Exact Quantum Query Complexity of EXACT and THRESHOLD*

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―――― **Abstract** ――――

A quantum algorithm is *exact* if it always produces the correct answer, on any input. Coming up with exact quantum algorithms that substantially outperform the best classical algorithm has been a quite challenging task.

In this paper, we present two new exact quantum algorithms for natural problems:

- for the problem EXACT_k^n in which we have to determine whether the sequence of input bits $x_1, \ldots, x_n$ contains exactly k values $x_i = 1$;
- for the problem THRESHOLD_k^n in which we have to determine if at least k of n input bits are equal to 1.

1 Introduction

We consider quantum algorithms in the query model. The algorithm needs to compute a given Boolean function $f : \{0,1\}^n \to \{0,1\}$ by querying its input bits until it is able to produce the value of the function, either with certainty, or with some error probability. The complexity of the algorithm is measured as the number of queries it makes (other kinds of computation needed to produce the answer are disregarded).

In the *bounded error* setting where the algorithm is allowed to give an incorrect answer with probability not exceeding a given constant ϵ, $0 < \epsilon < \frac{1}{2}$, many efficient quantum algorithms are known, with either a polynomial speed-up over classical algorithms (e.g., [12, 1, 9, 16, 4]), or, in the case of partial functions, even an exponential speed-up (e.g., [18, 17]).

Less studied is the *exact* setting where the algorithm must give the correct answer with certainty. Though for partial functions quantum algorithms with exponential speed-up are known (for instance, [8, 5]), the results for total functions up to recently have been much less spectacular: the best known quantum speed-up was just by a factor of 2.

Even more, as remarked in [13], all the known algorithms achieved this speed-up by the same trick: exploiting the fact that XOR of two bits can be computed quantumly with one query, while a classical algorithm needs two queries [8, 7, 10].

A step forward was made by [13] which presented a new algorithm achieving the speed-up by a factor of 2, without using the "XOR trick". The algorithm is for the Boolean function

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EXACT_2^4 which is true iff exactly 2 of its 4 input bits are equal to 1. It computes this function with 2 queries, while a classical (deterministic) algorithm needs 4 queries.

This function can be generalized to EXACT_k^n in the obvious way. Its deterministic complexity is n (due to its sensitivity being n, see [15]). [13] conjectured that its quantum query complexity is $\max\{k, n-k\}$.

In this paper we prove the conjecture. We also solve the problem for a similar function, THRESHOLD_k^n which is true iff *at least* k of the input bits are equal to 1. When $n = 2k-1$, this function is well-known as the MAJORITY function. The quantum query complexity of THRESHOLD_k^n turns out to be $\max\{k, n-k+1\}$, as conjectured in [13].

In a recent work [2], a function $f(x_1, \ldots, x_n)$ with the deterministic query complexity n and the exact quantum query complexity $O(n^{.8675\cdots})$ was constructed. The quantum advantage that is achieved by our algorithms is smaller but we think that our results are still interesting, for several reasons.

First, we present quantum algorithms for computational problems that are natural and simple to describe. Second, our algorithms contain new ideas which may be useful for designing other exact algorithms. Currently, the toolbox of ideas for designing exact quantum algorithms is still quite small. Expanding it is an interesting research topic.

2   Technical Preliminaries

We denote $[m] = \{1, 2, \ldots, m\}$. We assume familiarity with basics of quantum computation [14]. We now briefly describe the quantum query algorithm model.

Let $f : \{0, 1\}^n \to \{0, 1\}$ be the Boolean function to compute, with the input bit string $x = x_1 x_2 \ldots x_n$. The quantum query algorithm works in a Hilbert space with some fixed basis states. It starts in a fixed starting state, then performs on it a sequence of unitary transformations $U_1, Q, U_2, Q, \ldots, U_t, Q, U_{t+1}$. The unitary transformations U_i do not depend on the input bits, while Q, called the *query transformation*, does, in the following way. Each of the basis states corresponds to either one or none of the input bits. If the basis state $|\psi\rangle$ corresponds to the i-th input bit, then $Q|\psi\rangle = (-1)^{x_i}|\psi\rangle$. If it does not correspond to any input bit, then Q leaves it unchanged: $Q|\psi\rangle = |\psi\rangle$. For convenience in computations, we denote $\hat{x}_i = (-1)^{x_i}$.

