Early days following Grover’s quantum search algorithm

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Abstract

This is a note accompanying “CS 410/510: INTRO TO QUANTUM COMPUTING” I taught at Portland State University in Spring 2017. It is a review and summary of some early results related to Grover’s quantum search algorithm in a consistent way. I had to go back and forth among several books, notes and original papers to sort out various details when preparing the lectures, which was a pain. This is the motivation behind this note. I would like to thank Peter Høyer for valuable feedback on this note.

1 Introduction

This note has a simple purpose to serve: to sort out some of the early literature around Grover’s quantum search algorithm and to put them in context. If you note something interesting and/or significant that is worth adding or something incorrect here, please drop me an email. In the following, I will describe

• Quantum search algorithm when there are multiple marked items with or without the number of marked items known. (Section 2)

• Quantum counting, a nice application of Kitaev’s phase estimation technique. This also gives an alternative approach to searching with unknown number of solutions. (Section 3)

• A hybrid argument showing the optimality of Grover’s algorithm (based on [BBBV97]). This is pretty standard, but I want to point out a minor tweak that shows a stronger claim: unstructured search, in fact the decision version, is hard even on average, strengthening the worst-case hardness which is commonly seen in the literature. (Section 4)

Overview. Here is my narrative of the time-line based on my reading on early papers and information I collected elsewhere (books, lecture notes, and conversations with other researchers including some authors of these work).

I will start the story with Grover’s quantum algorithm for finding a marked item in a dataset, which achieves quadratic speedup over optimal classical algorithms in the query model. It was first published in STOC’96 [Gro96], a prestigious conference in theoretical computer science, under the relatively plain title “A fast quantum mechanical algorithm for database search”. He then worked out another version with the likely more popular title “Quantum mechanics helps in searching for a needle in a haystack” that was geared towards physicists and appeared in Phys.
Rev. Lett. [Gro97]. Note that a couple of years ago, Shor proposed his famous quantum factorization algorithm. Kitaev on the other continent (Russia) apparently heard about Shor’s result but was not able to get a copy of Shor’s paper back then. He instead reproduced Shor’s results on his own by a different approach, based on his elegant and powerful tool of phase estimation [Kit95].

Several papers followed Grover’s work immediately. Boyer, Brassard, Høyer, and Tapp (these names will appear many times) first gave a finer analysis of Grover’s algorithm. They also extended it to the setting of multiple marked items for both cases that the number of solutions are known and unknown [BBHT96]. Applications of Grover’s algorithm also came out soon, such as quantum algorithms finding the minimum in a dataset [DH96] and for finding collisions [BHT98a]. Another important application, quantum counting, was already outlined in [BBHT96], and its full description appeared a little later [BHT98b]. The algorithm combines Grover’s search algorithm and Shor’s order finding algorithm in a clever way, but the analysis was a bit complicated. They also phrased Grover’s search algorithm in the more general framework of amplitude amplification, which was formalized in an earlier work by Brassard and Høyer [BH97].

Meanwhile, Cleve, Ekert, Macchiavello and Mosca were unwrapping and extending Kitaev’s work, and they rephrased many early algorithms (Deutsch, order finding, etc.) under the phase estimation framework [CEMM98]. It turned out that quantum counting can be easily described and understood under the phase-estimation framework (in fact the proceedings version of [BHT98b] already indicated this easier perspective without providing a complete analysis in their original approach). With Mosca, Brassard, Høyer and Tapp completed a full version [BHMT02]. This basically culminated the early stage of developments related to quantum search.

As to the optimality of Grover’s search algorithm, an early manuscript in 1994 by Bennett, Bernstein, Brassard and Vazirani [BBBV97] actually preceded Grover’s paper. They systematically studied the strengths and limits of quantum algorithms. In particular, they employed a nice tool - hybrid argument to prove a lower bound on the necessary number of quantum queries to solve the search problem with bounded error. They also proposed using majority voting to amplify the success probability of a quantum algorithm, but this does not achieve the quadratic speedup in quantum amplitude amplification in [BHMT02]. Apparently, Grover was not aware of this work by Bennett et al. when he worked out his quantum search algorithm. [BBHT96] noticed that the constant in the lower bound of [BBBV97] was lower than that in Grover’s algorithm, and they improved it to an almost tight bound. Exact optimality was later proved by Zalka [Zal99] (see [DH09] for a more intuitive proof).

