Quantum Computing and Grover's Algorithm

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1 Motivation for Study of Quantum Computing

In the early 1980's physicist Richard Feynman observed that no classical computer could simulate quantum mechanical systems without incurring exponential slowdown. [WC98] At the same time, it seems reasonable that a computer which behaves in a manner consistent with quantum mechanics could, in principle, simulate such systems without exponential slowdown. This possible violation of the Polynomial Church-Turing thesis: "any reasonable attempt to model mathematically computer algorithms and their time performance is bound to end up with a model of computation and associated time cost that is equivalent to Turing machines within a polynomial." [EID00][Papadimitriou94] Piqued much interest in the field.

At the same time, the evolution of classical computers has seen the size of transistors and memory elements shrink exponentially. These components can not continue this trend indefinitely and still behave in a classical manner. At the current rate sometime around 2020 the number of atoms used to represent a single bit of information will be one. [WC 98] At this scale the quantum behavior of the memory element must be dealt with.

1.1 A "Killer App" for Quantum Computing

For many years the study of quantum computing was primarily an academic curiosity, that changed rapidly in 1994, when Peter Shor published his paper "Algorithms for quantum computation: Discrete logarithms and factoring." The primary result of the paper was a polynomial time algorithm for factoring large integers. [Shor94] It is not known if there is a classical algorithm for factoring large integers efficiently, but the best algorithms published thus far are super-polynomial. [WC98] This algorithm coupled with the prominence of cryptographic systems based on factoring large integers fueled study of quantum computation, both from a algorithmic and a manufacturing point of view.

Shortly after that, in 1996 L. K. Grover published his paper providing a $O(\sqrt{n})$ time algorithm for finding a single marked element in an unsorted database of n elements. [Grover96] The best possible classical algorithm will run in $O(n)$ time. This search problem was not the first problem for which a quantum computer was shown to be better than any possible classical computer, but it was the first problem of real utility found where a quantum computer outperforms a classical computer in an asymptotic sense. While Shor's algorithm may be of more immediate utility, Grover's algorithm seems more interesting in a theoretical sense, as it identifies substantial efficiency for a real world problem in quantum computation.

2 The Quantum Computer

2.1 The Qubit

The bit is the fundamental unit of storage in a classical computer, similarly, the basis of quantum computation is a qubit. The qubit is similar to a bit in that when measured its value will be either 0 or 1. It differs primarily in what it is doing when it is not being measured. In particular, a qubit can exist in any superposition of the 0 and 1 state simultaneously. When a qubit in such a state is measured the superposition will be destroyed. It will be found to be uniquely in the 0 or 1 state with some probability for each, determined by the particulars of the superposition prior to the measurement. [WC98]

2.2 The Quantum Register

A quantum register is just a group of qubits, all part of the same quantum mechanical system. Just as a n bit register is capable of representing 2^n distinct values, so too will a n bit quantum register assume one of 2^n basis states when measured. [WC98]

A quantum algorithm consists of a sequence of operations on that register, to transform it into a state which, when measured, yields the desired result with high probability.

Note that a n bit quantum register can store an exponential amount of information. The register as a whole can be in an arbitrary superposition of the 2^n base states which it can be measured to be in. While in this superposition, and computation applied to the register will be applied to each component of the superposition, this behavior follows from the linearity of operators on quantum mechanical systems. This behavior, called *quantum parallelism* is the basis for most quantum algorithms.

2.3 A Formal Description of a Quantum Register

The state of any quantum mechanical system is described by a state vector in an appropriate Hilbert space. A Hilbert space is a complex linear vector space. [Greenwood00] This is similar to more familiar vector spaces with the exception that vectors may have complex lengths. A linear vector space is one in which the sum or constant multiple of a vector within the space is within the space as well. [Griffiths95]

In the case of our n bit quantum register, our Hilbert space will be of dimension 2^n. The orthogonal basis for the Hilbert space can be conveniently chosen to be the 2^n possible basis states that the quantum register can be found in when measured.

With the chosen basis, the projection of the state vector on the i'th basis vector will be the amplitude of the portion of the wave function corresponding to the register being solely in the i'th state.

