A LECTURE ON GROVER’S QUANTUM SEARCH ALGORITHM VERSION 1.1

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Abstract. This paper is a written version of a one hour lecture given on Lov Grover’s quantum database search algorithm. It is based on [4], [5], and [9].

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1. Problem definition

We consider the problem of searching an unstructured database of $N = 2^n$ records for exactly one record which has been specifically marked. This can be rephrased in mathematical terms as an oracle problem as follows:

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Label the records of the database with the integers 
\[0, 1, 2, \ldots, N - 1,\]
and denote the label of the unknown marked record by \(x_0\). We are given an oracle which computes the \(n\) bit binary function
\[f : \{0, 1\}^n \rightarrow \{0, 1\}\]
defined by
\[
f(x) = \begin{cases} 
1 & \text{if } x = x_0 \\
0 & \text{otherwise}
\end{cases}
\]

We remind the readers that, as a standard oracle idealization, we have no access to the internal workings of the function \(f\). It operates simply as a blackbox function, which we can query as many times as we like. But with each such a query comes an associated computational cost.

**Search Problem for an Unstructured Database.** Find the record labeled as \(x_0\) with the minimum amount of computational work, i.e., with the minimum number of queries of the oracle \(f\).

From probability theory, we know that if we examine \(k\) records, i.e., if we compute the oracle \(f\) for \(k\) randomly chosen records, then the probability of finding the record labeled as \(x_0\) is \(k/N\). Hence, on a classical computer it takes \(O(N) = O(2^n)\) queries to find the record labeled \(x_0\).

## 2. The Quantum Mechanical Perspective

However, as Lov Grover so astutely observed, on a quantum computer the search of an unstructured database can be accomplished in \(O(\sqrt{N})\) steps, or more precisely, with the application of \(O(\sqrt{N}\lg N)\) sufficiently local unitary transformations. Although this is not exponentially faster, it is a significant speedup.

Let \(\mathcal{H}_2\) be a 2 dimensional Hilbert space with orthonormal basis
\[
\{|0\rangle, |1\rangle\};
\]
and let
\[
\{|0\rangle, |1\rangle, \ldots, |N - 1\rangle\}
\]
denote the induced orthonormal basis of the Hilbert space
\[ \mathcal{H} = \bigotimes_{0}^{N-1} \mathcal{H}_2. \]

From the quantum mechanical perspective, the oracle function \( f \) is given as a blackbox unitary transformation \( U_f \), i.e., by
\[ \mathcal{H} \otimes \mathcal{H}_2 \xrightarrow{U_f} \mathcal{H} \otimes \mathcal{H}_2 \]
\[ |x\rangle \otimes |y\rangle \mapsto |x\rangle \otimes |f(x) \oplus y\rangle \]
where ‘\( \oplus \)’ denotes exclusive ‘OR’, i.e., addition modulo 2.

Instead of \( U_f \), we will use the computationally equivalent unitary transformation
\[ I_{|x_0\rangle} (|x\rangle) = (-1)^f(x) |x\rangle = \begin{cases} -|x_0\rangle & \text{if } x = x_0 \\ |x\rangle & \text{otherwise} \end{cases} \]
That \( I_{|x_0\rangle} \) is computationally equivalent to \( U_f \) follows from the easily verifiable fact that
\[ U_f \left( |x\rangle \otimes \frac{|0\rangle - |1\rangle}{\sqrt{2}} \right) = (I_{|x_0\rangle} (|x\rangle)) \otimes \frac{|0\rangle - |1\rangle}{\sqrt{2}}, \]
and also from the fact that \( U_f \) can be constructed from a controlled-\( I_{|x_0\rangle} \) and two one qubit Hadamard transforms. (For details, please refer to [10], [11].)

The unitary transformation \( I_{|x_0\rangle} \) is actually an inversion \( \Box \) in \( \mathcal{H} \) about the hyperplane perpendicular to \( |x_0\rangle \). This becomes evident when \( I_{|x_0\rangle} \) is rewritten in the form
\[ I_{|x_0\rangle} = I - 2 |x_0\rangle \langle x_0|, \]
where ‘\( I \)’ denotes the identity transformation. More generally, for any unit length ket \( |\psi\rangle \), the unitary transformation
\[ I_{|\psi\rangle} = I - 2 |\psi\rangle \langle \psi| \]
is an inversion in \( \mathcal{H} \) about the hyperplane orthogonal to \( |\psi\rangle \).

