A Statistical Approach to Analyzing the Quantum Alternating Operator Ansatz with Grover Mixer *

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Abstract. *The Quantum Alternating Operator Ansatz (QAOA) is a promising quantum heuristic to combinatorial optimization, designed for the Noisy Intermediate-Scale Quantum (NISQ) era. A key quantum operator of the algorithm is the mixing, which introduces quantum interference. This work investigates analytically the performance of QAOA with the Grover mixer, a mixing operator inspired by Grover's algorithm. A critical feature of QAOA with Grover mixer is that it depends only on the probability distribution of the solutions, ignoring the structure of the problem. Due to this, it was conjectured that QAOA with this mixer is bounded to the quadratic speed-up of Grover's algorithm over the classical brute force on the unstructured search problem. On the other hand, this feature allows the development of a statistical approach, which we explore in this work. For a variant of QAOA called Grover mixing QAOA (GM-QAOA), the analysis leads to an expression for the expectation value whose number of terms depends exponentially on the number of layers of the QAOA. In contrast, for Grover mixer Threshold QAOA (GM-Th-QAOA), a simpler variant that has an intimate relationship with Grover's algorithm, we obtain a constant-time expression, which allows us to get bounds for different performance metrics, such as the statistical quantities of standard score and quantile. Subsequently, we generalized QAOA with the Grover mixer in a framework we called Grover-based QAOA. By using a contradiction argument with the optimality of Grover's algorithm, we extend all the bounds of GM-Th-QAOA to the general context of Grover-based QAOA. As a result, we get the main contribution of this work: the proof of the aforementioned conjecture on the performance of QAOA with Grover mixer. We apply our bounds to the class of complete bipartite graphs on the Max-Cut problem, demonstrating that we cannot obtain a polynomial-time algorithm with Grover-based QAOA for these instances, showing that the performance limitation of the Grover mixer can be very severe. Our results suggest that achieving competitive performance with QAOA requires a mixing operator capable of leveraging the structure of combinatorial optimization problems.*

1. Introduction

Quantum computing has theoretical run-time advantages over classical computing—most commonly known as quantum speed-up—for some problems, such as a quadratic speed-up for searching an unstructured database [Grover 1996] and exponential speed-up for

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integer factoring [Shor 1994]. However, despite these theoretical advantages, the practical application of quantum computers is limited by significant technological hurdles. Specifically, the current technology state of quantum computing is known as the Noisy Intermediate-Scale Quantum (NISQ) era [Preskill 2018, Cheng et al. 2023]. During the NISQ era, due to the technological difficulty of isolating physical systems from the environment, we need to handle the presence of quantum noise, which generates errors that limit the scalability of both the number of qubits and the depth of the quantum circuit. These errors still cannot be eliminated, since the protocols of quantum error correction, which require a large number of qubits for redundancy, are currently unfeasible. Thus, to achieve quantum speed-up on problems of practical interest with NISQ devices, algorithms must be designed with restrictions on the number of qubits and circuit depth.

One class of algorithms with the potential for quantum speed-up in the NISQ era is the so-called Variational Quantum Algorithms (VQA) [Cerezo et al. 2021]. These algorithms address the scalability limitations of current quantum devices through a hybrid classical quantum-classical approach. In particular, the VQAs use a parameterized quantum circuit within NISQ capabilities that are optimized to minimize or maximize a predefined cost function, which is computed from measurements of observables in the quantum system. That optimization procedure is driven by a classical optimizer using strategies that may include optimization and/or training techniques.

There is a wide range of variational algorithms, finding applications in several knowledge fields, including quantum chemistry, quantum physics, quantum information, mathematical applications, dynamical simulations, and machine learning [Cerezo et al. 2021]. A particularly interesting application is combinatorial optimization [Bernhard and Vygen 2012], an area of mathematics and computer science focused on finding optimal solutions to problems where the goal is to select the best combination of elements from a finite set. Numerous practical applications can be represented as abstract combinatorial optimization problems, spanning various fields, such as finance, logistics, manufacturing, transportation, telecommunications, and healthcare. Most combinatorial optimization problems with great theoretical and practical interest, such as the Traveling Salesman Problem and the Max-Cut Problem, are NP-Hard. This means that—unless P = NP—there are no polynomial-time algorithms that find the optimal solution. For these cases, the interest is in the search for approximate solutions that are sufficiently satisfactory under some criteria.