The state vector can be written $\Psi = (a_1, a_2, \ldots a_N)^T$, where $N = 2^n$. a_i is the amplitude of the wave function in the i'th state, or equivalently the projection of the state vector onto the i'th basis state. The probability of measuring the register in the i'th state is then:

$$\frac{|a_i|^2}{\sum_{j=1}^{N} |a_j|^2}$$

where $|c|^2 = c^*c$, here * is the complex conjugate operator, so if $c = a + b\sqrt{-1}$, $|c|^2 = a^2 + b^2$. [WC98] In general the amplitude of any component of the wave function may be complex, but Grover's algorithm itself does not use any complex amplitudes.

If we we insist that

$$\sum_{j=1}^{N} |a_j|^2 = 1$$

then the probability of measuring the register to be in the i'th state becomes simply $|a_i|^2$, where a_i is the i'th component of the state vector. In this case we say the vector is normalized.

In the absence of measurement the state vector of any quantum system, including our quantum register, will evolve according to the Schrödinger wave equation. The Schrödinger equation has the property that if the solution is normalized at any time, it is normalized at all times. [Griffiths95] Therefore if we initialize our quantum register to be normalized, we can be sure that at all future times the probability of measuring the quantum register in the i'th state will be given simply by $|a_i|^2$.

A consequence of the Schrödinger equation is that the evolution of the system must be reversible. At any point in time, if we know the solution to Schrödinger's equation, we can derive its solution at all past and future times. Thus any transformation we wish to perform on our system should be reversible. For our quantum register this means that for any operation we use, we must be able to say what the state of the register was before the operation, given the operation and the resulting state. [Grover00] These remarks apply only to quantum systems evolving in isolation of their environment. Any measurement of the register will irreversibly alter the system, collapsing its wave function into one of its base states.

3 Performing Computations

Given the above constraints, it is not clear how to proceed in order to have our quantum register undergo a transformation from an initial state to some final state which performs a useful calculation. Further, if we wish to make use of quantum parallelism, it is not clear if the amplitude of the desired state will be large enough for there to be a good chance of finding the register in this state.

Since an operation on our n bit quantum register is simply a process which transforms our state vector in our $N = 2^n$ dimensional Hilbert space from state

$\Psi = (a_1, a_2, \dots a_N)^T$ to another state $\Psi' = (a_1', a_2', \dots a_N')^T$, we can represent any possible operator $\hat{T}$ as a matrix:

$$T = \begin{pmatrix} T_{11} & T_{12} & \dots & T_{1N} \\ T_{21} & T_{22} & \dots & T_{2N} \\ \vdots & \vdots & & \vdots \\ T_{N1} & T_{N2} & \dots & T_{NN} \end{pmatrix}$$

The matrix element T_{ij} is the projection of the j'th component of the input onto the i'th component of the output due to the operator. [Griffiths95]

While mathematically any transformation can be achieved by assigning the appropriate values to the matrix elements, only a very small class of operators represent physically realizable operators on a quantum system. For a matrix to represent an operator which acts on a quantum mechanical system, its effect on the state vector must agree with conditions imposed by the Schrödinger equation, namely the operation must be reversible, and it must preserve normalization of the state vector.

Physically realizable quantum transformations are reversible, thus we are immediately restricted to consideration of operators whose matrix representations are invertable, if the matrix representing the operation $\hat{T}$ is singular (the determinant of $\hat{T}$'s matrix representation is 0), it has no inverse, and thus can not be reversed. So, invertability is a necessary, but not sufficient condition for a matrix representation of a legal operator.

If we further require that the sum of the kinetic and potential energy (called the Hamiltonian) of our system is not changing with time, then the matrix representing any legal transformation will be "unitary". A matrix T is unitary if the transpose of the complex conjugate of T is T^{-1}. [Griffiths95] So, we restrict our candidates for operators to ones whose matrices are unitary, which will be a necessary and sufficient condition for being a physically realizable transformation on a quantum mechanical system with a time independent Hamiltonian. Systems with time dependent Hamiltonians' are also feasible, but are not required to perform either Grover's or Shor's algorithm, and are not considered here.

Now the specification of a quantum algorithm is simply a specification for an initial normalized state vector of the quantum register, and a series of unitary matrices representing legal transformations on that state vector. Eventually we will measure our register, and if our operators are chosen well we will measure the register to be in a desired state with high probability.