\(^1\)Please note that \( U_f = (\nu \circ \iota)(f) \), as defined in sections 10.3 and 10.4 of [12].
3. Properties of the inversion $I_{|\psi\rangle}$

We digress for a moment to discuss the properties of the unitary transformation $I_{|\psi\rangle}$. To do so, we need the following definition.

**Definition 1.** Let $|\psi\rangle$ and $|\chi\rangle$ be two kets in $\mathcal{H}$ for which the bracket product $\langle \psi | \chi \rangle$ is a real number. We define

$$S_C = \text{Span}_C (|\psi\rangle, |\chi\rangle) = \{ \alpha |\psi\rangle + \beta |\chi\rangle \in \mathcal{H} | \alpha, \beta \in \mathbb{C} \}$$

as the sub-Hilbert space of $\mathcal{H}$ spanned by $|\psi\rangle$ and $|\chi\rangle$. We associate with the Hilbert space $S_C$ a real inner product space lying in $S_C$ defined by

$$S_R = \text{Span}_R (|\psi\rangle, |\chi\rangle) = \{ a |\psi\rangle + b |\chi\rangle \in \mathcal{H} | a, b \in \mathbb{R} \},$$

where the inner product on $S_R$ is that induced by the bracket product on $\mathcal{H}$. If $|\psi\rangle$ and $|\chi\rangle$ are also linearly independent, then $S_R$ is a 2 dimensional real inner product space (i.e., the 2 dimensional Euclidean plane) lying inside of the complex 2 dimensional space $S_C$.

**Proposition 1.** Let $|\psi\rangle$ and $|\chi\rangle$ be two linearly independent unit length kets in $\mathcal{H}$ with real bracket product; and let $S_C = \text{Span}_C (|\psi\rangle, |\chi\rangle)$ and $S_R = \text{Span}_R (|\psi\rangle, |\chi\rangle)$. Then

1) Both $S_C$ and $S_R$ are invariant under the transformations $I_{|\psi\rangle}$, $I_{|\chi\rangle}$, and hence $I_{|\psi\rangle} \circ I_{|\chi\rangle}$, i.e.,

$$I_{|\psi\rangle} (S_C) = S_C \quad \text{and} \quad I_{|\psi\rangle} (S_R) = S_R$$
$$I_{|\chi\rangle} (S_C) = S_C \quad \text{and} \quad I_{|\chi\rangle} (S_R) = S_R$$
$$I_{|\psi\rangle} I_{|\chi\rangle} (S_C) = S_C \quad \text{and} \quad I_{|\psi\rangle} I_{|\chi\rangle} (S_R) = S_R$$

2) If $L_{|\psi\rangle}$ is the line in the plane $S_R$ which passes through the origin and which is perpendicular to $|\psi\rangle$, then $I_{|\psi\rangle}$ restricted to $S_R$ is a reflection in (i.e., a Möbius inversion about) the line $L_{|\psi\rangle}$. A similar statement can be made in regard to $|\chi\rangle$.

3) If $|\psi\rangle$ is a unit length vector in $S_R$ perpendicular to $|\psi\rangle$, then

$$-I_{|\psi\rangle} = I_{|\psi\rangle}.$$

(Hence, $\langle \psi | \chi \rangle$ is real.)
Finally we note that, since $I|\psi\rangle = I - 2|\psi\rangle \langle \psi|$, it follows that

**Proposition 2.** If $|\psi\rangle$ is a unit length ket in $\mathcal{H}$, and if $U$ is a unitary transformation on $\mathcal{H}$, then

$$UI|\psi\rangle U^{-1} = I_U|\psi\rangle .$$

4. The method in Lov’s “madness”

Let $H : \mathcal{H} \rightarrow \mathcal{H}$ be the Hadamard transform, i.e.,

$$H = \bigotimes_{k=0}^{n-1} H^{(2)} ,$$

where

$$H^{(2)} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

with respect to the basis $|0\rangle, |1\rangle$.

We begin by using the Hadamard transform $H$ to construct a state $|\psi_0\rangle$ which is an equal superposition of all the standard basis states $|0\rangle, |1\rangle, \ldots, |N-1\rangle$ (including the unknown state $|x_0\rangle$), i.e.,

$$|\psi_0\rangle = H|0\rangle = \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} |k\rangle .$$

Both $|\psi_0\rangle$ and the unknown state $|x_0\rangle$ lie in the Euclidean plane $\mathcal{S}_{\mathbb{R}} = \text{Span}_{\mathbb{R}} (|\psi_0\rangle, |x_0\rangle)$. Our strategy is to rotate within the plane $\mathcal{S}_{\mathbb{R}}$ the state $|\psi_0\rangle$ about the origin until it is as close as possible to $|x_0\rangle$. Then a measurement with respect to the standard basis of the state resulting from rotating $|\psi_0\rangle$, will produce $|x_0\rangle$ with high probability.

