Evidence for Super-Polynomial Advantage of QAOA over Unstructured Search

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We compare the performance of several variations of the Quantum Alternating Operator Ansatz (QAOA) on constrained optimization problems. Specifically, we study the Clique, Ring, and Grover mixers as well as the traditional objective value and recently introduced threshold-based phase separators. These are studied through numerical simulation on k-Densest Subgraph, Maximum k-Vertex Cover, and Maximum Bisection problems of size up to \( n = 18 \) on Erdős-Renyi graphs. We show that only one of these QAOA variations, the Clique mixer with objective value phase separator, outperforms Grover-style unstructured search, with a potentially super-polynomial advantage.

**Introduction** — The Quantum Alternating Operator Ansatz (QAOA) [1] is a quantum-classical heuristic algorithm for finding approximately optimum solutions for combinatorial optimization problems. Starting from an initial superposition of feasible solution states, QAOA repeatedly applies a phase separator operator followed by a mixer operator for a given number of rounds. The phase separator gives a phase to solutions according to the objective function to be optimized, and the mixer operator generates interference amongst states in order to amplify high-quality solutions. QAOA can be applied to a wide variety of combinatorial optimization problems by choosing an appropriate mixer and phase separator.

Determining the optimal operators for each problem, and the amount of phasing and mixing for each round, generates a large number of parameters to tune. This is akin to classical meta-heuristics, such as Simulated Annealing, Tabu Search, or Basin-hopping. Such heuristics usually do not give performance guarantees, but can outperform provable methods in practice in terms of runtime and solution quality. A key open question is whether QAOA shows such a practical advantage over other quantum or classical approximation algorithms.

The first step in addressing this question is to determine a classical or quantum benchmark that is a fair apples-to-apples comparison. In this work we argue that a useful optimization scheme must, at a minimum, outperform unstructured search for good solutions via Grover’s algorithm. We first show how this unstructured optimization approach can be recast as a QAOA, and then show through extensive numerical simulations that many previously introduced QAOA implementations fail to pass this bar on a variety of constrained optimization problems. However, QAOA with the Clique mixer [1] shows a potentially exponential speed-up as compared to Grover’s algorithm.

**QAOA Review** — A QAOA algorithm begins with an objective function \( C(x) \) encoding the optimization problem under consideration and a set of feasible solutions \( S = \{x\} \). One defines the cost Hamiltonian \( H_C \) by

\[
H_C |x \rangle = C(x) |x \rangle.
\]

The goal is to prepare a state \( |\psi \rangle \) from which one can sample high-quality solutions.

For the QAOA approaches considered here, we take our initial state as the uniform superposition of all feasible states, \( |\psi_0 \rangle = |S\rangle^{-1/2} \sum_{x \in S} |x \rangle \). For an unconstrained optimization problem of size \( n \), \( S \) is the set of all \( n \)-qubit computational basis states. For constrained optimization, \( S \) is restricted to some feasible subspace.

The quantum subroutine in QAOA consists of applying an alternating series of phase separator and mixer operators, defined in terms of Hamiltonians \( H_P \) and \( H_M \) respectively, on the initial state. The user inputs a number of rounds \( p \) along with arrays of angles \( \beta = \{\beta_1, \ldots, \beta_p\} \), \( \gamma = \{\gamma_1, \ldots, \gamma_p\} \), from which a quantum computer prepares the state

\[
|\beta, \gamma \rangle = e^{-i\beta_p H_M} e^{-i\gamma_p H_P} \ldots e^{-i\beta_1 H_M} e^{-i\gamma_1 H_P} |\psi_0 \rangle. \tag{1}
\]

Most commonly, a classical optimizer is used to tune the parameters \( \beta, \gamma \) in order to maximize \( \langle H_C \rangle := \langle \beta, \gamma | H_C |\beta, \gamma \rangle \) [1–3], but other cost functions have been suggested [4–7]. For problems with objective values in the range \( 0, \ldots, m \), there is an overhead polynomial in \( m \) to, with high probability, (i) get a sample above \( \langle H_C \rangle - 1 \) [2] and (ii) estimate \( \langle H_C \rangle \) within \( \pm 1 \) [8]. Moving forward, we adopt the standard terminology for maximizing the approximation ratio, given by

\[
\langle H_C \rangle / \max_{x \in S} C(x) \quad [9, 10].
\]

To begin the ith round of the QAOA, the phase separator unitary applies a phase \( e^{-i\gamma_i H_P} \) to each state, determined by the angle \( \gamma_i \) as well as the phase separator Hamiltonian \( H_P \). The traditional definition of QAOA [1] uses an objective value-based phase separator, where each state is phased equal to the objective value for that state, \( H_P = H_C \).