4 Grover's Algorithm

Assume you have a system with $N = 2^n$ states labeled $S_1, S_2, \dots S_N$. These 2^n states are represented by n bit strings. Assume there is a unique marked element S_m that satisfies a condition $C(S_m) = 1$, and for all other states $C(S) = 0$. We assume that C can be evaluated in unit time. Our task is to devise an algorithm which minimizes the number of evaluations of C.

The idea of Grover's algorithm is to place our register in a equal superposition of all states, and then selectively invert the phase of the marked state, and then perform an inversion about average operation a number of times. The selective inversion of the marked state follows by the inversion about average steps have the effect of increasing the amplitude of the marked state by $O(1/\sqrt{N})$. Therefore after $O(\sqrt{N})$ operations the probability of measuring the marked state approaches 1. [Grover96]

Grover's algorithm is as follows:

1. Prepare a quantum register to be normalized and uniquely in the first state. Then place the register in an equal superposition of all states $\left(\frac{1}{\sqrt{N}}, \frac{1}{\sqrt{N}} \dots \frac{1}{\sqrt{N}}\right)$ by applying the Walsh-Hadamard operator $\hat{W}$. This means simply the state vector will be in an equal superposition of each state.

2. Repeat $O(\sqrt{N})$ times the following two steps (the precise number of iterations is important, and discussed below):

   (a) Let the system be in any state S. If $C(S) = 1$, rotate the phase by π radians, else leave system unaltered. It is worth noting that this operation has no classical analog. We do not observe the state of the quantum register, doing so would collapse the superposition. The selective phase rotation gate would be a quantum mechanical operator which would rotate only the amplitude proportional to the marked state within the superposition.

   (b) Apply the inversion about average operator $\hat{A}$, whose matrix representation is: $A_{ij} = 2/N$ if $i \neq j$ and $A_{ii} = -1 + 2/N$ to the quantum register.

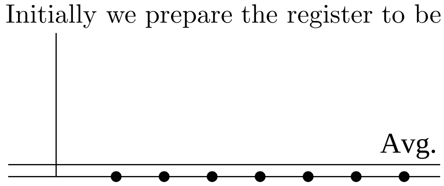
3. Measure the quantum register. The measurement will yield the n bit label of the marked state $C(S_M) = 1$ with probability at least $1/2$.

[Grover96]

4.1 An Illustration of Grover's Algorithm

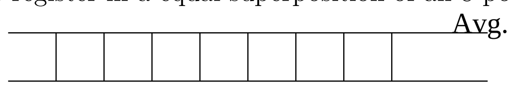
The following graphics illustrate the amplitudes of the varying states of a 3 bit quantum register undergoing the steps to Grover's algorithm:

Initially we prepare the register to be uniquely in the first state.



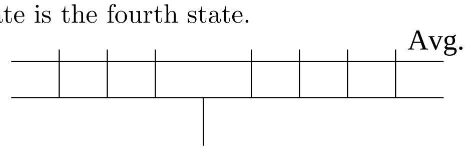
Register initially in first state

We then perform the Walsh-Hadamard transformation on the register, putting the register in a equal superposition of all 8 possible states.



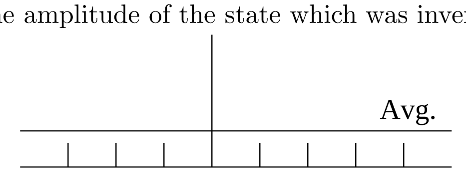
Register after Walsh−Hadamard

We then perform the selective phase inversion, which switches the sign of the amplitude of the marked state, for the purposes of this illustration the marked state is the fourth state.



Register after selective invert
4 is the desired state

Finally we perform the inversion about average operation, which increases the amplitude of the state which was inverted in the previous step.



Register after inversion about
average.

4.2 Outline of Proof of Correctness of Grover's Algorithm

To prove that Grover's algorithm successfully finds the unique marked state in $O(\sqrt{N})$ operations we must show the following:

1. That there is a operator to produce a equal superposition of states for part 1 of the algorithm. This operation is well known and referred to as the Walsh-Hadamard operator.

2. That there is a operator to rotate the phase of a given state.

3. That the definition of the matrix A : $A_{ij} = 2/N$ if $i \neq j$ and $A_{ii} = -1 + 2/N$ is an inversion about average operator.

4. That the matrix representations of all operators used are unitary. If this is the case then these transformations are physically realizable.

