Classical algorithms for Forrelation

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Abstract

We study the forrelation problem: given a pair of $n$-bit boolean functions $f$ and $g$, estimate the correlation between $f$ and the Fourier transform of $g$. This problem is known to provide the largest possible quantum speedup in terms of its query complexity and achieves the landmark oracle separation between the complexity class BQP and the Polynomial Hierarchy. Our first result is a classical algorithm for the forrelation problem which has runtime $O(n^{2^{n/2}})$. This is a nearly quadratic improvement over the best previously known algorithm. Secondly, we introduce a graph-based forrelation problem where $n$ binary variables live at vertices of some fixed graph and the functions $f, g$ are products of terms describing interactions between nearest-neighbor variables. We show that the graph-based forrelation problem can be solved on a classical computer in time $O(n^2)$ for any bipartite graph, any planar graph, or, more generally, any graph which can be partitioned into two subgraphs of constant treewidth. The graph-based forrelation is simply related to the variational energy achieved by the Quantum Approximate Optimization Algorithm (QAOA) with two entangling layers and Ising-type cost functions. By exploiting the connection between QAOA and the graph-based forrelation we were able to simulate the recently proposed Recursive QAOA with two entangling layers and 225 qubits on a laptop computer.

1 Introduction

Much of what is known about the power of quantum computers has been learned by studying the black-box model of quantum query complexity. Here one considers a kind of computational problem where the input is a binary string $x \in \{-1, 1\}^N$ and the goal is to compute some property of the input by accessing or querying as few bits of $x$ as possible. In a classical algorithm we may query the input bits one at a time, whereas in a quantum algorithm each query is performed by applying a unitary oracle $O_x$ satisfying $O_x|i\rangle = x_i|i\rangle$ for $i \in [N]$. Many computational problems have been shown to admit quantum speedups as measured by query complexity, including e.g., quantum search [1], period finding [2], and the hidden subgroup problem [3, 4]. These and other provable speedups in quantum query complexity inform the search for real-world quantum advantage. For example, Shor’s algorithm for integer factorization is based on the quantum algorithm for period finding [2]. The conjectured

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real-world speedup for this problem is predicated on the belief that the additional structure present in the integer factorization problem does not make it significantly easier for classical computers.

In this paper we study the forrelation problem which was introduced in Ref. [5]. Forrelation is a powerful computational primitive: it achieves an almost maximal quantum speedup as measured by query complexity [6, 7, 8] and it underlies the dramatic oracle separation between the complexity classes BQP and PH [9]. Moreover, a generalized \( k \)-fold forrelation problem is BQP-complete [6]. We note that the primary focus of these previous works was to lower bound the classical query complexity of forrelation and related problems. In this paper we develop new classical algorithms for forrelation. Firstly in the black-box setting, and then in an explicit graph-based setting which is related to the performance of certain quantum algorithms for optimization [10].

To describe our results in more detail, let us now define the forrelation problem, following Aaronson and Ambainis [5, 6]. The input to the problem is a pair of Boolean functions \( f, g : \{0, 1\}^n \to \{1, -1\} \). The forrelation between \( f \) and \( g \) is defined as

\[
\Phi(f, g) = 2^{-3n/2} \sum_{x,y \in \{0,1\}^n} f(x)g(y)(-1)^{x \cdot y}.
\]

The forrelation quantifies the correlations between \( f \) and the binary Fourier transform of \( g \). Approximating \( \Phi(f, g) \) with a small additive error is known as the forrelation problem.

Forrelation problem. Given \( f, g : \{0, 1\}^n \to \{1, -1\} \) and \( \epsilon > 0 \), compute an estimate \( \mu \) such that \(|\mu - \Phi(f, g)| \leq \epsilon\).

A simple quantum algorithm can approximate \( \Phi(f, g) \) by querying oracles \( U_f \) and \( U_g \) implementing diagonal unitary operators \( U_f|x\rangle = f(x)|x\rangle \) and \( U_g|x\rangle = g(x)|x\rangle \), as can be seen from the identity

\[
\Phi(f, g) = \langle 0^n|H^\otimes nU_fH^\otimes nU_gH^\otimes n|0^n \rangle.
\]

Using this identity, one can express the forrelation as \( \Phi(f, g) = 1 - 2p \) where \( p \) is the output probability of a quantum circuit that makes only 1 query to an \((n + 1)\)-bit oracle that computes either \( f \) or \( g \) depending on the value of an ancilla bit. This output probability can be estimated to within additive error \( \epsilon \) using amplitude estimation [11]. In this way we can solve the forrelation problem on a quantum computer using only \( O(\epsilon^{-1}) \) queries to the oracles \( U_f \) and \( U_g \).

While this algorithm approximates \( \Phi(f, g) \) to within a small constant error using \( O(1) \) quantum queries, Aaronson and Ambainis have shown that any classical algorithm achieving the same requires \( \Omega(n^{-12n/2}) \) queries. They also established that the output probability of any 1-query quantum algorithm can be approximated to a given constant error by a classical randomized algorithm using \( O(2^{n/2}) \) queries [6]. In other words—among tasks that can be solved with a bounded error using 1 quantum query—forrelation has an almost maximal randomized query complexity.

In fact, a very simple classical algorithm suggested by Aaronson in Ref. [5] (see Section 5 of that paper) is almost optimal in terms of query complexity. One first samples random
\( n \)-bit strings \( x_1, \ldots, x_L \) and \( y_1, \ldots, y_L \) and then computes the sample forrelation

\[
Z = L^{-2}2^{n/2} \sum_{i,j=1}^{L} f(x_i)g(y_j)(-1)^{x_i \cdot y_j}
\]  

(1)

It is easy to see that \( \mathbb{E}[Z] = \Phi(f, g) \) and one can also show that using \( L = O(\epsilon^{-1}2^{n/2}) \) samples suffices to ensure that \( Z \) approximates the forrelation within an additive error \( \epsilon \) with high probability. The total number of queries required by this algorithm is \( 2L \) which almost matches the lower bound on classical query complexity. However, computing Eq. (1) seems to require summing \( L^2 \) terms, and so the runtime of this algorithm is quadratically worse than the query complexity. Our first contribution provides the following improvement:

**Theorem 1.** There is a classical randomized algorithm that solves the forrelation problem with probability at least 99%. The algorithm has query complexity \( O(\epsilon^{-1}2^{n/2}) \) and runtime \( O(n\epsilon^{-1}2^{n/2}) \).

To prove the theorem, we approximate \( \Phi(f, g) \) using a variant of the sample-based forrelation Eq. (1) in which the sets \( \{x_1, \ldots, x_L\} \subseteq \mathbb{F}_2^n \) and \( \{y_1, \ldots, y_L\} \subseteq \mathbb{F}_2^n \) are chosen to be random affine subspaces with \( L = 2^\ell \) for suitably chosen \( \ell \approx n/2 \). To establish the claimed runtime bound we show that this estimator can equivalently be expressed as an amplitude of a quantum circuit acting on \( \ell \) qubits and computed using a runtime \( \sim 2^\ell \) using sparse matrix-vector multiplication.

Ref. [6] also introduces a more general \( k \)-fold forrelation of Boolean functions \( f_1, f_2, \ldots, f_k : \{0, 1\}^n \to \{-1, 1\} \) defined as

\[
\Phi(f_1, f_2, \ldots, f_k) = \langle 0^n | H^{\otimes n} U_{f_1} H^{\otimes n} U_{f_2} H^{\otimes n} \ldots U_{f_k} H^{\otimes n}|0^n \rangle.
\]  

(2)

As in the case \( k = 2 \) considered above, the \( k \)-fold forrelation can be expressed as \( 1 - 2p \) where \( p \) is the output probability of a quantum circuit that makes \( \lceil k/2 \rceil \) queries to the oracles. This output probability, and the forrelation, can be additively approximated by a quantum computation that makes \( O(ke^{-1}) \) queries. Using the well-known connection between quantum query algorithms and multilinear polynomials over \( \mathbb{F}_2 \) [12], Aaronson and Ambainis proved that any amplitude of a \( k \)-query quantum circuit—and consequently, the \( k \)-fold forrelation—can be additively approximated by a classical randomized algorithm which uses \( O(2^k e^{-2+\frac{k}{2}} 2^{n(1-\frac{1}{k})}) \) queries. They conjectured that a matching lower bound holds for each even \( k = O(1) \) and constant error \( \epsilon \). That is, their conjecture asserts that the \( k \)-fold forrelation should have maximal classical query complexity among quantities that can be expressed as the output probability of a \( k/2 \) query quantum algorithm. A slight relaxation of this conjecture was established by Bansal and Sinha who showed that for every positive integer \( k \), approximating the \( k \)-fold forrelation to within an error \( \epsilon \) satisfying \( \epsilon^{-1/k} = 64k^2 \log(k \cdot 2^n) \) requires \( \Omega(2^{n(1-\frac{1}{k})}/\text{poly}(n, k)) \) oracle queries using a classical computer [8].

Here we provide a simple classical algorithm which achieves an exponential improvement in terms of the scaling with \( k \) and improves the dependence on \( \epsilon \), as compared with Ref. [6].
Theorem 2. There exists a classical randomized algorithm which approximates $\Phi(f_1, f_2, \ldots, f_k)$ to within additive error $\epsilon$ with probability at least 99%, and uses $O(k\epsilon^{-2/k}2^{n(1-\frac{1}{k})})$ oracle queries.

Note that if we choose $\epsilon = \epsilon(n,k)$ as prescribed by Bansal and Sinha, then for each $k$ the randomized simulation matches their lower bound up to factors polynomial in $n$ and $k$. As in Ref. [6], our proof of Theorem 2 follows from a more general simulation of quantum query algorithms. In particular, in Section 2 we establish that any amplitude of a $k$-query quantum algorithm can be approximated by a classical algorithm with query complexity as described in Theorem 2.

Next we consider a graph-based forrelation problem with explicitly specified functions $f$ and $g$ that possess certain local features. Suppose $G = (V, E)$ is a fixed $n$-vertex graph. We place a binary variable $x_j$ at each vertex $j \in V$. We say that a function $f : \{0, 1\}^n \rightarrow \mathbb{S}^1$ is two-local on $G$ if it is a product of terms describing interactions between nearest-neighbor variables, as well as terms that depend on a single variable, that is,

$$f(x) = \prod_{\{u,v\} \in E} f_{uv}(x_u, x_v) \prod_{u \in V} f_u(x_u)$$

for some functions $f_{uv} : \{0, 1\}^2 \rightarrow \mathbb{S}^1$ and $f_u : \{0, 1\} \rightarrow \mathbb{S}^1$. Here $\mathbb{S}^1$ is the unit circle in the complex plane. We shall use the term two-local without specifying the underlying graph whenever it is clear from the context. A function $f(x)$ is said to be 1-local if it is a product of terms depending on a single variable.

Suppose $O_1, \ldots, O_n$ are single-qubit operators normalized such that $\|O_j\| \leq 1$ for all $j$. A graph-based forrelation associated with the graph $G$ and two-local functions $f, g$ is defined as a complex number

$$\Phi = \langle 0^n | H^\otimes n U_g (O_1 \otimes O_2 \otimes \cdots \otimes O_n) U_f H^\otimes n | 0^n \rangle. \quad (3)$$

As before, $U_f$ and $U_g$ are diagonal $n$-qubit unitary operators such that $U_f|x\rangle = f(x)|x\rangle$ and $U_g|x\rangle = g(x)|x\rangle$ for all $x$. Note that such operators can be implemented efficiently by quantum circuits for any two-local functions. Furthermore, the operators $O_j$ can be extended to two-qubit unitary operators using a block encoding, see e.g. Lemma 5 of [13]. Thus the graph-based forrelation can be efficiently approximated to a given additive error using a quantum computer. A natural question is whether or not it is classically hard to approximate a graph-based forrelation to within a given additive error. Unfortunately the exponential lower bound on the query complexity established in the black-box setting does not rule out an efficient classical algorithm that can “look inside” the black box.

Our interest in graph-based forrelation is partly motivated by its connection with algorithms for near-term quantum computers and restricted models of quantum computation. For example, one can show that the expected value of any tensor product operator on the output state of an $n$-qubit Clifford circuit can be expressed as a graph-based forrelation for a suitable $n$-vertex graph $G$ and two-local functions $f = g$ (in particular, an output

\[\text{This claim follows from the well-known fact [14] that the output state of any Clifford circuit acting on } n \text{-qubits is locally equivalent to a graph state } \prod_{(u,v) \in E} \text{CZ}_{u,v} H^\otimes n | 0^n \rangle \text{ for a suitable } n\text{-vertex graph } G = (V, E).\]
probability of a measurement based quantum computation [15] can be expressed as a graph-based forrelation). Similarly, an amplitude of any IQP circuit [16] composed of one- and two-qubit gates can be expressed as a graph-based forrelation with \( O_j = H \) for all \( j \). In Appendix A we provide more details and ascertain as a simple consequence that approximating a graph-based forrelation with a given relative error is \( \#P \)-hard, even when restricted to planar graphs.

A graph-based forrelation appears naturally in the study of Quantum Approximate Optimization Algorithm (QAOA) [10]. Namely, consider \( n \) qubits located at vertices of the graph \( G \) and a cost function Hamiltonian \( C = \sum_{\{u,v\} \in E} J_{u,v}Z_uZ_v \), where \( J_{p,q} \) are arbitrary coefficients. Level-\( k \) QAOA maximizes the expected energy \( \langle \psi | C | \psi \rangle \) over variational states

\[
|\psi\rangle = e^{-i\beta_k B}e^{-i\gamma_k C} \ldots e^{-i\beta_1 B}e^{-i\gamma_1 C}H^{\otimes n}|0^n\rangle,
\]

where \( B = X_1 + \ldots + X_n \) and \( \beta, \gamma \in \mathbb{R}^k \) are variational parameters. In Section 4 we show that the variational energy \( \langle \psi | C | \psi \rangle \) of level-2 QAOA states can be expressed as a linear combination of a few graph-based forrelations with suitable single-qubit operators \( O_j \) and 2-local functions \( f = g \) simply related to \( C \). Thus a polynomial-time classical algorithm for graph-based forrelation can be used to efficiently estimate the variational energy of level-2 QAOA states. Prior to our work such an algorithm was only known for the case of constant-degree graphs, or for level-1 QAOA states on general graphs [17].

Our main result is a classical algorithm for approximating graph-based forrelation with a given additive error. The algorithm is efficient whenever the vertices of \( G \) can be partitioned into two disjoint subsets \( A \) and \( B \) such that the subgraphs \( G_A \) and \( G_B \) induced by \( A \) and \( B \) have a small treewidth. Let \( w \) be the maximum width of these tree decompositions. Our algorithm is described in the following theorem.

**Theorem 3.** There is a classical randomized algorithm that outputs an estimate \( \mu \) satisfying \( |\mu - \Phi| \leq \epsilon \) with probability at least 99\%. The algorithm has runtime \( O(n^2 w 4^w \epsilon^{-2}) \).

