Quantum Lower Bounds by Polynomials*

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Abstract

We examine the number T of queries that a quantum network requires to compute several Boolean functions on $\{0,1\}^N$ in the black-box *model. We show that, in the black-box model, the exponential quantum speed-up obtained for* partial *functions (i.e. problems involving a promise on the input) by Deutsch and Jozsa and by Simon cannot be obtained for any* total *function: if a quantum algorithm computes some total Boolean function f with bounded-error using T black-box queries then there is a classical deterministic algorithm that computes f exactly with $O(T^6)$ queries. We also give asymptotically tight characterizations of T for all symmetric f in the exact, zero-error, and bounded-error settings. Finally, we give new precise bounds for AND, OR, and PARITY. Our results are a quantum extension of the so-called polynomial method, which has been successfully applied in classical complexity theory, and also a quantum extension of results by Nisan about a polynomial relationship between randomized and deterministic decision tree complexity.*

1 Introduction

The *black-box* model of computation arises when one is given a black-box containing an N-tuple of Boolean variables $X = (x_0, x_1, \ldots, x_{N-1})$. The box is equipped to output x_i on input i. We wish to determine some property of X, accessing the x_i only through the black-box. Such a black-box access is called a *query*. A property of X is any Boolean function that depends on X, i.e. a property is a function $f : \{0,1\}^N \to \{0,1\}$. We want to compute such properties using as few queries as possible.

Consider, for example, the case where the goal is to determine whether or not X contains at least one 1, so we want to compute the property $\mathrm{OR}(X) = x_0 \vee \ldots \vee x_{N-1}$. It is well known that the number of queries required to compute OR by any *classical* (deterministic or probabilistic) algorithm is $\Theta(N)$. Grover [15] discovered a remarkable *quantum* algorithm that, making queries in superposition, can be used to compute OR with small error probability using only $O(\sqrt{N})$ queries. This number of queries was shown to be asymptotically optimal [3, 5, 37].

Many other quantum algorithms can be naturally expressed in the black-box model, such as an algorithm due to Simon [32], in which one is given a function $X : \{0,1\}^n \to \{0,1\}^n$, which, technically, can also be viewed as a black-box $X = (x_0, \ldots, x_{N-1})$ with $N = n2^n$. The black-box X satisfies a particular promise, and the goal is to determine whether or not X satisfies some other property (the details of the promise and properties are explained in [32]). Simon's quantum algorithm is proven to yield an *exponential* speed-up over classical algorithms in that it makes $(\log N)^{O(1)}$ queries, whereas every classical randomized algorithm for the same function must make $N^{\Omega(1)}$ queries. The promise means that the function $f : \{0,1\}^N \to \{0,1\}$ is *partial*; it is not defined on all $X \in \{0,1\}^N$. (In the previous example of OR, the function is *total*; however, the quantum speed-up is only quadratic.) Some other quantum algorithms that are naturally expressed in the black-box model are described in [10, 4, 19, 5, 6, 17, 22, 9, 7, 21, 8].

Of course, *upper bounds* in the black-box model immediately yield upper bounds for the *circuit description* model in which the function X is succinctly described as a $(\log N)^{O(1)}$-sized circuit computing x_i from i. On the

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other hand, *lower bounds* in the black-box model do not imply lower bounds in the circuit model, though they can provide useful guidance, indicating what certain algorithmic approaches are capable of accomplishing. It is noteworthy that, at present, there is no known algorithm for computing OR (i.e. satisfiability) in the circuit model that is significantly more efficient than using the circuit solely to make queries (though, *proving* that no better algorithm exists is likely to be difficult, as it would imply $P \neq NP$).

It should also be noted that the black-box complexity of a function only considers the number of queries; it does not capture the complexity of the *auxiliary* computational steps that have to be performed in addition to the queries. In cases such as OR, PARITY, MAJORITY, this auxiliary work is not significantly larger than the number of queries; however, in some cases it may be much larger. For example, consider the case of factoring N-bit integers. The best known algorithms for this involve $\Theta(N)$ queries to determine the integer, followed by $2^{N^{\Omega(1)}}$ operations in the classical case but only $N^2(\log N)^{O(1)}$ operations in the quantum case [31]. Thus, the number of queries is apparently not of primary importance in the case of factoring.

In this paper, we analyze the black-box complexity of several functions and classes of functions in the quantum computation setting. In particular, we show that the kind of exponential quantum speed-up that Simon's algorithm achieves for a partial function cannot be obtained by any quantum algorithm for any total function: at most a polynomial speed-up is possible. We also tightly characterize the quantum black-box complexity of all symmetric functions, and obtain exact bounds for functions such as AND, OR, PARITY, and MAJORITY for various error models: exact, zero-error, bounded-error.

An important ingredient of our approach is a reduction that translates quantum algorithms that make T queries into multilinear polynomials over the N variables of degree at most $2T$. This is a quantum extension of the so-called polynomial method, which has been successfully applied in classical complexity theory (see [2] for an overview). Also, our polynomial relationship between the quantum and the classical complexity is analogous to earlier results by Nisan [23], who proved a polynomial relationship between randomized and deterministic decision tree complexity.

2 Summary of results

We consider three different settings for computing f on $\{0,1\}^N$ in the black-box model. In the *exact* setting, an algorithm is required to return $f(X)$ with certainty for every X. In the *zero-error* setting, for every X, an algorithm may return "inconclusive" with probability at most $1/2$, but *if* it returns an answer, this must be the correct value of $f(X)$ (algorithms in this setting are sometimes called *Las Vegas* algorithms). Finally, in the *two-sided bounded-error* setting, for every X, an algorithm must correctly return the answer with probability at least $2/3$ (algorithms in this setting are sometimes called *Monte Carlo* algorithms; the $2/3$ is arbitrary). Our main results are:[1]

1. In the black-box model, the quantum speed-up for *any* total function cannot be more than by a sixth-root. More specifically, if a quantum algorithm computes f with bounded-error probability by making T queries, then there is a classical deterministic algorithm that computes f exactly making at most $O(T^6)$ queries. If f is *monotone* then the classical algorithm needs at most $O(T^4)$ queries, and if f is *symmetric* then it needs at most $O(T^2)$ queries.

