Fast quantum algorithms for numerical integrals and stochastic processes[1]

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We discuss quantum algorithms that calculate numerical integrals and descriptive statistics of stochastic processes. With either of two distinct approaches, one obtains an exponential speed increase in comparison to the fastest known classical deterministic algorithms and a quadratic speed increase in comparison to classical Monte Carlo (probabilistic) methods. We derive a simpler and slightly faster version of Grover's mean algorithm, demonstrate how to apply quantum counting to the problem, develop some variations of these algorithms, and show how both (apparently quite different) approaches can be understood from the same unified framework. Finally, we discuss how the exponential speed increase appears to (but does not) violate results obtained via the method of polynomials, from which it is known that a bounded-error quantum algorithm for computing a total function can be only polynomially more efficient than the fastest deterministic classical algorithm.

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1 Introduction

Quantum algorithms have been discovered that can solve many problems faster than the best known classical algorithms. Most famous are Shor's factoring algorithm[12] and Grover's searching algorithm[7][8], but quantum computers can also be used to simulate physics with an exponential speedup[1], find means, and medians with a quadratic speedup [9], and solve a variety of artificial problems [5][13] exponentially faster than is possible classically. Still, due (perhaps) to the enormous technical challenges that must be overcome before a useful quantum computer can ever be built, there is a general sense that more applications must be found in order to justify attempts to construct a quantum computing device.

We suggest one possible application of a quantum computer, namely, computing the values of integrals. This problem can be solved in a fairly straightforward manner via either quantum counting [3], or Grover's mean estimation algorithm [9]. Although these algorithms are not new, this application may be the most useful one described to date. (Because N operations are required to retrieve N values from a classical database, the mean finding algorithm affords no speed-up when applied to a pre-existing data set. Indeed, even the original database search algorithm has only limited utility, because it can only be used to search a function space, not a true database. It not clear to how many real-life problems it could be applied [14]). We also show how these apparently different algorithms can be understood from a unified perspective, thereby explaining their equivalent computational complexity.

In addition, we suggest that a quantum computer may be used to determine various characteristics of stochastic processes (for example, stock prices). Frequently, such processes are used to generation distribution functions, and one wishes to know the mean, variance, and higher moments. One can apply quantum counting and mean estimation to obtain super-classical speedups for these problems as well.

On a quantum computer, one can find the value of a d-dimensional integral in $O(1/\epsilon)$ operations, where ϵ is the desired accuracy. It follows from the results of Nayak and Wu [11] that this is in fact a lower bound. Classically, one requires $O(1/\epsilon^2)$ operations to achieve the same accuracy using probabilistic methods, and requires $O(1/\epsilon^d)$ - *exponentially* more - operations to achieve the same accuracy deterministically. (More precisely, it is polynomial in the accuracy and exponential in the number of dimensions). Since real computers and all classical devices are in fact deterministic, this exponential speed increase is by no means a red herring. Indeed, there is a popular misconception that real computers can perform probabilistic algorithms with impunity by employing pseudo-random number generators. Of course, pseudo-random numbers are not truly random at all - and one must in fact be careful about treating them as such. For example, in 1992 Ferrenberg et al. found bugs in a supposedly good pseudo-random number generator when a numerical simulation of an Ising spin system failed due to hidden correlations in the "random" numbers [6]. The moral here is that one cannot rely upon a classical computing device to properly

execute a probabilistic algorithm. In some (more than merely technical) sense, the quantum algorithm for evaluating integrals provides an exponential speed increase.

The rest of this paper is organized as follows: first, we formalize the problems and discuss the relevant classical algorithms. We then review Grover's search algorithm from the more general perspective of amplitude amplification. We describe two different approaches to mean estimation, one using amplitude amplification and the other quantum counting, and provide a new, simpler, and slightly faster version of the former algorithm. We discuss some variations of these algorithms and show how they are essentially the same. Finally, we conclude with a discussion of the lower bounds set by the method of polynomials, and explain why they must be applied with greater care than one might first suppose.