A prominent variational algorithm, used mainly for heuristic optimization in combinatorial optimization, is the Quantum Approximate Optimization Algorithm [Farhi et al. 2014], generalized to the Quantum Alternating Operator Ansatz (QAOA) [Hadfield et al. 2019]. The operation of QAOA consists of a fixed number of layers where two parameterized operators are alternately applied. One is the phase separation operator, responsible for introducing bias based on the cost function through changing relative phases between solutions, while the other, called the mixing operator, introduces quantum interference between states, dealing with the amplitude transfer process. A convenient interpretation for operator mixing is provided by the Quantum Walk-based Optimization Algorithm (QWOA) [Marsh and Wang 2020], a generalization of QAOA that sees the mixing operator as a Continuous-time Quantum Walk (CTQW) operator. [1].

[1]CTQWs are the quantum analog to the classical continuous-time Markov chains [Portugal 2018].

There is already a wide range of designs for mixing operators in the literature, such as Refs. [Hadfield et al. 2019, Bärtschi and Eidenbenz 2020, Marsh and Wang 2020]. We can highlight the transverse field mixer [Farhi et al. 2014]—the original mixer of QAOA—which can be seen as a CTQW in a hypercube graph, and the Grover mixer [Bärtschi and Eidenbenz 2020], a variational version of the diffusion operator of Grover's algorithm [Grover 1996] [2] that, up to a rescaling of the operator parameter, consists of a CQTW in the complete graph. Two variants of QAOA that use the Grover mixer are of interest to discuss. The first is the Grover Mixer Quantum Alternating Operator Ansatz (GM-QAOA) [Bärtschi and Eidenbenz 2020], which combines the Grover mixer with the standard phase separation operator. The last is the Grover Mixer Threshold QAOA (GM-Th-QAOA) [Golden et al. 2021], which combines the Grover mixer with a phase separation operator that encodes a binary function that partitions the solution space into two parts, separated by a threshold value on the cost function. Notably, setting all optimization parameters to π simplifies GM-Th-QAOA to Grover's search for a set of marked states determined by the chosen threshold. An advantage of GM-Th-QAOA over GM-QAOA is that there is an efficient method to obtain the variational parameters, something unusual in VQAs since in many cases their associated classical optimization problems are NP-Hard [Cerezo et al. 2021].

The performance of QAOA remains poorly understood, especially its potential compared to the best classical algorithm counterparts. Much of the QAOA knowledge is empirical since analytical results are historically uncommon and scattered in the literature, largely due to quantum operators being analytically complex [Golden et al. 2023b]. In this context, the mixing operator seems to be a key aspect of understanding how QAOA works. Several works, such as Refs. [Akshay et al. 2020, Golden et al. 2023b, Golden et al. 2023a], empirically show that different mixers yield different results for the same input instances, making the understanding of the role of mixing for QAOA an important research topic in the field. However, despite empirical evidence, a solid theoretical understanding is lacking.

In this sense, the Grover mixer provides an insightful path to get analytical results for QAOA. Numerically, although it was observed that the Grover mixer performs better than the transversal field mixer for small instances [Akshay et al. 2020], a result explained by the ability of the Grover mixer to mix quickly that is provided by the maximum connection between edges on the complete graph [Benchasattabuse et al. 2023], experiments on larger instances indicated that the Grover mixer performs worse than the transverse field mixer [Golden et al. 2023b] and a mixer called clique [Golden et al. 2023a]—showing in the last case an impressive exponential difference of performance. From the theoretical side, an important feature of QAOA with the Grover mixer is that the outcome of QAOA with this mixer depends exclusively on how the costs of the solutions are distributed in the solution space—the expectation value of QAOA with the Grover mixer is invariant under any permutation of states [Headley and Wilhelm 2023]—meaning that the algorithm is incapable of perceiving any problem structure of the instance. Combining it with the