   As a by-product, we also improve the polynomial relation between the *decision tree complexity* $D(f)$ and the *approximate degree* $\widetilde{deg}(f)$ of [25] from $D(f) \in O(\widetilde{deg}(f)^8)$ to $D(f) \in O(\widetilde{deg}(f)^6)$.

2. We tightly characterize the black-box complexity of all non-constant symmetric functions as follows. In the exact or zero-error settings $\Theta(N)$ queries are necessary and sufficient, and in the bounded-error setting $\Theta(\sqrt{N(N-\Gamma(f))})$ queries are necessary and sufficient, where $\Gamma(f) = \min\{|2k-N+1| : f \text{ flips value if the Hamming weight of the input changes from } k \text{ to } k+1\}$ (this $\Gamma(f)$ is a number that is low if f flips for inputs with Hamming weight close to $N/2$ [27]). This should be compared with the *classical* bounded-error query complexity of such functions, which is $\Theta(N)$. Thus, $\Gamma(f)$ characterizes the speed-up that quantum algorithms give.

   An interesting example is the THRESHOLD$_M$ function which is 1 iff its input X contains at least M 1s. This has query complexity $\Theta(\sqrt{M(N-M+1)})$.

3. For OR, AND, PARITY, MAJORITY, we obtain the bounds in the table below (all given numbers are both necessary and sufficient). These results are all new, with the exception of the $\Theta(\sqrt{N})$-bounds for

	exact	zero-error	bounded-error
OR, AND	N	N	$\Theta(\sqrt{N})$
PARITY	$N/2$	$N/2$	$N/2$
MAJORITY	$\Theta(N)$	$\Theta(N)$	$\Theta(N)$

Table 1. Some quantum complexities

[1] All our results remain valid if we consider a *controlled* black-box, where the first bit of the state indicates whether the black-box is to be applied or not. (Thus such a black-box would map $|0,i,b,z\rangle$ to $|0,i,b,z\rangle$ and $|1,i,b,z\rangle$ to $|1,i,b\oplus x_i,z\rangle$.) Also, our results remain valid if we consider *mixed* rather than only pure states.

OR and AND in the bounded-error setting, which appear in [15, 3, 5, 37]. The new bounds improve by polylog(N) factors previous lower bound results from [8], which were obtained through a reduction from communication complexity. The new bounds for PARITY were independently obtained by Farhi *et al.* [12].

Note that lower bounds for OR imply lower bounds for *database search* (where we want to find an i such that $x_i = 1$, if one exists), so exact or zero-error quantum search requires N queries, in contrast to $\Theta(\sqrt{N})$ queries for the bounded-error case.

3 Preliminaries

Our main goal in this paper is to find the number of queries a quantum algorithm needs to compute some Boolean function by relating such networks to polynomials. In this section we give some basic definitions and properties of multilinear polynomials and Boolean functions, and describe our quantum setting.

3.1 Boolean functions and polynomials

We assume the following setting, mainly adapted from [25]. We have a vector of N Boolean variables $X = (x_0, \ldots, x_{N-1})$, and we want to compute a Boolean function $f : \{0,1\}^N \to \{0,1\}$ of X. Unless explicitly stated otherwise, f will always be total. The Hamming weight (number of 1s) of X is denoted by $|X|$. For convenience we will assume N even, unless explicitly stated otherwise. We can represent Boolean functions using N-variate polynomials $p : \mathbf{R}^N \to \mathbf{R}$. Since $x^k = x$ whenever $x \in \{0,1\}$, we can restrict attention to *multilinear* p. If $p(X) = f(X)$ for all $X \in \{0,1\}^N$, then we say p *represents* f. We use $deg(f)$ to denote the degree of a minimum-degree p that represents f (actually such a p is unique). If $|p(X) - f(X)| \leq 1/3$ for all $X \in \{0,1\}^N$, we say p *approximates* f, and $\widetilde{deg}(f)$ denotes the degree of a minimum-degree p that approximates f. For example, $x_0 x_1 \ldots x_{N-1}$ is a multilinear polynomial of degree N that represents the AND-function. Similarly, $1 - (1-x_0)(1-x_1)\ldots(1-x_{N-1})$ represents OR. The polynomial $\frac{1}{3}x_0 + \frac{1}{3}x_1$ approximates but does not represent AND on 2 variables.

Nisan and Szegedy [25, Theorem 2.1] proved a general lower bound on the degree of any Boolean function that depends on N variables:

Theorem 3.1 (Nisan, Szegedy) *If f is a Boolean function that depends on N variables, then $deg(f) \geq \log N - O(\log \log N)$.*

Let $p : \mathbf{R}^N \to \mathbf{R}$ be a polynomial. If π is some permutation and $X = (x_0, \ldots, x_{N-1})$, then $\pi(X) = (x_{\pi(0)}, \ldots, x_{\pi(N-1)})$. Let S_N be the set of all $N!$ permutations. The *symmetrization* p^{sym} of p averages over all permutations of the input, and is defined as:

$$p^{sym}(X) = \frac{\sum_{\pi \in S_N} p(\pi(X))}{N!}.$$

Note that p^{sym} is a polynomial of degree at most the degree of p. Symmetrizing may actually lower the degree: if $p = x_0 - x_1$, then $p^{sym} = 0$. The following lemma, originally due to [20], allows us to reduce an N-variate polynomial to a single-variate one.