2 Statement of the problem and classical algorithms

Without loss of generality, we consider integrals of a real-valued d-dimensional function $g(x_1, x_2, ...x_d)$ defined for x_i in the range $[0, 1]$ and where $g(x_1, x_2, ...x_d) \in [0, 1]$, for all values of x_i. Thus we seek to calculate

$$I = \int_0^1 \int_0^1 ... \int_0^1 g(x_1, x_2, ...x_d) dx_1 dx_2 ... dx_d \tag{1}$$

In the discussion that follows, we shall approximate g with a real-valued d-dimensional function $f(a_1, a_2, ...a_d)$ defined over integral values a_i in the range $[1, M]$ and where

$$f(a_1, a_2, ...a_d) = g(\frac{a_1}{M}, \frac{a_2}{M}, ...\frac{a_d}{M}) \tag{2}$$

Thus, we wish to find the sum

$$S = \frac{1}{M^d} \sum_{x_1=1}^{M} \sum_{x_2=1}^{M} ... \sum_{x_d=1}^{M} f(a_1, a_2, ...a_d) \tag{3}$$

Note that the sum S is identical to the average of f over all a_i. The accuracy with which the sum S approaches the integral I is obviously determined by the density of points M in each variable and the shape of the particular function. However[2], in what follows, our sole concern will be with approximating the sum S.

[2]Because the computational complexity of the quantum algorithms (and also the classical Monte Carlo algorithms, for that matter) depend only logarithmically on M, this approximation is not a limiting factor (as long as the function is not pathological).

A sum of this form can also be used to determine properties of a stochastic process. We describe a stochastic process by a sequence of values, $w_1, w_2, ..., w_N$, where each value w_i is chosen randomly from a distribution which may depend on some (or all) w_j for $j < i$. For example, a simple one dimensional random walk might be described by a sequence for which each w_i is either $(w_{i-1} + 1)$ or $(w_{i-1} - 1)$ with equal probability. Often, one is interested in a property of such a sequence that can be represented as a function $v(w_1, w_2, ..., w_N)$. (In many cases, the function v may depend only upon the final value w_N). One wishes to determine the mean, variance, skewness, and possibly higher moments of the function v over the space of all possible sequences. This problem is easily transformed into the form (1) through a change of variables: write each w_i as a function $w_i(r_i, w_1, w_2, ..., w_{i-1})$, where r_i is a random variable in the range [0,1]. Then we can write v as a function $v(r_1, r_2, ..., r_N)$ of the independent random variables r_i , scale the output so that it fits within the desired range, and we have a function in the form g above. The mean value of the stochastic process is then simply the integral (1). Once again, we represent the integral as a discrete sum. (For some stochastic processes, the problem may in fact be discrete from the beginning). Thus the problem again reduces to finding the sum S in (3).

One can find higher moments of a stochastic process by simply applying the above approach to a calculation of the mean of v^2, v^3, etc. This method can of course also be applied to calculate moments of any distribution function (even if it is not the result of a stochastic process) as long as it can be represented in closed form.

It should be intuitively obvious that without any knowledge of the function f, one requires classically $O(M^d)$ operations to evaluate the sum. More precisely, if we view f as an oracle (or "black-box"), then one requires at least $M^d/2$ queries to determine S to within $\pm\frac{1}{4}$. (This is because it is possible that the remaining $M^d/2$ unqueried function values may be either all 0's or all 1's, one of which will always shift the mean by at least $\frac{1}{4}$). It follows that an ordinary classical Turing machine requires exponentially many operations to determine S with accuracy ϵ for any $\epsilon < \frac{1}{4}$.

However, if one is allowed to employ a probabilistic algorithm, then one can randomly sample values of the function f for various $a_1, a_2, ...a_d$; as long as the values of a_i are chosen randomly (and provided that you are not exceedingly unlucky), it is possible to quickly approximate S to any desired precision. Indeed, it is a straightforward consequence of the central limit theorem that one can determine S with accuracy ϵ (with bounded probability) using only $O(1/\ \epsilon^2)$ operations. Note that the number of trials does not depend at all upon the size of the function's domain - as it did in the deterministic case - but only on the desired accuracy. This is in fact how Monte Carlo integrals are computed, and is essentially the only practical way to calculate integrals of functions with high dimensionality. (It is also why we are not concerned with the approximation of the integral I with the sum S - one can make M essentially as large as one desires, paying only a logarithmic cost in computational complexity). Unfortunately, Monte Carlo integrals on classical devices require the use of a pseudo-random number generator, and as mentioned previously, there is no guarantee that one

will obtain "good" random numbers. One obvious way to solve this dilemma would be to use a simple quantum event to produce a string of truly random numbers; but once one introduces quantum mechanics into the problem, we can find an even more effective solution.