Now let’s get to the technical meat.

2 Search with multiple marked items

Let’s set up Grover’s search problem in the standard way. The presentation here is adapted from Watrous’s lecture note\(^1\). Let \( f : \{0,1\}^n \to \{0,1\} \) be a function\(^2\) and let \( N = 2^n \). We are given access to the oracle \( O_f \) that implements \( f \) as an unitary as usual:

\[
| x \rangle | y \rangle \xrightarrow{O_f} | x \rangle | y \oplus f(x) \rangle.
\]

Define the two sets representing the “marked” and “unmarked” items:

\(^1\)https://cs.uwaterloo.ca/~watrous/CPSC519/LectureNotes/12.pdf

\(^2\)We consider \( \{0,1\}^n \) for the sake of simplicity. For a domain \( [N] \), we will need quantum Fourier transform on \( \mathbb{Z}_N \) rather than the simple Hadamard gate.
\[ A := \{ x \in \{0,1\}^n : f(x) = 1 \}, \quad B := \{ x \in \{0,1\}^n : f(x) = 0 \}. \]

Then let \( a = |A| \) and \( b = |B| \) and define two orthonormal states:

\[ |A\rangle := \frac{1}{\sqrt{a}} \sum_{x \in A} |x\rangle, \quad |B\rangle := \frac{1}{\sqrt{b}} \sum_{x \in B} |x\rangle. \]

Grover’s algorithm start by preparing a state in uniform superposition

\[ |h\rangle = H^\otimes n |0^n\rangle = \sum_{x \in \{0,1\}^n} |x\rangle. \]

Two reflection operations are at the heart of Grover’s algorithm:

\[ R_h = -H^\otimes n Z_0 H^\otimes n \quad \& \quad R_B := Z_f \]

where

\[ Z_0 |x\rangle := \begin{cases} -|x\rangle & \text{if } x = 0^n \\ |x\rangle & \text{if } x \neq 0^n \end{cases} \quad \& \quad Z_f |x\rangle := (-1)^{f(x)} |x\rangle. \]

Note that \( Z_f \) is just the “phase”-oracle of \( f \) that computes \( f(x) \) in the phase. It can be implemented from \( O_f \) with one auxiliary qubit by the standard “phase-kick-back” trick. \( Z_0 \) can be implemented in a similar fashion (i.e., phase oracle for function \( \delta_0 \)).

Consider the two dimensional plane spanned by \( \{ |A\rangle, |B\rangle \} \). Observe that on this plane

- \( R_h = -H^\otimes n Z_0 H^\otimes n \): reflects a state about \( |h\rangle \). This can be seen by noting that \( H \) brings \( \{ |h\rangle, |h^\perp\rangle \} \) to \( \{ |0\rangle, |0^\perp\rangle := H^\otimes n |h^\perp\rangle \} \), where \( |h^\perp\rangle \) denotes the state orthogonal to \( |h\rangle \) on the plane of \( \{ |A\rangle, |B\rangle \} \), and \(-Z_0\) flips the sign of all standard basis vectors except \( |0^n\rangle \). Algebraically, \( R_h = H^\otimes n (-Z_0) H^\otimes n = 2 |h\rangle \langle h| - I \). Grover interpreted \( R_h \) as “inversion about the mean”, which gives an intuitive explanation how the amplitude on the marked item grows. \( R_h \) is sometimes also called the Grover diffusion operator, probably preferred by physicists.

- \( R_B = Z_f \): reflects a state about \( |B\rangle \) in the plane defined by \( \{ |A\rangle, |B\rangle \} \).