[2] Grover's algorithm (or Grover's search) is an algorithm that was developed for the called unstructured search problem, which, in its generalized form, aims to find m elements in an unstructured list of M using as few queries as possible. The number of queries that Grover's algorithm requires to find out a marked element with high probability is $\Theta(\sqrt{M/m})$, which is a quadratic speed-up over the best classical algorithm, the brute force, that finds the marked elements, in average, with $\Theta(M/m)$ queries.

empirical results, it was conjectured in Refs. [Golden et al. 2023b, Golden et al. 2023a] that QAOA with the Grover mixer could not surpass the limits of the unstructured search [3]. This barrier would prevent the algorithm from being competitive in larger instances, since it would correspond to a modest quadratic speed-up over a classical brute force algorithm, such as random sampling. If the conjecture holds, the superior performance of transverse field and clique mixers in the numerical experiments must be linked to their ability to exploit the underlying problem structure.

Despite the limitations potentially caused by the independence of the problem structure of the QAOA with Grover mixer, it can significantly simplify the analysis and open the path for the development of analytical methods for the QAOA. In this sense, Headley and Wilhelm [Headley and Wilhelm 2023] developed a statistical approach that, using random variables to model the problem, obtained an analytical expression of the expectation value of QAOA depending only on the probability distribution associated with the solution space. Despite the significant simplifications that this method provides, the complexity of the resulting expression scales exponentially with the depth of the quantum circuit (i.e., the number of layers of QAOA), which makes it difficult to scale the studies in the number of rounds. On the other hand, it does not depend on the number of qubits (i.e., the entry size of the optimization problem) and, because of this, given that the asymptotic probability distribution of some class of instances is known, we can analytically compute the optimal parameters by taking the size limit. This was done by the authors for the Number Partition Problem assuming that the numbers are chosen under i.i.d. conditions.

1.1. Contributions

The main focus of this dissertation is to investigate the performance of QAOA with the Grover mixer— especially the conjecture that the Grover mixer restricts QAOA to the bound of the unstructured search problem. Firstly, we get equivalent results to the aforementioned statistical approach of Headley and Wilhelm [Headley and Wilhelm 2023] for GM-QAOA [4]. These results are shown in Section 3 of the present document. The subsequent results of the dissertation correspond to the paper of Bridi and Marquezino [Bridi and Marquezino 2024] and are shown in Sections 4 and 5 of the present document. This paper considers the application of the statistical approach to the GM-Th-QAOA and to a more general framework of QAOA with the Grover mixer we called *Grover-based QAOA*, providing original contributions and insights not only about the performance of these variants but about the QAOA in general.

2. Quantum alternating operator ansatz and Grover mixer

The Quantum Alternating Operator Ansatz (QAOA) [Hadfield et al. 2019] is defined as follows.

Definition 2.1 (Quantum Alternating Operator Ansatz) *Consider an instance of a combinatorial optimization problem defined on a domain S with a cost function (the objective function) $c(k) : S \to \mathbb{R}$ be minimized. For some Hilbert space known as configuration space, the algorithm acts in some subspace called feasible subspace spanned by*

[3] For the unstructured search problem, Grover's search is optimal in the average probability of measuring marked elements for any number of queries [Zalka 1999, Hamann et al. 2021].

[4] We develop it while working independently in the context of QWOA on the complete graph before becoming aware of the existence of the paper of Headley and Wilhelm.