3 Principle of Amplitude Amplification

Both of the quantum algorithms discussed in this paper require a generalized version of Grover searching. The treatment below follows that of Grover [9]; similar ideas have also been described by Brassard et. al. [3] and various others.

All quantum algorithms consist of unitary operations applied in series. Any sequence of unitary operations can be viewed as a single unitary operator. Consider a particular unitary operator U which has amplitude U_{ts} between a starting state $|s\rangle$ and a target state $|t\rangle$. If the computer is initially in the state $|s\rangle$, then after one application of U the computer will be found in the state $|t\rangle$ with amplitude U_{ts}, and if the state of the computer is measured in the canonical basis, the probability of obtaining the state $|t\rangle$ will therefore be $|U_{ts}|^2$. We seek to $amplify$ the amplitude of the state $|t\rangle$. (Increasing the amplitude of this state increases the chances that it will be found upon measurement and thereby allows for fast searching).

Amplitude amplification in its simplest form requires the inversion operator I_x which inverts the phase of the state $|x\rangle$. We compose the unitary operators I and U to form the unitary operator G in the following way:.

$$G = -I_s U^{-1} I_t U \tag{4}$$

It can be easily verified that the operator G leaves invariant the subspace spanned by $|s\rangle$ and $U^{-1}|t\rangle$. In particular, one finds that

$$G\left(\alpha|s\rangle + \beta U^{-1}|t\rangle\right) = \left\{(1 - 4\,|U_{ts}|^2)\alpha + 2U_{ts}\beta\right\}|s\rangle + \left\{-2U_{ts}^*\alpha + \beta\right\}U^{-1}|t\rangle \tag{5}$$

which is approximately a rotation by $2\,|U_{ts}|$ radians. It follows that by applying $O(1/\,|U_{ts}|)$ iterations, one can obtain the state $U^{-1}|t\rangle$ with near certainty.

The original fast searching algorithm [8] applies the above steps with $U = W$, where W is the Walsh-Hadamard transform - that is, a $\pi/2$ rotation of each qubit. If the initial state $|s\rangle = |00...0\rangle$, then $|U_{ts}| = |W_{ts}| = 1/\sqrt{N}$ for all possible target states $|t\rangle$. The unitary operation I_t selectively inverts the phase of the actual target state $|t\rangle$ for which we are searching. After one application of W, the probability of measuring $|t\rangle$ would be only $\frac{1}{N}$, the same as one would obtain classically by guessing. However, it follows immediately from the above that the amplitude $|t\rangle$ can be amplified to nearly 1 by applying only $O(\sqrt{N})$ operations.

4 Integrals via Amplitude Amplification

To evaluate the integral I in (1) (or alternatively the sum S in (3)), one can use the mean estimation algorithm described by Grover in [9]. We provide a simpler variation on this algorithm, which distills the essential features from the original algorithm, but eliminates unnecessary unitary operations and qubits while retaining the essentials of the approach.

The algorithm works by refining a series of approximations. One can obtain an intuitive understanding of the approach by employing an analogy to classical coin-flipping: although it is tricky to describe, the algorithm is actually quite simple in practice. Consider a coin, which, when tossed, comes up heads with probability $p_1 = S$. By the central limit theorem, one can determine S with accuracy δ using $O(1/\ \delta^2)$ trials. Let us call the first estimate so obtained E_1 and the error δ_1. Then with high probability $E_1 - \delta/2 < p_1 < E_1 + \delta/2$. We now wish to "zoom in" on this interval and determine S more accurately within these bounds. We thus define the difference $D_{\ 1} = S - (E_1 - \delta/2)$, that is, the distance that S is from the bottom of the interval. Thus with high probability D_1 is bounded by 0 and δ. We "zoom in" by rescaling this value so that it is bounded by $[0, 1]$ and call this value p_2, that is $p_2 = D_1/\delta$.