5. That repeated applications of step 2 of the algorithm increase the amplitude of the marked state, such that after $O(\sqrt{N})$ iterations the probability of measuring the marked state is at least 1/2.

4.3 Operator to Create Equal Superposition of States

An equal superposition of states is created by the application of the well known Walsh-Hadamard operator. The matrix representing the Walsh-Hadamard operator for an n bit quantum register is a $2^n \times 2^n$ matrix whose elements are defined to be: $W_{ij} = 2^{-n/2}(-1)^{\bar{i}\cdot\bar{j}}$, where $\bar{i}$ is the binary representation of i, and $\bar{i} \cdot \bar{j}$ is the bitwise dot product of the n bit strings i and j, i and j range from 0 to $(N-1)$, [Grover96] Put another way, $W_{ij} = \pm 2^{-n/2}$, where the sign is positive if the bitwise AND of i and j has an even number of 1's and negative otherwise. [Grover00]

The reason the Walsh-Hadamard operator inverts the sign (or rotates the phase π radians) in certain states is to allow it to be reversible. We are asking for an operator which places a quantum system in an equal superposition of states. For a classical probabilistic system this would necessarily be a irreversible process, as the resultant state would be the same for any input. Since the amplitudes of a quantum state can be complex, the probability of measuring the a system in a given state is the absolute square of the amplitude in the given state. Thus the Walsh-Hadamard operation can encode information in the phases of the states to make it reversible, while still placing the register in a state where if measured any basis state will be found with equal probability. [Grover00]

We may assume that prior to step 1 of our algorithm that our state is prepared to be identically in one of the $N = 2^n$ basis states. Assume that we place our register initially in the state where each of the bits is zero, then the state vector for our n bit register is: $\Psi = (1, 0, 0, \ldots 0)^T$. As a reminder, the state vector Ψ has $N = 2^n$ components, representing each of the states our n bit quantum register can be measured in. After application of the Walsh-Hadamard transformation the j'th element of the state vector is $W_{0j} = 2^{n/2}(-1)^{\bar{0}\cdot\bar{j}}$, note that the bitwise dot product of the zero vector and any j vector is 0, thus the sign of each amplitude is positive.

The result is an equal superposition of each state, all with positive amplitude. This was attained by performing the Walsh-Hadamard operator to the register prepared solely in the first state.

Note that this can be done for a n bit quantum register in $O(n) = O(\lg N)$ time, although to simulate this on a classical computer we must perform no less than $O(N)$ operations. Here we see an example of the kind of exponential slowdown in classical simulation of quantum systems that Feynman observed.

4.4 Operator to Rotate Phase

The matrix representing an arbitrary rotation operator is very simple. It takes the form of a diagonal matrix with $R_{ij} = 0$ if $i \neq j$, and $R_{ii} = e^{\sqrt{-1}\phi_i}$. Here ϕ_i is an arbitrary real number, and from Euler's formula we know the diagonal entries may be equivalently written as $\cos\phi_i + \sqrt{-1}\sin\phi_i$. [Grover96]

For the selective phase rotation we will need such a matrix which rotates only the phase of the marked state π radians. This will be diagonal matrix with all ones on the diagonal, except the k'th diagonal element will be -1 when the marked state is the k'th state. Obviously we can not construct anything like this operator classically, as to do so we would need to know the marked state in advance.

How such a gate would be implemented in quantum mechanical system is a little murky, I will leave it in Grover's own words:

> "In a practical implementation this would involve one portion of the quantum system sensing the state and then deciding whether or not to rotate the phase. It would do it in a way so that no trace of the state of the system be left after this operation (so as to ensure that paths leading to the same final state were indistinguishable and could interfere). The implementation does *not* involve a classical measurement." [Grover96]

We shall take the existence of such a gate as a given for the remainder of the paper.