For example, suppose \( G \) is a bipartite graph. Then we may take the subgraphs \( G_A \) and \( G_B \) to have no edges. In this case \( w = 1 \) and our algorithm has a runtime \( O(n^2 \epsilon^{-2}) \). A more sophisticated application is obtained by considering planar graphs \( G \). As discussed in Section 3.1, the requisite partition of vertices with \( w = 2 \) can be computed efficiently for any planar graph \( G \) and thus our algorithm has runtime \( O(n^2 \epsilon^{-2}) \). The same runtime scaling holds for any family of graphs with a fixed forbidden minor [18]. Thus Theorem 3 provides an efficient classical method for calculating variational energies of the level-2 QAOA for any bipartite or any planar graph. As a demonstration, we report a classical simulation of the recently proposed Recursive QAOA [19] on planar graphs with the level-2 variational states, see Section 4 for details. For example, simulating the Recursive QAOA with \( n = 225 \) qubits on a laptop computer took less than one day. To accomplish this simulation we had to solve about 300,000 instances of the graph-based forrelation problem.

In order to convey the main ideas, let us now describe how the algorithm claimed in Theorem 3 works in the simplest case where \( G \) is a bipartite graph and all operators \( O_j \) are unitary. Partition the vertices of \( G \) as \( V = A \cup B \) such that every edge of \( G \) connects a vertex in \( A \) and a vertex in \( B \). Note that the subgraphs \( G_A \) and \( G_B \) are trivial in this case (each subgraph has an empty set of edges). Let \( O_A \) and \( O_B \) be the tensor products of operators
and we describe how our algorithm for graph-based forrelation can be used to estimate the variational energy of level-2 QAOA algorithms.

Thus it suffices to approximate the mean value of a random variable $R(x)$ with $x$ sampled from $P(x)$. Fix an integer $S \gg 1$ and let $x^1, \ldots, x^S \in \{0,1\}^n$ be independent samples from $P(x)$. Define the desired estimate of $\Phi$ as an empirical mean value of $R(x)$ over the observed samples, $\mu = (R(x^1) + R(x^2) + \ldots + R(x^S))/S$. The random variable $R(x)$ has the mean value $\Phi$ and its variance is bounded as

$$\text{Var}(R) \leq \sum_{x \in \{0,1\}^n} P(x)|R(x)|^2 = \sum_{x \in \{0,1\}^n} |\langle x | \beta \rangle|^2 = 1. \quad (4)$$

By the Chebyshev inequality, $|\mu - \Phi| \leq \epsilon$ with probability at least 0.99 if we choose $S = 100\epsilon^{-2}$.

The above algorithm is efficient whenever efficient subroutines are available for computing amplitudes of the states $|\alpha\rangle$, $|\beta\rangle$ and for sampling the probability distribution $|\langle x | \alpha \rangle|^2$. In Section 3 we prove Theorem 3 by constructing the desired subroutines for more general (non-bipartite) graphs that admit a partition into two subgraphs with a small treewidth. We leave as an open question complexity of the graph-based forrelation problem on general graphs.

The remainder of the paper is organized as follows. Our results concerning oracle-based forrelation, i.e., the proofs of Theorems 1 and 2, are provided in Section 2. In Section 3 we describe the classical algorithm for graph-based forrelation and prove Theorem 3. Finally, in Section 4 we describe how our algorithm for graph-based forrelation can be used to estimate the variational energy of level-2 QAOA algorithms.
2 Oracle-based forrelation

In this section we consider the forrelation problem in which functions $f, g$ are accessed via oracle queries. We begin by proving Theorem 1, restated below.

Theorem 1. There is a classical randomized algorithm that solves the forrelation problem with probability at least 99%. The algorithm has query complexity $O(\epsilon^{-1}2^{n/2})$ and runtime $O(n\epsilon^{-1}2^{n/2})$.

Proof. Let $\epsilon > 0$ be given. If $\epsilon \leq 2^{-n/2}$ then we use a very naive algorithm to compute $\Phi(f, g)$ exactly using the desired total runtime $O(n2^n)$ and $O(2^n)$ queries. Indeed, in this case it suffices to exactly compute a length $2^n$ vector $H^{\otimes n}U_gH^{\otimes n}U_fH^{\otimes n}|0^n\rangle$ using matrix vector multiplication. Applying each single-qubit Hadamard gate using sparse matrix-vector multiplication requires a runtime $O(2^n)$ while applying each gate $U_f$ or $U_g$ uses $O(2^n)$ queries. The forrelation $\Phi(f, g)$ is then obtained as the $0^n$ entry of this vector.

In the following we consider the case $\epsilon \geq 2^{-n/2}$.

Let $A_{n,k}$ be the set of all affine spaces $S \subseteq \mathbb{F}_2^n$ with $|S| = 2^k$. For each $S \in A_{n,k}$ define a normalized $n$-qubit stabilizer state $|S\rangle = 2^{-k/2} \sum_{x \in S} |x\rangle$.

For any pair $S, T \in A_{n,k}$, define

$$\mu(S, T) = 2^{n-k} \langle S|U_fH^{\otimes n}U_g|T\rangle.$$ (6)

Claim 1. Suppose $S, T \in A_{n,k}$ are drawn uniformly at random. Then

$$\mathbb{E}(\mu(S, T)) = \Phi(f, g) \quad \text{and} \quad \text{Var}(\mu(S, T)) \leq 2^{n-2k} + \frac{2}{2^k}. \quad (7)$$

Proof. For any $x \in \mathbb{F}_2^n$, let $\chi_S(x) = 1$ if $x \in S$ and $\chi_S(x) = 0$ otherwise. Then

$$\mathbb{E}_S(\chi_S(x)) = \frac{|S|}{2^n} = 2^{k-n}. \quad (8)$$

Likewise, for any pair of binary strings $x, y \in \mathbb{F}_2^n$ such that $x \neq y$ we have

$$\sigma_2 \equiv \mathbb{E}_S(\chi_S(x)\chi_S(y)) = \frac{|S|(|S| - 1)}{2^n(2^n - 1)} = \frac{4^{k-n}(1 - 2^{-k})}{1 - 2^{-n}} \leq 4^{k-n}. \quad (9)$$

To see this, note that for any $n$-qubit state $|v\rangle$, each entry of $(H \otimes I_{n-1})|v\rangle$ is a sum of two entries of $|v\rangle$. 

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Using Eq. (7) we get
\[ \mathbb{E}_S(|S|) = 2^{(k-n)/2} |+^n| \]
where \(|+^n| = H^\otimes n |0^n|\), and consequently
\[ \mathbb{E}_S \mathbb{E}_T \mu(S, T) = \Phi(f, g). \quad (9) \]

Using Eq. (8) we get
\[ \mathbb{E}_S(|S\rangle\langle S|) = a \cdot I + b \cdot |+^n\rangle\langle +^n| \quad a \equiv 2^{-n} - 2^{-k} \sigma_2 \quad b \equiv 2^{n-k} \sigma_2. \quad (10) \]
and
\[ \mathbb{E}_S \mathbb{E}_T (\mu(S, T))^2 = 4^{n-k} \mathbb{E}_S \mathbb{E}_T \text{Tr} \left( |S\rangle\langle S| U_f H^\otimes n U_g^\dagger |T\rangle\langle T| U_g H^\otimes n U_f^\dagger \right) \]
\[ = 2^{3n-2k} a^2 + 4^{n-k} b^2 \Phi(f, g)^2 + 2 \cdot 4^{n-k} ab \]
\[ \leq 2^{n-2k} + \Phi(f, g)^2 + \frac{2}{2k}. \quad (11) \]
where we used the upper bounds \(a \leq 2^{-n}\) and \(b \leq 2^{k-n}\). Combining Eqs. (9, 11) gives
\[ \text{Var}(\mu(S, T)) = \mathbb{E}_S \mathbb{E}_T (\mu(S, T))^2 - (\mathbb{E}_S \mathbb{E}_T \mu(S, T))^2 \leq 2^{n-2k} + \frac{2}{2k}. \]

Now let us fix \(k\) to be an integer satisfying
\[ 2^{18} \cdot 2^n \epsilon^{-2} \geq 2^{2k} \geq 2^{16} \cdot 2^n \epsilon^{-2}. \quad (12) \]
We shall choose our estimate \(\mu \equiv \mu(S, T)\) where the affine subspaces \(S, T \in A_{n,k}\) are drawn uniformly at random. Note that the random selection of these affine spaces can be performed using a runtime \(O(\text{poly}(n))\), resulting in a parameterization
\[ S = \{Ax + b : x \in \{0, 1\}^k\} \quad T = \{Cx + d : x \in \{0, 1\}^k\} \quad (13) \]
where \(A\) and \(C\) are \(n \times k\) binary matrices and \(b, d \in \{0, 1\}^n\), and addition is performed over \(\mathbb{F}_2\).

Using Claim 1 and Eq. (12) we get
\[ \text{Var}(\mu(S, T)) \leq \frac{\epsilon^2}{2^{16}} + \frac{\epsilon^2}{2^7} 2^{-n/2} \leq \epsilon^2 \left( \frac{1}{2^{16}} + \frac{1}{2^7} \right) \leq \frac{\epsilon^2}{100}, \]
where in the second inequality we used Eq. (5). Applying Chebyshev’s inequality we see that
\[ \Pr(|\mu(S, T) - \Phi(f, g)| \geq \epsilon) \leq 1/100, \]
as desired. Below we show that there is a classical algorithm which, given \(S, T \in A_{n,k}\) (as in Eq. (13)), computes \(\mu(S, T)\) exactly using a runtime \(O(k^2 n + n 2^k)\) and \(O(2^k)\) queries. Using Eq. (12) we see that the total runtime is \(O(n 2^{n/2} \epsilon^{-1})\) and the total number of queries is \(O(2^{n/2} \epsilon^{-1})\).
Let us now describe how to compute \(\mu(S,T)\) using the stated runtime and number of queries. Using Eqs. (13,6) we may write

\[
\mu(S,T) = 2^{n/2-2k} \sum_{x,y \in \{0,1\}^k} f(Ax + b)g(Cy + d)(-1)^{y^T C^T Ax + x^T A^T d + b^T Cy + b^T d}
\]

To compute this sum on a classical computer we first initialize the following vector of length \(2^k\)

\[
|\psi_1\rangle = \sum_{x \in \{0,1\}^k} f(Ax + b)(-1)^{x^T A^T d}|x\rangle.
\]

We compute the entries of this vector one at a time using a Gray code ordering. Applying a single Hadamard gate to a \(2^k\)-qubit state stored in classical computer memory takes a runtime \(O(2^k)\). We initialize \(\psi_1\) can be performed using \(O(nk + n2^k)\) runtime and \(O(2^k)\) queries.

In the next step we compute a vector

\[
|\psi_2\rangle = \sum_{x \in \{0,1\}^k} f(Ax + b)(-1)^{x^T A^T d}|C^T Ax\rangle.
\]

We first compute the matrix \(C^T A\) which takes a runtime \(O(k^2 n)\). We initialize \(|\psi_2\rangle\) as a vector of length \(2^k\) with every entry equal to zero. Then, using our Gray code order we compute \(C^T Ax_1, C^T Ax_2, \ldots, C^T Ax_{2^k}\). Each time we compute a vector \(z_i = A^T Cx_i\) we set

\[
\langle z_i | \psi_2 \rangle \leftarrow \langle z_i | \psi_2 \rangle + \langle x_i | \psi_1 \rangle.
\]

The total runtime for this step is \(O(k^2 n + k2^k)\) since \(C^T A\) is a \(k \times k\) matrix.

Viewing \(\psi_2\) as a \(k\)-qubit state, we then apply a Hadamard gate on each qubit to obtain

\[
|\psi_3\rangle = H^\otimes k |\psi_2\rangle = 2^{-k/2} \sum_{x,y \in \{0,1\}^k} f(Ax + b)(-1)^{x^T A^T d}(-1)^{y^T C^T Ax}|y\rangle.
\]

Applying a single Hadamard gate to a \(k\)-qubit state stored in classical computer memory takes a runtime \(O(2^k)\) using sparse matrix-vector multiplication. The total runtime to compute \(\psi_3\) using a sequential application of the \(k\) Hadamard gates is then upper bounded as \(O(k2^k)\).

Finally, we compute a vector \(\psi_4\) defined by

\[
\langle y | \psi_4 \rangle = \langle y | \psi_3 \rangle \cdot 2^{n/2-3k/2}(-1)^{b^T d} g(Cy + d)(-1)^{b^T Cy} \quad y \in \{0,1\}^k.
\]

Performing this step using a Gray code ordering can be done using \(O(nk + n2^k)\) total runtime and \(O(2^k)\) queries (similar to the procedure used to initialize \(\psi_1\)). Here

\[
|\psi_4\rangle = 2^{n/2-2k} \sum_{x,y \in \{0,1\}^k} f(Ax + b)(-1)^{x^T A^T d}(-1)^{y^T C^T Ax} g(Cy + d)(-1)^{b^T Cy}(-1)^{b^T d}|y\rangle.
\]

Finally, \(\mu(S,T)\) is obtained by summing all entries of the vector \(\psi_4\) using a runtime \(O(2^k)\).

In total, this algorithm uses \(O(2^k)\) queries and \(O(k^2 n + n2^k)\) runtime, as claimed. \(\square\)
Now let us turn our attention to the $k$-fold forrelation $\Phi(f_1, f_2, \ldots, f_k)$ defined in Eq. (2). Here $f_1, f_2, \ldots, f_k : \{0, 1\}^n \rightarrow \{-1, 1\}^n$ are $n$-bit boolean functions. Letting $m \geq n$ we shall describe a randomized classical algorithm which is capable of estimating a more general $m$-qubit amplitude of the form

$$q = \langle 0^m | M_1 U_{f_1} M_2 U_{f_2} \ldots U_{f_k} M_{k+1} | 0^m \rangle.$$  

(14)

where $M_1, \ldots, M_{k+1}$ are $m$-qubit operators such that $\|M_j\| \leq 1$ for all $1 \leq j \leq k + 1$, and $U_{f_j} |x\rangle |y\rangle = f_j(x) |x\rangle |y\rangle$ for each $x \in \{0, 1\}^n$, $y \in \{0, 1\}^{m-n}$. Clearly the $k$-fold forrelation $\Phi(f_1, f_2, \ldots, f_k)$ can be expressed as in Eq. (14) with $m = n$. Amplitudes of the form Eq. (14) can also express output probabilities of quantum query algorithms. Indeed, suppose $p$ is the probability of measuring an output qubit in the state $|1\rangle$ at the output of a quantum algorithm that makes $t$ quantum queries to an oracle. Then $p$ can be expressed as as in Eq. (14) with $k = 2t$.

Aaronson and Ambainis described a randomized classical algorithm which approximates an amplitude of the form Eq. (14). Their result is summarized as follows.

**Theorem 4 ([6]).** There exists a classical randomized algorithm which, given $\epsilon > 0$, outputs an estimate $\tilde{q}$ such that

$$|\tilde{q} - q| \leq \epsilon$$

with probability at least 99%. The algorithm uses $O(2^k \epsilon^{-2+\frac{2}{k}} 2^{n(1-\frac{1}{k})})$ oracle queries.