To achieve this objective, we use the oracle $I_{|x_0\rangle}$ to construct the unitary transformation

$$Q = -HI_{|0\rangle}H^{-1}I_{|x_0\rangle} ,$$

which by proposition 2 above, can be reexpressed as

$$Q = -I_{|\psi_0\rangle}I_{|x_0\rangle} .$$

Let $|x_0^\perp\rangle$ and $|\psi_0^\perp\rangle$ denote unit length vectors in $\mathcal{S}_{\mathbb{R}}$ perpendicular to $|x_0\rangle$ and $|\psi_0\rangle$, respectively. There are two possible choices for each of $|x_0^\perp\rangle$ and $|\psi_0^\perp\rangle$. 

and $|ψ₀^⟩$ respectively. To remove this minor, but nonetheless annoying,
ambiguity, we select $|x₀^⟩$ and $|ψ₀⊥⟩$ so that the orientation of the plane $S_R$
induced by the ordered spanning vectors $|ψ₀⟩$, $|x₀⟩$ is the same orientation
as that induced by each of the ordered bases $|x₀^⟩$, $|x₀⟩$ and $|ψ₀⟩$, $|ψ₀⊥⟩$.

(Please refer to Figure 2.)

**Remark 1.** *The removal of the above ambiguities is really not essential.
However, it does simplify the exposition given below.*

![Figure 2](image)

Figure 2. The linear transformation $Q|S_R$ is reflection in the line $L|x₀^⟩$
followed by reflection in the line $L|ψ₀⟩$ which is the same as rotation by the
angle $2β$. Thus, $Q|S_R$ rotates $|ψ₀⟩$ by the angle $2β$ toward $|x₀⟩$.

We proceed by noting that, by the above proposition 1, the plane $S_R$
lying in $H$ is invariant under the linear transformation $Q$, and that, when
$Q$ is restricted to the plane $S_R$, it can be written as the composition of two
inversions, i.e.,

$$Q|S_R = I|ψ₀⊥⟩I|x₀⟩.$$  

In particular, $Q|S_R$ is the composition of two inversions in $S_R$, the first in
the line $L|x₀^⟩$ in $S_R$ passing through the origin having $|x₀⟩$ as normal, the
second in the line $L|ψ₀⟩$ through the origin having $|ψ₀⊥⟩$ as normal.

We can now apply the following theorem from plane geometry:

---

2The line $L|x₀^⟩$ is the intersection of the plane $S_R$ with the hyperplane in $H$ orthogonal
to $|x₀⟩$. A similar statement can be made in regard to $L|ψ₀⟩$. 

**Theorem 1.** If $L_1$ and $L_2$ are lines in the Euclidean plane $\mathbb{R}^2$ intersecting at a point $O$; and if $\beta$ is the angle in the plane from $L_1$ to $L_2$, then the operation of reflection in $L_1$ followed by reflection in $L_2$ is just rotation by angle $2\beta$ about the point $O$.

Let $\beta$ denote the angle in $S_\mathbb{R}$ from $L_{|x_0^\perp\rangle}$ to $L_{|\psi_0\rangle}$, which by plane geometry is the same as the angle from $|x_0^\perp\rangle$ to $|\psi_0\rangle$, which in turn is the same as the angle from $|x_0\rangle$ to $|\psi_0^\perp\rangle$. Then by the above theorem $Q|S_\mathbb{R} = I|\psi_0^\perp\rangle I|x_0\rangle$ is a rotation about the origin by the angle $2\beta$.

The key idea in Grover’s algorithm is to move $|\psi_0\rangle$ toward the unknown state $|x_0\rangle$ by successively applying the rotation $Q$ to $|\psi_0\rangle$ to rotate it around to $|x_0\rangle$. This process is called amplitude amplification. Once this process is completed, the measurement of the resulting state (with respect to the standard basis) will, with high probability, yield the unknown state $|x_0\rangle$. This is the essence of Grover’s algorithm.

But how many times $K$ should we apply the rotation $Q$ to $|\psi_0\rangle$? If we applied $Q$ too many or too few times, we would over- or undershoot our target state $|x_0\rangle$.