We now imagine a second iteration, where we are provided with a second coin which lands heads with probability p_2. Of course, one could not actually make such a coin without knowing S ahead of time, which would defeat the purpose. However, in the analogous quantum problem it will be possible, so we shall imagine that someone can in fact provide for us the coin with probability p_2. As with p_1, one can determine p_2 with accuracy δ using $O(1/\ \delta^2)$ trials. Call this estimate E_2; then $E_2 - \delta/2 < p_2 < E_2 + \delta/2$ with high probability. However, because $p_2 = D_1/\delta$, an estimate of p_2 with accuracy δ is an estimate of D_1 with accuracy δ^2. Since $S = D_{\ 1} + (E_1 - \delta/2)$, we thus obtain an estimate of S to accuracy δ^2.

We continue this process with further iterations. Let $D_2 = S - (E_1 - \delta/2) - (E_2 - \delta/2)\delta$, which is evidently bounded by $[0, \delta^2]$; we define p_3 by rescaling D_2: that is, $p_3 = D_2/\delta^2$, which is bounded by $[0, 1]$. We imagine a third coin with probability of heads p_3 and determine this probability to accuracy δ using $O(1/\ \delta^2)$ trials, as before. But since $p_3 = D_2/\delta^2$, this implies an estimate of D_2 to accuracy δ^3, which implies an estimate of S to accuracy δ^3. We then let $D_3 = S - (E_1 - \delta/2) - (E_2 - \delta/2)\delta - (E_3 - \delta/2)\delta^2$, etc. Each iteration requires the same number of coin tosses, but improves our estimate by a factor of δ. With $O(n/\ \delta^2)$ tosses, we estimate S with accuracy δ^n. Phrased differently, the required number of coin tosses scales only as the log of the desired accuracy. However, let us reiterate that this classical algorithm could not actually be used in practice; it is discussed only to serve as an analogy to the quantum algorithm, described below. It highlights the fact that the final complexity of the algorithm will not be limited by the number of trials (which we have seen is only logarithmic in the desired accuracy), but by the fact that $O(1/\ \epsilon)$ quantum logic operations are required to prepare the final coin-like-state (that reveals S to accuracy ϵ).

We will now describe the quantum algorithm. Let E be the current best estimate for S; that is

$$E = (E_1 - \delta/2) + (E_2 - \delta/2)\delta + (E_3 - \delta/2)\delta^2 + ... + (E_k - \delta/2)\delta^{k-1} \quad (6)$$

As before, let $D = S - E$. We wish to obtain an estimate for D with accuracy δ^k. To begin, we define a new function $f' = f - E$. Recall that

$$D = S - E \quad (7)$$

$$= \left(\frac{1}{M^d} \sum_{a_1,a_2,...a_d=0}^{M-1} f(a_1, a_2, ...a_d) \right) - E \quad (8)$$

$$= \frac{1}{M^d} \sum_{a_1,a_2,...a_d=0}^{M-1} f'(a_1, a_2, ...a_d) \quad (9)$$

In other words, D is the average value of f'. The essential quantum part of the algorithm is to estimate the average value of f'; from this, we will simply iterate to obtain finer estimates. To calculate the average, consider a quantum computer with $d \log_2 M + 1$ qubits. Label the states $|r\rangle|a_1, a_2, ...a_d\rangle$ where the first qubit r is a work qubit and the remaining qubits indicate a value in the domain of f. The computer is placed initially in the zero state: $|0\rangle|00....0\rangle$. We begin by applying a Walsh-Hadamard transform to the function qubits in order to obtain an equal superposition of all possible values for the a_i:

$$|\Psi_1\rangle = \frac{1}{\sqrt{M^d}} \sum_{a_1,a_2,...a_d=0}^{M-1} |0\rangle|a_1, a_2, ...a_d\rangle \quad (10)$$

Next we rotate the first qubit by an amount f'. The state is then

$$|\Psi_2\rangle = \frac{1}{\sqrt{M^d}} \sum_{a_1,a_2,...a_d=0}^{M-1} \sqrt{1 - f'(a_1, a_2, ...a_d)^2}|0\rangle|a_1, a_2, ...a_d\rangle + f'(a_1, a_2, ...a_d)|1\rangle|a_1, a_2, ...a_d\rangle \quad (11)$$