An alternative approach is to apply a phase only to states with an objective value above a threshold [11]. This threshold-based phase separator is defined for a given threshold parameter \( th \) as

\[
H_{Th} |x \rangle = \begin{cases} 0 & \text{if } C(x) \leq th, \\ |x \rangle & \text{otherwise.} \end{cases} \tag{2}
\]
This threshold is an additional parameter to be tuned to optimize QAOA performance.

After the phase separator unitary has applied a phase to each basis state, the mixing unitary $e^{-i\beta_j H_{Mj}}$ generates constructive and destructive interference between the states. Here we consider three implementations of the mixing operator. The Clique and Ring mixers [1], $H_{C_l}$ and $H_R$, are given by

$$H_{C_l} = \sum_{j>i} X_iX_j + Y_iY_j, \quad H_R = \sum_{j=i+1} X_iX_j + Y_iY_j. \quad (3)$$

Here $X$ and $Y$ refer to the standard Pauli operators. The Clique mixer sums over all pairs of qubits, while the Ring mixer includes only adjacent qubits along a chain with periodic boundary. The Grover mixer $H_G$ [12, 13] is given by

$$H_G = |\psi_0\rangle \langle \psi_0|. \quad (4)$$

The QAOA framework works with any combination of these mixers and phase separator operators. We refer to each choice by the name of the mixer followed by “-Obj” to refer to the objective value-based phase separator $H_{C_l}$, and “-Th” refers to the threshold-based phase separator $H_{Th}$.

Setting $\beta = \pi$ with the Grover mixer gives Grover’s diffusion operator, $e^{-i\pi|\psi_0\rangle \langle \psi_0|} = I - 2|\psi_0\rangle \langle \psi_0|$. Similarly, setting $\gamma = \pi$ with the threshold phase separator gives a phase of -1 to all states with objective value above the threshold and +1 to states below the threshold. Therefore the Grover-Th implementation QAOA with all angles set to $\pi$ is exactly equivalent to Grover’s search for states above a given threshold [14]. Furthermore, it was shown in [11] that $\beta_j = \gamma_j = \pi$ are the optimal angles for Grover-Th. This is distinct from the Grover-like QAOA implementation of [15] in that the circuit-level implementation is indistinguishable from Grover, and it is applicable to both constrained and unconstrained problems [12, 13].

Since the asymptotic scaling of Grover’s algorithm is known, this provides a natural benchmark to test other QAOA variants against. In making this comparison, we use the number of rounds $p$ as a proxy for algorithmic runtime. This ignores two additional sources of complexity: finding good angles and thresholds as well as the depth of the circuit-level implementations. We discuss angle-finding in a later section, and threshold-finding in the Appendix. All of these mixers and phase separators can be implemented exactly with polynomial-size circuits for the optimization problems we consider (see Appendix for a description of the circuits) although their precise complexity is an active research topic [16–18]. An approximate implementation through Trotterization largely eliminates size differences, and so it is common in QAOA analysis to compare different mixers purely on a per-round basis [8, 13].

Results — We performed numerical simulations of all six combinations of mixers and phase separators – Clique-Obj, Clique-Th, Ring-Obj, Ring-Th, Grover-Obj, and Grover-Th – on three constrained optimization problems. Of these combinations, only Clique-Obj consistently outperformed Grover-Th, as shown in Fig. 1.

The problems we considered were $k$-Densest Subgraph, Maximum $k$-Vertex Cover, and Maximum Bisection. These problems are defined on an undirected graph $G(V, E)$ with $|V| = n$. $k$-Densest Subgraph is the problem of finding the subgraph with $k$ vertices that contains the most edges, while Max $k$-Vertex Cover is the problem of finding the $k$ vertices that cover the most edges. Max Bisection is defined only for $k = n/2$ and asks for the
partition of the graph into two equal subgraphs with the most edges crossing between partitions. If the adjacent vertices of $e \in E$ are labeled as $v_1^e$ and $v_2^e$, these problems are formally defined as
\[ \text{maximize} \sum_{e \in E} f(v_1^e \in V', v_2^e \in V') \tag{5} \]
over all $V' \subset V$ with $|V'| = k < n$, where $f = \text{AND, OR, XOR}$ for $k$-Densest Subgraph, Max $k$-Vertex Cover and Max Bisection respectively.

