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Quantum Approximate Optimization Algorithm (QAOA)

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1 Introduction

Quantum optimization is an emerging field hoping to solve optimization problems with the help of quantum algorithms running on quantum devices. What many scientists strive to find is, in fact, the evidence of *quantum advantage*; that is, a quantum computer with a tailored quantum algorithm can efficiently perform a task that its classical counterparts cannot [37]. In a classical setting, an algorithm is usually specified as a high-level list of instructions that needs to be translated into basic gate operations applied to bit strings. In contrast, a quantum algorithm in the quantum circuit model refers to a quantum circuit in which *unitary operators* and basic quantum gates are applied to quantum registers [35].

One of the well-known quantum algorithms is the *quantum approximate optimization algorithm* (QAOA) proposed by Farhi et al. [17]. QAOA aims to solve the problem of maximizing the number of satisfied clauses in the *max satisfiability* problem. However, QAOA can be employed to solve any *polynomial unconstrained binary optimization* (PUBO) formulations since they can be viewed as special cases of the max satisfiability problem. Consider the following PUBO problem

$$\max_{x\in\{0,1\}^n} f(x) \tag{1}$$

with $f(x) : \{0,1\}^n \to \mathbb{R}$ and $f(x) \coloneqq \sum_{j=1}^{m} w_j f_j(x)$. Here, $w_j \in \mathbb{R}$ and $m = \mathcal{O}(\text{poly}(n))$ and Boolean functions $f_j(x)$ have a bounded degree such that $\deg(f) = d$ [23].

Farhi et al. [17] showed that under certain conditions (hard to satisfy), QAOA finds approximate solutions to combinatorial optimization problems. The potential and challenges of this algorithm have drawn the attention of many researchers, including [6, 29, 44], to name a few. QAOA is inspired by the *quantum adiabatic algorithm* (QAA) that aims to find the smallest eigenvalue of a Hermitian matrix called *ground state energy* [17, 19, 20]. QAA starts with a Hermitian matrix (with a known ground state) and gradually evolves into another Hermitian matrix with an unknown ground state while tracing the ground state. The evolution time of QAA can be exponential, making it computationally expensive [17]. Further, the success probability of QAA is generally not a monotonic function of the running time, while QAOA's performance with optimal parameters improves as the number of iterations (called levels) grows [17].

2 QAOA Circuit

QAOA starts with a quantum state $|s\rangle$, a *superposition* (combination) of all bit strings. The measurement of a superposition on a computational basis is equivalent to sampling from a uniform distribution. A bit string x corresponds to a vector called *computational basis state* $|x\rangle \in \mathbb{C}^{2^n}$ with one of its entries being one and the rest being zeros. This superposition can be constructed by applying *Hadamard* gates (H) on a zero state $|0\rangle^{\otimes n}$ (Tensor product of n zero qubits); that is

$$|s\rangle = H^{\otimes n}|0\rangle^{\otimes n} = \frac{1}{\sqrt{2^n}} \sum_{x\in\{0,1\}^n} |x\rangle.$$

Here, there are 2^n different states with n being the number of quantum bits (qubits). A QAOA circuit is designed as an iterative framework in which each level has the same structure with different parameter values. Each level of the algorithm has two types of unitary operators: (i) phase separation operator (U_P) and (ii) mixing operator (U_M). Consider problem (1), a Hermitian operator called *Hamiltonian* H_f [23] defined as follows

$$H_f|x\rangle \coloneqq f(x)|x\rangle.$$

The optimal objective value is a special case of the extremal eigenvalues of a H_f. Hadfield [23] provides a general framework for converting the classical representation of a Boolean objective function f into its Hamiltonian H_f. The phase separation operator is defined as $U_P(\gamma) \coloneqq e^{-i\gamma H_f}$ with $\gamma \in [0, 2\pi]$ and i be the imaginary unit. The phase separation operator U_P simulates Hamiltonian H_f with n qubits and $\mathcal{O}(md\,\mathrm{poly}(n))$ basic quantum gates assuming any Boolean function f_j acts at most on $\mathcal{O}(\log n)$ bits [23]. In particular, if $d = \mathcal{O}(1)$, QAOA's circuit requires $\mathcal{O}(mn^d)$ basic gates [23].

Hamiltonian H_f is a diagonal matrix, thus, phase separation operator U_P, by itself, will not change the probability distribution of the output of QAOA. Accordingly, QAOA requires the mixing operator U_M that does not commute phase separation operator U_P (i.e., $U_M U_P \neq U_P U_M$); this indicates that they do not share all their eigenstates [24, 25]. The interaction of both operators modifies the probability distribution of QAOA's output.