Finally, we perform the inverse of the Walsh-Hadamard transform used in the first step. It is easy to see that the amplitude of the state $|1\rangle|00...0\rangle$ will then be D (because each state $|1\rangle|a_1, a_2, ...a_d\rangle$ contributes amplitude $\frac{1}{\sqrt{M^d}} f'(a_1, a_2, ...a_d)$ to the state $|1\rangle|00...0\rangle$). An estimate for D can therefore be obtained by making measurements of the state of the system in repeated trials, and counting the frequency of the result $|1\rangle|00...0\rangle$. To obtain an accuracy ϵ requires $O(1/\ \epsilon^2)$ measurements.

However, we can use amplitude amplification to increase the accuracy of our estimate. The steps described above can be viewed as a single unitary operation U that has amplitude $|U_{ts}|$ between the starting state $|s\rangle = |0\rangle|00...0\rangle$ and the target state $|t\rangle = |1\rangle|00...0\rangle$. It follows that one can use amplitude amplification to increase the probability of measuring the state $|1\rangle|00...0\rangle$. By performing only

$O(N)$ operations, one can increase the amplitude of $|t\rangle$ to $N * D$. The largest value one can choose for N is $O(1/\delta^k)$ (because the magnitude of D is $O(\delta^k)$ and the norm of the amplified amplitude is bounded by one). In this case, the probability amplitude for the target state is then roughly D/δ^{k3}. Borrowing from our earlier classical analogy, this is the scaled ("zoomed-in") value p_{k+1}. With the same $O(1/\ \epsilon^2)$ trials, we thus determine $p_{k+1}$with accuracy ϵ, but this provides an estimate of D with accuracy $\epsilon^* = \epsilon/N = \epsilon\delta^k$. If we vary N and fix ϵ, we perform only $O(1/\epsilon^*)$ operations to find D with accuracy ϵ^*.

Because of the limit on the size N, the algorithm requires several iterations. Initially, D may be any value between 0 and 1, and hence N can be at most 1. (That is, we cannot use amplitude amplification at all). As the estimates become more accurate, then the value of D becomes correspondingly smaller, and one can choose larger and larger N.

Just as in the classical case, each estimate p_k is determined with a fixed number of trials, but since the corresponding estimates of D (and S) become exponentially more accurate with each iteration, the total number of trials is only a logarithmic function of the desired accuracy. Hence, the significant contribution to the computational complexity is not the number of trials. Instead, the complexity is determined by the amplitude amplification. Within a polylogarithmic factor, the entire cost of the algorithm occurs on the last iteration (because each iteration takes exponentially more time). The computational complexity of the entire algorithm is therefore the same as the amplitude amplification of the last iteration: $O(1/\ \epsilon^*)$ operations are required, where ϵ^* is the desired accuracy.

It is interesting to note that, as with the classical Monte Carlo method, the quantum algorithm depends only upon the desired accuracy: the size of the function's domain (M^d) is irrelevant.

5 Integrals via Quantum Counting

There is another algorithm which can be used to evaluate the sum S in (3), based upon the idea of quantum counting [3]. To use this method, one must first convert the real-valued function $f(a_1, a_2, ...a_d)$ into a boolean valued function. This is accomplished via the addition of an extra parameter q. The parameter takes on integral values in the range [1,Q] where Q is determined by the desired accuracy. We then define

$$b(a_1, a_2, ...a_d, q) = \begin{array}{l} 1 \text{ if } q \leq f(a_1, a_2, ...a_d) * Q \\ 0 \text{ if } q > f(a_1, a_2, ...a_d) * Q \end{array} \tag{12}$$

In other words, for a given $a_1, a_2, ...a_d$,the fraction of the Q values for which $b(a_1, a_2, ...a_d, q) = 1$ is the best approximation to $f(a_1, a_2, ...a_d)$. It follows that the average value of b is identical to the average value of f. However, since b is a boolean-valued function, one can estimate the average value of b via

[3]Because the amplitude amplification process is not exactly linear, the final amplitude is not exactly D/δ^k. However, this difference can be easily accounted for and has no effect on the computational complexity of the algorithm.