Lemma 3.2 (Minsky, Papert) *If $p : \mathbf{R}^n \to \mathbf{R}$ is a multilinear polynomial, then there exists a polynomial $q : \mathbf{R} \to \mathbf{R}$, of degree at most the degree of p, such that $p^{sym}(X) = q(|X|)$ for all $X \in \{0,1\}^N$.*

Proof Let d be the degree of p^{sym}, which is at most the degree of p. Let V_j denote the sum of all $\binom{N}{j}$ products of j different variables, so $V_1 = x_0 + \ldots + x_{N-1}$, $V_2 = x_0x_1 + x_0x_2 + \ldots + x_{N-1}x_{N-2}$, etc. Since p^{sym} is symmetrical, it can be written as

$$p^{sym}(X) = a_0 + a_1 V_1 + a_2 V_2 + \ldots + a_d V_d,$$

for some $a_i \in \mathbf{R}$. Note that V_j assumes value $\binom{|X|}{j} = |X|(|X|-1)(|X|-2)\ldots(|X|-j+1)/j!$ on X, which is a polynomial of degree j of $|X|$. Therefore the single-variate polynomial q defined by

$$q(|X|) = a_0 + a_1\binom{|X|}{1} + a_2\binom{|X|}{2} + \ldots + a_d\binom{|X|}{d}$$

satisfies the lemma. □

A Boolean function f is *symmetric* if permuting the input does not change the function value (i.e., $f(X)$ only depends on $|X|$). Paturi has proved a powerful theorem that characterizes $\widetilde{deg}(f)$ for symmetric f. For such f, let $f_k = f(X)$ for $|X| = k$, and define

$$\Gamma(f) = \min\{|2k-N+1| : f_k \neq f_{k+1} \text{ and } 0 \leq k \leq N-1\}.$$

$\Gamma(f)$ is low if f_k "jumps" near the middle (i.e., for some $k \approx N/2$). Now [27, Theorem 1] gives:

Theorem 3.3 (Paturi) *If f is a non-constant symmetric Boolean function on $\{0,1\}^N$, then $\widetilde{deg}(f) \in \Theta(\sqrt{N(N-\Gamma(f))})$.*

For functions like OR and AND, we have $\Gamma(f) = N-1$ and hence $\widetilde{deg}(f) \in \Theta(\sqrt{N})$. For PARITY (which is 1 iff $|X|$ is odd) and MAJORITY (which is 1 iff $|X| > N/2$), we have $\Gamma(f) = 1$ and $\widetilde{deg}(f) \in \Theta(N)$.

3.2 The framework of quantum networks

Our goal is to compute some Boolean function f of $X = (x_0, \ldots, x_{N-1})$, where X is given as a black-box: calling the black-box on i returns the value of x_i. We want to use as few queries as possible.

A classical algorithm that computes f by using (adaptive) black-box queries to X is called a *decision tree*, since it can be pictured as a binary tree where each node is a query, each node has the two outcomes of the query as children, and the leaves give answer $f(X) = 0$ or $f(X) = 1$. The *cost* of such an algorithm is the number of queries made on the worst-case X, so the cost is the depth of the tree. The *decision tree complexity* $D(f)$ of f is the cost of the best decision tree that computes f. Similarly we can define $R(f)$ as the expected number of queries on the worst-case X for *randomized* algorithms that compute f with bounded-error.

A *quantum network* with T queries is the quantum analogue to a classical decision tree with T queries, where queries and other operations can now be made in quantum superposition. Such a network can be represented as a sequence of unitary transformations:

$$U_0, O_1, U_1, O_2, \ldots, U_{T-1}, O_T, U_T,$$

where the U_i are arbitrary unitary transformations, and the O_j are unitary transformations which correspond to queries to X. The computation ends with some measurement or observation of the final state. We assume each transformation acts on m qubits and each qubit has basis states $|0\rangle$ and $|1\rangle$, so there are 2^m basis states for each stage of the computation. It will be convenient to represent each basis state as a binary string of length m or as the corresponding natural number, so we have basis states $|0\rangle, |1\rangle, |2\rangle, \ldots, |2^m - 1\rangle$. Let K be the index set $\{0, 1, 2, \ldots, 2^m - 1\}$. With some abuse of notation, we will sometimes identify a set of numbers with the corresponding set of basis states. Every state $|\phi\rangle$ of the network can be uniquely written as $|\phi\rangle = \sum_{k \in K} \alpha_k |k\rangle$, where the α_k are complex numbers such that $\sum_{k \in K} |\alpha_k|^2 = 1$. When $|\phi\rangle$ is measured in the above basis, the probability of observing $|k\rangle$ is $|\alpha_k|^2$. Since we want to compute a function of X, which is given as a black-box, the initial state of the network is not very important and we will disregard it hereafter (we may assume the initial state to be $|0\rangle$ always).

The queries are implemented using the unitary transformations O_j in the following standard way. The transformation O_j only affects the leftmost part of a basis state: it maps basis state $|i, b, z\rangle$ to $|i, b \oplus x_i, z\rangle$ ($\oplus$ denotes XOR). Here i has length $\lceil \log N \rceil$ bits, b is one bit, and z is an arbitrary string of $m - \lceil \log N \rceil - 1$ bits. Note that the O_j are all equal.

How does a quantum network compute a Boolean function f of X? Let us designate the rightmost bit of the final state of the network as the output bit. More precisely, the output of the computation is defined to be the value we observe if we measure the rightmost bit of the final state. If this output equals $f(X)$ with certainty, for every X, then the network computes f *exactly*. If the output equals $f(X)$ with probability at least $2/3$, for every X, then the network computes f with bounded error probability at most $1/3$. To define the zero-error setting, the output is obtained by observing the *two* rightmost bits of the final state. If the first of these bits is 0, the network claims ignorance ("inconclusive"), otherwise the second bit should contain $f(X)$ with certainty. For every X, the probability of getting "inconclusive" should be less than $1/2$. We use $Q_E(f)$, $Q_0(f)$ and $Q_2(f)$ to denote the minimum number of queries required by a quantum network to compute f in the exact, zero-error and bounded-error settings, respectively. Note that $Q_2(f) \leq Q_0(f) \leq Q_E(f) \leq D(f) \leq N$.

4 General lower bounds on the number of queries

In this section we will provide some general lower bounds on the number of queries required to compute a Boolean function f on a quantum network, either exactly or with zero- or bounded-error probability.

4.1 Bounds for error-free computation

The next lemmas relate quantum networks to polynomials; they are the key to most of our results.

Lemma 4.1 *Let $\mathcal{N}$ be a quantum network that makes T queries to a black-box X. Then there exist complex-valued N-variate multilinear polynomials $p_0, \ldots, p_{2^m-1}$, each of degree at most T, such that the final state of the network is the superposition*

$$\sum_{k \in K} p_k(X)|k\rangle,$$

for any black-box X.