The algorithm from Ref. [6] is based on the polynomial method [12]. In particular, identifying each $n$-bit function $f_j$ with a string $x_j \in \{-1, 1\}^{2^n}$, the function $q(x_1, x_2, \ldots, x_k)$ can be expressed as a multilinear polynomial $q : \{-1, 1\}^{k \cdot 2^n} \rightarrow [-1, 1]$ [12]. Crucially, the coefficients of $q$ are independent of the oracles and can be computed without using any queries. The algorithm from Ref. [6] first transforms the polynomial $q$ into a new polynomial $q'$ with $L = O(2^k 2^n \epsilon^{-2})$ variables and whose coefficients satisfy a certain balancedness property that is used in the analysis. This step requires no queries. The desired amplitude $q(x_1, x_2, \ldots, x_k)$ is equal to a suitable value of $q'$, which is approximated using a Monte Carlo algorithm that queries the oracles $O(L^{1-1/k})$ times.

Here we show that the scaling with $k$ and $\epsilon$ can be sharpened as follows.

**Theorem 5.** There exists a classical randomized algorithm which, given $\epsilon > 0$, outputs an estimate $\tilde{q}$ such that

$$|\tilde{q} - q| \leq \epsilon$$

with probability at least 99%. The algorithm uses $O(k \epsilon^{-2+2^{-k}2^{n(1-\frac{1}{k})}})$ oracle queries.

**Proof.** In the following we shall write

$$\Pi(z) = |z\rangle \langle z| \otimes I \quad z \in \{0, 1\}^n,$$

where the identity acts on $m - n$ qubits. For any nonzero complex vector $\alpha$ of length $2^m$, define a probability distribution over $n$-bit strings

$$p_\alpha(z) = \|\alpha\|^{-2} \|\Pi(z) |\alpha\rangle\|^2 \quad z \in \{0, 1\}^n.$$  

(15)
Define $|\phi_0\rangle = |0^m\rangle$ and then for each $1 \leq j \leq k$ construct a (possibly un-normalized) state $\phi_j$ as follows. First sample binary strings $z_1, z_2, \ldots, z_L$ independently from the distribution $p_{M_j}^{\dagger}|\phi_{j-1}\rangle$ (see Eq. (15)). We will fix $L$ later. Then define

$$|\phi_j\rangle = \frac{1}{L} \sum_{i=1}^{L} f_j(z_i) \Pi(z_i) M_j^\dagger |\phi_{j-1}\rangle$$

(16)

Note that

$$\mathbb{E}(|\phi_j\rangle) = U_{f_j} M_j^\dagger |\phi_{j-1}\rangle$$

(17)

and we have the operator inequality

$$\mathbb{E}( |\phi_j\rangle \langle \phi_j|) = \left(\frac{L-1}{L}\right) U_{f_j} M_j^\dagger |\phi_{j-1}\rangle \langle \phi_{j-1}| M_j U_{f_j} + \frac{||\phi_{j-1}||^2}{L} \sum_{z \in \{0,1\}^n} \Pi(z) M_j^\dagger |\phi_{j-1}\rangle \langle \phi_{j-1}| M_j \Pi(z) M_j^\dagger |\phi_{j-1}\rangle$$

$$\leq U_{f_j} M_j^\dagger |\phi_{j-1}\rangle \langle \phi_{j-1}| M_j U_{f_j} + \frac{||\phi_{j-1}||^2}{L} \cdot I.$$ 

(19)

Using Eq. (19) we see that

$$\mathbb{E}(||\phi_j||^2) = Tr(\mathbb{E}(|\phi_j\rangle \langle \phi_j|)) \leq \left(1 + \frac{2^n}{L}\right) ||\phi_{j-1}||^2$$

(21)

where to bound the first term we used the fact that $||M_j|| \leq 1$. For each $0 \leq r \leq k$ define a complex-valued random variable

$$X_r = \langle \phi_r | M_{r+1} U_{f_{r+1}} M_{r+2} \ldots U_{f_k} M_{k+1} |0^m\rangle.$$ 

Note that $X_0 = q$ is the desired amplitude. Using Eq. (17) we see that

$$\mathbb{E}(X_k) = \mathbb{E}(X_{k-1}) = \ldots = \mathbb{E}(X_0) = q.$$ 

Note that $X_k$ can be computed using $L$ queries to each of the given oracles $f_1, f_2, \ldots, f_k$.

**Lemma 1.**

$$\mathbb{E}(|X_k|^2) - |q|^2 \leq 2^{n(k-1)} L^{-k} \left(1 + \frac{L}{2^n}\right)^k.$$ 

(22)

**Proof.** Let us write $\mathbb{E}_j$ for the expectation over all random variables used in generating the states $\phi_1, \phi_2, \ldots, \phi_j$. Then, for all $1 \leq r \leq k$ we have

$$\mathbb{E}(|X_r|^2) = \mathbb{E}_r(|X_r|^2) = \mathbb{E}_{r-1} \mathbb{E}_{\phi_r} \left( |\langle \phi_r | M_{r+1} U_{f_{r+1}} M_{r+2} \ldots U_{f_k} M_{k+1} |0^m\rangle|^2 \right) \leq \mathbb{E}_{r-1} \left(|X_{r-1}|^2\right) + \frac{1}{L} \mathbb{E}_{r-1} \left(||\phi_{r-1}||^2\right)$$
where in the last line we used Eq. (20). The second term above can be computed using a repeated application of Eq. (21), which gives, for each $1 \leq r \leq k$,

$$\mathbb{E}(|X_r|^2) - \mathbb{E}(|X_{r-1}|^2) \leq \frac{1}{L} \left(1 + \frac{2^n}{L}\right)^{r-1}$$

Since $X_0 = q$ we get

$$\mathbb{E}(|X_k|^2) - |q|^2 = \sum_{r=1}^{k} \left(\mathbb{E}(|X_r|^2) - \mathbb{E}(|X_{r-1}|^2)\right) \leq 2^{-n} \left(1 + \frac{2^n}{L}\right)^k - 1$$

Discarding the subtracted term in the parentheses, we arrive at Eq. (22).

Now let us fix $B$ as follows

$$B = 2k \cdot \left[2^{n(1-1/k)}(\epsilon^2/400)^{-1/k}\right] \quad (23)$$

This will be our query budget. There are two cases to consider. If $B \geq k \cdot 2^n$ then we can simply query each oracle at all $2^n$ possible binary strings and output an exact computation of $q$. If instead $B \leq k \cdot 2^n$ then we compute the estimator $\tilde{q} = X_k$ with the choice $L = B/k$. In this case we have $L \leq 2^n$ and therefore Eq. (22) gives

$$\mathbb{E}(|X_k|^2) - |q|^2 \leq 2^{n(k-1)}L^{-k}2^k \leq \epsilon^2/400$$

where in the second inequality we lower bounded $L = B/k$ using Eq. (23). Therefore

$$\text{Var}(\text{Re}(\tilde{q})) + \text{Var}(\text{Im}(\tilde{q})) = \mathbb{E}(|X_k|^2) - |q|^2 \leq \frac{\epsilon^2}{400}.$$ 

By Chebyshev’s inequality we see that $|\text{Re}(\tilde{q}) - \text{Re}(q)| \leq \epsilon/\sqrt{2}$ with probability at least 0.995. The same arguments show that $|\text{Im}(\tilde{q}) - \text{Im}(q)| \leq \epsilon/\sqrt{2}$ with probability at least 0.995. By a union bound, we have $|q - \tilde{q}| \leq \epsilon$ with probability at least 0.99.

### 3 Graph-based forrelation

The algorithm for estimating a graph-based forrelation $\Phi$ described in the Introduction has a polynomial runtime whenever efficient subroutines are available for computing amplitudes of the states $|\alpha\rangle$ and $|\beta\rangle$ such that $\Phi = \langle \beta | \alpha \rangle$ and for sampling the probability distribution $|\langle x | \alpha \rangle|^2$. Here we establish Theorem 3 by constructing such subroutines for more general (non-bipartite) graphs that admit a partition into two subgraphs with a small treewidth.

Section 3.1 provides relevant background concerning tree decompositions. Section 3.2 describes an efficient subroutine for computing a sum $\sum_x h(x)$, where $h(x)$ is a two-local function on a graph with a small treewidth. Section 3.3 combines these ingredients and completes the proof of Theorem 3.
3.1 Low treewidth partitions of planar graphs

**Definition 1 (Tree decomposition).** Let $G = (V, E)$ be a graph. A tree decomposition of $G$ consists of a tree $T = (W, F)$, along with a bag $B_i \subseteq V$ for each node $i \in W$, such that the following properties hold:

- For each $v \in V$, there exists a node $i \in W$ such that $v \in B_i$.
- For each $\{u, v\} \in E$, there exists a node $i \in W$ such that $u \in B_i$ and $v \in B_i$.
- For each $v \in V$, the subgraph $T_v$ of $T$ induced by the set of nodes $i \in W$ such that $v \in B_i$ is a tree.

We shall use the shorthand $T, B$ to denote a tree decomposition, where $B = \{B_i : i \in W\}$ is the set of bags. The *width* $w$ of a tree decomposition is defined as

$$w = \max_{i \in W} |B_i| - 1.$$ 

The *treewidth* of a graph $G$ is defined as the minimal width of any tree decomposition of it.

**Definition 2.** A graph $G$ is said to be outerplanar if it admits a planar embedding in which all vertices are incident to the outer face.

Boedlaender has shown that outerplanar graphs have tree decompositions of width at most 2 that can be computed in linear time.

**Theorem 6 (Boedlaender [21, 22]).** If $G$ is an outerplanar graph then its treewidth is $\leq 2$ and a tree decomposition of width $\leq 2$ can be computed in linear time.

We refer the reader to Ref. [21] which provides a straightforward inductive proof that the treewidth is at most 2, and Ref. [22] which gives a linear time algorithm to compute such a tree decomposition. In this paper it will suffice for us to use the slower quadratic time Algorithm 1 (implicit in Ref. [21]).

The following theorem states that the vertices of any planar graph can be partitioned into two subsets, each of which induce a graph of low treewidth. For completeness, we include the simple proof below, following Ref. [23]. An example is depicted in Fig. 1.

**Theorem 7 (Chartrand, Geller, Hedetniemi 1971 [23]).** If $G = (V, E)$ is a planar graph then there exists a partition $V = A \cup B$ such that the induced subgraphs $G_A$ and $G_B$ are outerplanar graphs. Moreover, the partition can be computed in linear time from a planar embedding of $G$.

**Proof.** We begin by defining a sequence of planar graphs $G_k = (V_k, E_k)$ for $0 \leq k \leq p$, where $p \leq |V|$ depends on $G$. Let $V_0 = V$, $E_0 = E$, and $G_0 = G$. For each $k$ let us write $V_k^{\text{out}} \subseteq V_k$ for the vertices incident to the outer face of $G_k$. If $V_k \neq V_k^{\text{out}}$ we define

$$V_{k+1} = V_k \setminus V_k^{\text{out}}$$

and let $G_{k+1}$ be the subgraph of $G_k$ induced by $V_{k+1}$. The process terminates at some graph $G_p$ for which $V_p = V_p^{\text{out}}$ (an outerplanar graph). Note that $G_{k+1}$ has fewer vertices than $G_k$, so the process stops after $p \leq |V|$ steps.
Figure 1: Illustration of Theorem 7. A planar graph and a partition of its vertices into subsets $A$ and $B$ shown in red and blue. The induced subgraphs $G_A$ and $G_B$ are outerplanar graphs.

The vertex set of $G$ can be partitioned as $V = A \cup B$ where

$$A = V_0^{\text{out}} \cup V_2^{\text{out}} \cup V_4^{\text{out}} \ldots \quad B = V_1^{\text{out}} \cup V_3^{\text{out}} \cup V_5^{\text{out}} \ldots$$

Finally, we show that the induced subgraphs $G_A$ and $G_B$ are outerplanar. For each $j = 0, 1, \ldots, p$ let $H_j$ be the induced subgraph of $G$ on vertices $V_j^{\text{out}}$. By construction, $G_A$ consists of disconnected copies of $H_0, H_2, H_4, \ldots$ and $G_B$ consists of disconnected copies of $H_1, H_3, H_5, \ldots$. To complete the proof we show that each graph $H_j$ is outerplanar. Observe that $H_j$ is the induced subgraph of the graph $G_j$ on the vertices incident to its outer face. Therefore all vertices of $H_j$ are on its outer face and we are done.

### 3.2 Summation of two-local functions

Suppose $G = (V, E)$ is a graph with $m = |V|$ vertices and $\Gamma$ is a finite set. We shall say that $h : \Gamma^m \to \mathbb{C}$ is a two-local function on $G$ if it can be written as

$$h(x) = \prod_{\{u,v\} \in E} h_{uv}(x_u, x_v) \prod_{u \in V} h_u(x_u)$$

for some functions $h_{uv} : \Gamma^2 \to \mathbb{C}$ and $h_u : \Gamma \to \mathbb{C}$. Here $x = x_1 x_2 \ldots x_m$ with $x_j \in \Gamma$ for $1 \leq j \leq m$. Note that if $G$ has no isolated vertices then the vertex terms $\{h_u\}$ can be folded into the edge terms $\{h_{uv}\}$ and need not explicitly appear in Eq. (24).

**Lemma 2.** Suppose we are given a two-local function $h : \Gamma^m \to \mathbb{C}$ on an $m$-vertex tree $T$. There is a classical algorithm which computes $\sum_{x \in \Gamma^m} h(x)$ using a runtime $O(m |\Gamma|^2)$.

**Proof.** Write $T = (W, F)$. Suppose $u \in W$ is a leaf of the tree and is incident to $v \in W$. Let $T' = (W', F')$ where $W' = W \setminus \{u\}$ and $F' = F \setminus \{u, v\}$ be the tree obtained by removing $u$ and its incident edge from $T$. We may compute a new two-local function $h'$ on $T'$ such that

$$\sum_{y \in \Gamma^{m-1}} h'(y) = \sum_{x \in \Gamma^m} h(x).$$

This is depicted in Fig. 2. Indeed, define $h'_{r,s} = h_{r,s}$ for all edges $\{r, s\} \in F'$, $h'_r = h_r$ for all vertices $r \in W' \setminus \{v\}$, and

$$h'_v(x_v) = \sum_{x_u \in \Gamma} h_{uv}(x_u, x_v) h_v(x_v).$$

(25)
Figure 2: (a) Depiction of a two-local function \( h \) on a tree with 4 vertices. (b) The two-local function resulting from contraction of a leaf vertex \( u \). Here \( h'_v(x_v) = \sum x_u h_{uv}(x_u, x_v) h_v(x_v) \) can be computed in time \( O(|\Gamma|^2) \).

We can compute the new function \( h' \) from \( h \) by evaluating the sum Eq. (25) for each \( x_v \in \Gamma \). Each such evaluation requires \( O(|\Gamma|) \) additions and multiplications, so the total runtime is \( O(|\Gamma|^2) \). To evaluate the sum \( \sum x h(x) \) we repeat this process \( m \) times until we have removed all vertices of \( T \). The total runtime is \( O(m|\Gamma|^2) \).