The decision versions of these problems are NP-hard for general graphs; the optimization variants considered here cover a broad spectrum in their known complexity results: Max Bisection is MaxSNP-complete [19] and the approximation hardness carries over from Max Cut, i.e. there is no polynomial-time approximation better than $\approx 0.941$ unless $P = NP$ [20], or better than $\approx 0.878$ under the Unique Games Conjecture [21]. The current best polynomial-time approximation ratio $0.8776$ is achieved with estimated runtime $O(n^{0.1004})$ [22]. For Max $k$-Vertex Cover, the corresponding known upper and lower bounds on polynomial-time approximation are $(1 - \delta)$ for a small $\delta$ [23, NP-hardness], $0.944$ [24, 25, UGC-hardness], $0.92$ [25, approximation algorithm]. Similarly, $k$-Densest Subgraph has no PTAS (polynomial-time approximation scheme) under various complexity-theoretic assumptions [26, 27], and the best known polynomial-time achievable approximation ratio is $n^{-1/4-\epsilon}$ for all $\epsilon > 0$ [28].

For these problems, the QAOA algorithm uses $n$ qubits and only computational basis states with Hamming weight $k$, i.e. exactly $k$ qubits set to 1, represent feasible solutions. This gives a total of $n \choose k$ feasible solutions, and the equal superposition of them is the Dicke state $|D^n_k\rangle$, which can be prepared in depth $O(n)$ [18]. We focus on these constrained optimization problems be-

FIG. 2. Round-by-round performance comparison for all QAOA implementations under consideration across $k$-Densest Subgraph, Max $k$-Vertex Cover, and Max Bisection for $n = 8, 10, 12$ and $k = n/2$, averaged over 12 problem instances on graphs of type $G(n, 0.5)$. 
cause the Clique, Ring, and Grover mixers preserve Ham-
ing weight and provide transitions between all feasible states.

Our metric for performance in these comparisons is the number of rounds necessary to achieve an approximation ratio of 0.99 (we also give results for the lower target of 0.95 in the Appendix). With such a high approximation target, we can clearly observe in Fig. 1 the expected Grover-Th scaling of \( O\left(\frac{\alpha}{n^{1/2}}\right) \) as problem size increases.

Clique-Obj outperforms Grover-Th with a potentially super-polynomial speedup for all three problem classes, with fewer data-points collected for Max Bisection due to less efficient angle finding, discussed in the next Section.

For each problem class we evaluated the number of rounds necessary to reach .99 approximation ratio across 40 random instances for each \( n \). We then performed a weighted least squares fit of this data to both a logarithm ansatz, \( a \log(bn + c) \) and a polynomial ansatz, \( an^p + c \). As seen in Fig. 1, the logarithm ansatz provided a very close fit for \( k \)-Densest Subgraph and Max \( k \)-Vertex Cover, while Max Bisection could only be fit to the polynomial ansatz. Both \( k \)-Densest Subgraph and Max \( k \)-Vertex Cover could also be fit to the polynomial ansatz, with exponent \( \leq 0.075 \) at 95% confidence level. Hence independent of the choice of fit, the data heavily suggests that for large graph problems, e.g. \( 10^{10} \) nodes, the mean number of rounds to achieve a high approximation ratio for these problems is \( O(100) \).

We found that Grover-Th consistently outperformed the remaining QAOA operator choices – Clique-Th, Grover-Obj, Ring-Th, and Ring-Obj. We compared the mean performance over 12 random instances for each operator combination across the three problem classes at \( n = 8, 10, 12 \) with \( k = n/2 \), see Fig. 2. For \( n = 8 \), Grover-Th is the best performing mixer for all problem classes, however by \( n = 10 \) Clique-Obj has largely surpassed Grover-Th. Meanwhile, the remaining mixers remain below Grover-Th, without a clear indication of an improvement as \( n \) increases. We give more details on the performance of these other approaches, and potential for future study, in the following section.

Discussion — The approximation ratios of the different QAOA implementations generally followed the pattern Clique-Obj \( \geq \) Grover-Th \( \geq \) Clique-Th \( \geq \) Grover-Obj \( \geq \) Ring-Obj \( \geq \) Ring-Th, though some difference in rankings is present at lower \( n \). For Clique and Ring mixers, the -Obj phase separator outperformed the -Th version. This is in contrast to the Grover mixer, where Grover-Th always beat Grover-Obj (consistent with findings from [11], which extend up to \( n = 40 \)). Clique-Obj performed almost identically to Grover-Th for Max Bisection, but was worse for \( k \)-Densest Subgraph and Max \( k \)-Vertex Cover.