4.5 Inversion About Average Operator

We define the inversion about average operation on our state vector as an operator that takes the amplitude of the i'th state, and increases or decreases it so that it is as much above or below the average as it was below or above the average before the operation. [Grover96]

The matrix representation of the inversion about average operator $\hat{A}$ is defined: $A_{ij} = 2/N$ if $i \neq j$ and $A_{ii} = -1 + 2/N$. Note that $A = -I + 2P$ where I is the identity matrix, and P is the matrix with each element is equal to $1/N$. Observe that P has the following two properties, first $P^2 = P$, and second Pv, for any vector v, results in a vector $v^{'}$ with each element being the arithmetic average of the the elements of v. [Grover96]

Now we can examine the operation of A on an arbitrary vector v. $Av = (-I + 2P)v = -v + 2Pv$, By the second property of P above, note that Pv is a vector with each element equal to a where a is the arithmetic average of the elements of v. Therefore the i'th component of the vector is $(-v_i + 2a)$ which can be rewritten $a + (a - v_i)$. Thus the i'th element is exactly as much above/below average as it was below/above average before the operation. [Grover96]

4.6 Proof that Operations are Unitary

If the above matrices not unitary, they will not be physically realizable, at least for systems with time independent Hamiltonians, which are the only ones being considered here. It must be shown that each of the above operations is unitary. As a reminder, a unitary matrix is one whose inverse is the same as the transpose of its complex conjugate, and unitary matrices represent reversible operators that preserve normalization.

The Walsh-Hadamard transformation is one of the fundamental unitary transformations used in quantum computing. The proof is simply a great deal of linear algebra, showing $W^2 = I$ (since W is real and symmetric) and is omitted for brevity.

The rotation matrix R with $R_{ij} = 0$ if $i \neq j$, and $R_{ii} = e^{\sqrt{-1}\phi_i}$. Here ϕ_i is an arbitrary real number.

It is easy to see R's complex conjugate transposed is the inverse of R. When R is multiplied by it's complex conjugate, the only non-zero elements are on the diagonal, and when the diagonal elements are multiplied the powers of e will cancel, resulting in $e^0 = 1$ on the diagonal, the identity matrix. [Grover96]

To show the inversion about average matrix A is unitary, recall that A may be written as $A = -I + 2P$ where:

- I is the identity matrix
- P is the matrix with each element is equal to $1/N$

Recall that $P^2 = P$.

A is real and symmetric, so A is its own transposed complex conjugate, and we must show $A^2 = I$.

$A^2 = (-I + 2P)^2 = I^2 - 2P - 2P + 4P^2 = I - 4P + 4P = I$

[Grover96]

4.7 Proof that Algorithm Increases Amplitude of Desired State

Having established that the transformations in question are unitary, and thus physically realizable, it is left to establish that iterations of Grover's algorithm increase the amplitude of the marked state $C(S_m) = 1$ enough that the probability of measuring state S_m is at least 1/2 in $O(\sqrt{N})$ operations.

We start by examining the effect of the inversion about average operator A.

4.7.1 Theorem 1

Theorem 1: Given the state vector of our register with one state with amplitude k, and every other state with amplitude l, after an application of A:

- the amplitude in the one state is $k' = \left(\frac{2}{N} - 1\right) k + 2\frac{(N-1)}{N} l$
- the amplitude of the remaining $(N-1)$ states is $l' = \frac{2}{N} k + \frac{(N-1)}{N} l$

Proof: Given the definition of A as $A_{ij} = 2/N$ if $i \neq j$ and $A_{ii} = -1 + 2/N$, it follows from the definition of matrix multiplication of k and l by A that:

- $k' = \left(\frac{2}{N} - 1\right) k + 2\frac{(N-1)}{N} l$
- $l' = \frac{2-N}{N} l + \frac{2}{N} k + \frac{2(N-2)}{N} l$

The second expression simplifies to $l' = \frac{2}{N} k + \frac{(N-2)}{N} l$ with some simple algebraic manipulation. [Grover96]

4.7.2 Corollary 1.1

Corollary 1.1: We seek to show that after applying A, both $k^{'}$ and $l^{'}$ are positive, under the following conditions:

Let the state vector for:

- one state have amplitude k
- each of the remaining $(N-1)$ states the amplitude is l

And let:

- k and l be real
- k be negative, and l be positive
- $\left|\frac{k}{l}\right| < \sqrt{N}$
- $N \geq 9$

Then, after applying A, both $k^{'}$ and $l^{'}$ are positive.