Proof Let $|\phi_i\rangle$ be the state of the network (using some black-box X) just before the ith query. Note that $|\phi_{i+1}\rangle = U_i O_i |\phi_i\rangle$. The amplitudes in $|\phi_0\rangle$ depend on the initial state and on U_0 but not on X, so they are polynomials of X of degree 0. A query maps basis state $|i, b, z\rangle$ to $|i, b \oplus x_i, z\rangle$. Hence if the amplitude of $|i, 0, z\rangle$ in $|\phi_0\rangle$ is α and the amplitude of $|i, 1, z\rangle$ is β, then the amplitude of $|i, 0, z\rangle$ *after* the query becomes $(1 - x_i)\alpha + x_i\beta$ and the amplitude of $|i, 1, z\rangle$ becomes $x_i\alpha + (1 - x_i)\beta$, which are polynomials of degree 1. (In general, if the amplitudes before a query are polynomials of degree $\leq j$, then the amplitudes after the query will be polynomials of degree $\leq j + 1$.) Between

the first and the second query lies the unitary transformation U_1. However, the amplitudes after applying U_1 are just linear combinations of the amplitudes before applying U_1, so the amplitudes in $|\phi_1\rangle$ are polynomials of degree at most 1. Continuing in this manner, the amplitudes of the final states are found to be polynomials of degree at most T. We can make these polynomials multilinear without affecting their values on $X \in \{0,1\}^N$, by replacing all x_i^k by x_i. □

Note that we have not used the assumption that the U_j are unitary, but only their linearity. The next lemma is also implicit in the combination of some proofs in [13, 14].

Lemma 4.2 *Let $\mathcal{N}$ be a quantum network that makes T queries to a black-box X, and B be a set of basis states. Then there exists a real-valued multilinear polynomial $P(X)$ of degree at most $2T$, which equals the probability that observing the final state of the network with black-box X yields a state from B.*

Proof By the previous lemma, we can write the final state of the network as

$$\sum_{k \in K} p_k(X)|k\rangle,$$

for any X, where the p_k are complex-valued polynomials of degree $\leq T$. The probability of observing a state in B is

$$P(X) = \sum_{k \in B} |p_k(X)|^2.$$

If we split p_k into its real and imaginary parts as $p_k(X) = pr_k(X) + i \cdot pi_k(X)$, where pr_k and pi_k are real-valued polynomials of degree $\leq T$, then $|p_k(X)|^2 = (pr_k(X))^2 + (pi_k(X))^2$, which is a real-valued polynomial of degree at most $2T$. Hence P is also a real-valued polynomial of degree at most $2T$, which we can make multilinear without affecting its values on $X \in \{0,1\}^N$. □

Letting B be the set of states that have 1 as rightmost bit, it follows that we can write the acceptance probability of a network as a degree-$2T$ polynomial $P(X)$ of X. In the case of exact computation of f we must have $P(X) = f(X)$ for all X, so P represents f and we obtain $2T \geq deg(f)$.

Theorem 4.3 *If f is a Boolean function, then $Q_E(f) \geq deg(f)/2$.*

Combining this with Theorem 3.1, we obtain a general lower bound:

Corollary 4.4 *If f depends on N variables, then $Q_E(f) \geq (\log N)/2 - O(\log \log N)$.*

For *symmetric* f we can prove a much stronger bound. Firstly for the zero-error setting:

Theorem 4.5 *If f is non-constant and symmetric, then $Q_0(f) \geq (N+1)/4$.*

Proof We assume $f(X) = 0$ for at least $(N+1)/2$ different Hamming weights of X; the proof is similar if $f(X) = 1$ for at least $(N+1)/2$ different Hamming weights. Consider a network that uses $T = Q_0(f)$ queries to compute f with zero-error. Let B be the set of basis states that have 11 as rightmost bits. By Lemma 4.2, there is a real-valued multilinear polynomial P of degree $\leq 2T$, such that for all X, $P(X)$ equals the probability that the output of the network is 11 (i.e., that the network answers 1). Since the network computes f with zero-error and f is non-constant, $P(X)$ is non-constant and equals 0 on at least $(N+1)/2$ different Hamming weights (namely the Hamming weights for which $f(X) = 0$). Let q be the single-variate polynomial of degree $\leq 2T$ obtained from symmetrizing P (Lemma 3.2). This q is non-constant and has at least $(N+1)/2$ zeroes, hence degree at least $(N+1)/2$, and the result follows. □

Thus functions like OR, AND, PARITY, threshold functions etc., all require at least $(N+1)/4$ queries to be computed exactly or with zero-error on a quantum network. Since N queries always suffice, even classically, we have $Q_E(f) \in \Theta(N)$ and $Q_0(f) \in \Theta(N)$ for non-constant symmetric f.

Secondly, for the exact setting, we can use results by Von zur Gathen and Roche [36, Theorems 2.6 and 2.8]:

Theorem 4.6 (Von zur Gathen, Roche) *If f is non-constant and symmetric, then $deg(f) = N - O(N^{0.548})$. If, in addition, $N+1$ is prime, then $deg(f) = N$.*

Corollary 4.7 *If f is non-constant and symmetric, then $Q_E(f) \geq N/2 - O(N^{0.548})$. If, in addition, $N+1$ is prime, then $Q_E(f) \geq N/2$.*

In Section 6 we give more precise bounds for some particular functions. In particular, this will show that the $N/2$ lower bound is tight, as it can be met for PARITY.

4.2 Bounds for computation with bounded-error

Here we use similar techniques to get bounds on the number of queries required for *bounded-error* computation of some function. Consider the acceptance probability of a T-query network that computes f with bounded-error, written as a polynomial $P(X)$ of degree $\leq 2T$. If $f(X) = 0$ then we should have $P(X) \leq 1/3$, and if $f(X) = 1$ then $P(X) \geq 2/3$. Hence P approximates f, and we get:

Theorem 4.8 *If f is a Boolean function, then $Q_2(f) \geq \widetilde{deg}(f)/2$.*

This result implies that a quantum algorithm that computes f with bounded error probability can be at most polynomially more efficient (in terms of number of queries) than a classical deterministic algorithm: Nisan and Szegedy proved that $D(f) \in O(\widetilde{deg}(f)^8)$ [25, Theorem 3.9], which together with the previous theorem implies $D(f) \in O(Q_2(f)^8)$. The fact that there is a polynomial relation between the classical and the quantum complexity is also implicit in the generic oracle-constructions of Fortnow and Rogers [14]. In Section 5 we will prove the stronger result $D(f) \in O(Q_2(f)^6)$.