**Lemma 3.** Let \( G = (V, E) \) be an \( m \)-vertex graph. Suppose we are given a two-local function \( h: \{0, 1\}^m \to \mathbb{C} \) on \( G \), along with a tree decomposition of \( G \) of width \( w \) and containing \( N \) nodes. There is a classical algorithm which computes

\[
\sum_{x \in \{0, 1\}^m} h(x)
\]

using a runtime \( O(Nw2^w) \).

**Proof.** Let us write \( T = (W, F) \) and \( B = \{B_i : i \in W\} \) for the given tree decomposition. With this notation we have \( N = |W| \) and \( w + 1 = \max_i |B_i| \). To simplify notation in the following we redefine \( w \leftarrow w + 1 \) to be the width of the tree decomposition plus one.

For each bag \( B_i \) with \( i \in W \) we define a variable \( y_i \in \{0, 1\}^w \). Here \( y_i \) contains a bit labeled by each vertex of \( G \) in bag \( i \) (i.e., each element of \( B_i \)), and also contains \( w - |B_i| \) ancilla bits. These ancilla bits are only present to ensure, for convenience, that all variables \( y_i \) are of the same length. We say that \( y_i \) and \( y_j \) are consistent if, (a) for each \( v \in B_i \cap B_j \) the corresponding bit of \( y_i \) agrees with that of \( y_j \), and (b) all ancilla bits of \( y_i \) are 0 and all ancilla bits of \( y_j \) are 0.

Let \( \Gamma = \{0, 1\}^w \). We now show how to compute a function \( Q: \Gamma^N \to \mathbb{C} \) which is two-local on \( T \) and such that

\[
\sum_{y \in \Gamma^N} Q(y) = \sum_{x \in \{0, 1\}^m} h(x).
\]

By definition, such a two-local function is of the form

\[
Q(y) = \prod_{\{i,j\} \in F} Q_{ij}(y_i, y_j) \prod_{i \in W} Q_i(y_i).
\]
We choose
\[ Q_{ij}(y_i, y_j) = \begin{cases} 1 & y_i \text{ and } y_j \text{ are consistent} \\ 0 & \text{otherwise.} \end{cases} \]

With this choice, the binary strings \( y \) such that
\[ \prod_{\{i,j\} \in F} Q_{ij}(y_i, y_j) = 1 \]
are in one-to-one correspondence with assignments \( x \in \{0,1\}^m \) of bits to each vertex of \( G \). Let us write \( x \sim y \) for this correspondence. We choose the functions at each node so that
\[ \prod_{i \in W} Q_i(y_i) = h(x) = \prod_{\{u,v\} \in E} h_{uv}(x_u, x_v) \prod_{u \in V} h_u(x_u) \quad \text{for} \quad x \sim y. \tag{28} \]
which then ensures Eq. \((27)\). To satisfy Eq. \((28)\), note that (by definition of a tree decomposition) for each edge \( \{u,v\} \in E \), there is a node \( i \) such that \( u \in B_i \) and \( v \in B_i \). The weight \( h_{uv}(x_u, x_v) \) can then be incorporated into the function \( Q_i \). Likewise, the weight \( h_u(x_u) \) can be incorporated into any function \( Q_i \) such that \( u \in B_i \).

Let’s now upper bound the time needed to compute the truth table of each \( Q_i \). First, we can compute \( Q_i(0\ldots0) \) in \( O(w^2) \) time since there are at most \( O(w^2) \) terms of \( h \) on \( w \)-many vertices. Notice that if we compute \( Q_i(0\ldots01) \), there are \( O(w) \) terms of \( h \) whose contribution to \( Q_i \) changes. That is, given \( Q_i(0\ldots0) \), computing \( Q_i(0\ldots01) \) can be done in \( O(w) \) time. Of course, this argument generalizes for any two inputs which differ in a single input bit. Therefore, we sequentially compute \( Q_i(y_i) \) for \( y_i \in \{0,1\}^w \) in Gray code order (i.e., each \( y_i \) differs in at most 1 bit from the previously computed bit), leading to an \( O(Nw2^w) \) time algorithm to compute \( Q_i(y_i) \) for all \( i \in W \) and \( y_i \in \{0,1\}^w \).

Since \( Q \) is two-local on the tree \( T \), we may then apply Lemma 2 which gives a classical algorithm to evaluate the sum Eq. \((27)\) in time \( O(N4^w) \). However, we can speed up this algorithm using the fact that \( Q_{ij}(y_i, y_j) \) is particularly simple. Using the same algorithm from Lemma 2, we must compute
\[ Q'_v(y_v) = Q(y_v) \sum_{y_u \in \{0,1\}^w} Q_{uv}(y_u, y_v)Q_u(y_u) \]
when we are contracting a child \( u \) to its parent \( v \) in the tree. Suppose that node \( v \) and node \( u \) share \( k \) many vertices, and for simplicity, let’s assume that these are the first \( k \) bits of both \( y_u \) and \( y_v \). These \( k \) bits partition \( \sum_{y_u \in \{0,1\}^w} Q_{uv}(y_u, y_v)Q_u(y_u) \) into \( 2^k \) non-overlapping sums. For example, if the first \( k \) bits of \( y_v \) are \( 0^k \), then
\[ \sum_{y_u \in \{0,1\}^w} Q_{uv}(y_u, y_v)Q_u(y_u) = \sum_{x \in \{0,1\}^{w-k}} Q_u(0^kx) \]
where we have ignored the ancilla bits since we can always just set those bits to be 0. If the first \( k \) bits of \( y_v \) are \( z \neq 0^k \), then we get the sum \( \sum_{x \in \{0,1\}^{w-k}} Q_u(zx) \) instead. Therefore, computing \( \sum_{y_v \in \{0,1\}^w} Q_{uv}(y_u, y_v)Q_u(y_u) \) for all the possible \( k \)-bit prefixes of \( y_v \) can be done in time \( O(2^w) \). Finally, to compute \( Q'(y_v) \) we must also multiply by the factor \( Q(y_v) \). Once again, we iterate over all \( y_v \) in time \( O(2^w) \). Repeating this process for each node, we get a total runtime of \( O(N2^w) \), which completes the proof. \( \square \)
3.3 Classical algorithm for graph-based forrelation

In this section we prove Theorem 3. We first consider the special case in which all operators $O_j$ are unitary; at the end of this section we show how to handle the more general case. As discussed in Section 3, it suffices to give efficient algorithms for computing amplitudes of a state

$$|\alpha\rangle = (O_A \otimes I_B)U_H^{\otimes n}|0^n\rangle.$$  

and for sampling the probability distribution $|\langle x|\alpha\rangle|^2$. This is accomplished in Lemmas 4,5 below. Let $G_A = (A, E_A)$ be the subgraph of $G$ induced by $A$. By assumption, we are given a tree decomposition $T, B$ of $G_A$ of width $w$ such that $T$ has $O(n)$ nodes.

Lemma 4. There is a classical algorithm which, given $x \in \{0, 1\}^n$, computes an amplitude $\langle x|\alpha\rangle$ using a runtime $O(nw2^w)$.

Proof. Below we use notation introduced in Section 3.1. Let us begin by writing

$$\langle x|\alpha\rangle = 2^{-n/2} \sum_{y_A} \langle x_A|O_A|y_A\rangle f(y_A x_B).$$  

Partition the edges of $G$ as $E = E_A \cup E_{\text{cut}} \cup E_B$ where $E_A$ are the edges with both endpoints in $A$, $E_B$ are the edges with no endpoints in $A$, and $E_{\text{cut}}$ are the edges with exactly one endpoint in $A$. Since $f$ is a two-local function on $G$ we may write

$$f(y_A x_B) = \prod_{\{u,v\} \in E_A} f_{uv}(y_u, y_v) \prod_{\{u,v\} \in E_{\text{cut}}} f_{uv}(y_u, x_v) \prod_{\{u,v\} \in E_B} f_{uv}(x_u, x_v) \prod_{u \in A} f_u(y_u) \prod_{u \in B} f_u(x_u).$$

We claim that for any fixed $x = x_A x_B$,

$$h(y_A) = 2^{-n/2} \langle x_A|O_A|y_A\rangle f(y_A x_B), \quad y_A \in \{0, 1\}^{|A|}$$

defines a two-local function on $G_A$. Indeed, we may write

$$h(y_A) = \omega \prod_{\{u,v\} \in E_A} h_{uv}(y_u, y_v) \prod_{u \in A} h_u(y_u)$$  

where

$$h_{uv}(y_u, y_v) = f_{uv}(y_u, y_v), \quad h_u(y_u) = \langle x_u|O_u|y_u\rangle f_u(y_u) \prod_{v: \{u,v\} \in E_{\text{cut}}} f_{uv}(y_u, x_v)$$

and $\omega = 2^{-n/2} \prod_{\{u,v\} \in E_B} f_{uv}(x_u, x_v) \prod_{u \in B} f_u(x_u) \in \mathbb{C}$ can be absorbed into (say) one of the functions $h_u$ to make Eq. (30) of the form Eq. (24). We then apply Lemma 3 which completes the proof. \qed

Lemma 5. There is a classical algorithm which samples a binary string $x \in \{0, 1\}^n$ from the distribution $P(x) = |\langle x|\alpha\rangle|^2$ using a runtime $O(n^2 w 4^w)$.  

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Proof. It will be convenient to order the bits of \( x \) as \( x_Bx_A \), that is, all bits of \( B \) appear first. We shall use the well-known linear time reduction from sampling to computing marginal probabilities. That is, for each \( \ell \in [n] \) and binary string \( x_1x_2\ldots x_\ell \), we define a marginal probability
\[
P_\ell(x_1x_2\ldots x_\ell) = \sum_{x_{\ell+1}x_{\ell+2}\ldots x_n} P(x).
\]

To sample from \( P(x) \) we first sample \( x_1 \in \{0,1\} \) from \( P_1(x_1) \), then we sample \( x_2 \) from \( P_2(x_1x_2)/P_1(x_1) \), then \( x_3 \) from \( P_3(x_1x_2x_3)/P_2(x_1x_2) \), and so on. To complete the proof, below we show that each marginal Eq. (31) can be computed using a runtime \( O(nw4^w) \).

If \( \ell \leq |B| \), then
\[
P_\ell(x_1x_2\ldots x_\ell) = \langle 0^n|H^{\otimes n}U_f^\dagger(|x_1x_2\ldots x_\ell\rangle \otimes I_{|B|-\ell} \otimes O_A^\dagger O_A)U_f H^{\otimes n}|0^n \rangle.
\]

Since all operators \( O_j \) are unitary, one can replace \( O_A^\dagger O_A \) with the identity. Then \( U_f^\dagger \) and \( U_f \) cancel each other since \( U_f \) commutes with any diagonal operator. Thus
\[
P_\ell(x_1x_2\ldots x_\ell) = \langle 0^n|H^{\otimes n}(|x_1x_2\ldots x_\ell\rangle \otimes I_{n-\ell})H^{\otimes n}|0^n \rangle = \frac{1}{2^{\ell}}.
\]

Suppose now that \( \ell \geq |B| + 1 \). Define a partition \( A = CD \), where \( C = A \cap \{1,2,\ldots,\ell\} \) includes all bits of \( A \) that contribute to the marginal probability and \( D \) includes all bits of \( A \) that are traced out. Then \( x_1x_2\ldots x_\ell = x_Bx_C \). Using Eq. (29) we may write
\[
P_\ell(x_Bx_C) = 2^{-n} \sum_{x_D} \left| \sum_{y_A} \langle x_Cx_D|O_A|y_A \rangle f(x_By_A) \right|^2
\]
\[
= 2^{-n} \sum_{x_D, y_A, z_A} \langle x_Cx_D|O_A|y_A \rangle^* \langle x_Cx_D|O_A|z_A \rangle f^*(x_By_A)f(x_Bz_A).
\]

For any subset of qubits \( M \) we shall write \( O_M \) for the tensor product of \( O_j \) over \( j \in M \). Then \( O_A = O_C \otimes O_D \) and thus
\[
\sum_{x_D} \langle x_Cx_D|O_A|y_A \rangle^* \langle x_Cx_D|O_A|z_A \rangle = \langle x_C|O_C|y_C \rangle^* \langle x_C|O_C|z_C \rangle \sum_{x_D} \langle x_D|O_D|y_D \rangle^* \langle x_D|O_D|z_D \rangle.
\]

The unitarity of \( O_j \) implies
\[
\sum_{x_D} \langle x_D|O_D|y_D \rangle^* \langle x_D|O_D|z_D \rangle = \langle y_D|O_D^\dagger O_D|z_D \rangle = \langle y_D|z_D \rangle = \delta_{y_D,z_D}.
\]

We arrive at
\[
P_\ell(x_Bx_C) = 2^{-n} \sum_{y_C,y_D} \langle x_C|O_C|y_C \rangle^* \langle x_C|O_C|y_D \rangle f^*(x_By_D) f(x_By_Cy_D)
\]
\[
= \sum_{y_C,y_D} h(y_C,y_D), \tag{33}
\]
where
\[ h(y_C, y'_C, y_D) = 2^{-n} \langle x_C|O_C y_C \rangle^* \langle x_C|O_C y'_C \rangle f^*(x_B y_C y_D) f(x_B y'_C y_D). \]

We claim that \( h \) is a two-local function on a certain augmented graph \( \tilde{G} = (\tilde{V}, \tilde{E}) \) with vertex set \( \tilde{V} = V \cup C' \cup D \), where \( C' \) is a second copy of \( C \). To construct this graph, start with a disjoint union of \( G_A \) and \( G_C \) (the induced subgraphs of \( G \) on vertices in \( A \), \( C' \) respectively). For each edge \( \{u, v\} \in E_A \) with \( u \in C \) and \( v \in D \), we then add a new edge \( \{u', v\} \) between \( u \) and the copy \( u' \in C' \). Since \( f \) is two-local on \( G \), a direct inspection shows that each two-local term in \( f^*(x_B y_C y_D) \) or \( f(x_B y'_C y_D) \) that depends on the variables \( y \) or \( y' \) involves nearest-neighbor variables in the augmented graph \( \tilde{G} \). The remaining two-local terms in \( f^*(x_B y_C y_D) \) or \( f(x_B y'_C y_D) \) that depend on at least one variable \( x \) become 1-local since \( x_B \) is fixed. Furthermore, the matrix elements \( \langle x_C|O_C y_C \rangle \) and \( \langle x_C|O_C y'_C \rangle \) are 1-local functions of \( y_C \) and \( y'_C \). Thus \( h \) is a two-local function on the augmented graph \( \tilde{G} \).