The observation that Clique-Obj significantly outperforms Grover-Th is dependent on two important elements: robust angle finding and large problem size.

Angle Finding: Our initial studies employed the traditional basin-hopping approach [16], which uses a random initial collection of angles to begin optimizing for a \( p \)-round QAOA. However we observed improved performance by using an inductive approach, partially inspired by [8]. Specifically, for a given problem we take the optimal angles for the \( (p - 1) \)-round QAOA, \( \beta_{p-1} = \{\beta_1, \ldots, \beta_{p-1}\} \), \( \gamma_{p-1} = \{\gamma_1, \ldots, \gamma_{p-1}\} \), and begin our basin-hopping search for angles for the \( p \)-round QAOA with

\[
\beta_p = \{\beta_1, \ldots, \beta_{p-1}, \beta_p\}, \quad \gamma_p = \{\gamma_1, \ldots, \gamma_{p-1}, \gamma_p\}.
\]

For example, at \( n = 12 \) Clique-Obj with our extrapolated basin-hopping approach outperforms Grover-Th, whereas Clique-Obj with random basin-hopping does not, see Fig. 3.

For the specific case of Clique-Obj on \( k \)-Densest Subgraph and Max \( k \)-Vertex Cover, we observed over thousands of examples that the basin-hopping algorithm never left the local optimum it arrived at after starting at the extrapolated point. Therefore, in order to accelerate our analysis we found the angles for round \( p \) by just using Gradient Descent beginning at Eq. (6).

Due to the optimality of Grover’s algorithm for unstructured search, the performance gains from Clique-Obj must come from exploiting the structure of each individual problem instance via angle-finding. A common concern for asymptotic QAOA performance is the complexity of finding good angles. These results show that relatively simple and low-complexity angle-finding heuristics can exist for problems of interest up to roughly 30 rounds. There are several additional sources of overhead which in our experience did not significantly contribute: finding angles for rounds \( 1, \ldots, p-1 \) before the angles for round \( p \) can be found, the cost of Gradient

![FIG. 3. Relative performance difference for Clique-Obj with basin-hopping from an extrapolated initial point versus a random initial point, averaged over 12 \( k \)-Densest Subgraph problem instances with \( n = 12, k = 6 \).](image)
Descent for each round, and the cost of finding the optimal threshold for Grover-\(\text{Th}\) for a given round. See the Appendix for more information on angle- and threshold-finding.

**Problem Size:** The simplified angle-finding heuristic described above reduced our simulation time by a factor of 100 for Clique-\(\text{Obj}\) on \(k\)-Densest Subgraph and Max \(k\)-Vertex Cover, which allowed us to analyze problems up to \(n = 18\) and \(p \approx 30\), with the largest problem instances taking \(\mathcal{O}(1 \text{ day})\) compute time on an NVIDIA RTX A6000 with 48GB of memory. For Max Bisection we required the full basin-hopping approach to get good results, and thus were only able to extend our results to \(n = 14\). Analyzing problems of this size proved critical, as the improved performance of Clique-\(\text{Obj}\) is only evident for \(n \geq 12\). This emphasizes the need for future study at large \(n\).

In this work we have only studied random graphs with edge probability = 0.5 and we have restricted to the cases \(k = n/2\) for \(k\)-Densest Subgraph and Max \(k\)-Vertex Cover. Additional analysis is necessary to see if the relative QAOA implementation performance persists in other graph types, particularly since dense graphs often admit a classical PTAS [29]. However, we note that in [11] Grover-\(\text{Obj}\) was compared against Grover-\(\text{Th}\) on the same problem classes as well as Max Cut, with differing edge probabilities and \(k\) values. In these comparisons there was little variation in relative performance (with Grover-\(\text{Th}\) always outperforming Grover-\(\text{Obj}\)) across this more diverse set of problems.

The results for Clique-\(\text{Th}\), Ring-\(\text{Th}\), and Ring-\(\text{Obj}\) for \(n \leq 12\) do not suggest a high likelihood of outperforming Grover-\(\text{Th}\), however we cannot rule this possibility out. For example, we see in Fig. 2 that in the final round of Max Bisection results at \(n = 12\), Clique-\(\text{Th}\) outperformed Grover-\(\text{Th}\). Extending these results to even higher \(n\), or discovering improved angle-finding techniques, may show further relative performance gains.