Let $Q \coloneqq \{1, \cdots, n\}$ be the set of qubits. For every qubit $j \in Q$, let X_j be the basic *Pauli* gate X applied to qubit j. Pauli gates are the basic operations applied on qubits [35]. We define $B \coloneqq \sum_{j\in Q} X_j$. The mixing operator can be written as $U_M(\beta) \coloneqq e^{-i\beta B}$ with $\beta \in [0, \pi]$. The choice of mixing operator is however not unique, and the use of different mixing operators has been explored [26, 43]. Fig. 1 illustrates a general scheme of QAOA with p levels, denoted by QAOA$_p$ [24]. Let $\vec{\gamma} = (\gamma_1, \cdots, \gamma_p)$ and $\vec{\beta} = (\beta_1, \cdots, \beta_p)$. The *ansatz* – an estimate of the solution – of QAOA is denoted by $|\psi(\vec{\beta}, \vec{\gamma})\rangle$ and defined as

$$|\psi(\vec{\beta}, \vec{\gamma})\rangle = U_M(\beta_p)U_P(\gamma_p)\cdots U_M(\beta_1)U_P(\gamma_1)|s\rangle.$$

The last step of the algorithm is the *measurement* which is a realization of the quantum state in a classical form. The expected result after this step is

$$F_p(\vec{\beta}, \vec{\gamma}) = \langle\psi(\vec{\beta}, \vec{\gamma})|H_f|\psi(\vec{\beta}, \vec{\gamma})\rangle,$$

that is, the inner product of $|\psi(\vec{\beta}, \vec{\gamma})\rangle$ and $H_f|\psi(\vec{\beta}, \vec{\gamma})\rangle$. Function $F_p(\vec{\beta}, \vec{\gamma})$ represents the expectation of H_f in state $|\psi(\vec{\beta}, \vec{\gamma})\rangle$. After the measurement step, a QAOA circuit generates a bit string

representing a solution. In practice, $F_p(\vec{\beta}, \vec{\gamma})$ can be calculated as the expected objective value of solutions in a set of algorithm runs. The QAOA's performance depends on the number of levels; given optimal parameters of QAOA, the algorithm asymptotically converges to optimal solutions as the number of levels grows [17].

Theorem 1 ([17]). *Consider the PUBO problem (1). Let $f^* \coloneqq \max_x f(x)$ be its optimal objective value and $F_p(\vec{\beta}, \vec{\gamma})$ be the expected output of QAOA$_p$. Then,*

$$\lim_{p \to \infty} \max_{\vec{\beta}, \vec{\gamma}} F_p(\vec{\beta}, \vec{\gamma}) = f^*.$$

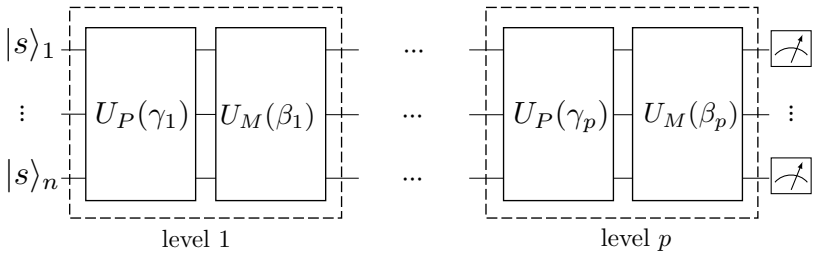

Figure 1: The QAOA$_p$ quantum circuit [see 24, Figure 5.1].

3 Parameters Tuning

QAOA requires tuning the parameters to maximize the expected objective value for a given number of levels.

$$(\vec{\beta}^*, \vec{\gamma}^*) = \operatorname*{argmax}_{\vec{\beta}, \vec{\gamma}} F_p(\vec{\beta}, \vec{\gamma}).$$

This parameter tuning problem is nonconvex and NP-hard. In general, the only available information for optimizing the parameters is the objective values of samples. Numerous practical ideas with no theoretical guarantees have been proposed to address this requirement, such as employing derivative-free methods [22, 40, 42, 44, 45]. Fig. 2 illustrates the nonconvex, nonlinear, and periodic nature of $F_1(\vec{\beta}, \vec{\gamma})$ for an instance of the weighted max cut problem. The optimal value of parameters for a given number of levels can be different from others, but still, they provide a good starting point to optimize circuits with more levels [45]. Zhou et al. [45] posited that the optimal value of parameters converges to a fixed set of values as the number of levels increases. Fig. 2 shows that even with one level, the gradient of $F_p(\vec{\beta}, \vec{\gamma})$ vanishes rapidly; this phenomenon is known as the barren plateau [1, 3, 34]. The barren plateau expands exponentially as the number of qubits grows, making the tuning process even more challenging [34]. As illustrated in Fig. 2, the choice of parameters – even choosing locally optimal parameters – significantly affects the performance of QAOA. This effect is often overlooked in many studies while evaluating the efficacy of different ideas.