Combining Theorem 4.8 with Paturi's Theorem 3.3 gives a lower bound for *symmetric* functions in the bounded-error setting: if f is non-constant and symmetric, then $Q_2(f) = \Omega(\sqrt{N(N-\Gamma(f))})$. We can in fact prove a matching upper bound, using the following result, which follows immediately from [7] as noted by Mosca [21]. It shows that we can *count* the number of 1s in X exactly, with bounded error probability:

Theorem 4.9 (Brassard, Høyer, Tapp; Mosca) *There exists a quantum algorithm that returns $t = |X|$ with probability at least $3/4$ using expected time $\Theta(\sqrt{(t+1)(N-t+1)})$, for all $X \in \{0,1\}^N$.*

Actually, the algorithms given in [7, 21] are classical algorithms which use some quantum networks as subroutines; the notion of *expected* time for such algorithms is the same as for classical ones. This counting-result allows us to prove the matching upper bound:

Theorem 4.10 *If f is non-constant and symmetric, then $Q_2(f) \in \Theta(\sqrt{N(N-\Gamma(f))})$.*

Proof Let f be some non-constant Boolean function. We will sketch a strategy that computes f with bounded error probability $\leq 1/3$. Let $f_k = f(X)$ for X with $|X| = k$. First note that since $\Gamma(f) = \min\{|2k - N + 1| : f_k \neq f_{k+1} \text{ and } 0 \leq k \leq N-1\}$, f_k must be identically 0 or 1 for $k \in \{(N-\Gamma(f))/2, \ldots, (N+\Gamma(f)-2)/2\}$. Consider some X with $|X| = t$. In order to be able to compute $f(X)$, it is sufficient to know t exactly if $t < (N-\Gamma(f))/2$ or $t > (N+\Gamma(f)-2)/2$, or to *know* that $(N-\Gamma(f))/2 \leq t \leq (N+\Gamma(f)-2)/2$ otherwise.

Run the counting algorithm for $\Theta(\sqrt{(N-\Gamma(f))N/2})$ steps to count the number of 1s in X. If $t < (N-\Gamma(f))/2$ or $t > (N+\Gamma(f)-2)/2$, then with high probability the algorithm will have terminated and will have returned t. If it has not terminated after $\Theta(\sqrt{(N-\Gamma(f))N/2})$ steps, then we know $(N-\Gamma(f))/2 \leq t \leq (N+\Gamma(f)-2)/2$ with high probability.

From this application of the counting algorithm, we now have obtained the following with bounded error probability:

- If $t < (N-\Gamma(f))/2$ or $t > (N+\Gamma(f)-2)/2$, then the counting algorithm gave us an exact count of t.
- If $(N-\Gamma(f))/2 \leq t \leq (N+\Gamma(f)-2)/2$, then we know this, and we also know that f_t is identically 0 or 1 for all such t.

Thus with bounded error probability we have obtained sufficient information to compute $f_t = f(X)$, using only $O(\sqrt{N(N-\Gamma(f))})$ queries. Repeating this procedure some constant number of times, we can limit the probability of error to at most $1/3$. We can implement this strategy in a quantum network with $O(\sqrt{N(N-\Gamma(f))})$ queries to compute f. □

This implies that the above-stated result about quantum counting (Theorem 4.9) is optimal, since a better upper bound for counting would give a better upper bound on $Q_2(f)$ for symmetric f, whereas we already know that Theorem 4.10 is tight. In contrast to Theorem 4.10, it can be shown that a randomized classical strategy needs $\Theta(N)$ queries to compute any non-constant symmetric f with bounded-error.

After reading a first version of this paper, where we proved that most functions cannot be computed exactly using significantly fewer than N (i.e., $o(N)$) queries, Andris Ambainis [1] extended this to the bounded-error case: *most* functions cannot be computed with bounded-error using significantly fewer than N queries.

On the other hand, Wim van Dam [34] recently proved that with good probability we can learn all N variables in the black-box using only $N/2 + \sqrt{N}$ queries. This implies the general upper bound $Q_2(f) \leq N/2 + \sqrt{N}$ for *any* f. This bound is almost tight, as we will show later on that $Q_2(f) = N/2$ for $f = \text{PARITY}$.

4.3 Lower bounds in terms of block sensitivity

Above we gave lower bounds on the number of queries used, in terms of degrees of polynomials that represent or approximate the function f that is to be computed. Here we give lower bounds in terms of the *block sensitivity* of f.

Definition 4.11 *Let $f : \{0,1\}^N \to \{0,1\}$ be a function, $X \in \{0,1\}^N$, and $B \subseteq \{0, \ldots, N-1\}$ a set of indices. Let X^B denote the vector obtained from X by flipping the variables in B. We say that f is* sensitive *to B on X if $f(X) \neq f(X^B)$. The* block sensitivity *$bs_X(f)$ of f on X is the maximum number t for which there exist t disjoint sets of indices $B_1, \ldots, B_t$ such that f is sensitive to each B_i on X. The* block sensitivity *$bs(f)$ of f is the maximum of $bs_X(f)$ over all $X \in \{0,1\}^N$.*

For example, $bs(\text{OR}) = N$, because if we take $X = (0,0,\ldots,0)$ and $B_i = \{i\}$, then flipping B_i in X flips the value of the OR-function from 0 to 1.