$M = |S|$ basis states (the feasible states) codifying the solutions of S. The state final of QAOA, denoted $|\psi^{(r)}\rangle$, is given by $|\psi^{(r)}\rangle = \prod_{k=1}^{r} U_M(\beta_k)U_P(\gamma_k)|\psi\rangle$. Here, r is the number of rounds/layers of QAOA; $|\psi\rangle$ is a generic initial state; $U_P(\gamma) = e^{-i\gamma H_Q}$ is the phase separation operator, where H_Q is a Hamiltonian that encodes a real-valued function $q(k)$ compiled from the cost function such that $H_Q|k\rangle = q(k)|k\rangle$ for any feasible state $|k\rangle$; $U_M(\beta) = e^{-i\beta H_M}$ is the mixing operator, where H_M is mixer Hamiltonian; sets $\boldsymbol{\beta} = (\beta_1, \ldots, \beta_r)$ and $\boldsymbol{\gamma} = (\gamma_1, \ldots, \gamma_r)$ are the optimization parameters (or angles).

To this work, we assume as the goal of QAOA to minimize the expectation value $\langle\psi^{(r)}|H_C|\psi^{(r)}\rangle$, where the Hamiltonian H_C, diagonal in the computational basis, encodes the cost function of a combinatorial optimization problem such that $H_C|k\rangle = c(k)|k\rangle$. Both variants of QAOA of interest, GM-QAOA and the GM-Th-QAOA, are particular cases of QAOA that have as mixer Hamiltonian the Grover mixer, given by $H_M = |s\rangle\langle s|$, and the initial state, denoted by $|s\rangle$, is given by a uniform superposition over all feasible states. The difference between both is that while the phase separation operator of GM-QAOA codifies the own cost function ($q(k) = c(k)$ and $H_Q = H_C$), the phase separation of GM-Th-QAOA codifies the threshold function $T_h(k)$ given by $T_h(k) = -1$ if $c(k) \leq t$ and 0 otherwise, for a threshold value t that must be optimized. In particular, we denote the expectation value of GM-QAOA and GM-Th-QAOA by $E_r(\boldsymbol{\beta}, \boldsymbol{\gamma})$ and $E_r(t)$, respectively.

3. The statistical approach for GM-QAOA

To statistically model the combinatorial optimization problems, we define X as the random variable of uniformly sampling an element on the set S and calculating the cost function. The function $f_X(x) = |\{k \in S : c(k) = x\}|/M$ is the probability distribution of X, and the support R_X of X is a countable subset of real numbers. We denote the mean, standard deviation, and minimum value of X by $\mu = \mathrm{E}[X]$, $\sigma = \sqrt{\mathrm{E}[X-\mu]^2}$, and R_X^{min}, respectively, and assume $0 < \sigma < \infty$. Furthermore, we also define the random variables Y and Z as $Y = X - \mu$ and $Z = (X - \mu)/\sigma$.

We compute the expectation value from the definition $E_r(\boldsymbol{\beta}, \boldsymbol{\gamma}) = \langle\psi^{(r)}|H_C|\psi^{(r)}\rangle$ by replacing $|\psi^{(r)}\rangle = \prod_{k=1}^{r} U_M(\beta_k)U_P(\gamma_k)|\psi\rangle$ and $U_M(\beta) = \mathbb{I} + (-1 + e^{-i\beta})|s\rangle\langle s|$, where $\mathbb{I}$ is the identity matrix. For a single layer, at some point in the calculations, the quantity $\langle s|U_P(\gamma)|s\rangle = \frac{1}{M}\sum_{k\in S} e^{-i\gamma c(k)}$ appears. The summation can be equivalently expressed by counting the number of solutions where $c(k) = x$ for each possible cost $x \in R_X$, i.e., $Mf_X(x)$. Consequently, we introduce the random variable X in the expression with $\langle s|U_P(\gamma)|s\rangle = \varphi_X^*(\gamma)$, where as $\varphi_X(\gamma) = \sum_{x\in R_X} f_X(x)e^{-i\gamma x}$ is the characteristic function of X with argument γ. Similarly, we have the quantity $\langle s|H_C U_P(\gamma)|s\rangle = \frac{1}{M}\sum_{k\in S} c(k)e^{-i\gamma c(k)}$, which is replaced by $i\varphi_X'^*(\gamma) = \sum_{x\in R_X} x f_X(x)e^{-i\gamma x}$. For an arbitrary number of layers, we follow the same substitution principle for similar quantities resulting in characteristic functions and derivatives of characteristic functions with more complicated arguments. The final expression, whose notation is too loaded to be introduced in this document, can be found in Equation 4.42 of Bridi [Bridi 2024], consisting of a summation with a number of terms of order $\mathcal{O}(4^r)$. The exponential complexity restricts the simulation to something in the order of a dozen layers.