Wang et al. [42] derived the closed formula of $F_1(\vec{\beta}, \vec{\gamma})$ for the case of $p = 1$ as a function of parameters for the *max cut* problem that seeks to maximize the sum of the weight of edges connecting two complementary sets of vertices in a graph. Similarly, Hadfield et al. [25] derived

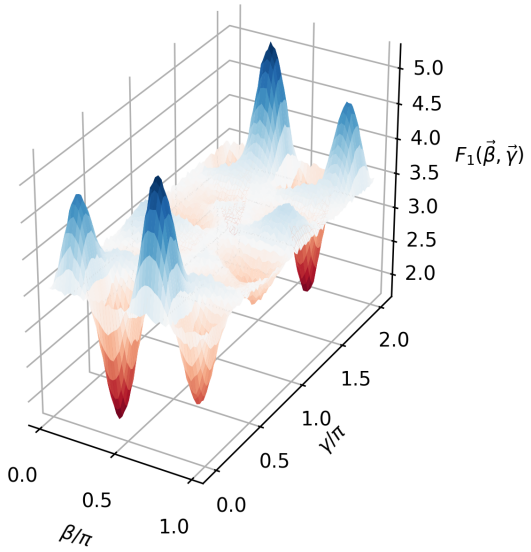

Figure 2: $F_1(\vec{\beta}, \vec{\gamma})$ for an instance of the weighted max cut problem with 8 vertices and 23 edges.

the closed formula of $F_1(\vec{\beta}, \vec{\gamma})$ for a general *quadratic unconstrained binary optimisation* (QUBO) problem.

4 Complexity

Farhi et al. [18] showed that QAOA_1 outperforms existing classical algorithms on a class of instances of the *bounded occurrence constraint* problem in which every variable appears in at most 3 constraints. Very soon Barak et al. [5] proposed a better classical algorithm, however, Farhi et al. [18] demonstrated QAOA's potential. Farhi and Harrow [21] later proved that, under reasonable complexity assumptions, classical sampling cannot efficiently simulate the output distribution of QAOA_1 circuits. QAOA is not expected to solve either any NP-hard problem to optimality in polynomial-time or even outperform the best classical approximation ratios for all NP-hard problems [6]. Many researchers are still interested in finding a class of problems and instances in which either a classical algorithm or QAOA outperforms the other [4, 6, 8, 28, 33]. Specifically, it is an open question whether QAOA can achieve a quantum advantage over all classical algorithms, regardless of the size of the instance, for a class of instances of the max cut problem [6, 30].

Let graph G be the corresponding graph to problem (1) in which each vertex represents a variable, and an edge is drawn between two vertices if their corresponding variables appear in a function $f_j(x)$. QAOA_p is a *p-local* algorithm where its output depends only on the vertex's radius p neighborhood [32]. This characteristic is known as *locality*. As a result, QAOA is effective when the number of levels p is sufficiently large [8, 11, 15, 16]. Recent studies show that the QAOA's level p needs to grow at least logarithmically with problem size n for specific combinatorial optimization problems [15]. Similar studies have been conducted for the max cut problem on several instance classes [8, 6, 32]. Motivated by this property, a *recursive* QAOA (RQAOA) has been proposed that fixes two variables' correlation at each recursion step and reduces QAOA's circuit size [7, 8]. Akshay

et al. [1, 2] investigated the effect of ρ (the ratio of the number of constraints to the number of variables) on QAOA's performance. They introduced the *reachability deficit* as a QAOA limitation in solving instances with large ρ. QAOA's locality may also explain this issue.

Besides the theoretical convergence of QAOA, scientists hope that advancements in developing high-quality qubits accelerate the potential speed-up of the QAOA in solving practical problems [22]. The number of qubits at hand is not the primary barrier of quantum computers, rather, it is their noisy behavior that impedes the scalability [37]. Moreover, the dissimilarity of the problem structure with hardware design has been diagnosed to increase the compilation time on quantum computers [27].

Quantum algorithms, by nature, differ from randomized algorithms. However, they are still dealing with inherent randomness in their final results. QAOA evaluates a sample of runs indicating a distribution of solutions [17]. It is guaranteed that an ϵ-precise estimation of the expected objective value of samples can be obtained with $\mathcal{O}\left(\frac{\|H_f\|^2}{\epsilon^2}\right)$ runs of QAOA circuits [38]. As an optimal or best solution in a sample is often desired, selecting an appropriate sample size remains a question, especially during the parameter tuning process.

5 Conclusions

It is worth noting that the *variational quantum eigensolver* (VQE) method is a similar quantum approximation algorithm developed independently from QAOA. The VQE is designed to find a state with high ground state overlap of a Hamiltonian [36]. In essence, both algorithms aim to find a ground state of a Hamiltonian with a slightly different approach [17, 36].

A number of ideas have been proposed for improving QAOA's performance. Although the initial uniform combination of bit strings is essential to QAOA's theoretical convergence, several researchers investigated its *warm-starting* to improve the algorithm's performance [13, 41]. Egger et al. [13] used both rounded and unrounded semidefinite optimization relaxation of a QUBO problem as an initial state instead of the original superposition. They adjusted the QAOA mixing unitaries so that the warm-start QAOA converges to optimal solutions as the number of levels approaches infinity. However, in the rounded case, it is not guaranteed that the warm-start QAOA converges to optimal solutions as the number of levels approaches infinity [9]. Indeed, the warm-start fails when QAOA starts with a single bit string instead of a superposition of all bit strings regardless of the quality of its corresponding solution [9].

Most papers have examined the behavior of QAOA on the well-known max-cut problem. Nevertheless, QAOA can be applied to any PUBO problem [10, 26]. Several researchers have attempted to find PUBO formulations that yield the best QAOA performance for different combinatorial optimization problems [10, 12, 14, 31, 39].

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