We claim that the treewidth \( \tilde{w} \) of \( \tilde{G} \) satisfies \( \tilde{w} \leq 2w + 1 \). Indeed, let \( T, B \) be the given tree decomposition of \( G_A \) of width \( w \). Define a tree decomposition \( \tilde{T}, \tilde{B} \) of \( \tilde{G} \) as follows. First set \( \tilde{T} = T \). Then, for each node \( i \) of \( T \), let \( S_i = B_i \cap C \) be the set of vertices of \( C \) that appear in \( B_i \). Let \( S_i' \) contain the corresponding vertices of \( C' \), and define
\[ \tilde{B}_i = B_i \cup S_i'. \]

One can straightforwardly check that this defines a tree decomposition \( \tilde{T}, \tilde{B} \) of \( \tilde{G} \). The upper bound \( \tilde{w} \leq 2w + 1 \) follows from the fact that each bag can at most double in size.

To complete the proof, we apply Lemma 3 which allows us to compute the sum Eq. (33) using a runtime \( O(n(2w + 1)2^{2w+1}) = O(nw4^w) \). Since sampling \( x \) from \( P(x) \) requires computation of \( n \) marginal probabilities the overall runtime of the algorithm is \( O(n^2w4^w) \). \( \square \)

Let \( \mathcal{A} \) be a randomized algorithm that samples a bit string \( x \in \{0,1\}^n \) from the distribution \( |\langle x|\alpha\rangle|^2 \) and outputs the quantity \( \mu = \langle \beta|x\rangle/|\langle \alpha|x\rangle| \). We have \( \mathbb{E}(\mu) = \langle \beta|\alpha \rangle = \Phi \) and \( \mathbb{E}(|\mu|^2) = |\langle \beta|\beta \rangle| \leq 1 \). Thus \( \mu \) is an unbiased estimator of \( \Phi \) with variance at most one. Lemmas 4,5 imply that \( \mathcal{A} \) has runtime \( O(n^2w4^w) \). By generating \( S = 100e^{-2} \) independent samples of \( \mu \) using \( \mathcal{A} \) calls to the algorithm \( \mathcal{A} \) and computing the sample mean value one can approximate \( \Phi \) with an additive error \( \epsilon \) in time \( O(n^2w4^w\epsilon^{-2}) \), as claimed.

So far we have assumed that \( O_j \) are unitary operators. Now let us consider the more general case where we only require \( \|O_j\| \leq 1 \) for all \( j \). Using the singular value decomposition one can write any \( 2 \times 2 \) matrix \( M \) as
\[ M = \|M\| \cdot U \begin{bmatrix} 1 & 0 \\ 0 & s \end{bmatrix} V \]
for some \( 0 \leq s \leq 1 \) and some \( 2 \times 2 \) unitary matrices \( U, V \). The identity
\[ \begin{bmatrix} 1 & 0 \\ 0 & s \end{bmatrix} = \frac{(1+s)}{2} I + \frac{(1-s)}{2} Z \]
gives \( M = \|M\|(q_0 M_0 + q_1 M_1) \), where \( M_0 = UV \) and \( M_1 = UZV \) are unitary, \( q_0 = (1+s)/2 \), and \( q_1 = (1-s)/2 \). Applying this decomposition to each operator \( O_j \) one gets
\[ \Phi = \omega \sum_{z \in \{0,1\}^n} q(z)\Phi(z), \]
for some \( \omega \).
where \( \omega = \prod_{j=1}^{n} \| O_j \| \leq 1 \) is the normalization constant, \( q(z) \) is a product distribution, and
\[
\Phi(z) = \langle 0^n | H^\otimes n U_g (O_{1,z_1} \otimes O_{2,z_2} \otimes \cdots \otimes O_{n,z_n}) U_f H^\otimes n | 0^n \rangle,
\]
for some unitary operators \( O_{j,0} \) and \( O_{j,1} \). As shown above, there exists a randomized algorithm \( A \) that takes as input a bit string \( z \in \{0, 1\}^n \) and outputs a random variable \( \mu(z) \in \mathbb{C} \) such that \( \mathbb{E}(\mu(z)) = \Phi(z) \) and \( \mathbb{E}(|\mu(z)|^2) \leq 1 \). Here the mean values are taken over the internal randomness of \( A \). We can now estimate \( \Phi \) by Monte Carlo method. Generate \( S = 100\epsilon^{-2} \) independent samples \( z^1, \ldots, z^S \) from the distribution \( q(z) \). For each sample \( z^j \) call the algorithm \( A \) to obtain the estimator \( \mu(z) \). Finally, approximate \( \Phi \) by the quantity
\[
\eta = \frac{\omega}{S} \sum_{j=1}^{S} \mu(z^j).
\]
One can straightforwardly check that \( \mathbb{E}(\eta) = \Phi \). Furthermore,
\[
\text{Var}(\eta) = \frac{\omega^2}{S} \text{Var}(\mu(z^1)) \leq \frac{1}{S} \sum_{z} q(z) \mathbb{E}(|\mu(z)|^2) \leq \frac{1}{S} = \frac{\epsilon^2}{100}.
\]
By the Chebyshev inequality, \( |\eta - \Phi| \leq \epsilon \) with probability at least 0.99.

## 4 Applications to quantum approximate optimization

In this section we discuss the connection between the classical algorithm for graph-based forrelation and certain quantum approximate optimization algorithms (QAOA) \[10\]. In particular, in Section 4.1 we show how graph-based forrelation can be be used to calculate the variational energies for the level-2 QAOA algorithm on planar and bipartite graphs. In Section 4.2, we describe an implementation of this algorithm that can accurately estimate these energies. Finally, in Section 4.3, we discuss the recursive QAOA algorithm \[19\] for which our graph-based forrelation approach can give a complete classical simulation. We then combine our implementation for computing level-2 QAOA energies with the recursive QAOA algorithm to show that our algorithm can be leveraged for solving large optimization problems.

### 4.1 Quantum mean value problem for level-2 QAOA

Suppose \( G = (V, E) \) is a graph with \( n \) vertices. We place a qubit at each vertex of \( G \). Consider a diagonal \( n \)-qubit Hamiltonian
\[
C = \sum_{\{p,q\} \in E} J_{p,q} Z_p Z_q
\]
where \( J_{p,q} \) are real coefficients. It describes a classical Ising-type cost function defined on the graph \( G \). Note that \( \langle z | C | z \rangle \) is a 2-local function on \( G \). The Quantum Approximate Optimization Algorithm (QAOA) introduced in \[10\] maximizes the expected value \( \langle \psi | C | \psi \rangle \) over
a suitable class of $n$-qubit variational states $\psi$ that depend on a few parameters. Once the optimal variational state $\psi$ is found, a bit string $x \in \{0, 1\}^n$ is sampled from the distribution $|\langle x | \psi \rangle|^2$ obtained by measuring every qubit of $\psi$. The expected value of the cost function $\langle x | C | x \rangle$ coincides with the optimal variational energy $\langle \psi | C | \psi \rangle$.

Here we focus on the level-2 version of QAOA. The corresponding variational states are generated by a quantum circuit with two entangling layers,

$$|\psi\rangle = e^{-i\beta_2 B} e^{-i\gamma_2 C} e^{-i\beta_1 B} e^{-i\gamma_1 C} |+_n\rangle.$$

Here, $\beta_\ell, \gamma_\ell \in \mathbb{R}$ are variational parameters, $|+_n\rangle = H^\otimes n |0^n\rangle$, and $B = X_1 + X_2 + \ldots + X_n$. Consider the first step of QAOA – computing the expected value $\langle \psi | C | \psi \rangle$. By linearity, it suffices to compute the expected value $\langle \psi | Z_s Z_t | \psi \rangle$ for some fixed edge $\{s, t\} \in E$. The standard lightcone argument shows that $\langle \psi | Z_s Z_t | \psi \rangle$ only depends on coefficients $J_{p,q}$ such that the edge $\{p,q\}$ is incident to $s$, or $t$, or one of nearest neighbors of $s$, $t$. The remaining edges are irrelevant and can be removed from the graph. Below we assume that the graph has been truncated such that all irrelevant edges are removed.

Inserting the identity decompositions on qubits $s, t$ between the first $B$-layer and the second $C$-layer one gets

$$\langle \psi | Z_s Z_t | \psi \rangle = \sum_{x \in \{0,1\}^4} \mu(x)$$

where

$$\mu(x) = \langle +^n | e^{i\gamma_1 C} e^{i\beta_1 B} | x_1 x_2 \rangle \langle x_1 x_2 | s,t e^{i\gamma_2 C} e^{i\beta_2 B} Z_s Z_t e^{-i\beta_2 B} e^{-i\gamma_2 C} | x_3 x_4 \rangle \langle x_3 x_4 | s,t e^{-i\beta_1 B} e^{-i\gamma_1 C} | +^n \rangle$$

Using the fact that $X^\otimes n$ commutes with $B, C, Z_s Z_t$ and $X^\otimes n | +^n \rangle = | +^n \rangle$ one can easily check that $\mu(x)$ has symmetries $\mu(x \oplus 1111) = \mu(x)$ and $\mu(x_3 x_4 x_1 x_2) = \mu^*(x_1 x_2 x_3 x_4)$. Since $\langle \psi | Z_s Z_t | \psi \rangle$ is real, one can write

$$\langle \psi | Z_s Z_t | \psi \rangle = \text{Re} \left[ 2 \mu(0000) + 4 \mu(0010) + 4 \mu(0001) + 2 \mu(0111) + 2 \mu(0110) + 2 \mu(0101) \right].$$

(34) Let us show that the quantity $\mu(x)$ can be expressed as a graph-based forrelation, namely,

$$\mu(x) = \langle x_1 x_2 | U | x_3 x_4 \rangle \cdot \langle +^n | e^{i\gamma_1 C} O_1(x) \otimes O_2(x) \otimes \cdots \otimes O_n(x) e^{-i\gamma_1 C} | +^n \rangle$$

(35) for some single-qubit operators $O_j(x)$ such that $\|O_j(x)\| \leq 1$ and a two-qubit operator

$$U = e^{i\gamma_2 J_s t Z \otimes Z} e^{i\beta_2 J_s t Z \otimes Z} Z \otimes Z e^{-i\beta_2 J_s t Z \otimes Z} e^{-i\gamma_2 J_s t Z \otimes Z}.$$  

(36) Indeed, a simple algebra shows that

$$\mu(x) = \langle x_1 x_2 | U | x_3 x_4 \rangle \cdot \langle +^n | e^{i\gamma_1 C} e^{i\beta_1 B} e^{i\gamma_2 C'} | x_1 x_2 \rangle \langle x_3 x_4 | s,t e^{-i\gamma_2 C'} e^{-i\beta_1 B} e^{-i\gamma_1 C} | +^n \rangle$$

where $C'$ is obtained from $C$ by retaining only the edges incident to exactly one of the vertices $s, t$. In other words,

$$C' = \sum_{p \in V \setminus \{s,t\}} J_{s,p} Z_s Z_p + J_{t,p} Z_t Z_p.$$
Replacing $Z_s$ and $Z_t$ in $C'$ by their eigenvalues leads to Eq. (35) where
\[
O_s(x) = e^{i\beta_1 X} |x_1\rangle \langle x_3| e^{-i\beta_1 X},
\]
(37)
\[
O_t(x) = e^{i\beta_1 X} |x_2\rangle \langle x_4| e^{-i\beta_1 X},
\]
(38)
and
\[
O_p(x) = e^{i\beta_1 X} e^{i\gamma_2 (J_{s,p}(-1)^{x_1} + J_{t,p}(-1)^{x_2} - J_{s,p}(-1)^{x_3} - J_{t,p}(-1)^{x_4})} Z e^{-i\beta_1 X}
\]
(39)
for all $p \notin \{s,t\}$. Combining Eqs. (34,35,36,37,38,39) shows that computing the mean value $\langle \psi | Z_s Z_t | \psi \rangle$ can be reduced to solving six instances of the graph-based forrelation problem.

Finally, although there are efficient classical algorithms for maximizing Ising cost functions over planar graphs [24], we note that for Ising cost functions with non-zero magnetic fields (i.e., the Hamiltonian contains $J_a Z_a$ terms) no such polynomial-time algorithm is known. Furthermore, the above reduction from level-2 QAOA to graph-based forrelation can be easily extended to these more general cost functions $C$ that contain both quadratic and linear terms.

As a consequence, our classical algorithm for graph-based forrelation problems can be deployed to efficiently compute mean values $\langle \psi | C | \psi \rangle$ for level-2 QAOA on planar and bipartite graphs. This allows one to study the performance of these QAOA algorithms using a classical computer. Note that it does not provide a classical simulation of the full QAOA algorithm—a quantum computer is still needed to sample from the variational state $|\psi\rangle$ once a suitable choice of variational parameters has been found.

### 4.2 Numerical estimation of quantum mean values

We implemented our graph-based forrelation algorithm and used it to calculate level-2 QAOA variational energies. To test our implementation, we calculated $\langle \psi | C | \psi \rangle$ where $C$ is the 2-local Hamiltonian with randomly-selected $\pm 1$ couplings over the 10-qubit triangular lattice shown below:

![Triangular Lattice](image)

A green edge corresponds to a $+1$ coupling, while a red edge corresponds to a $-1$ coupling. The triangular lattice was chosen over the usual square lattice due to the fact that it is not bipartite, and therefore requires the more sophisticated partitioning of vertices used in the graph-based forrelation algorithm for general planar graphs.

In Figure 3, we graph the accuracy of the estimate as a function of $\epsilon$ where $\epsilon^{-2}$ samples were taken for each unitary graph-based forrelation instance. Recall, however, that we estimate each local term of the Hamiltonian separately (of which there are 18 in the example). We randomly chose the variational angles in the range $[0, 2\pi)$ ($\beta_1 = 1.44433$, $\beta_2 = 3.56786$, $\gamma_1 = 0.937498$, and $\gamma_2 = 4.93861$). These choices were fixed for all $\epsilon$. The exact energy ($-4.35917$) was calculated explicitly using Mathematica.
Figure 3: Additive estimation error for the energy of the triangular lattice as a function of accuracy parameter $\epsilon$. Each data point is the average of 10 trials with variance shown by the error bars. The parameters $\beta_1 = 1.44433$, $\beta_2 = 3.56786$, $\gamma_1 = 0.937498$, and $\gamma_2 = 4.93861$ were fixed for all $\epsilon$, and the exact energy $-4.35917$ was calculated by brute force. We note that we expect linear scaling with $\epsilon$.

4.3 The level-2 RQAOA algorithm and implementation

Recall that the ability to optimize the variational parameters of the QAOA algorithm does not immediately confer the ability to carry out the entire QAOA heuristic due to the fact that a quantum computer is needed to sample from the variational state $|\psi\rangle$. Instead, we turn to the Recursive QAOA algorithm (RQAOA) of Bravyi, Kliesch, König, and Tang [19] which can be simulated entirely given an algorithm to compute expected values and optimize variational angles. The algorithm has also been shown to perform well in certain cases in which the usual QAOA is provably suboptimal.