Finally, the algorithm performs a full measurement in the standard basis. Depending on the result of the measurement, it outputs either 0 or 1 which must be equal to $f(x)$.

By the principle of delayed measurement, sometimes a measurement performed in the middle of computation is equivalent to it being performed at the end of computation [14]. We will use that in our algorithms, because they are most easily described as recursive algorithms with the following structure: perform unitary U_1, query Q, unitary U_2, then measure; depending on the result of measurement, call a smaller (by 2 input bits) instance of the algorithm. The principle of delayed measurement ensures that such recursive algorithm can be transformed by routine techniques into the commonly used query algorithm model described above.

The minimum number of queries made by any quantum algorithm computing f is denoted by $Q_E(f)$. We use $D(f)$ to denote the minimum number of queries used by a deterministic algorithm that computes f.

3 Algorithm for EXACT

▶ **Definition 1.** The function $EXACT_k^n$ is a Boolean function of n variables being true iff *exactly k* of the variables are equal to 1.

▶ **Theorem 2.**

$$Q_E(EXACT_k^{2k}) \leq k$$

Proof. We present a recursive algorithm. When $k = 0$ the algorithm returns 1 without making any queries. Suppose $k = m$. For the recursive step we will use basis states $|0\rangle$, $|1\rangle$, ..., $|n\rangle$ and $|i, j\rangle$ with $i, j \in [2m]$, $i < j$. The i-th input bit will be queried from the state $|i\rangle$. We begin in the state $|0\rangle$ and perform a unitary transformation U_1:

$$U_1 |0\rangle \rightarrow \sum_{i=1}^{2m} \frac{1}{\sqrt{2m}} |i\rangle.$$

Next we perform a query:

$$\sum_{i=1}^{2m} \frac{1}{\sqrt{2m}} |i\rangle \xrightarrow{Q} \sum_{i=1}^{2m} \frac{\hat{x}_i}{\sqrt{2m}} |i\rangle.$$

Finally, we perform a unitary transformation U_2, such that

$$U_2 |i\rangle = \sum_{j>i} \frac{1}{\sqrt{2m}} |i, j\rangle - \sum_{j<i} \frac{1}{\sqrt{2m}} |j, i\rangle + \frac{1}{\sqrt{2m}} |0\rangle$$

One can verify that such a unitary transformation exists by checking the inner products:

1) for any $i \in [2m]$,

$$\langle i | U_2^\dagger U_2 |i\rangle = \sum_{j>i} \frac{1}{2m} + \sum_{j<i} \frac{1}{2m} + \frac{1}{2m} = 1.$$

2) for any $i, j \in [2m]$, $i \neq j$,

$$\langle j | U_2^\dagger U_2 |i\rangle = \left(\sum_{l>j} \frac{1}{\sqrt{2m}} \langle j, l| - \sum_{l<j} \frac{1}{\sqrt{2m}} \langle l, j| + \frac{1}{\sqrt{2m}} \langle 0| \right) \cdot$$
$$\left(\sum_{l>i} \frac{1}{\sqrt{2m}} |i, l\rangle - \sum_{l<i} \frac{1}{\sqrt{2m}} |l, i\rangle + \frac{1}{\sqrt{2m}} |0\rangle \right) = 0$$

The resulting quantum state is

$$\sum_{i=1}^{2m} \frac{\hat{x}_i}{\sqrt{2m}} |i\rangle \xrightarrow{U_2} \sum_{i=1}^{2m} \frac{\hat{x}_i}{2m} |0\rangle + \sum_{i<j} \frac{\hat{x}_i - \hat{x}_j}{2m} |i, j\rangle.$$

If we measure the state and get $|0\rangle$, then $EXACT_m^{2m}(x) = 0$. If on the other hand we get $|i, j\rangle$, then $x_i \neq x_j$ and $EXACT_m^{2m}(x) = EXACT_{m-1}^{2m-2}(x \setminus \{x_i, x_j\})$, therefore we can use our algorithm for $EXACT_{m-1}^{2m-2}$.

