence properties. We can model finite shot noise as a random variable for the $k^{th}$ step in the annealing chain that depends on the state being measured,

$$X_k = \left( \frac{1}{N} \sum_{\ell=1}^N f_\xi(x_\ell) - J(x_\ell) \right) - \left( \frac{1}{N} \sum_{\ell=1}^N f_\xi(x_\ell) - J(x_i) \right),$$

(6)

where $J(m) = \langle m | C | m \rangle$ and $f_\xi$ is the $\ell^{th}$ evaluation on the quantum computer - i.e. the $\ell^{th}$ shot. One of the conditions for convergence given in (28) is that $\sigma_k \in o(T_k)$, where $\sigma_k$ is the standard deviation of $X_k$, $T_k$ is the annealing temperature and $o(\cdot)$ is the standard asymptotic notation for a strict upper bound. Likewise in what follows, $O(\cdot)$ denotes an asymptotic upper bound with possible equality, $\omega(\cdot)$ denotes a strict asymptotic lower bound, $\Omega(\cdot)$ denotes an asymptotic lower bound with possible equality and $\Theta(\cdot)$ means both $O(\cdot)$ and $\Omega(\cdot)$.

From (11) we know that the values of the sampled cost function are concentrated about their mean $C(\gamma, \beta)$, with variance, $\sigma^2$ upper bounded by

$$\sigma^2 \leq 2 e \left( v - 1 \right) (2p+2) - 1 \left( v - 1 \right) - 1,$$

(7)

for a graph with $e$ edges and $v$ vertices. Thus

$$\sigma^2 = \sigma^2/N \in O(e/N),$$  

(8)

where $\sigma^2$ is the variance of sample mean. This shows that we should expect the number of shots required to be at worst proportional to the number of edges in the graph.

From (28), we expect the modified annealing algorithm to work if $\sqrt{N/e} \in \omega(1/T_k)$. We will show, however, in Sec. IV that even without modifying dual annealing, it can find the local maxima with a single shot per point in parameter space.

The implementation details of the dual annealing algorithm can be found in (24) and theoretical details can be found in (30). We reproduce some relevant details here. In particular, the algorithm uses a distorted Cauchy-Lorentz distribution for the “visiting temperature”

$$g_{q_v}(\Delta x(t)) \propto \frac{[T_{q_v}(t)]^{-\frac{1}{2q_v}}}{[1 + (q_v - 1) \frac{\Delta x(t)^2}{T_{q_v}(t)}]^{\frac{1}{2q_v} + \frac{1}{2}}}.$$

(9)
where \( x(t) \) is a jumping distance, and \( D \) is the dimension of the optimization problem \([20]\). For the \( p = 1 \) QAOA \( D = 2 \), since there are only two values to optimize, \( \gamma \) and \( \beta \). This temperature is annealed according to

\[
T_{q_a}(t) = T_{q_a}(1) \frac{2^{q_v}-1}{(1+t)^{2^{q_v}-1}-1},
\]

and new points are accepted with probability

\[
p_{q_a} = \min\{1, [1-q_a] \Delta E/T_{q_a} \}^{1/\gamma}.
\]

\( q_a \) and \( q_v \) are called the acceptance and visiting parameters, and are hyperparameters used to control how exploratory the annealing algorithm is. This annealing routine is accompanied by local search at the end of each annealing attempt and a number of restart attempts. Simulated annealing, and hence dual annealing, benefits from a wealth of analysis and convergence guarantees \([31]\).

### III. CHOICE OF GRAPH

While the primary purpose of this paper is to discuss the choice of classical optimizer in the QAOA, we need to choose a problem instance. So as to avoid solving a problem that is known to be trivial, we give a heuristic argument for our choice of graph. The particular problem we choose due to its simple-to-implement Hamiltonian and abundance in the quantum computing community is MAX-CUT. The difficulty of MAX-CUT depends on the family of graphs being considered, and the general problem has been well-studied classically - the Goemans-Williamson (GW) algorithm gives an optimal approximation ratio assuming the unique games conjecture \([32-34]\). Therefore one would like to identify a collection of graphs that classical computers perform worst on.

In this work we choose random graphs \( G(v, e) \) on \( v \) vertices with \( e \) edges chosen at random from all possible edges. MAX-CUT on these graphs has a phase transition when \( e/v = 1/2 \), in the following sense: below \( 1/2 \) there are efficient classical algorithms for solving the problem, however above \( 1/2 \) there seem to be hard instances \([33, 34]\). Furthermore, if we consider signed graphs, then if the cover number of the positively signed edges is near \( \sqrt{v} \), the problem becomes strongly NP hard \([37]\). A problem is strongly NP hard if the problem remains NP hard when its numerical parameters are bounded by a polynomial in the input size. This means that hard instances are, roughly speaking, easy to generate, and so in particular randomly generating instances should result in graphs that may be more challenging for classical algorithms.

The cover number of the positively signed edges is the minimum size of a subset \( V \) of the vertices, such that every edge with positive weight has at least one endpoint in \( V \). In particular, \([38]\) shows this family is strongly NP hard for graphs with cover number \( \Omega(v^{-k}) \), with \( k \) a positive integer. We have already specified \( e \in \Theta(v) \) so that \( k = 2 \) is the smallest \( k \) that is guaranteed to be compatible. This suggests that algorithms like the GW algorithm may perform less favorably on these graphs. An example of this graph is shown in Fig. 2. Similar graphs have been considered in \([22]\).