Proof:

First we will show that $k^{'}$ is positive:

- From theorem 1 we know $k^{'} = \left(\frac{2}{N} - 1\right) k + 2\frac{(N-1)}{N} l$.
- By assumption k is negative. Since $N > 2$ by assumption, $\left(\frac{2}{N} - 1\right)$ is negative.
- By assumption l is positive. Since $N > 2$ by assumption, $2\frac{(N-1)}{N}$ is positive.
- Thus the expression for $k^{'}$ is of the form $negative * negative + positive * positive$, which must be positive.

Next we will show that $l^{'}$ is positive:

- From theorem 1 we know $l^{'} = \frac{2}{N}k + \frac{(N-2)}{N}l$.
- By assumption $\left|\frac{k}{l}\right| < \sqrt{N}$
- For $N \geq 9$, $\frac{(N-2)}{2} > \sqrt{N}$. Therefore when $N \geq 9$: $\frac{(N-2)}{2} > \sqrt{N} > \left|\frac{k}{l}\right|$, and:

$$l^{'} = \frac{2}{N}k + \frac{(N-2)}{N}l > \frac{2}{N}k + \left|\frac{k}{l}\right| l$$

- Because k is negative and l is positive by assumption, $\left|\frac{k}{l}\right| = \frac{-k}{l}$.
- Therefore:

$$l^{'} = \frac{2}{N}k + \frac{(N-2)}{N}l > \frac{2}{N}k + \frac{-k}{l}l = (\frac{2}{N} - 1)k$$

- It follows that $l^{'}$ is positive because k is positive and $\frac{2}{N} - 1 > 0$ for $N \geq 3$ (and by assumption $N \geq 9$).

[Grover96]

4.7.3 Corollary 1.2

Corollary 1.2: Let the state vector be as follows:

- For the marked state S_m such that $C(S_m) = 1$, the amplitude is k
- For all other $(N-1)$ states the amplitude is l

Then after the application of A:

$$k^2 + (N-1)l^2 = k^{'2} + (N-1)l^{'2}$$

Proof: This follows directly from the fact that A is unitary, and that unitary transformations preserve normalization of the state vector. That means precisely that the sum of the absolute squares of the components is the same before and after the operation. Since we never deal with any complex amplitudes in the processing of Grover's algorithm, corollary 1.2 follows directly. [Grover96]

4.7.4 Theorem 2

Theorem 2: Let the state vector before step 2a of Grover's algorithm be as follows:

- For the unique marked state S_m which satisfies $C(S_m) = 1$ the amplitude is k such that $0 < k < 1/\sqrt{2}$
- For each of the remaining $(N-1)$ states the amplitude is l such that $l > 0$

In this case we seek to prove both:

- The change in k, Δk after steps 2a and 2b in Grover's algorithm is bounded below by $\Delta k > \frac{1}{2\sqrt{N}}$
- After steps 2a and 2b in Grover's algorithm $l > 0$

Proof: Let the initial amplitudes be k and l, let the amplitudes after the selected phase inversion step 2a be $k^{'}$ and $l^{'}$, let the amplitudes after the inversion about average step 2b be $k^{''}$ and $l^{''}$.

By theorem 1 we know $k^{''} = \left(1 - \frac{2}{N}\right) k + 2\frac{(N-1)}{N} l$ (note the reversal of terms in the coefficient of k, this is due to the phase inversion of k in step 2a), therefore $\Delta k = k^{''} - k = -\frac{2k}{N} + 2\left(1 - \frac{1}{N}\right) l$. By the assumption $0 < k < 1/\sqrt{2}$ and Corollary 1.2 it follows that $|l| > \frac{1}{\sqrt{2N}}$. By assumption l is positive, thus $l > \frac{1}{\sqrt{2N}}$. Combining this with $\Delta k = k^{''} - k = -\frac{2k}{N} + 2\left(1 - \frac{1}{N}\right) l$. it follows that $\Delta k > \frac{1}{2\sqrt{N}}$. [Grover96]

To show $l^{''}$ positive consider after step 2a of the algorithm, after the selective phase inversion, but before the inversion about average. At this point $k^{'} < 0$ and $l^{'} > 0$, since $\left(0 < k < \frac{1}{2\sqrt{N}}\right)$ and $|l| > \frac{1}{\sqrt{2N}}$ (from previous paragraph) that $\left|\frac{k^{'}}{l^{'}}\right| < \sqrt{N}$. This means that after step 2a our register is in a state covered by Corollary 1.1, which states after the inversion about average operation $l^{''}$ will be positive.