Let us briefly describe this algorithm. Suppose we have some cost function $C: \{-1, 1\}^n \rightarrow \mathbb{R}$ we would like to maximize. For our purposes, let us also suppose that $C$ is an Ising cost function of the form

$$C(z) = \sum_{\{p,q\} \in E} J_{p,q} z_p z_q$$

where $E$ is the edge set of some graph, and the $J_{p,q}$ are real coefficients. As in the QAOA algorithm, we promote the cost function to a Hamiltonian, i.e., $C = \sum_{\{p,q\} \in E} J_{p,q} Z_p Z_q$, and optimize the variational parameters of the state

$$|\psi\rangle = e^{-i\beta_2 B} e^{-i\gamma_2 C} e^{-i\beta_1 B} e^{-i\gamma_1 C} |+^n\rangle$$

to maximize $\langle \psi | C | \psi \rangle$. Given these parameters, we compute the values

$$M_{p,q} = \langle \psi | Z_p Z_q | \psi \rangle$$
for each edge \( \{p, q\} \in E \). We then choose whichever edge \( \{p, q\} \) showed the strongest correlation, that is,
\[
\{p, q\} = \arg \max_{\{a, b\} \in E} |M_{a,b}|.
\]
Finally, we impose the constraint \( z_p = \text{sgn}(M_{p,q})z_q \) and eliminate \( z_p \) from the cost function so that we obtain a new Ising cost function on \( n - 1 \) variables. That is, after eliminating variable \( z_p \), the term \( J_{r,p}z_rz_p \) in the cost function becomes \( J_{r,p}\text{sgn}(M_{p,q})z_rz_q \). We recurse on this smaller instance (finding the new optimal parameters, choosing an edge, etc.) until some threshold number of variables is met, after which we simply brute force the optimal solution.

The RQAOA algorithm has an important property of preserving planarity of the underlying graph \( G \). Namely, the variable elimination step of the algorithm, i.e., constraining \( z_p \) and \( z_q \) to be (anti)correlated, corresponds to a contraction of the edge \( \{p, q\} \) in the graph \( G \) —the term \( J_{p,q}z_pz_q \) in the cost function disappears and becomes a constant energy shift, and all edges incident to those two vertices become incident to the merged node. It is well-known that edge contractions preserve planarity.\(^3\) Thus, recursive steps in RQAOA generate a family of Ising cost functions defined on planar graphs, as long as the initial cost function is defined on a planar graph.

Let us now describe our implementation of the level-2 RQAOA algorithm on 2D grid graphs. We optimize the variational angles in two phases. First, we set \( \beta_2 = \gamma_2 = 0 \) and optimize \( \beta_1 \) and \( \gamma_1 \) using the solution for level-1 QAOA \(^{[19]}\). We fix the optimal \( \beta_1 \) and \( \gamma_1 \) obtained at this step. Second, we search over a grid of possible \( \beta_2 \) and \( \gamma_2 \) values and choose whichever angles yield the largest energy using our algorithm for calculating 2-level variational energies. We note that this approach ensures that the energy computed at each step is at least the energy computed by the level-1 QAOA algorithm. Indeed, we observe empirically that the energy we obtain is almost always strictly greater than the level-1 energy. That said, our approach does not guarantee we obtain the largest possible level-2 variational energy.

The second step above is aided by the following observation: for fixed angles \( \beta_1, \gamma_1, \gamma_2 \), the value of \( \beta_2 \) which maximizes the variational energy can be computed by calculating the energy at only three different values of \( \beta_2 \). Therefore, the two-dimensional search in the second step above essentially reduces to a one-dimensional search. We describe this reduction in Appendix B.

Finally, in order to more efficiently probe larger and more complex optimization problems using level-2 RQAOA, we supplement our graph-based forrelation algorithm for calculating the variational energies with an explicit brute force solution. It is simple to see that the expected value of a particular \( Z_sZ_t \) term only depends on neighbors of the neighbors of the edge \( \{s, t\} \)—that is, the lightcone of the \( Z_sZ_t \) term. When this set of qubits is small, we can brute force the expected values by explicitly writing out the state of the system. On the other hand, when this set of qubits is large, the exponential running time of the brute force algorithm becomes prohibitive and we must turn to our graph-based forrelation algorithm.

\(^3\)For example, one can appeal to Wagner’s theorem which states that a finite graph is planar iff it excludes \( K_5 \) and \( K_{3,3} \) as minors. By definition, taking minors involves contracting edges, and so if the minor was excluded before then it is clearly excluded after contracting an edge.
Figure 4: The graphs above depict a single run of the level-2 RQAOA algorithm on a 15 × 15 grid with random ±1 couplings. We set the parameters ε = .03, brute force the solution when 10 vertices remain, and search over 30 possible values of γ2 to optimize the level-2 variational angles. The algorithm returned an optimal assignment to the vertices to maximize the cost function. *Left:* The running time of the algorithm at each step of the RQOA algorithm. *Right:* The number of calls we make to our graph-based forrelation algorithm (e.g., a value of 0 implies that only the brute-force algorithm was used).

We describe our exact brute force algorithm (which is more sophisticated than the one hinted at above) in Appendix C.

Notice that although the 2D grid graph has low degree, the graph obtained by contracting various edges does not in general remain low degree. Therefore, while the earlier steps of the RQAOA algorithm can be computed by brute force, the later steps must be computed by our graph-based forrelation algorithm. This phenomenon can be observed in Figure 4.

We test this implementation of the level-2 RQAOA on 10 × 10 and 15 × 15 grid graphs with random ±1 couplings. In both tests, we set ε = .03 (once again, taking ε⁻² many samples), brute force the solution when 10 vertices remain, and search over a grid of 30 points to optimize the level-2 variational angles. In ten random instances on the 10 × 10 grid, there was only one for which our implementation did not yield an optimal solution (and even in this case, the solution obtained was 98% of the optimal value). While impressive, we note that the level-1 RQAOA algorithm also performs very well on such instances, and so we do not attempt to make a qualitative comparison between the two. That said, we stress that we know of no faster method for calculating the level-2 variational energies and that the energies given by our level-2 algorithm are greater than those given by the level-1 algorithm. Finally, we tested a single random instance on the 15 × 15 grid and give a detailed breakdown of its runtime in Figure 4. The algorithm found an optimal assignment to the vertices to maximizes the cost function, which we computed explicitly using Gurobi’s integer quadratic programming software [25].
5 Conclusions

Quantum computers available today may already be capable of certain specialized tasks that are too hard for existing classical computers. A convincing demonstration of a quantum computational advantage requires evidence that the task is hard for classical computers. Even if we focus on problems which admit asymptotic quantum speedups, one would like to ensure that the problem size is large enough to defeat existing classical machines. This requires an accurate estimate of the runtime required by classical algorithms. Our work provides such estimates for the forrelation problem — a powerful computational primitive that achieves nearly maximal quantum speedup, as measured by query complexity. We developed classical algorithms both for the oracle-based and for an explicitly defined graph-based forrelation problems. In the oracular setting our algorithm is almost optimal as its runtime nearly matches the query complexity lower bound. This provides a nearly quadratic speedup \((2^{n/2} vs 2^n)\) compared with the best previously known algorithms reported in Refs. [5, 6]. In the graph-based setting our algorithm has a polynomial runtime for a large family of graphs including any bipartite or any planar graph. This extends a line of work studying classical algorithms for problems that promise a quantum advantage such as boson sampling [26], random circuit sampling [27], or IQP circuits [28]. Our work also provides a new tool to study the performance of quantum approximate optimization algorithms. The ability to calculate the variational energy of QAOA states classically eliminates the need to prepare the state on a quantum device while optimizing the QAOA parameters. Alternatively, our classical simulator can be used to benchmark QAOA on large problem sizes that are not yet accessible in the experiment.

While we have provided strong evidence that a relative-error version of graph-based forrelation is intractable, an intriguing open question is whether or not the standard additive-error version is hard for classical machines. Alternatively, one may attempt to improve or extend the reach of our efficient classical algorithms. A modest goal would be to improve the error dependence of the classical algorithm for graph-based forrelation on planar graphs from \(\epsilon^{-2}\) to \(\epsilon^{-1}\), matching the error scaling of our algorithm for oracle-based forrelation. Such an improvement would likely provide a substantial enhancement of the practical performance of QAOA simulation.

A related open question is whether some special instances of the graph-based forrelation problem can be used to demonstrate a computational quantum advantage with an efficient classical verification. For example, suppose \(G = (V, E)\) is an \(n\)-vertex graph that admits a partition of vertices \(V = AB\) such that the subgraphs \(G_A\) and \(G_B\) induced by \(A\) and \(B\) have treewidth \(O(\log n)\). Suppose also that finding a low-treewidth partition as above from scratch is a classically hard problem. The forrelation \(\Phi\) based on such graph \(G\) can be efficiently (in time polynomial in \(n\)) approximated by the classical algorithm of Section 3 only if a low-treewidth partition \(AB\) is explicitly specified. Meanwhile, a quantum computer can efficiently approximate the forrelation \(\Phi\) in all cases. Imagine a classical verifer in possession of a secret low-treewidth partition \(V = AB\) and a prover who claims to have a quantum computer. The verifier can challenge the prover to approximate the forrelation \(\Phi\) without access to the secret partition \(AB\). Once the prover provides an estimate of \(\Phi\), the verifier can efficiently test whether this estimate is accurate enough using the algorithm of Section 3. The ability to pass this test may serve as a proof of quantumness, assuming that graphs \(G\)
with the desired properties indeed exist.

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References

[1] Lov K Grover. Quantum mechanics helps in searching for a needle in a haystack. Physical review letters, 79(2):325, 1997.

[2] Peter W Shor. Polynomial-time algorithms for prime factorization and discrete logarithms on a quantum computer. SIAM review, 41(2):303–332, 1999.

[3] Michele Mosca and Artur Ekert. The hidden subgroup problem and eigenvalue estimation on a quantum computer. In NASA International Conference on Quantum Computing and Quantum Communications, pages 174–188. Springer, 1998.

[4] Mark Ettinger, Peter Høyer, and Emanuel Knill. The quantum query complexity of the hidden subgroup problem is polynomial. Information Processing Letters, 91(1):43–48, 2004.

[5] Scott Aaronson. BQP and the polynomial hierarchy. In Proceedings of the forty-second ACM symposium on Theory of computing, pages 141–150, 2010.

[6] Scott Aaronson and Andris Ambainis. Forrelation: A problem that optimally separates quantum from classical computing. SIAM Journal on Computing, 47(3):982–1038, 2018.

[7] Avishay Tal. Towards optimal separations between quantum and randomized query complexities. arXiv preprint arXiv:1912.12561, 2019.

[8] Nikhil Bansal and Makrand Sinha. k-forrelation optimally separates quantum and classical query complexity. arXiv eprint arXiv:2008.07003, 2020.

[9] Ran Raz and Avishay Tal. Oracle separation of bqp and ph. In Proceedings of the 51st Annual ACM SIGACT Symposium on Theory of Computing, pages 13–23, 2019.

[10] Edward Farhi, Jeffrey Goldstone, and Sam Gutmann. A quantum approximate optimization algorithm. arXiv preprint arXiv:1411.4028, 2014.
[11] Gilles Brassard, Peter Hoyer, Michele Mosca, and Alain Tapp. Quantum amplitude amplification and estimation. *Contemporary Mathematics*, 305:53–74, 2002.

[12] Robert Beals, Harry Buhrman, Richard Cleve, Michele Mosca, and Ronald De Wolf. Quantum lower bounds by polynomials. *Journal of the ACM (JACM)*, 48(4):778–797, 2001.

[13] Sergey Bravyi, David Gosset, and Ramis Movassagh. Classical algorithms for quantum mean values. *arXiv preprint arXiv:1909.11485*, 2019.

[14] Maarten Van den Nest, Jeroen Dehaene, and Bart De Moor. Graphical description of the action of local Clifford transformations on graph states. *Physical Review A*, 69(2):022316, 2004.

[15] Robert Raussendorf and Hans J Briegel. A one-way quantum computer. *Physical Review Letters*, 86(22):5188, 2001.

[16] Michael J Bremner, Richard Jozsa, and Dan J Shepherd. Classical simulation of commuting quantum computations implies collapse of the polynomial hierarchy. *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 467(2126):459–472, 2011.

[17] Zhihui Wang, Stuart Hadfield, Zhang Jiang, and Eleanor G Rieffel. Quantum approximate optimization algorithm for MaxCut: A fermionic view. *Physical Review A*, 97(2):022304, 2018.

[18] Matt DeVos, Guoli Ding, Bogdan Oporowski, Daniel P Sanders, Bruce Reed, Paul Seymour, and Dirk Vertigan. Excluding any graph as a minor allows a low tree-width 2-coloring. *Journal of Combinatorial Theory, Series B*, 91(1):25–41, 2004.

[19] Sergey Bravyi, Alexander Kliesch, Robert Koenig, and Eugene Tang. Obstacles to variational quantum optimization from symmetry protection. *Physical Review Letters*, 125:260505, 2020.

[20] M Nest. Simulating quantum computers with probabilistic methods. *arXiv preprint arXiv:0911.1624*, 2009.

[21] Hans Bodlaender. Planar graphs with bounded treewidth. Technical Report RUUCS-88-14, Department of Computer Science, Utrecht University, the Netherlands (1988).

[22] Hans L Bodlaender. A linear-time algorithm for finding tree-decompositions of small treewidth. *SIAM Journal on computing*, 25(6):1305–1317, 1996.

[23] Gary Chartrand, Dennis Geller, and Stephen Hedetniemi. Graphs with forbidden subgraphs. *Journal of Combinatorial Theory, Series B*, 10(1):12–41, 1971.

[24] Nicol Schraudolph and Dmitry Kamenetsky. Efficient exact inference in planar ising models. *Advances in Neural Information Processing Systems*, 21:1417–1424, 2008.
In the following we consider the problem of approximating a correlation $\Phi(f, g)$ to within a given relative error, where $f, g$ are two-local functions.

Firstly, let us see how to establish hardness of approximation for graph-based correlations arising from stabilizer states [29]. As was shown in [14], for any $n$-qubit stabilizer state $|\psi\rangle$ where exists an $n$-vertex graph $G = (V, E)$ and single-qubit Clifford operators $C_1, \ldots, C_n$ such that

$$|\psi\rangle = (C_1 \otimes C_2 \otimes \cdots \otimes C_n)U_f H^\otimes n|0^n\rangle,$$

$$f(x) = \prod_{\{u, v\} \in E} (-1)^{x_u x_v}.$$ 

Clearly, $f$ is a two-local function on $G$. Thus the expected value of any tensor product operator on any $n$-qubit stabilizer state can be expressed as a graph-based correlation for a suitable $n$-vertex graph and two-local functions $f = g$. As a corollary, approximating a graph-based correlation with a small relative error is #P-hard, even on a two-dimensional grid graph $G$. This follows from the facts that (a) any output probability of a quantum circuit can be expressed as the expected value of a tensor product observable on a 2D cluster state using measurement-based quantum computing [15], and (b) estimating the output probabilities of quantum circuits with a small relative error is #P-hard [30].

In the remainder of this section we show that this hardness persists for the standard correlation problem with $O_j = H$ for all $j$. In the following we write $S^1$ for the unit circle in the complex plane.