We can adapt the proof of [25, Lemma 3.8] on lower bounds of polynomials to get lower bounds on the number of queries in a quantum network in terms of block sensitivity.[2] The proof uses a theorem from [11, 28]:

Theorem 4.12 (Ehlich, Zeller; Rivlin, Cheney) *Let $p : \mathbf{R} \to \mathbf{R}$ be a polynomial such that $b_1 \leq p(i) \leq b_2$ for every integer $0 \leq i \leq N$, and $|p'(x)| \geq c$ for some real $0 \leq x \leq N$. Then $deg(p) \geq \sqrt{cN/(c + b_2 - b_1)}$.*

Theorem 4.13 *If f is a Boolean function, then $Q_E(f) \geq \sqrt{bs(f)/8}$ and $Q_2(f) \geq \sqrt{bs(f)/16}$.*

Proof We will prove the theorem for bounded-error computation, the case of exact computation is completely analogous but slightly easier. Consider a network using $T = Q_2(f)$ queries that computes f with error probability $\leq 1/3$. Let P be the polynomial of degree $\leq 2T$ that approximates f, obtained as for Theorem 4.8. Note that $P(X) \in [0,1]$ for all $X \in \{0,1\}^N$, because P represents a probability. Let $b = bs(f)$, and X and $B_0, \ldots, B_{b-1}$ be the input and sets which achieve the block sensitivity. We assume without loss of generality that $f(X) = 0$.

Consider variable $Y = (y_0, \ldots, y_{b-1}) \in \mathbf{R}^b$. Define $Z = (z_0, \ldots, z_{N-1}) \in \mathbf{R}^N$ as: $z_j = y_i$ if $x_j = 0$ and $j \in B_i$, $z_j = 1 - y_i$ if $x_j = 1$ and $j \in B_i$, and $z_j = x_j$ if $j \notin B_i$ (the x_j are fixed). Note that if $Y = \vec{0}$ then $Z = X$, and if Y has $y_i = 1$ and $y_j = 0$ for $j \neq i$ then $Z = X^{B_i}$. Now $q(Y) = P(Z)$ is a b-variate polynomial of degree $\leq 2T$, such that

- $q(Y) \in [0,1]$ for all $Y \in \{0,1\}^b$ (because P gives a probability).
- $|q(\vec{0}) - 0| = |P(X) - f(X)| \leq 1/3$, so $0 \leq q(\vec{0}) \leq 1/3$.
- $|q(Y) - 1| = |P(X^{B_i}) - f(X^{B_i})| \leq 1/3$ if Y has $y_i = 1$ and $y_j = 0$ for $j \neq i$.
  Hence $2/3 \leq q(Y) \leq 1$ if $|Y| = 1$.

Let r be the single-variate polynomial of degree $\leq 2T$ obtained from symmetrizing q over $\{0,1\}^b$ (Lemma 3.2). Note that $0 \leq r(i) \leq 1$ for every integer $0 \leq i \leq b$, and for some $x \in [0,1]$ we have $r'(x) \geq 1/3$ because $r(0) \leq 1/3$ and $r(1) \geq 2/3$. Applying the previous theorem we get $deg(r) \geq \sqrt{b/4}$, hence $T \geq \sqrt{b/16}$. □

We can generalize this result to the computation of *partial* Boolean functions, which only work on a domain $\mathcal{D} \subseteq \{0,1\}^N$ of inputs that satisfy some promise, by generalizing the definition of block sensitivity to partial functions in the obvious way.

[2] This theorem can also be proved by an argument similar to the lower bound proof for database searching in [3].

5 Polynomial relation between classical and quantum complexity

Here we will compare the classical complexities $D(f)$ and $R(f)$ with the quantum complexities. Some separations: as we show in the next section, if $f =$ PARITY then $Q_2(f) = N/2$ while $D(f) = N$; if $f =$ OR then $Q_2(f) \in \Theta(\sqrt{N})$ by Grover's algorithm, while $R(f) \in \Theta(N)$ and $D(f) = N$, so we have a quadratic gap between $Q_2(f)$ on the one hand and $R(f)$ and $D(f)$ on the other.[3]

By a well-known result, the best randomized decision tree can be at most polynomially more efficient than the best deterministic decision tree: $D(f) \in O(R(f)^3)$ [23, Theorem 4]. As mentioned in Section 4, we can prove that also the *quantum* complexity can be at most polynomially better than the best deterministic tree: $D(f) \in O(Q_2(f)^8)$. Here we give the stronger result that $D(f) \in O(Q_2(f)^6)$. In other words, if we can compute some function quantumly with bounded-error using T queries, we can compute it classically error-free with $O(T^6)$ queries.

To start, we define the *certificate complexity* of f:

Definition 5.1 *Let $f : \{0,1\}^N \to \{0,1\}$ be a function. A* 1-certificate *is an assignment $C : S \to \{0,1\}$ of values to some subset S of the N variables, such that $f(X) = 1$ whenever X is consistent with C. The* size *of C is $|S|$. Similarly we define a* 0-certificate.

The certificate complexity *$C_X(f)$ of f on X is the size of a smallest $f(X)$-certificate that agrees with X. The* certificate complexity *$C(f)$ of f is the maximum of $C_X(f)$ over all X. The* 1-certificate complexity *$C^{(1)}(f)$ of f is the maximum of $C_X(f)$ over all X for which $f(X) = 1$.*

For example, if f is the OR-function, then the certificate complexity on $(1,0,0,\ldots,0)$ is 1, because the assignment $x_0 = 1$ already forces the OR to 1. The same holds for the other X for which $f(X) = 1$, so $C^{(1)}(f) = 1$. On the other hand, the certificate complexity on $(0,0,\ldots,0)$ is N, so $C(f) = N$.

The first inequality in the next lemma is obvious from the definitions, the second inequality is [23, Lemma 2.4]. We give the proof for completeness.

Lemma 5.2 (Nisan) $C^{(1)}(f) \leq C(f) \leq bs(f)^2$.

Proof Consider an input $X \in \{0,1\}^N$ and let $B_1, \ldots, B_b$ be disjoint *minimal* sets of variables that achieve the block sensitivity $b = bs_X(f) \leq bs(f)$. We will show that C :

[3] In the case of randomized decision trees, no function is known for which there is a quadratic gap between $D(f)$ and $R(f)$. The best known separation is for complete binary AND/OR-trees, where $D(f) = N$ and $R(f) \in \Theta(N^{0.753\ldots})$, and it has been conjectured that this is the best separation possible. This holds both for zero-error randomized trees [29] and for bounded-error trees [30].