4.8 A Special Case

It is instructive to consider the special case of $N = 4$. In this special case, the precise number of iterations needed to attain the correct measurement with unit certainty is one. Thus it can provide some intuition as to the manner in which Grover's algorithm exploits interference between the states to raise the probability of the the desired state. [Grover00]

In the case of $N = 4$ then, the entire Grover's algorithm is simply:

1. Qureg $= (1, 0, 0, 0)^T$ (Quantum register in state 00 with probability 1)
2. Apply Walsh-Hadamard transformation to Qureg
3. if (C(Qureg) == 1) Apply Phase Inversion
4. Apply A transformation to Qureg (A is inversion about average)
5. Measure state of Qureg

   Let us trace the evolution of our quantum register through the algorithm. Let us assume the state we are searching for is the state three. We will denote the state of our quantum register like this: $(a, b, c, d)^T$, where the probability of measuring the register to be in the state 00 is a^2, the probability of measuring state 01 is b^2, the probability of measuring state 10 is c^2, and the probability of measuring state 11 is d^2. In general, the amplitudes could be complex, but no complex amplitudes are used in Grover's algorithm, so $a^2 = |a|^2$.

   For a 4 state system, the Walsh-Hadamard transformation is represented by the matrix:

$$W = \frac{1}{2}\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix}$$

   The inversion about average transformation is represented by the matrix:

$$A = \frac{1}{2}\begin{pmatrix} -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 \end{pmatrix}$$

After step 1 of our algorithm the quantum register is in the state $(1, 0, 0, 0)^T$.
After step 2 of our algorithm the quantum register is in the state $W{*}(1, 0, 0, 0)^T = (.5, .5, .5, .5)^T$
After step 3 of our algorithm the quantum register is in the state $(.5, .5, -.5, .5)^T$. Remember, the marked element in this example is the third one.
After step 4 of our algorithm the quantum register is in the state $A{*}(.5, .5, -.5, .5)^T = (0, 0, 1, 0)^T$.
Now comes step 5, the measurement step, we can see that with unit probability we will measure the state 3, which was the marked state.

Now, this is an exceptional case, in general we will not attain unit probability after any number of iterations. By theorem 2 we can see that there is some number of iterations m that is $O(\sqrt{N})$ such that the probability of measuring the marked state is at least 1/2. Note that the result for monotonic increasing probability of the marked state proved in theorem 2 only applies so long as the amplitude of the marked state is less than $\frac{1}{\sqrt{2}}$. Once the amplitude is greater than that further applications of A cause it to shrink, it will then oscillate back and fourth as more applications of the inner loop are executed. [BBHT96]

5 Open Questions

There are several open questions in Grover's paper. Foremost among these is how many times exactly should we iterate step 2 of Grover's algorithm. Grover proves the existence of some $m \in O(\sqrt{N})$, such that after m iterations of step 2 of the algorithm the probability of finding the register in the marked state is greater than 1/2. Since the amplitude of the desired state, and hence the of probability of measuring the desired state, is not monotonic increasing after m iterations, it is not enough to know know the existence of m, it's value must be determined.

5.1 How Many Iterations are Required

Our initial state $\Psi_0 = (1/\sqrt{N}, 1/\sqrt{N}, \ldots, 1/\sqrt{N})$, is attained by performing the Walsh-Hadamard transformation on the register in the zero state.

Let (k, l) denote denote the state of our vector, where k is the amplitude of the marked state, and l is the amplitude of each of the remaining $(N-1)$ states. It is the case in Grover's algorithm that the unmarked states always have the same amplitude, so we can use this shorthand.

After the first application of the Walsh-Hadamard operator to place us in an equal superposition of states let us say we are in state $\Psi_0 = (k_0, l_0)$.