approximate counting. That is, $S = \langle b \rangle = \frac{r}{M^d Q}$, where r is the number of solutions $b(a_1, a_2, ...a_d, q) = 1$. To count the number of solutions r, we recall that during the amplitude amplification process, the state of the system rotates within the subspace spanned by $|s\rangle$ and $U^{-1}|t\rangle$ at a rate which is proportional to $|U_{ts}|$. Moreover, we recall that by using the Walsh-Hadamard transform for U (as in the Grover search algorithm), the magnitude of U_{ts} is exactly $|U_{ts}| = |W_{ts}| = 1/\sqrt{N}$ for any given target state $|i\rangle$. But if the target state is a sum over all basis vectors for which $b(i) = 1$, that is, $|t\rangle = \sum_{i \in b(i)=1} |i\rangle$, then the amplitude of $|U_{ts}| = \sqrt{r/N}$. Hence the amplitudes of the states $|s\rangle$ and $U^{-1}|t\rangle$ will oscillate with a frequency that depends on r. It is therefore a simple matter to create a superposition

$$|\Psi >= \frac{1}{\sqrt{A}} \sum_{j=0}^{A-1} |j\rangle G^j |s\rangle \tag{13}$$

and determine the value of r by performing a fast Fourier transform on the first register. The accuracy $1/A$ will depend linearly upon the number of points used in the FFT, as will the number of quantum logic operations (because it takes $O(1)$ operations to perform G, one requires $O(A)$ operations to create the state $|\Psi\rangle$ above). It follows that one can determine the value of the integral f to accuracy ϵ with $O(1/\epsilon)$ operations, as in the previous algorithm. Also as above, we find that the number of operations does not depend upon the size of the domain of f, but only upon the desired accuracy.

6 Discussion

At first, it may appear surprising that these two very different quantum algorithms should both require $O(1/\epsilon)$ operations. However, by exploring some variations of these algorithms, we find that, while not identical, they are both quite similar.

First, we note that there is a trivial variation of quantum counting, which is simply to measure the state of the system in repeated trials, and count the number of times one obtains the target state (or more precisely, a state for which $b(a_1, a_2, ...a_d, q) = 1$.) That is, we determine the fraction $\frac{r}{M^d Q} = \langle b \rangle = S$ through random sampling. This technique is directly analogous to the way, in Grover mean estimation, we find the probability p_1 through repeated trials (counting the number of times we measure the target state $|1\rangle|00...0\rangle$). In both cases, $O(1/\epsilon^2)$ operations would be required to obtain an accuracy ϵ. The difference is that using the Grover method, one can subtract the most recent estimate from each term in the sum (to obtain the function f'), and then perform amplitude amplification to increase the probability of obtaining the target state. By amplifying this difference, the precision of the algorithm is limited by the (nearly) linear amplitude amplification process rather than by the quadratic sampling process. In the case of quantum counting, one can also apply the

amplitude amplification process to the target state (indeed, this is exactly what the quantum counting algorithm does). However, one cannot subtract the most recent estimate from each term in the sum: specifically, for a given $a_1, a_2, ...a_d$, there can be no less than zero values of q for which $b(a_1, a_2, ...a_d, q) = 1$. In the Grover method, individual terms in the sum may be negative, even though the sum of all the terms is always positive. The counting method does not allow this possibility. It is therefore impossible to use the technique of iterated, refined estimates to increase the precision of the approximation.

The relationship can be viewed from another perspective by considering a variation of Grover's method. As presented earlier, the technique depends upon measuring the amplitude of the target state $|1\rangle|00...0\rangle$. This is accomplished through repeated measurements. However, one can also determine this amplitude with a quantum FFT. Recalling once again that during the amplitude amplification process the state of the system rotates within the subspace spanned by $|s\rangle$ and $U^{-1}|t\rangle$, at a rate which is proportional to $|U_{ts}|$ (which in this case is equal to p_k), we see that one could also use an FFT to determine $|U_{ts}|$ (and therefore p_k). As in the case of quantum counting, one requires $O(1/\epsilon)$ operations to obtain the result with accuracy ϵ. Moreover, because the FFT measures the frequency of the rotation, one does not need to perform the iterated estimates (which previously ensured that the initial amplitude $|U_{ts}|$ was sufficiently small that it would in fact be amplified throughout the entire process).