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Note that we can delay the measurements by using $|i, j\rangle$ as a starting state for the recursive call of the algorithm.

For the sake of completeness, we include the following corollary already given in [13]:

▶ **Corollary 3.** *[13]*

$$Q_E(EXACT_k^n) \leq \max\{k, n - k\}$$

Proof. Assume that $k < \frac{n}{2}$. The other case is symmetric. Then we append the input x with $n - 2k$ ones producing x' and call $EXACT_{n-k}^{2n-2k}(x')$. Then concluding that there are $n - k$ ones in x' is equivalent to there being $(n-k) - (n-2k) = k$ ones in the original input x. ◄

The lower bound can be established by the following fact:

▶ **Proposition 4.** *If g is a partial function such that $g(x) = f(x)$ whenever g is defined on x, then $Q_E(g) \leq Q_E(f)$.*

▶ **Proposition 5.**

$$Q_E(EXACT_k^n) \geq \max\{k, n - k\}$$

Proof. Assume that $k \leq \frac{n}{2}$. The other case is symmetric. Define

$$g(x_{k+1}, \ldots, x_n) = EXACT_k^n(1, \ldots, 1, x_{k+1}, \ldots, x_n).$$

Observe that g is in fact negation of the OR function on $n - k$ bits which we know [3] to take $n - k$ queries to compute. Therefore by virtue of Proposition 4 no algorithm for $EXACT_k^n$ may use less than $n - k$ queries. ◄

4 Algorithm for THRESHOLD

We will abbreviate THRESHOLD as Th.

▶ **Definition 6.** The function Th_k^n is a Boolean function of n variables being true iff *at least* k of the variables are equal to 1.

The function Th_{k+1}^{2k+1} is commonly referred to as MAJ_{2k+1} or $MAJORITY_{2k+1}$ because it is equal to the majority of values of input variables.

Remarkably an approach similar to the one used for $EXACT$ works in this case as well.

▶ **Theorem 7.**

$$Q_E(MAJ_{2k+1}) \leq k + 1.$$

Proof. Again, a recursive solution is constructed as follows. The base case $k = 0$ is trivial to perform with one query, because the function returns the value of the single variable. The recursive step $k = m$ shares the states, unitary transformation U_1 and the query with our algorithm for $EXACT$, but the unitary U_2 is slightly different:

$$U_1 |0\rangle \rightarrow \sum_{i=1}^{2m+1} \frac{1}{\sqrt{2m+1}} |i\rangle.$$

$$\sum_{i=1}^{2m+1} \frac{1}{\sqrt{2m+1}} |i\rangle \xrightarrow{Q} \sum_{i=1}^{2m+1} \frac{\hat{x}_i}{\sqrt{2m+1}} |i\rangle.$$

$$U_2 \left|i\right\rangle = \sum_{j>i} \frac{\sqrt{2m-1}}{2m} \left|i,j\right\rangle - \sum_{j<i} \frac{\sqrt{2m-1}}{2m} \left|j,i\right\rangle + \sum_{j\neq i} \frac{1}{2m} \left|j\right\rangle.$$

The resulting state is

$$\sum_{i=1}^{2m+1} \frac{\hat{x}_i}{\sqrt{2m+1}} \left|i\right\rangle \xrightarrow{U_2} \sum_{i=1}^{2m+1} \sum_{j\neq i} \frac{\hat{x}_j}{2m\sqrt{2m+1}} \left|i\right\rangle + \sum_{i<j} \frac{(\hat{x}_i - \hat{x}_j)\sqrt{2m-1}}{2m\sqrt{2m+1}} \left|i,j\right\rangle.$$

We perform a complete measurement. There are two kinds of outcomes:

1) If we get state $\left|i\right\rangle$, then either

   a) x_i is the value in the majority which according to the polynomial $\sum_{j\neq i}\hat{x}_j$ not being zero implies that in $x \setminus \{x_i\}$ the number of ones is greater than the number of zeroes by at least 2; or

   b) x_i is a value in the minority.