From theorem 1 we see the j'th iteration will produce the state $\Psi_j = (k_j, l_j)$, where $k_0 = l_0 = 1/\sqrt{N}$, further:

$$k_{j+1} = \frac{N-2}{N} k_j + \frac{2(N-1)}{N} l_j$$

$$l_{j+1} = \frac{N-2}{N} l_j - \frac{2}{N} k_j$$

With a little work on the recurrence relation we an solve for closed form solutions of k and j. Let the angle θ be defined so that $\sin^2 \theta = 1/N$. It can be shown through mathematical induction that:

$$k_{j+1} = \sin((2j+1)\theta)$$

$$l_{j+1} = \frac{1}{\sqrt{N-1}} \cos((2j+1)\theta)$$

[BBHT96]

We are interested in the number of iterations for k to have near unit probability. Evidently, we will find the register to be in the target state with unit probability when $(2m+1)\theta = \pi/2$, or when $m = (\pi - 2\theta)/4\theta$. We can only perform an integer number of iterations, but the probability of failure is less than $1/N$ if we iterate $\lfloor \pi/4\theta \rfloor$ times, which is very close to $\frac{\pi}{4}\sqrt{N}$ when N is large ($1/\sqrt{N} = \sin\theta \approx \theta$). [BBHT96] For the 50 percent probability called for by Grover's algorithm we need only $\frac{\pi}{8}\sqrt{N}$ iterations. [BBHT96]

5.2 Searching for More Than One Item

Grover briefly mentions that his algorithm can work in a setting where there is more than one state such that $C(S_i) = 1$. In fact this poses no difficulty whatsoever, and regardless of the number of marked states we retain our superior performance over classical algorithms.. If there are t marked states, we can find one of the marked states in $O(\sqrt{N/t})$ time. This presumes that we know the number of marked elements in advance. [BBHT96]

Another interesting special case comes when $t = N/4$, in this case just as in the special case where $N = 4$, we will find a solution with unit probability after only one iteration, which is twice as fast as the expected running time for a classical algorithm, and exponentially faster than the worst case classical running time. [BBHT96]

5.3 Optimality of Grover's Algorithm

It is not directly proved, but simply stated in Grover's 1996 paper that his result was optimal.

It was established in [BBBV96] that any quantum algorithm can not identify a single marked element in fewer than $\Omega(\sqrt{N})$. Grover's algorithm takes $O(\sqrt{n})$ iterations, and is thus asymptotically optimal.

It has been shown since that any quantum algorithm would require at least $\pi/4\sqrt{N}$ queries, which is precisely the number queries required by Grover's algorithm. [Grover99]

5.4 Implications on P = NP

A common fallacious argument made is that since any quantum algorithm takes $\Omega(\sqrt{N})$ operations to identify a single marked element in a database of N elements, a quantum computer can not be used to attain exponential speed up in a search problem.

This argument is incorrect because this lower bound applies only to queries of the type used in Grover's algorithm, whose queries ask only about a single database element at a time. [Grover97]

Various novel approaches can be used to get around the $\Omega(\sqrt{N})$ queries barrier which still leave hope for a finding some exponential speed up of an NP-Hard problem. These approaches generally try to capitalize on some structure of the problem at hand, which Grover's algorithm does not do at all.

Grover provides an algorithm which will locate a single marked element in a N element database in exactly 1 query. It does however require $O(N \log N)$ pre and post processing time. While much slower in overall running time for the best classical and quantum algorithms for the same task, it does demonstrate that the $\Omega(\sqrt{N})$ query limit is not necessarily rule out exponential speed up of quantum computers in a search problem. [Grover97]

It has also been shown that nonlinear quantum mechanics imply polynomial time solutions for NP-complete problems, however the same paper notes that: "Such nonlinearity is purely hypothetical: all known experiments confirm the linearity of quantum mechanics to a high degree of accuracy" [Abrams98]

6 Conclusion

Quantum computation allows for exponential speed up and storage in a quantum register via quantum parallelism. The more basis states represented within the register, and hence the more speed up due to parallelism in the register, the more improbable it is that a desired state can be measured. Grover's algorithm handles this problem by relying on transformations which cause the amplitude of the marked state to increase at the expense of the non marked states, in a manner ways this is analogous to interference of waves.

Grover's algorithm is unique among quantum algorithms in that it shows a useful calculation that a quantum computer can calculate in fewer operations than any classical computer possibly can. At the heart of Grover's algorithm are two unitary transformations, the first is a selective phase inversion, which makes the sign of the amplitude of the target negative. The second unitary transformation is an inversion about average operation. Initially we place the amplitude of all states at the same positive value, each phase switch and inversion about average increases the amplitude of the target state. The exact number of times we perform these transformations is roughly $\pi/4\sqrt{N}$ for sufficiently large N. For a classical algorithm the best time bound is $O(n)$.

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