The situation is in many ways similar to the relationship between Shor's algorithm and Kitaev's algorithm[10]. In the Kitaev algorithm, one estimates the phase of an eigenvalue ϕ of a unitary operator $\widehat{U}$. The number of operations required to estimate ϕ grows polynomially with the desired precision, but Kitaev obtains exponential precision by considering $\widehat{U}^2, \widehat{U}^4, \widehat{U}^8$,etc. This process is analogous to the refined estimates used in the Grover method. In [4], Cleve et. al. describe how to modify Kitaev's algorithm so that it uses an FFT to estimate the phase. The resulting algorithm is then identical to Shor's.

A final variation of these mean finding algorithms arises naturally from the following considerations[4]. In (our version of) the Grover algorithm, we apply the unitary operators $W^{-1}RW$, where W is the Walsh-Hadamard transformation and R is the rotation by f' (which maps $|\Psi_1\rangle$ to $|\Psi_2\rangle$ in the previous description). The three unitary operators $W^{-1}RW$ take the initial zero state into a target state with an amplitude proportional to D, the number we seek to estimate. In the quantum counting algorithm, we begin with the zero state, and apply only the operator W to obtain a (different) target state, also with an amplitude that is proportional to the (square root of the) number we wish to estimate. In the final variation, we apply the operators $\widehat{R}W$: that is, we leave out the final inverse Walsh-Hadamard, and (to compensate) use a slightly different rotation $\widehat{R}$. Because it is the rotation R that shifts the amplitude according to the function we are trying to estimate, the final W is in some sense an extra, unnecessary step. However, if we use the original rotation R from the modified Grover algorithm and consider the target state to be all those states

[4]This last variation on quantum counting was suggested by Peter Hoyer.

where the first qubit is $|1\rangle$, the amplitude of the target state would then be proportional to the sum (or mean) of all values of f squared – which is not quite what we desire. Hence we simply perform a modified rotation $\widehat{R}$. which rotates by $\sqrt{f}$, in which case the target state will occur with probability proportional to the sum of all values of $\sqrt{f}$ squared, i.e., to the mean of f. By repeated iterations of this process, we can perform an FFT (as in quantum counting) and determine the mean of f with the same linear scaling that we obtain with the other approaches.

It is worth noticing that in this last variation, as with the original quantum counting, one cannot use the method of iterated estimates (like we did in the original Grover technique) because – once again – it is not possible to account for negative values of f'. It is also interesting to compare this method with the original algorithms and ask why we need to introduce the square root? With respect to the original Grover technique, this is because of the difference between summing and then squaring (as we do in the original algorithm) and squaring and then summing (which we do in the later algorithm). However, in the case of quantum counting, the amplitude of the final state is determined by squaring and then summing as well. But since the original quantum counting applies to boolean values, all components of the superposition occur with equal weight, and the result is the same.

The algorithms described above are summarized by the following chart:

$\|\mathbf{s}\rangle$	$\|\mathbf{t}\rangle$	**U**	$\|U_{ts}\|$	**Method**	**Complexity**
$\|0\rangle\|00....0\rangle$	$\|1\rangle\|00....0\rangle$	$W^{-1}RW$	S	Sampling with iterated estimates	$O(1/\epsilon)$
$\|0\rangle\|00....0\rangle$	$\|1\rangle\|00....0\rangle$	$W^{-1}RW$	S	FFT	$O(1/\epsilon)$
$\|00....0,0\rangle$	$\sum_{i\in b(i)=1} \|i\rangle$	W	$\sqrt{S}$	Sampling (no iterated estimates)	$O(1/\epsilon^2)$
$\|00....0,0\rangle$	$\sum_{i\in b(i)=1} \|i\rangle$	W	$\sqrt{S}$	FFT	$O(1/\epsilon)$
$\|0\rangle\|00....0\rangle$	$\sum_{a_i=0}^{M-1} \sqrt{f}\|1\rangle\|a_1,a_2,...a_d\rangle$	$\widehat{R}W$	$\sqrt{S}$	Sampling (no iterated estimates)	$O(1/\epsilon^2)$
$\|0\rangle\|00....0\rangle$	$\sum_{a_i=0}^{M-1} \sqrt{f}\|1\rangle\|a_1,a_2,...a_d\rangle$	$\widehat{R}W$	$\sqrt{S}$	FFT	$O(1/\epsilon)$