   In both of these cases, for all $j : j \neq i$ it is true that $MAJ_{2m+1}(x) = MAJ_{2m-1}(x \setminus \{x_i, x_j\})$. Therefore, we can solve both cases by removing x_i and one other arbitrary input value and calculating majority from the remaining values.

2) If we get state $\left|i,j\right\rangle$, then it is even better: we know that $x_i \neq x_j$ and therefore $MAJ_{2m+1}(x) = MAJ_{2m-1}(x \setminus \{x_i, x_j\})$.

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▶ **Corollary 8.** *If $0 < k < n$, then*

$$Q_E(Th_k^n) \leq \max\{k, n-k+1\}.$$

Proof. Assume that $k \leq \frac{n}{2}$. The other case is symmetric. Then we append the input x with $n - 2k + 1$ ones producing x' and call $MAJ_{2n-2k+1}(x')$. Then x' containing at least $n - k + 1$ ones is equivalent to x containing at least $(n-k+1) - (n-2k+1) = k$ ones. ◄

▶ **Proposition 9.**

$$Q_E(Th_k^n) \geq \max\{k, n-k+1\}$$

Proof. Assume that $k \leq \frac{n}{2}$. The other case is symmetric. Define

$$g(x_k, x_{k+1}, \ldots, x_n) = Th_k^n(1, \ldots, 1, x_k, x_{k+1}, \ldots, x_n).$$

Observe that g is in fact the OR function on $n - k + 1$ bits which we know [3] takes $n - k + 1$ queries to compute. Therefore by virtue of Proposition 4 no algorithm for Th_k^n may use less than $n - k + 1$ queries. ◄

5   Conclusion

Coming up with exact quantum algorithms that are substantially better than any classical algorithm has been a difficult open problem. Until a few months ago, no example of total Boolean function with $Q_E(f) < D(f)/2$ was known and the examples of functions with $Q_E(f) = D(f)/2$ were almost all based on one idea: applying 1-query quantum algorithm for $x_1 \oplus x_2$ as a subroutine.

The first exact quantum algorithm with $Q_E(f) < D(f)/2$ (for a total f) was constructed in [2]. However, no symmetric function with $Q_E(f) < D(f)/2$ is known. It has been proven

that if $f(x)$ is a symmetric, non-constant function of n variables, then $Q_E(f) \geq n/2 - o(n)$ [11, 6].

In this paper, we construct exact quantum algorithms for two symmetric functions: *EXACT* and *THRESHOLD*. Both of those algorithms achieve $Q_E(f) = D(f)/2$ (exactly or in the limit) and use new ideas. At the same time, our algorithms are quite simple and easy to understand.

The main open problem is to come with more algorithmic techniques for constructing exact quantum algorithms. Computer experiments via semidefinite optimization [13] show that there are many functions for which exact quantum algorithms are better than deterministic algorithms. Yet, in many of these cases, the only way to construct these algorithms is by searching the space of all quantum algorithms, using semidefinite optimization as the search tool.

For example, from the calculations in [13] (based on semidefinite optimization) it is apparent that there are 3 symmetric functions of 6 variables for which $Q_E(f) = 3$: *PARITY*, $EXACT_3^6$ and $EXACT_{2,4}^6$ (exactly 2 or 4 of 6 variables are equal to 1).

Unlike for the first two functions, we are not aware of any simple quantum algorithm or lower bounds for $EXACT_{2,4}^6$. Based on the evidence from semidefinite optimization, we conjecture that if n is even and $2k < n$ then the quantum query complexity of $EXACT_{k,n-k}^n$ is $n - k - 1$. In particular, this would mean that the complexity of $EXACT_{n/2-1,n/2+1}^n$ is $\frac{n}{2}$ and this function also achieves a gap of $Q_E(f) = D(f)/2$.

At the moment, we know that this conjecture is true for $k = 0$ and $k = 1$. Actually, both of those cases can be solved by a classical algorithm which uses the 1-query algorithm for $x_1 \oplus x_2$ as a quantum subroutine. This approach fails for $k \geq 1$ and it seems that the approach in the current paper is also not sufficient — without a substantial new component.

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