We determine the integer $K$ as follows:

Since

$$|\psi_0\rangle = \sin \beta |x_0\rangle + \cos \beta |x_0^\perp\rangle,$$

the state resulting after $k$ applications of $Q$ is

$$|\psi_k\rangle = Q^k |\psi_0\rangle = \sin [(2k + 1) \beta] |x_0\rangle + \cos [(2k + 1) \beta] |x_0^\perp\rangle.$$

Thus, we seek to find the smallest positive integer $K = k$ such that

$$\sin [(2k + 1) \beta]$$

is as close as possible to 1. In other words, we seek to find the smallest positive integer $K = k$ such that

$$(2k + 1) \beta$$
is as close as possible to $\pi/2$. It follows that\footnote{The reader may prefer to use the \textit{floor} function instead of the \textit{round} function.}

$$K = k = \text{round} \left( \frac{\pi}{4\beta} - \frac{1}{2} \right),$$

where "\textit{round}" is the function that rounds to the nearest integer.

We can determine the angle $\beta$ by noting that the angle $\alpha$ from $|\psi_0\rangle$ and $|x_0\rangle$ is complementary to $\beta$, i.e.,

$$\alpha + \beta = \pi/2,$$

and hence,

$$\frac{1}{\sqrt{N}} = \langle x_0 | \psi_0 \rangle = \cos \alpha = \cos(\frac{\pi}{2} - \beta) = \sin \beta.$$

Thus, the angle $\beta$ is given by

$$\beta = \sin^{-1} \left( \frac{1}{\sqrt{N}} \right) \approx \frac{1}{\sqrt{N}} \text{ (for large } N \text{)},$$

and hence,

$$K = k = \text{round} \left( \frac{\pi}{4 \sin^{-1} \left( \frac{1}{\sqrt{N}} \right)} - \frac{1}{2} \right) \approx \text{round} \left( \frac{\pi}{4 \sqrt{N}} - \frac{1}{2} \right) \text{ (for large } N \text{).}$$

5. \textbf{Summary of Grover’s algorithm}

In summary, we provide the following outline of Grover’s algorithm:
**Grover’s Algorithm**

| STEP 0. | (Initialization) |
|---------|------------------|
| $|\psi\rangle \leftarrow H |0\rangle = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} |j\rangle$ |
| $k \leftarrow 0$ |

| STEP 1. | Loop until $k = \text{round} \left( \frac{\pi}{4} \sin^{-1} \left( \frac{1}{\sqrt{N}} \right) - \frac{1}{2} \right) \approx \text{round} \left( \frac{\pi}{4} \sqrt{N} - \frac{1}{2} \right)$ |
|---------|---------------------------------|
| $|\psi\rangle \leftarrow Q |\psi\rangle = -HI|0\rangle HI|x_0\rangle |\psi\rangle$ |
| $k \leftarrow k + 1$ |

| STEP 2. | Measure $|\psi\rangle$ with respect to the standard basis $|0\rangle, |1\rangle, \ldots, |N-1\rangle$ to obtain the marked unknown state $|x_0\rangle$ with probability $\geq 1 - \frac{1}{N}$. |

We complete our summary with the following theorem:

**Theorem 2.** With a probability of error\footnote{If the reader prefers to use the floor function rather than the round function, then probability of error becomes $\text{Prob}_E \leq \frac{4}{N} - \frac{4}{\pi^2}$.}

$$\text{Prob}_E \leq \frac{1}{N},$$

Grover’s algorithm finds the unknown state $|x_0\rangle$ at a computational cost of

$$O \left( \sqrt{N} \lg N \right)$$

**Proof.**

Part 1. The probability of error $\text{Prob}_E$ of finding the hidden state $|x_0\rangle$ is given by

$$\text{Prob}_E = \cos^2 \left[ (2K + 1) \beta \right],$$

where

$$\begin{cases} 
\beta &= \sin^{-1} \left( \frac{1}{\sqrt{N}} \right) \\
K &= \text{round} \left( \frac{\pi}{4} \sqrt{N} - \frac{1}{2} \right) 
\end{cases}$$
where “round” is the function that rounds to the nearest integer. Hence,

\[
\pi/4 - 1 \leq K \leq \pi/4 \implies \frac{\pi}{2} - \beta \leq (2K + 1)\beta \leq \frac{\pi}{2} + \beta
\]

\[
\implies \sin \beta = \cos \left(\frac{\pi}{2} - \beta\right) \geq \cos \left((2K + 1)\beta\right) \geq \cos \left(\frac{\pi}{2} + \beta\right) = -\sin \beta
\]

Thus,

\[
Prob_E = \cos^2 \left((2K + 1)\beta\right) \leq \sin^2 \beta = \sin^2 \left(\sin^{-1} \left(\frac{1}{\sqrt{N}}\right)\right) = \frac{1}{N}
\]

Part 2. The computational cost of the Hadamard transform \( H = \bigotimes_{0}^{n-1} H^{(2)} \) is \( O(n) = O(\lg N) \) single qubit operations. The transformations \(-I_0\) and \(I_{x_0}\) each carry a computational cost of \( O(1) \).