(14)

We see, therefore that the two apparently distinct algorithms are in fact both very closely related. In both cases, we perform a sequence of unitary operations that generate an operator with amplitude $|U_{ts}|$ to make a transition from the $|0\rangle$ state to the target state $|t\rangle$, where the value of $|U_{ts}|$ depends directly on the sum S. In both cases, we can use a quantum FFT to estimate the value of $|U_{ts}|$ and approximate S with accuracy ϵ in $O(1/\ \epsilon)$ operations. In both cases, we can estimate the value of $|U_{ts}|$ directly through repeated measurements and then approximate S with accuracy ϵ in $O(1/\ \epsilon^2)$ operations. The only difference is that in Grover's method, the particular form of the operator U allows one to consider negative values f', which in turn allows one to use the process of iterated, refined estimates and thus to obtain linear precision directly with repeated measurements instead of with the fast Fourier transform.

7 Conclusion

To briefly summarize: we have proposed two new applications for quantum computation: evaluating integrals and calculating descriptive statistics of stochastic process. Whereas $O(M^d)$ operations are required on a classical deterministic Turing machine, and $O(1/\ \epsilon^2)$ operations are required with a classical probabilistic algorithm, one can obtain the same accuracy on a quantum computer

with only $O(1/\epsilon)$ quantum operations, using two different algorithms. We have provided a simpler (and slightly more efficient) version of Grover's mean-finding algorithm, demonstrated how quantum counting can be applied to mean estimation, derived some variations of both algorithms, and shown how the two are very closely related.

In concluding, we would like to make two points. The first is that, while these algorithms are probabilistic in nature, the mean estimation algorithms employing FFTs do not rely upon sampling the function space, as do classical Monte Carlo methods. The quantum algorithms in some sense consider the entire (exponentially large) domain of the function all in one shot, and, with high probability, return the mean to within the desired accuracy.

Second, it is interesting to consider our results in light of the work by Beals et. al. [2], where it is proven (using the method of polynomials) that a bounded-error quantum algorithm for computing a total function can be only polynomially more efficient than the fastest deterministic classical algorithm. A boolean function $b(a_1, a_2, ...a_d, q)$ such as the one described in Section 5 can be described as a sequence of $M^d q$ boolean values; the average of b is a function of those $M^d q$ boolean values, and it is a total function, since it is well-defined for all possible input functions b. In order to phrase mean-estimation as a decision problem, we can ask: "Is the average value of b within the range $[E- \epsilon, E+ \epsilon]$?" (for some chosen E and ϵ). Naively, it appears that the results of [2] would imply that this problem cannot be speed up more than polynomially on a quantum computer (vs. a classical deterministic computer) - whereas we have just finished demonstrating an exponential separation. It appears that there is a contradiction.[5]

The (in fact quite simple) resolution of this problem is that the decision question posed above does not quite correspond to mean-estimation. According to the question given, a function with mean just slightly (infinitesimally) more than $E+ \epsilon$ does not have a mean that is approximately E, whereas a function that has mean exactly $E+ \epsilon$ does. Of course, our quantum algorithms cannot reliably differentiate between these two cases in polynomial time any better than the classical deterministic algorithms can. The decision question that one can associate with mean-estimation would be a probabilistic one; the answer should be sometimes yes and sometimes no with a probability that depends (perhaps as a gaussian function) upon the distance the true mean is from the estimate E. Such a question is not a function (although it can be viewed as the average value of a weighted ensemble of functions). Thus, the results obtained in [2] do not apply to our problem, and there is no contradiction.

In concluding therefore the authors would like to make the following point. It is easy for results such as those in [2] to cause one to be disheartened about the prospects of quantum computing. However, sometimes the "real" problems we wish to solve have special properties that can make them easier than the general cases. Calculating approximate integrals is one such example - and there are likely others waiting to be discovered.

[5] Actually, this issue applies equally to the exponential separation between the classical deterministic and probabilistic algorithms.

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