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Appendix

Mixer & Phase Separator Circuit Implementation

All of the mixers and phase separators considered in this work can be implemented in polynomial depth:

- **Objective Value Phase Separator**: $H_C$ consists of Quadratic and (except for Max Bisection) Linear Pauli-Z terms, which pairwise commute, and hence can be implemented individually (e.g. with depth at most $O(n)$ using a SWAP network [3, 30]).

- **Threshold Phase Separator**: The cost $C(x)$ can be added into a Two’s Complement [31] ancilla register, initialized with $-th - 1$. Phasing can then be done simply by (inverse) phasing of the leading qubit which encodes the sign information, followed by an uncomputation of the register.

- **Ring Mixer**: The Jordan Wigner Transform maps the Ring Mixer Hamiltonian to a quadratic fermionic Hamiltonian [16]. If $n$ is a power of two and the Hamming weight is odd, this Hamiltonian can be diagonalized using the fermionic fast Fourier transformation [32, 33], a method which can be extended if $n$ has only small prime factors [34]. Otherwise, one can also use a Givens’ rotation network [35].

- **Clique Mixer**: The Clique Mixer, as a permutation-invariant qubit Hamiltonian [17], can be diagonalized using the Schur Transform [36]. In particular, this results in phasing according to the total angular momentum.

- **Grover Mixer**: For Hamming-weight constrained problems, the Grover Mixer [12] can be implemented with a $n$-controlled phase shift together with Dicke State preparation unitaries [18].

Angle and Threshold Finding

See Fig. 4 for results comparing the extrapolated basin-hopping angle-finding scheme, Eq. 6, against basin-hopping from a random initial point.

Threshold-based phase separators require an algorithm for determining the optimal threshold for a given number of rounds $p$. The simplest approach is to try every possible threshold value. This is generally not too computationally onerous as constrained optimization problems, such as those considered in this work, have a number of distinct objective values which grows at-worst polynomially with problem size. For example, $k$-Densest Subgraph, Max $k$-Vertex Cover, and Max Bisection can have at most $O(n^2)$ distinct objective values. However, robust numerical experimentation points to the several improvements that can be made over this brute force search. As an example see Fig. 5, where we plot approximation ratio as a function of threshold for a single $n = 8, k = 4$ $k$-Densest Subgraph problem over 8 rounds. This example showcases several salient points which we can use to improve our threshold-finding.

First, for all mixers the threshold which produces the highest approximation ratio for a given round $p$ is always greater than or equal to the threshold which produced the highest approximation ratio for round $p - 1$. In practice, this heavily constrains the search space as even for $p = 1$ the threshold which produces the highest approximation ratio tends to be reasonably large.

Second, with Grover-Th, for a given round the approximation ratio as a function of threshold monotonically increases up to a peak value, then monotonically decreases. This peak structure allows for a modified binary search, as introduced in [11].

Third, Clique-Th and Ring-Th do not necessarily follow this peak structure, therefore at round $p$ one must conduct an exhaustive search of all threshold values above the optimal $p - 1$ threshold value.

**Results for 0.95 Approximation Ratio**

In Fig. 6 we give results for Clique-Obj and Grover-Th with a target of 0.95 approximation ratio. This better captures the performance for truly approximate optimization, as opposed to the 0.99 approximation ratio, which for the problems under consideration is very close to optimal. In these results, the expected exponential scaling for Grover-Th is less obvious, due to the relatively large fraction and highly varied distribution of high-quality solutions in low-$n$-problem instances. However, Clique-Obj starts to outperform Grover-Th at even
FIG. 4. Comparing angle finding with basin-hopping starting at random initial point versus an extrapolated initial point. This is averaging results over 12 random $n = 8$, $k = 4$ $k$-Densest Subgraph problems, and 100 basin-hopping iterations per round.

FIG. 5. Approximation ratio as a function of threshold for Clique-Th, Ring-Th, and Grover-Th over 8 rounds on a single $n = 8$, $k = 4$ $k$-Densest Subgraph problem.

smaller problem sizes than in the 99% target approximation plots in Figure 1.
FIG. 6. Performance comparison for Clique-Obj and Grover-Th on $k$-Densest Subgraph and Max $k$-Vertex Cover from $n = 4$ through $n = 18$, and Max Bisection from $n = 4$ through $n = 14$. Square points represent average performance across 40 problem instances per $n$ on graphs of type $G(n, 0.5)$, except for $n = 4$ where we study all 64 possible four-vertex graphs. Vertical bars represent standard deviation across the problem instances.