$\cup_i B_i \to \{0,1\}$ which sets variables according to X, is a certificate for X of size $\leq bs(f)^2$.

Firstly, if C were not an $f(X)$-certificate then let X' be an input that agrees with C, such that $f(X') \neq f(X)$. Let $X' = X^{B_{b+1}}$. Now f is sensitive to B_{b+1} on X and B_{b+1} is disjoint from $B_1, \ldots, B_b$, which contradicts $b = bs_X(f)$. Hence C is an $f(X)$-certificate.

Secondly, note that for $1 \leq i \leq b$ we must have $|B_i| \leq bs_{X^{B_i}}(f)$: if we flip one of the B_i-variables in X^{B_i} then the function value must flip from $f(X^{B_i})$ to $f(X)$ (otherwise B_i would not be minimal), so every B_i-variable forms a sensitive set for f on input X^{B_i}. Hence the size of C is $|\cup_i B_i| = \sum_{i=1}^{b} |B_i| \leq \sum_{i=1}^{b} bs_{X^{B_i}}(f) \leq bs(f)^2$. □

The crucial lemma is the following, which we prove along the lines of [23, Lemma 4.1].

Lemma 5.3 $D(f) \leq C^{(1)}(f) bs(f)$.

Proof The following describes an algorithm to compute $f(X)$, querying at most $C^{(1)}(f)bs(f)$ variables of X (in the algorithm, by a "consistent" certificate C or input Y at some point we mean a C or Y that agrees with the values of all variables queried up to that point).

1. Repeat the following at most $bs(f)$ times:
   Pick a consistent 1-certificate C and query those of its variables whose X-values are still unknown (if there is no such C, then return 0 and stop); if the queried values agree with C then return 1 and stop.

2. Pick a consistent $Y \in \{0,1\}^N$ and return $f(Y)$.

The nondeterministic "pick a C" and "pick a Y" can easily be made deterministic by choosing the first C resp. Y in some fixed order. Call this algorithm **A**. Since **A** runs for at most $bs(f)$ stages and each stage queries at most $C^{(1)}(f)$ variables, **A** queries at most $C^{(1)}(f)bs(f)$ variables.

It remains to show that **A** always returns the right answer. If it returns an answer in step 1, this is either because there are no consistent 1-certificates left (and hence $f(X)$ must be 0) or because X is found to agree with a particular 1-certificate C; in both cases **A** gives the right answer.

Now consider the case where **A** returns an answer in step 2. We will show that all consistent Y must have the same f-value. Suppose not. Then there are consistent Y, Y' with $f(Y) = 0$ and $f(Y') = 1$. **A** has queried $b = bs(f)$ 1-certificates $C_1, C_2, \ldots, C_b$. Furthermore, Y' contains a consistent 1-certificate C_{b+1}. We will derive from these C_i disjoint sets B_i such that f is sensitive to each B_i on Y. For every $1 \leq i \leq b+1$, define B_i as the set of variables on which Y and C_i disagree. Clearly, each B_i is non-empty. Note that Y^{B_i} agrees with C_i, so $f(Y^{B_i}) = 1$ which shows that f is sensitive to each B_i on Y. Let v be a variable in some B_i ($1 \leq i \leq b$), then $X(v) = Y(v) \neq C_i(v)$. Now for $j > i$, C_j has been chosen consistent with all variables queried up to that point (including v), so we cannot have $X(v) = Y(v) \neq C_j(v)$, hence $v \notin B_j$. This shows that all B_i and B_j are disjoint. But then f is sensitive to $bs(f)+1$ disjoint sets on Y, which is a contradiction. Accordingly, all consistent Y in step 2 must have the same f-value, and **A** returns the right value $f(Y) = f(X)$ in step 2, because X is one of those consistent Y. □

The inequality of the previous lemma is tight, because if $f = \text{OR}$, then $D(f) = N, C^{(1)}(f) = 1, bs(f) = N$.

The previous two lemmas imply $D(f) \leq bs(f)^3$. Combining this with Theorem 4.13 ($bs(f) \leq 16\, Q_2(f)^2$), we obtain the main result:

Theorem 5.4 *If f is a Boolean function, then $D(f) \leq 4096\, Q_2(f)^6$.*

We do not know if the $O(Q_2(f)^6)$-relation is tight, and suspect that it is not. The best separation we know is for OR and similar functions, where $D(f) = N$ and $Q_2(f) \in \Theta(\sqrt{N})$. However, for such symmetric Boolean function we can do no better than a quadratic separation: $D(f) \leq N$ always holds, and we have $Q_2(f) \in \Omega(\sqrt{N})$ by Theorem 4.10, hence $D(f) \in O(Q_2(f)^2)$ for symmetric f. For *monotone* Boolean functions, where the function value either increases or decreases monotonically if we set more input bits to 1, we can use [23, Proposition 2.2] ($bs(f) = C(f)$) to prove $D(f) \leq 256\, Q_2(f)^4$. For the case of exact computation we can also give a better result: Nisan and Smolensky (unpublished [24]) proved $D(f) \leq 2\, deg(f)^4$ for any f, which together with our Theorem 4.3 yields $D(f) \leq 32\, Q_E(f)^4$.

As a by-product, we improve the polynomial relation between $D(f)$ and $\widetilde{deg}(f)$. Nisan and Szegedy [25, Theorem 3.9] proved $\widetilde{deg}(f) \leq D(f) \leq 1296\, \widetilde{deg}(f)^8$. Using our result $D(f) \leq bs(f)^3$ and Nisan and Szegedy's $bs(f) \leq 6\, \widetilde{deg}(f)^2$ [25, Lemma 3.8] we get

Corollary 5.5 $\widetilde{deg}(f) \leq D(f) \leq 216\, \widetilde{deg}(f)^6$.