4. The statistical approach for GM-Th-QAOA

To explore the theoretical capabilities of the Grover mixer in combinatorial optimization, it is helpful to consider a more tractable scenario. As we have seen, the expression obtained with the statistical approach for GM-QAOA has a number of terms that grow exponentially with the number of rounds, making it difficult to obtain bounds on the performance of the algorithm. Given this challenge, it is natural to investigate a simplified variant of QAOA with the Grover mixer. This leads us to GM-Th-QAOA. Given the close relationship of that variant with Grover's algorithm and the unstructured search problem, we can use the well-known formula of the probability of Grover's algorithm and establish the optimality of the optimization parameter as a consequence of the optimality of Grover's search on average probability for the unstructured search [Zalka 1999, Hamann et al. 2021]. As a consequence, we provide in Theorem 4.1 an expression for the expectation value whose complexity is independent of the number of rounds, which allows the study of the algorithm's behavior asymptotically, something unfeasible for GM-QAOA. Instead of the characteristic function, the key statistical quantity here is the conditional expected value. Specifically, the expectation of X given $X \leq x$ is $\mathrm{E}[X|X \leq x] = G_X(x)/F_X(x)$, where $G_X(x) = \sum_{k \in R_X : k \leq x} k f_X(k)$ and $F_X(x) = \sum_{k \in R_X : k \leq x} f_X(k)$ is the cumulative distribution function (cdf).

Theorem 4.1 *For any number r of layers in GM-Th-QAOA with optimal angles,*

$$E_r(t) = \mu - G_Y(t-\mu)\frac{1 - P(\rho, r)/F_Y(t-\mu)}{1 - F_Y(t-\mu)}, \tag{1}$$

where $\rho = F_Y(t-\mu)$ and $P(\rho, r)$ is given by $\sin^2\left((2r+1)\arcsin\left(\sqrt{\rho}\right)\right)$ if $\rho \leq \sin^2\left(\pi/(4r+2)\right)$ and 1 otherwise.

Note that the statistical quantities of Eq. 1 are expressed in terms of the random variable Y, and the mean of the distribution is abstract with trivial term μ.

The success of the aforementioned efficient method of Golden et al. [Golden et al. 2021] in finding the optimal optimization parameters depends on a conjecture. The closed-form expression given by Eq.(1) allows us to address this open problem. The conjecture concerns the behavior of the function we called *threshold curve*, which is the curve of $E_r(t)$ versus t, fixing optimal $\boldsymbol{\beta}$ and $\boldsymbol{\gamma}$ for the given t. In particular, it was numerically observed by Golden et al. [Golden et al. 2021] that the threshold curve decreases monotonically until reaching a minimum value, after which it increases monotonically. This behavior, which we have proven to be valid in general, allows us to apply a modified binary search to find the optimal threshold, yielding an exponential improvement over the otherwise required standard linear search.

In sequence, we prove bounds on the performance using two different statistical quantities as metrics, the standard scores and the quantile. In the first one, in an analogous way to what we did for the mean using the random variable Y, we abstract the standard deviation with the help of random variable Z, concluding that GM-Th-QAOA (it also holds GM-QAOA) is invariant over the two first statistical moments. That way, it becomes natural to abstract the expectation value in the quantity $C_r(t)$ such that $E_r(t) = \mu - C_r(t)\sigma$, which is the negative of what is called the standard score in statistics. To get bounds on the $C_r(t)$, we define $C^{Th}(r)$ as the maximum possible value achievable by