### IV. NUMERICS

We simulate the \( p = 1 \) QAOA on a graph sampled from the family of graphs discussed in Sec. [III] using quimb \([39]\). We emphasize that the purpose of this paper is to demonstrate the performance of the optimizers with low shot rates. The \( p = 1 \) QAOA has been well-studied, and its performance is well-understood analytically \([11, 30, 41]\). Thus, our emphasis is that these techniques allow for the demonstration and benchmarking of a quantum computer - for the case of \( p = 1 \) optimization, one should use the known-optimal choice of angles if the goal is produce a best approximate solution to the
FIG. 2. Example Graph from Section III. Above we see a graph on $v = 20$ vertices, generated according to the distribution described in Sec. III. Edgeless vertices are omitted from the figure. We sample $e = 3v/5$ edges at random, and edge weights are chosen uniformly at random from $[-1, 1]$.

problem being studied. In certain problem instances of MAX-CUT, we can reduce the search space for both $\gamma$ and $\beta$ to the range $[0, \pi]$. In general we see this is not possible, since scaling the edge weight by a factor of $1/c$ moves the maximum in $\gamma$ by a factor of $c$. Nevertheless, we restrict our search space, since we are interested primarily showing that optimization is possible. For our example, we choose a graph on $v = 20$ vertices, which has $n = 16$ qubits that interact with at least one other qubit. We note that $n = 16$ is a non-trivial example for initial demonstrations of new quantum computing architectures.

The particular graph considered in this section is shown in Fig. 2 and is sampled from the distribution described in Sec. III. The graph is chosen from a distribution with $e = 3v/5$ edges, with $v = 20$, and therefore only contains 16 vertices with edges. Such a graph would be useful for demonstrating the QAOA on an architecture of a $4 \times 4$ grid of atoms. As mentioned in Sec. III, rather than minimizing Eq. 3, we maximize $-C(\gamma, \beta)$.

In Fig. 3 we see the performance of dual annealing on the graph in Fig. 2. We use one shot per point in parameter space ($N = 1$) and allow the dual annealing algorithm ten opportunities to restart and re-anneal. In total the optimizer sampled 326 times. For a clock rate of 5Hz this would take just over a minute to run. Fig. 3 also provides two kernel density estimates of the distribution of sampled points which highlights that there are two distinct attractors over $\beta$, and one over $\gamma$, corresponding to the optima of the landscape. Kernel density estimates use Gaussian kernels to produce a non-parametric estimate of the sampling distribution that is given by

$$\hat{f}_h(x) = \frac{1}{nh} \sum \exp\left(-\frac{(x - x_i)^2}{h^2}\right), \quad (12)$$

where the bandwidth $h$ given by

$$h = n^{-1/(d+4)}, \quad (13)$$

and $n$ is the number of samples (326) and $d$ is the dimension (1) as suggested in [42]. This demonstrates that the dual annealing optimizer not only can find a good cut, but also is taking advantage of the structure of the optimization landscape.

Another interesting feature of single-shot optimization, which we leave to future work, is the behavior of the single-shot performance statistics. While many optimizers attempt to estimate and maximize the QAOA energy, the goal of the QAOA is to optimize the single best observed bitstring. The shot to shot energy is plotted against the cumulative best energy in Fig. 4. While the optimizer quickly finds a good cut and Fig. 3 shows that the optimizer samples preferentially from the basins of attraction of the optima, it can be seen that the single shot data varies substantially. The maximum value in the grid of values produced in Fig. 3 is 3.78, however the optimum reported by the optimizer is 4.13. This is in fact the sum of the positive weights, and hence the maximum cut.

We see that dual annealing is able to perform with just a single shot per choice of angle pair $\gamma$ and $\beta$. For quantum computers with low shot rates this provides a tractable method for performing closed-loop quantum-classical optimization, with noisy estimates of the energy at each point.

V. CONCLUSION

Due to its easy implementation and interpretation, the QAOA is an appealing holistic benchmark for quantum computers. However, different quantum computing architectures place different requirements on the classical
optimization subroutine of the QAOA. In particular, neutral atom quantum computers often have substantially slower measurement rates than conventional superconducting quantum computers. To use the QAOA as a benchmark for these platforms thus requires choosing a classical optimizer that can use noisy estimates of the QAOA energy.

In this paper, we have demonstrated an optimization technique that is well-suited for this problem, dual annealing. Dual annealing searches the parameter space in a thermal way, accepting transitions if the cost is lower or if the annealing temperature is sufficiently high to allow jumps to worse points. We have shown that this algorithm can use a single shot per point in parameter space while still finding good cut values for the MAX-CUT problem on as many as $n = 16$ qubits.

Additionally, we have suggested a new family of graphs which have a phase transition in their known classical hardness. There are several straightforward analyses to extend this work - including realistic noise models, scaling to larger numbers of qubits and extending the algorithm considered here to model the shot uncertainty explicitly $^{29}$, as described in Sec. $^4$. Finally, while the intention of this work was to discuss the optimizer choice for demonstrating the performance of NISQ hardware, and thus focused on $p = 1$, exploring the increased dimensionality of the search space for higher $p$ is an interesting direction for future research.

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