To this end, we consider so-called IQP circuits [16]. In Ref.[16] it is shown that given an $N$-qubit, $m$-gate quantum circuit $C$ we may efficiently compute $n \leq N + m$ and a two-local function $h : \{0, 1\}^n \to S^1$ on a two-dimensional grid graph such that

$$\langle 0^n | H^\otimes n U_h H^\otimes n | 0^n \rangle = \sqrt{2^{n-N}} \langle 0^N | C | 0^N \rangle.$$
This is used in Ref.[16] to show that postselected IQP circuits on planar graphs are as powerful as postBQP. Hardness of approximation for IQP circuit amplitudes then follows from the well known fact that a quantum circuit amplitude \(\langle 0^n|C|0^n\rangle\) is \#P-hard to approximate to a given relative error.

**Lemma 6 ([16]).** Given a two-local function \(h : \{0,1\}^n \to \mathbb{S}^1\) on a planar graph \(G\) and \(\epsilon > 0\), it is \#P-hard to compute an approximation \(Z\) such that

\[
(1 - \epsilon)\langle 0^n|H^\otimes nU_hH^\otimes n|0^n\rangle \leq Z \leq (1 + \epsilon)\langle 0^n|H^\otimes nU_hH^\otimes n|0^n\rangle.
\]

To establish the following lemma, we show that approximating forrelation of two-local functions on a planar graph is as hard as approximating IQP circuit amplitudes.

**Lemma 7.** Given \(\epsilon > 0\) and two-local functions \(f, g : \{0,1\}^n \to \mathbb{S}^1\) on a planar graph \(G\), it is \#P-hard to compute an approximation \(\tilde{\Phi}\) such that

\[
(1 - \epsilon)\Phi(f,g) \leq \tilde{\Phi} \leq (1 + \epsilon)\Phi(f,g).
\]

**Proof.** Suppose we are given a two-local function \(h : \{0,1\}^n \to \mathbb{S}^1\) on a planar graph \(G\). Below we (efficiently) construct two-local functions \(f,g : \{0,1\}^n \to \mathbb{S}^1\) on \(G\) such that

\[
\langle 0^n|H^\otimes nU_fH^\otimes nU_gH^\otimes n|0^n\rangle = \langle 0^n|H^\otimes nU_hH^\otimes n|0^n\rangle.
\]  \(\text{(40)}\)

The claimed hardness of approximation then follows immediately from Lemma 6.

To prove Eq. (40) we use the one-qubit identity

\[
e^{-i\pi/4}SHS = HS^\dagger H,
\]  \(\text{(41)}\)

where \(S = \text{diag}(1,i)\) is the phase gate. Define functions \(f, g\) such that \(U_g = (S^\dagger)^\otimes n\) and \(U_f = e^{i\pi n/4}U_hU_g\). Note that both \(f\) and \(g\) are two-local on \(G\). Then

\[
\langle 0^n|H^\otimes nU_fH^\otimes nU_gH^\otimes n|0^n\rangle = e^{-i\pi n/4}\langle 0^n|H^\otimes nU_fS^\otimes nH^\otimes n|0^n\rangle = \langle 0^n|H^\otimes nU_hH^\otimes n|0^n\rangle,
\]

where in the first equality we used Eq. (41). This establishes Eq. (40) and completes the proof.

The graph \(G\) in lemmas 6 and 7 may be taken to be a two-dimensional grid graph without loss of generality.
B Simplifying level-2 QAOA variational optimization

Let \( G = (V, E) \) be a graph with \( n \) vertices,
\[
B = \sum_{p \in V} X_p \quad \text{and} \quad C = \sum_{\{p, q\} \in E} J_{p, q} Z_p Z_q.
\]

For level-2 QAOA, we would like to set \( \beta_1, \beta_2, \gamma_1, \gamma_2 \) to maximize the energy
\[
E(\beta_1, \beta_2, \gamma_1, \gamma_2) = \langle +^n | W^\dagger CW | +^n \rangle,
\]
where \( W = e^{-i\beta_2 B} e^{-i\gamma_2 C} e^{-i\beta_1 B} e^{-i\gamma_1 C} \) is the QAOA circuit with two entangling layers.

Our goal for this section will be to show that if you fix the values of \( \beta_1, \gamma_1 \) and \( \gamma_2 \), then the value of \( \beta_2 \) that maximizes the energy \( E \) can be computed analytically using the energy at three distinct values of \( \beta_2 \).

To show this, let us first focus on the contribution to the energy by single \( Z \) terms of \( C \). Since \( e^{-i\beta_2 B} \) is a product of single-qubit operations, the conjugation of \( Z \) by \( e^{-i\beta_2 B} \) only depends on the gates on qubits \( s \) and \( t \). We get
\[
e^{i\beta_2 B} Z_s Z_t e^{-i\beta_2 B} = e^{i\beta_2 (X_s + X_t)} Z_s Z_t e^{-i\beta_2 (X_s + X_t)} = e^{2i\beta_2 (X_i + IX)} ZZ
\]
\[
= \left( \cos^2(2\beta_2) I + i \sin(2\beta_2) \cos(2\beta_2) (IX + XI) - \sin^2(2\beta_2) XX \right) ZZ
\]
\[
= \frac{1 + \cos(4\beta_2)}{2} ZZ + \frac{\sin(4\beta_2)}{2} (ZY + YZ) + \frac{1 - \cos(4\beta_2)}{2} YY.
\]

By linearity, this implies that we can write the expectation as
\[
E(\beta_1, \beta_2, \gamma_1, \gamma_2) = a \cos(4\beta_2) + b \sin(4\beta_2) + c
\]
for some real coefficients \( a, b, \) and \( c \) which are complicated functions of \( \beta_1, \gamma_1, \) and \( \gamma_2 \). We can compute these coefficients exactly using only three evaluations of the expectation function:
\[
E(\beta_1, \pi/8, \gamma_1, \gamma_2) = b + c
\]
\[
E(\beta_1, -\pi/8, \gamma_1, \gamma_2) = -b + c
\]
\[
E(\beta_1, 0, \gamma_1, \gamma_2) = a + c.
\]

So, \( a, b, \) and \( c \) can be calculated easily by solving the system of equations. Once the values are known, we can calculate the max energy over \( \beta_2 \) using some elementary trigonometry:
\[
\max_{\beta_2} E(\beta_1, \beta_2, \gamma_1, \gamma_2) = c + \sqrt{a^2 + b^2}
\]
where the optimal \( \beta_2 \) is found by solving
\[
\tan(4\beta_2) = b/a
\]
\[
a \cos(4\beta_2) \geq 0
\]
\[
b \sin(4\beta_2) \geq 0.
\]

As a final remark, we note that this calculation also shows that the optimal value for \( \beta_2 \) is between \([0, \pi/2)\) since \( \arctan(b/a) \in [0, 2\pi) \).
**C Simulation of level-2 QAOA for low-degree graphs**

Let $G = (V, E)$ be a graph with $n$ vertices,

$$B = \sum_{p \in V} X_p \quad \text{and} \quad C = \sum_{\{p,q\} \in E} J_{p,q} Z_p Z_q.$$  

Consider some fixed edge $\{s, t\} \in E$. Our goal is to compute a quantum mean value

$$\mu = \langle +^n | W^\dagger Z_s Z_t W | +^n \rangle,$$

where $W = e^{-i \beta_2 B} e^{-i \gamma_2 C} e^{-i \beta_1 B} e^{-i \gamma_1 C}$ is the QAOA circuit with two entangling layers. In this section we give two classical algorithms $A'$ and $A''$ that compute the mean value $\mu$ using the Schrödinger and the Heisenberg pictures respectively. The runtime of these algorithms scales exponentially with the size of certain local neighborhoods of the vertices $s$ and $t$ defined as follows. Suppose $M \subseteq V$ is a subset of vertices and $r \geq 0$ is an integer. Let $N_r(M)$ be the set of all vertices $i \in V$ such that the graph distance between $i$ and $M$ is at most $r$. Let $n_r(M) = |N_r(M)|$. The runtime of our algorithms depends on $n_2(s)$, $n_2(t)$, $n_1(s,t)$, and $n_2(s,t)$. For example, suppose each vertex of $G$ has at most $d$ neighbors. Then $n_2(j) \leq 1 + d^2$ for any vertex $j$, $n_1(s,t) \leq 2d$, and $n_2(s,t) \leq 2(d^2 - d + 1)$. These bounds are tight if $G$ is a $d$-regular tree.

The unitary operator $W$ can be implemented by a quantum circuit with two layers of single-qubit $X$-rotations and two entangling layers composed of nearest-neighbor $ZZ$-rotations. Such circuit can propagate information from a qubit $j \in V$ only within the lightcone $N_2(j)$. Accordingly, the mean value $\mu$ can be computed by restricting the circuit $W$ onto the lightcone $N_2(s,t)$. The restricted version of $W$ acting on $n_2(s,t)$ qubits contains $O(n_2(s,t))$ single-qubit gates and two diagonal unitary operators describing a time evolution under the restricted version of $C$. Such circuit can be simulated using the standard methods in time $O(n_2(s,t)2^{n_2(s,t)})$. Once the state $W|+^n\rangle$ has been obtained, computing the expected value of $Z_s Z_t$ on this state takes time $O(2^{n_2(s,t)})$. Thus a naive algorithm for computing $\mu$ that exploits the lightcone structure has runtime $O(n_2(s,t)2^{n_2(s,t)})$. Below we show how to improve upon this naive algorithm.

**Lemma 8.** There exist classical algorithms $A'$ and $A''$ that compute the mean value Eq. (42) in time

$$T' = O(n_2(s)2^{n_2(s)} + n_2(t)2^{n_2(t)}) \quad \text{and} \quad T'' = O(n_1(s,t)4^{n_1(s,t)} + n_2(s,t)3^{n_1(s,t)}) \quad (43)$$

respectively.

For simplicity here we assume that arithmetic operations with real numbers and evaluation of the standard trigonometric functions can be performed with an infinite precision in a unit time. Under this assumption the algorithms $A'$ and $A''$ compute the mean value $\mu$ exactly. For a given problem instance one can estimate the runtimes using Eq. (43) and pick the algorithm with the smallest runtime. In the rest of this section we prove Lemma 8 by explicitly describing the two algorithms.
Algorithm $\mathcal{A}':$ Consider a vertex $j \in \{s, t\}$. Write $C = C_{\text{loc}}(j) + C_{\text{else}}(j)$, where $C_{\text{loc}}(j)$ is the sum of all terms $J_{p,q}Z_pZ_q$ with $p, q \in \mathcal{N}_2(j)$ and $C_{\text{else}}(j)$ is the sum of all remaining terms. Since all terms in $C$ pairwise commute, the standard lightcone argument shows that
\[
W^\dagger Z_j W = W_{\text{loc}}(j)^\dagger Z_j W_{\text{loc}}(j)
\]
where
\[
W_{\text{loc}}(j) = e^{-i\beta_2 B} e^{-i\gamma_2 C_{\text{loc}}(j)} e^{-i\beta_1 B} e^{-i\gamma_1 C_{\text{loc}}(j)}.
\]
Note that $W_{\text{loc}}(j)$ acts non-trivially only on $\mathcal{N}_2(j)$. Thus $W^\dagger Z_j W|+\rangle = |\psi_j\rangle \otimes |+^{n_2(j)}\rangle$, where
\[
|\psi_j\rangle = W_{\text{loc}}(j)^\dagger Z_j W_{\text{loc}}(j)|+^{n_2(j)}\rangle
\]
is a state supported in $\mathcal{N}_2(j)$. One can compute a lookup table of the function $C_{\text{loc}}(j) : \{0, 1\}^{n_2(j)} \to \mathbb{R}$ in time $O(n_2(j)2^{n_2(j)})$ by iterating over the set $\{0, 1\}^{n_2(j)}$ using Gray code. Indeed, since $C_{\text{loc}}(j)$ is a quadratic function, updating its value upon flipping a single bit of the input bit string takes time $O(n_2(j))$. The quantum circuit $W_{\text{loc}}(j)^\dagger Z_j W_{\text{loc}}(j)$ contains $O(n_2(j))$ single-qubit $X$-rotations and $O(1)$ diagonal unitary operators implementing the time evolution under $C_{\text{loc}}(j)$. The latter can be simulated in time $O(2^{n_2(j)})$ since the lookup table of $C_{\text{loc}}(j)$ is available. Each single-qubit $X$-rotation can be simulated in time $O(2^{n_2(j)})$ using a sparse matrix-vector multiplication. Thus the full vector specifying the state $|\psi_j\rangle$ can be computed in time $O(n_2(j)2^{n_2(j)})$. We have
\[
\mu = \langle +^{n} | (W^\dagger Z_s W)(W^\dagger Z_t W)|+^{n} \rangle = \langle \psi'_j | \psi'_t \rangle
\]
where $|\psi'_j\rangle$ is a state obtained from $|\psi_j\rangle$ by projecting all qubits $i \notin \mathcal{N}_2(s) \cap \mathcal{N}_2(t)$ onto the $|+\rangle$ state. Once a qubit is projected onto the $|+\rangle$ state, it is discarded. The state $|\psi'_j\rangle$ can be computed in time $O(2^{n_2(j)})$, as follows from the proposition below.

**Proposition 1.** Given a state $|\psi\rangle \in (\mathbb{C}^2)^\otimes n$ and an integer $k \in \{1, 2, \ldots, n\}$, let $|\psi'\rangle \in (\mathbb{C}^2)^\otimes n-k$ be a (possibly unnormalized) state obtained from $|\psi\rangle$ by projecting the first $k$ qubits onto the $|+\rangle$ state, that is,
\[
\langle y | \psi' \rangle = 2^{-k/2} \sum_{x \in \{0,1\}^k} \langle x, y | \psi \rangle, \quad y \in \{0, 1\}^{n-k}.
\]

Then one can compute $|\psi'\rangle$ in time $O(2^n)$.

**Proof.** If $k = 1$ then compute all amplitudes $\langle y | \psi' \rangle$ by iterating over $y \in \{0, 1\}^{n-1}$ and using Eq. (44). This takes time $O(2^n)$. Applying the same step inductively $k$ times takes time
\[
\sum_{i=1}^{k} O(2^{n-i}) \leq O(2^n) \sum_{i=1}^{\infty} 2^{-i} = O(2^n).
\]

Here we noted that the number of qubits is reduced by one at each step. \qed
Computing the inner product $\mu = \langle \psi'_1 | \psi'_n \rangle$ takes time $2^{|\mathcal{N}_2(s) \cap \mathcal{N}_2(t)|}$ which is negligible compared with the earlier steps of the algorithm. The overall runtime of algorithm $\mathcal{A}'$ is therefore $T' = O(n_2(s)2^{n_2(s)} + n_2(t)2^{n_2(t)})$.