$C_r(t)$ on r layers. In particular, we prove with the assistance of Jensen's inequality that $C^{Th}(r)$ is asymptotically bounded by $\mathcal{O}(r)$. As an immediate consequence, we bound the number of layers to achieve a fixed approximation ratio $\lambda = E_r(t)/R_X^{min}$. Provided that $R_X^{min} \neq 0$ and $|R_X^{min}| < \infty$, we get

$$r \geq \frac{\mu - \lambda R_X^{min}}{(C^{Th}(r)/r)\sigma}, \tag{2}$$

where $C^{Th}(r)/r = \mathcal{O}(1)$. Worth mentioning that Eq. (2), in addition to being inserted in a more general context of combinatorial optimization, improves by a constant factor the bound of the Theorem 3 on Benchasattabuse et al. [Benchasattabuse et al. 2023] paper.

The other statistical bound is an asymptotic tight bound on the quantity $F_X(E_r(t))$, which represents the quantile where the expectation value of GM-Th-QAOA lies. A key advantage of this metric is its ability to directly relate the algorithm's performance to the underlying spectral distribution, enabling an equitable comparison across various probability distributions and optimization problems. To simplify the discussion on quantiles, we assume that X is a continuous random variable. This assumption is not merely a matter of convenience but is well justified, as QAOA primarily targets NP-hard optimization problems that exhibit enough scalability for this to be a reasonable approximation. Additionally, we assume that $f_X(R_X^{min})$ is finite and nonzero, another reasonable assumption since all target problems of QAOA have a finite optimal value. Under these conditions, we prove the following theorem.

Theorem 4.2 *For GM-Th-QAOA, if X is a continuous distribution and $f_X(R_X^{min}) = a$, where $0 < a < \infty$, then $F_X(E_r(t)_{opt}) = \Theta(1/r^2)$.*

Theorem 4.2 formally establishes a tight quadratic speed-up over classical brute force in the asymptotic limit, since with r round we achieve a quantile of order $1/r^2$, whereas a random sampling procedure would attain, in average, a quantile of order $1/r$.

To finish the analytical discussion of GM-Th-QAOA, we combine both statistical bounds, concluding that since Theorem 4.2 provides a fixed asymptotic scale of $1/r^2$ for the quantile, the evolution of the standard score $C_r(t)$ as the number of layers increases depends on how cdf behaves as approach the minimum value R_X^{min}. More precisely, we state that $C_r(t) = \Theta(|F_Z^{-1}(1/r^2)|)$. This result implies that the standard score of a distribution with cdf $F_Z(x)$ that presents an exponential decay must evolve logarithmically. It holds for key distributions in the literature, such as the normal distribution. Consequently, for an optimization problem where the probability distribution exhibits exponential decay, the number of rounds required to reach a fixed approximation ratio must grow exponentially larger than the tight bound of Eq. 2.

Other interesting bounds were obtained, such as the minimum number of rounds to measure an optimal solution with probability equal to 1 (i.e., exact optimization), given by $r = \Omega(1/\sqrt{f_X(R_X^{min})})$, another demonstration of quadratic speed-up.

As an additional study, to emphasize important aspects of the analytical results, we provide numerical experiments computing the expectation value expression of GM-QAOA and GM-Th-QAOA with different probability distributions, such as normal, gamma, and binomial distributions.

5. The statistical approach for Grover-based QAOA

A natural question is about the generality of the Theorem 4.2 to the context of QAOA with Grover mixer: is the quadratic speed-up over classical brute force the best we can extract from QAOA when we adopt Grover mixer? To address this, we extend the framework to a more general setting, introducing *Grover-based QAOA*, a variant of QAOA that, beyond Grover mixer and initial state $|s\rangle$, encompass a phase separation operator that encodes any real-valued function $q(k)$. In particular, we denote by E_r the expectation value of Grover-based QAOA. Using that generalization, we firstly prove in Lemma 5.1 that the amplification of the probability (i.e., the ratio between the probabilities on the final and the initial state of QAOA) over any set of degenerate states is quadratically bounded on the number of rounds. To prove this lemma, we use an argument by contradiction, showing that an amplification greater than that claimed to be the upper bound implies the existence of an algorithm for the unstructured search problem with greater average probability than Grover's algorithm, which we know to be optimal [Zalka 1999, Hamann et al. 2021].