6 Some particular functions

First we will consider the OR-function, which is related to database search. By Grover's well-known search algorithm [15, 5], if at least one x_i equals 1, we can find an index i such that $x_i = 1$ with high probability of success in $O(\sqrt{N})$ queries. This implies that we can also compute the OR-function with high success probability in $O(\sqrt{N})$: let Grover's algorithm generate an index i, and return x_i. Since $bs(\text{OR}) = N$, Theorem 4.13 gives us a lower bound of $\frac{1}{4}\sqrt{N}$ on computing the OR with bounded error

probability,[4] so we have $Q_2(\text{OR}) \in \Theta(\sqrt{N})$, where classically we require $\Theta(N)$ queries. Now suppose we want to get rid of the probability of error: can we compute the OR exactly or with zero-error using $O(\sqrt{N})$ queries? If not, can quantum computation give us at least *some* advantage over the classical deterministic case? Both questions have a negative answer:

Proposition 6.1 $Q_0(\text{OR}) = N$.

Proof Consider a network that computes OR with zero-error using $T = Q_0(\text{OR})$ queries. By Lemma 4.1, there are complex-valued polynomials p_k of degree at most T, such that the final state of the network on black-box X is

$$|\phi^X\rangle = \sum_{k \in K} p_k(X)|k\rangle.$$

Let B be the set of all basis states ending in 10 (i.e., where the output is the answer 0). Then for every $k \in B$ we must have $p_k(X) = 0$ if $X \neq \vec{0} = (0, \ldots, 0)$, otherwise the probability of getting the incorrect answer 0 on $|\phi^X\rangle$ would be non-zero. On the other hand, there must be at least one $k' \in B$ such that $p_{k'}(\vec{0}) \neq 0$, since the probability of getting the correct answer 0 on $|\phi^{\vec{0}}\rangle$ must be non-zero. Let $p(X)$ be the real part of $1 - p_{k'}(X)/p_{k'}(\vec{0})$. This polynomial p has degree at most T and represents OR. But then p must have degree at least $deg(\text{OR}) = N$, so $T \geq N$. □

Corollary 6.2 *A quantum network for exact or zero-error search requires N queries.*

Under the promise that the number of solutions is either 0 or K, for some fixed known K, exact search can be done in $O(\sqrt{N/K})$ queries [18, 21]. A partial block sensitivity argument (see the comment following Theorem 4.13) shows that this is optimal up to a multiplicative constant.

Like the OR-function, PARITY has $deg(f) = N$, so by Theorem 4.3 exact computation requires at least $N/2$ queries. This is also sufficient. It is well known that the XOR of 2 variables can be computed using only one query [9]. We can group the N variables of X as $N/2$ pairs: $(x_0, x_1), (x_2, x_3), \ldots, (x_{N-2}, x_{N-1})$, and compute the XOR of all $N/2$ pairs using $N/2$ queries. The parity of X is the parity of these $N/2$ XOR values, which can be computed without any further queries. If we allow bounded-error, then $N/2$ queries of course still suffice. It follows from Theorem 4.8 that this cannot be improved, because $\widetilde{deg}(\text{PARITY}) = N$ [20]:

Lemma 6.3 (Minsky, Papert) $\widetilde{deg}(\text{PARITY}) = N$.

[4] This $\Omega(\sqrt{N})$ lower bound on search is actually quite well known [3, 15], and is given in a tighter form in [5, 37], but the way we obtained it here is rather different from existing proofs.

Proof Let f be PARITY on N variables. Let p be a polynomial of degree $\widetilde{deg}(f)$ that approximates f. Since p approximates f, its symmetrization p^{sym} also approximates f. By Lemma 3.2, there is a polynomial q, of degree at most $\widetilde{deg}(f)$, such that $q(|X|) = p^{sym}(X)$ for all inputs. Thus we must have $|f(X) - q(|X|)| \leq 1/3$, so

$$q(0) \leq 1/3, q(1) \geq 2/3, \ldots, q(N-1) \geq 2/3,$$
$$q(N) \leq 1/3 \text{ (assuming } N \text{ even)}.$$

We see that the polynomial $q(x) - 1/2$ must have at least N zeroes, hence q has degree at least N and $\widetilde{deg}(f) \geq N$. □

Proposition 6.4 *If f is PARITY on $\{0,1\}^N$, then $Q_E(f) = Q_0(f) = Q_2(f) = N/2$.*[5]

For *classical* deterministic or randomized methods, N queries are necessary in both the exact and the zero-error setting. ($R(\text{PARITY}) = \lceil N/3 \rceil$ because for $R(f)$ we count *expected* number of queries.) Note that while computing PARITY on a quantum network is much harder than OR in the *bounded-error* setting ($N/2$ versus $\Theta(\sqrt{N})$), in the *exact* setting PARITY is actually easier ($N/2$ versus N).

The upper bound on PARITY uses the fact that the XOR connective can be computed with only one query. Using polynomial arguments, it turns out that XOR and its negation are the *only* examples among all 16 connectives where quantum gives an advantage over classical computation.

Since the AND of N variables can be reduced to MAJORITY on $2N - 1$ variables (if we set the first $N - 1$ variables to 0, then the MAJORITY of all variables equals the AND of the last N variables) and AND, like OR, requires N queries to be computed exactly or with zero-error, MAJORITY takes at least $(N + 1)/2$ queries. Van Melkebeek [35] and Hayes and Kutin [16] independently found an exact quantum algorithm that uses at most $N + 1 - e(N)$ queries, where $e(N)$ is the number of 1s in the binary representation of N; this can save up to $\log N$ queries. For the zero-error case, the $(N + 1)/2$ lower bound applies; Van Melkebeek, Hayes and Kutin have found an algorithm that works in roughly $\sqrt{0.5}N$ queries. For the bounded-error case, we can apply Theorem 4.10: if $f = \text{MAJORITY}$, then $\Gamma(f) = 1$, so we need $\Theta(N)$ queries. The best upper bound we have here is $N/2 + \sqrt{N}$, which follows from [34].

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[5] Recently, this has also been proved by Farhi, Goldstone, Gutmann, and Sipser [12], using a different technique. As noted independently by Terhal [33] and [12], this result immediately implies results by Ozhigov [26] to the effect that no quantum computer can significantly speed up the computation of *all* functions (this follows because no quantum computer can significantly speed up the computation of PARITY).

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