\text{STEP 1} is the computationally dominant step. In \text{STEP 1} there are \( O\left(\sqrt{N}\right) \) iterations. In each iteration, the Hadamard transform is applied twice. The transformations \(-I_0\) and \(I_{x_0}\) are each applied once. Hence, each iteration comes with a computational cost of \( O(\lg N) \), and so the total cost of \text{STEP 1} is \( O(\sqrt{N} \lg N) \).

6. An example of Grover’s algorithm

As an example, we search a database consisting of \( N = 2^n = 8 \) records for an unknown record with the unknown label \( x_0 = 5 \). The calculations for this example were made with OpenQuacks, which is an open source quantum simulator Maple package developed at UMBC and publically available.

We are given a blackbox computing device

\[
\text{In } \rightarrow \begin{array}{c}
\text{I[?]}
\end{array} \rightarrow \text{Out}
\]
that implements as an oracle the unknown unitary transformation

\[
I_{|x_0\rangle} = I_5 = \begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1
\end{bmatrix}
\]

We cannot open up the blackbox \(\square I_{|?\rangle}\) to see what is inside. So we do not know what \(I_{|x_0\rangle}\) and \(x_0\) are. The only way that we can glean some information about \(x_0\) is to apply some chosen state \(|\psi\rangle\) as input, and then make use of the resulting output.

Using of the blackbox \(\square I_{|?\rangle}\) as a component device, we construct a computing device \(-HI_{|0\rangle}HI_{|?\rangle}\) which implements the unitary operator

\[
Q = -HI_{|0\rangle}HI_{|x_0\rangle} = \frac{1}{4} \begin{bmatrix}
-3 & 1 & 1 & 1 & -1 & 1 & 1 & 1 \\
1 & -3 & 1 & 1 & -1 & 1 & 1 & 1 \\
1 & 1 & -3 & 1 & -1 & 1 & 1 & 1 \\
1 & 1 & 1 & -3 & -1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 3 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & -1 & -3 & 1 & 1 \\
1 & 1 & 1 & 1 & -1 & 1 & -3 & 1 \\
1 & 1 & 1 & 1 & -1 & 1 & 1 & -3
\end{bmatrix}
\]

We do not know what unitary transformation \(Q\) is implemented by the device \(-HI_{|0\rangle}HI_{|?\rangle}\) because the blackbox \(\square I_{|?\rangle}\) is one of its essential components.

**STEP 0.** We begin by preparing the known state

\[
|\psi_0\rangle = H |0\rangle = \frac{1}{\sqrt{8}} (1, 1, 1, 1, 1, 1, 1, 1)^{\text{transpose}}
\]
We proceed to loop

\[ K = \text{round} \left( \frac{\pi}{4 \sin^{-1} \left( \frac{1}{\sqrt{8}} \right)} - \frac{1}{2} \right) = 2 \]

times in STEP 1.

Iteration 1. On the first iteration, we obtain the unknown state

\[ |\psi_1\rangle = Q |\psi_0\rangle = \frac{1}{4\sqrt{2}} (1, 1, 1, 1, 5, 1, 1) \text{transpose} \]

Iteration 2. On the second iteration, we obtain the unknown state

\[ |\psi_2\rangle = Q |\psi_1\rangle = \frac{1}{8\sqrt{2}} (-1, -1, -1, -1, 11, -1, -1) \text{transpose} \]

and branch to STEP 2.

STEP 2. We measure the unknown state \(|\psi_2\rangle\) to obtain either

\[ |5\rangle \]

with probability

\[ \text{Prob}_{\text{Success}} = \sin^2 ((2K + 1) \beta) = \frac{121}{128} = 0.9453 \]

or some other state with probability

\[ \text{Prob}_{\text{Failure}} = \cos^2 ((2K + 1) \beta) = \frac{7}{128} = 0.0547 \]

and then exit.

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