Lemma 5.1 *For any number of layers in Grover-based QAOA, the amplification of the probability of measuring elements of a set of degenerated states is bounded by* $(2r+1)^2$.

On the constrained framework established by Lemma 5.1, we explicitly obtain the minimum expectation value by maximally amplifying the states with lower costs, resulting in an upper bound on the performance of Grover-based QAOA given by Theorem 5.1.

Theorem 5.1 *For any number* r *of layers in Grover-based QAOA,*

$$E_r \geq G_X(\tau_1)(2r+1)^2 + \tau_2(1 - F_X(\tau_1)(2r+1)^2), \tag{3}$$

where τ_1 *is the maximum element of the support of* X *in which* $F_X(t) \leq 1/(2r+1)^2$ *and* τ_2 *is the minimum element in which* $F_X(t) > 1/(2r+1)^2$.

The equality of Eq. (3) results in the same asymptotic behavior as GM-Th-QAOA in all metrics considered in this dissertation, including the bounds on the standard score and the quantile. The second mentioned metric is particularly important since under the same assumptions of Theorem 4.2, the quantile on Grover-based QAOA is bounded by $F_X(E_r) = \Omega(1/r^2)$, which implies that Grover-based QAOA is asymptotically limited to the quadratic a speed-up over classical brute force. This result is the most important contribution of this work, once proves the conjecture that the choice of Grover mixer restricts QAOA to the bound of the unstructured search problem.

To show the severity of our results, we apply it to the Max-Cut, a combinatorial optimization problem widely studied in the context of QAOA [Blekos et al. 2024]. By considering the particular class of the complete bipartite graphs, we use a combinatorial characterization of solution space without the explicit probability distribution to argue that the cdf must have a trend of exponential decay. Therefore, as the discussion done for GM-Th-QAOA applies to Grover-based QAOA, the number of layers required to achieve a fixed approximation ratio must grow exponentially with the number of vertices/edges of the graph. This limitation is quite critical since it is not possible to obtain a polynomial-time algorithm that guarantees any approximation ratio. Moreover, this construction indicates that the same phenomenon is likely to occur in other graph classes and even in different combinatorial optimization problems. This result contrasts with known results from other mixers, such as the approximation ratio guaranteed by the single layer QAOA with transverse field mixer on 3-regular graphs for Max-Cut problem [Farhi et al. 2014].

6. Concluding remarks

The results of this dissertation extend the margins of the knowledge of the theoretical potential of the Grover mixer as a mixing operator for QAOA. Among several bounds with different metrics of performance, the most significant culminates in the formal proof that the QAOA with Grover mixer has the performance bounded by the quadratic bound of the unstructured search, a limiting severe for combinatorial optimization, as evidenced by the application on Max-Cut. Nevertheless, the possibility of QAOA competing with classical computing remains. Recall the numerical evidence of exponential gain of QAOA with clique mixer over Grover mixer variants, provided by Golden et al. [Golden et al. 2023a]. However, the insights provided in this work highlight that to achieve competitive results, we need to work with algorithms that are capable of exploring the structure of combinatorial optimization problems. In the particular case of QAOA and its variants, this is necessarily linked to the choice of the mixing operator, since this operator provides the quantum interference between states encoding the solutions to the problem. Indeed, the clique mixer is a structure-dependent mixing operator. Therefore, future research should be focused on understanding the mechanisms by which mixing operator mixers can take advantage of the structure of combinatorial optimization problems. This research path was opened by Headley [Headley 2023], which extends the statistical approach to the transverse field mixer and a mixer called line (both structure-dependents).

The contributions of this work also are significant within a broader context. Despite the QAOA being a prominent quantum algorithm for combinatorial optimization, much of our knowledge of its general performance, as it was discussed, is empirical. Thereby, this work signifies a pivotal step towards a solid understanding of the performance and limitations of this class of algorithms, consequently providing insights into the potential of quantum computing for tackling combinatorial optimization problems.

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