**Algorithm $\mathcal{A}''$:** Our starting point is the expression for the mean value $\mu$ derived in Section 4.1, namely

$$\mu = \text{Re} \left[ 2\mu(0000) + 4\mu(0010) + 4\mu(0001) + 2\mu(0111) + 2\mu(0110) + 2\mu(0101) \right],$$

(45)

where

$$\mu(v) = \langle v_1 v_2 | U | v_3 v_4 \rangle \cdot \langle + | e^{i\gamma_1 C} O_1(v) \otimes O_2(v) \otimes ... \otimes O_n(v) e^{-i\gamma_1 C} | + \rangle,$$

(46)

$$U = e^{i\gamma_2 J \otimes Z \otimes Z} e^{i\beta_2 (X \otimes I + I \otimes X)} Z \otimes Z e^{-i\gamma_2 J \otimes Z \otimes Z},$$

(47)

and $O_j(v)$ are single-qubit operators defined by

$$O_s(v) = e^{i\beta_1 X} | v_1 \rangle \langle v_3 | e^{-i\beta_1 X},$$

(48)

$$O_t(v) = e^{i\beta_1 X} | v_2 \rangle \langle v_4 | e^{-i\beta_1 X},$$

(49)

$$O_p(v) = e^{i\beta_1 X} e^{i\gamma_2 (J_{s,p}(-1)^{v_1} + J_{t,p}(-1)^{v_2} - J_{s,p}(-1)^{v_3} - J_{t,p}(-1)^{v_4})} Z e^{-i\beta_1 X}$$

(50)

for $p \notin \{s, t\}$. Below we use shorthand notations $\mathcal{N}_r \equiv \mathcal{N}_r(s, t)$ and $n_r = |\mathcal{N}_r(s, t)|$, where $r = 1, 2$. We begin by observing that

$$O_p(v) = I \quad \text{for all } p \notin \mathcal{N}_1.$$ (51)

Indeed, if $p \notin \mathcal{N}_1$ then $J_{s,p} = J_{t,p} = 0$ and $O_p(v) = e^{i\beta_1 X} e^{-i\beta_1 X} = I$, see Eq. (50). Fix a bit string $v \in \{0, 1\}^4$ and let $O_{\mathcal{N}_1}$ be the tensor product of all operators $O_p(v)$ with $p \in \mathcal{N}_1$. From Eqs. (46,51) one gets $\mu(v) = \langle v_1 v_2 | U | v_3 v_4 \rangle \eta(v)$, where

$$\eta(v) = \langle + | e^{i\gamma_1 C} (O_{\mathcal{N}_1} \otimes I_{\text{else}}) e^{-i\gamma_1 C} | + \rangle.$$ (52)

It suffices to show that $\eta(v)$ can be computed in time $T''$ defined in Eq. (43). The standard lightcone argument shows that $\eta(v)$ depends only on the subgraph $G_{\mathcal{N}_1}$ induced by $\mathcal{N}_2$ and the restricted cost function that includes only the terms $J_{p,q} Z_p Z_q$ with $p, q \in \mathcal{N}_2$. To ease the notations, below we ignore all the remaining terms and assume that $G = G_{\mathcal{N}_2}, n = n_2$, and $C = \sum_{p,q \in \mathcal{N}_2} J_{p,q} Z_p Z_q$. Let us write

$$C = C_{\text{loc}} + C_{\text{ent}} + C_{\text{else}},$$ (53)

where $C_{\text{loc}}$ includes all terms $J_{p,q} Z_p Z_q$ with $p, q \in \mathcal{N}_1$, $C_{\text{ent}}$ includes all terms $J_{p,q} Z_p Z_q$ with $p \in \mathcal{N}_1, q \notin \mathcal{N}_1$, and $C_{\text{else}}$ includes all the remaining terms. Using the fact that all terms in $C$ pairwise commute and that $C_{\text{else}}$ commutes with $O_{\mathcal{N}_1} \otimes I_{\text{else}}$, one can rewrite Eq. (52) as

$$\eta(v) = \text{Tr} \left( O_{\mathcal{N}_1} e^{-i\gamma_1 C_{\text{loc}}} \rho e^{i\gamma_1 C_{\text{loc}}} \right)$$ (54)

where $\rho$ is a (mixed) $n_1$-qubit state defined as

$$\rho = \text{Tr}_{\mathcal{N}_1^c} \left( e^{-i\gamma_1 C_{\text{ent}}} | + \rangle \langle + | e^{i\gamma_1 C_{\text{ent}}} \right).$$ (55)

Here $\mathcal{N}_1^c$ is the complement of $\mathcal{N}_1$ and $\text{Tr}_{\mathcal{N}_1^c}$ denotes the partial trace over $\mathcal{N}_1^c$.
Proposition 2. There exists a classical algorithm that computes the matrix of \( \rho \) in the standard basis in time \( O(n_14^{n_1} + n^{3^{n_1}}) \).

Proof. Assume wlog that \( \mathcal{N}_1 = \{1, 2, \ldots, n_1\} \). Let \( m = |\mathcal{N}_1^c| \) and \( p(j) \) be the \( j \)-th qubit of \( \mathcal{N}_1^c \), where \( j = 1, \ldots, m \). Define \( n_1 \)-qubit states \( \rho_0, \rho_1, \ldots, \rho_m \) such that \( \rho_0 = |+^{n_1}\rangle\langle+^{n_1}| \) and

\[
\rho_j = \text{Tr}_{\text{anc}} \left[ e^{-i\gamma_1 \sum_{q \in \mathcal{N}_1} J_{p(j),q} Z_q Z_{\text{anc}}} (\rho_{j-1} \otimes |+\rangle\langle+|) e^{i\gamma_1 \sum_{q \in \mathcal{N}_1} J_{p(j),q} Z_q Z_{\text{anc}}} \right]
\]  

(56)

for all \( j = 1, 2, \ldots, m \). Here we consider a system of \( n_1 + 1 \) qubits with the first \( n_1 \) qubits describing \( \mathcal{N}_1 \) and the last qubit serving as ancilla. The notation \( \text{Tr}_{\text{anc}} \) means the partial trace over the ancilla. We claim that \( \rho_m = \rho \) is the state defined in Eq. (55). Indeed, one can consider the righthand side of Eq. (55) as the output state of a quantum channel that takes as input the state \( \rho_0 = |+^{n_1}\rangle\langle+^{n_1}| \), introduces \( m = n - n_1 \) ancillary qubits initialized in the \( |+\rangle\langle+| \) state, couples \( \mathcal{N}_1^c \) with the ancillary qubits by \( e^{-i\gamma_1 C_{\text{ent}}} \), and finally traces out the ancillas. Since all terms in \( C_{\text{ent}} \) pairwise commute, the same quantum channel can be implemented sequentially such that the \( j \)-th step introduces a single ancilla qubit \( p(j) \in \mathcal{N}_1^c \) initialized in the state \( |+\rangle\langle+| \), applies all interactions in \( C_{\text{ent}} \) that act non-trivially on \( p(j) \), and traces out \( p(j) \). This is described by Eq. (56).

A simple algebra shows that Eq. (56) is equivalent to

\[
\langle x|\rho_j|y \rangle = \langle x|\rho_{j-1}|y \rangle \cdot \cos \left( 2 \gamma_1 \sum_{q \in \mathcal{N}_1} J_{p(j),q}(x_q - y_q) \right)
\]  

for all \( x, y \in \{0, 1\}^{n_1} \). Recalling that \( \rho_0 = |+^{n_1}\rangle\langle+^{n_1}| \) and \( \rho = \rho_m \) one arrives at

\[
\langle x|\rho|y \rangle = 2^{-n_1} \prod_{j=1}^{m} \cos \left( 2 \gamma_1 \sum_{q \in \mathcal{N}_1} J_{p(j),q}(x_q - y_q) \right)
\]  

(58)

Define a function \( f : \{-1, 0, +1\}^{n_1} \to \mathbb{R} \) such that

\[
f(z) = 2^{-n_1} \prod_{j=1}^{m} \cos \left( 2 \gamma_1 \sum_{q \in \mathcal{N}_1} J_{p(j),q}z_q \right)
\]

From Eq. (58) one infers that \( \langle x|\rho|y \rangle = f(x - y) \) for all \( x, y \in \{0, 1\}^{n_1} \). Let us compute the matrix of \( \rho \) by iterating over strings \( z \in \{-1, 0, +1\}^{n_1} \) using ternary Gray code. In other words, each iteration changes only one component of \( z \). We shall maintain a list of values of \( m \) linear functions

\[
\ell_j(z) = 2 \gamma_1 \sum_{q \in \mathcal{N}_1} J_{p(j),q}z_q, \quad j = 1, 2, \ldots, m.
\]

Updating the value of each function \( \ell_j(z) \) upon changing a single component \( z_q \) takes a constant time. Thus updating the value of \( f(z) = 2^{-n_1} \prod_{j=1}^{m} \cos (\ell_j(z)) \) takes time \( O(m) \). The number of pairs \( x, y \in \{0, 1\}^{n_1} \) such that \( z = x - y \) is equal to \( 2^w(z) \), where \( w(z) \) is the number of zeros in \( z \). Identifying all such pairs \( x, y \) and recording the value \( f(z) \) to the
matrix elements $\langle x | \rho | y \rangle$ takes time $O(n_1 2^{w(z)})$ for a fixed $z$. We conclude that computing the full matrix of $\rho$ takes time

$$O(m 3^{n_1}) + \sum_{z \in \{-1,0,+1\}^{n_1}} O(n_1 2^{w(z)}) = O(m 3^{n_1} + n_1 4^{n_1}) = O(n 3^{n_1} + n_1 4^{n_1}).$$

In the last equality we noted that $m = n - n_1 \leq n$. \hfill \square

From Eq. (54) one gets $\eta(v) = \text{Tr}(O_{N_1} \tilde{\rho})$, where

$$\tilde{\rho} = e^{-i \gamma_1 C_{\text{loc}}} \rho e^{i \gamma_1 C_{\text{loc}}}.$$

The next step is to compute the matrix of $\tilde{\rho}$ in the standard basis. We have

$$\langle x | \tilde{\rho} | y \rangle = \langle x | \rho | y \rangle \cdot e^{-i \gamma_1 \langle x | C_{\text{loc}} | x \rangle + i \gamma_1 \langle y | C_{\text{loc}} | y \rangle}. \quad (59)$$

A lookup table of the function $\langle x | C_{\text{loc}} | x \rangle$ with $x \in \{0,1\}^{n_1}$ can be computed in time $O(n_1 2^{n_1})$ by iterating over $x$’s using Gray code. Then one can compute the matrix of $\tilde{\rho}$ using Eq. (59) in time $O(4^{n_1})$ by the brute force method.

It remains to compute $\eta(v) = \text{Tr}(O_{N_1} \tilde{\rho})$. We claim that this can be done in time $O(4^{n_1})$, assuming that the matrix of $\tilde{\rho}$ is already available. Indeed, let $N_1 = AB$, where $A$ and $B$ are subsets of size at most $(n_1 + 1)/2$. Let $O_A$ and $O_B$ be the tensor products of the single-qubit operators $O_p(v)$ with $p \in A$ and $p \in B$ respectively. Then $O_{N_1} = O_A \otimes O_B$. Compute the matrix of $O_A$ and $O_B$ in the standard basis. This takes time $O(|A|^4|A| + |B|^4|B|) = O(n_1 2^{n_1})$ if one uses the brute force method. Finally, we have

$$\eta(v) = \text{Tr}(O_{N_1} \tilde{\rho}) = \sum_{a,a' \in \{0,1\}^{|A|}} \sum_{\beta,\beta' \in \{0,1\}^{|B|}} \langle \alpha' | O_A | \alpha \rangle \cdot \langle \beta' | O_B | \beta \rangle \cdot \langle \alpha, \beta | \tilde{\rho} | \alpha', \beta' \rangle.$$

This sum can be computed by the brute force method in time $O(4^{|A|} + |B|) = O(4^{n_1})$ since the matrices of $O_A, O_B$, and $\tilde{\rho}$ are already available.

Summing up the runtime of each step in the algorithm and recalling that $n = n_2$ after restricting the problem to the subgraph induced by $N_2$ gives the overall runtime $T''$ in Eq. (43).

Comment: Numerical data for RQAOA reported in Section 4.3 was generated by combining three algorithms for computing expected values of observables ZZ on the QAOA states: the forrelation-based algorithm described in Section 3 and Section 4.1, algorithm $A'$, and a simplified version of algorithm $A''$. The latter computes the matrix $\rho$ defined in Eq. (58) in time $O(n_2(s,t) 4^{n_1(s,t)})$ by iterating over bit strings $x, y$ in Eq. (58) using the binary Gray code. This is only a minor slowdown compared with the algorithm based on ternary Gray code described above which computes $\rho$ in time $O(n_1(s,t) 4^{n_1(s,t)} + n_2(s,t) 3^{n_1(s,t)})$. Algorithms $A'$ or $A''$ were selected only if their estimated runtime is below a cutoff value of 0.1 second. Otherwise, the forrelation-based algorithm was selected.

### D Tree decomposition algorithm
Algorithm 1 Tree decomposition of an outerplanar graph [21]

1: function OUTERPLANARTD($G$)
2: if all vertices of $G$ have degree zero then
3: \hspace{1em} return $T = (V, \emptyset), B = \{B_v = \{v\} : v \in V\}$
4: else if $G$ has a degree-1 vertex then
5: \hspace{1em} Choose any degree-1 vertex $v \in V$.
6: \hspace{2em} Let $u \in V$ be the unique neighbor of $v$.
7: \hspace{2em} $V' \leftarrow V \setminus \{v\}$
8: \hspace{2em} $E' \leftarrow E \setminus \{v, u\}$
9: \hspace{2em} $G' \leftarrow (V', E')$
10: \hspace{2em} $T = (W, F), B = \{B_i : i \in V_T\} \leftarrow$ OuterplanarTD($G'$)
11: \hspace{2em} Find a node $i \in W$ such that $u \in B_i$.
12: \hspace{2em} $W' \leftarrow W \cup \alpha$
13: \hspace{2em} $B_\alpha \leftarrow \{u, v\}$
14: \hspace{2em} $F' \leftarrow F \cup \{i, \alpha\}$ return $T' = (W', F'), B' = B \cup B_\alpha$
15: else if $G$ has a degree-2 vertex then
16: \hspace{1em} Choose any degree-2 vertex $v \in V$.
17: \hspace{2em} Let $u, w \in V$ be the two distinct neighbors of $v$.
18: \hspace{2em} $V' \leftarrow V \setminus \{v\}$
19: \hspace{2em} $E' \leftarrow (E \setminus \{(v, u), (v, w)\}) \cup \{u, w\}$
20: \hspace{2em} $G' \leftarrow (V', E')$
21: \hspace{2em} $T = (W, F), B = \{B_i : i \in V_T\} \leftarrow$ OuterplanarTD($G'$)
22: \hspace{2em} Find a node $i \in W$ such that $w \in B_i$ and $u \in B_i$.
23: \hspace{2em} $W' \leftarrow W \cup \alpha$
24: \hspace{2em} $B_\alpha \leftarrow \{u, v, w\}$
25: \hspace{2em} $F' \leftarrow F \cup \{i, \alpha\}$ return $T' = (W', F'), B' = B \cup B_\alpha$
26: end if
27: end function