The composition \( G := R_f R_B = -H^\otimes n Z_0 H^\otimes n Z_f \) thus rotates a state towards \( |A\rangle \) by \( 2\theta_a \) (Exercise: verify it pictorially) where \( \theta_a := \sin^{-1}(\langle h|A\rangle) = \sin^{-1}(\sqrt{\frac{a}{N}}) \).

Grover’s quantum search algorithm is then easy to describe

**Algorithm 1** Grover’s quantum search algorithm (number of solutions known)

**Input**: \( O_f \) with \( f(x) = 1 \) iff. \( x \in A \). \( \lambda = 6/5 \).

**Output**: \( x \in A \), a marked item.

1. **Initialization**: \( |h\rangle := H^\otimes n |0^n\rangle = \sum_{x \in \{0,1\}^n} |x\rangle \).
2. **Iteration**: apply \( G = (-H^\otimes n Z_0 H^\otimes n)Z_f \) on \( |h\rangle \) \( k \) times (the number of iterations \( k \) is crucial and we will specify it later).
3. Measure and obtain candidate solution \( x \).

The effect of \( G \) gives the very intuitive geometric interpretation of Grover’s algorithm: starting from \( |h\rangle \), each iteration (i.e., application of \( G \)) rotates the current state by \( 2\theta_a \) towards \( |A\rangle \). After
sufficiently many iterations, we’d hope that we are close to $|A\rangle$ enough so we are likely to measure an element in $A$. More precisely

$$|h\rangle = \sin \theta_a |A\rangle + \cos \theta_a |B\rangle,$$

$$G^k |h\rangle = \sin((2k+1)\theta_a) |A\rangle + \cos((2k+1)\theta_a) |B\rangle.$$

How many iterations are sufficient? If we know $a$, the number of solutions, then it is easy to decide. We have

$$\gamma_k := \Pr[\text{finding an } x \in A \text{ after } k \text{ iterations}] = \left| \langle A| G^k |h\rangle \right|^2 = \sin^2((2k+1)\theta_a).$$

We would like to have $(2k+1)\theta_a$ as close to $\pi/2$ as possible. Let us pick $k^* := \left\lfloor \frac{\pi/2 - \theta_a}{2\theta_a} \right\rfloor$,

and let $\eta := \pi/2 - (2k^*+1)\theta_a$ (|$\eta$| $\leq \theta_a$). Then one finds an $x \in A$ successfully with probability at least

$$\gamma_k = \sin^2((2k+1)\theta_a) = \sin^2(\pi/2 - \eta) = \cos^2(\eta) \geq \cos^2(\theta_a) \geq 1 - \frac{a}{N}.$$

If we just repeat the entire algorithm a few times, we can amplify the success probability close to 1. Hence the number of queries we need is

$$O(k^*) = O\left(\frac{\pi/2 - \theta_a}{2\theta_a}\right) \leq O\left(\frac{1}{\sin \theta_a}\right) = O\left(\sqrt{\frac{N}{a}}\right).$$

### 2.1 Number of marked items unknown

We can pick $k$ according to $\theta_a$ when we know $a$. But what if we do not know $a$, the number of marked items? This is answered in [BBHT96]. We need a simple but crucial lemma.

**Lemma 1.** Let $\theta_a$ be as before (i.e., $\sin^2(\theta_a) = a/N$. Let $m$ be an integer and pick $k \leftarrow \{0, \ldots, m-1\}$ uniformly at random. Then after applying $G$ on $|h\rangle$ $k$ times, the probability of measuring an $x \in A$ is

$$P_m = \frac{1}{2} - \frac{\sin(4m\theta_a)}{4m \sin(2\theta_a)}.$$

In particular, when $m \geq 1/\sin(2\theta_a)$, $P_m \geq \frac{1}{4}$.

This inspires a simple trick. We start from $m = 1$, and slowly but exponentially increment $m$, so that we can reach the right region for $m$ without spending too many unnecessary queries\(^3\). In the algorithm below, we assume that $a \leq N/2$. When there are more solutions, it is easy to sample classically to find a marked item.

**Theorem 2.** Algorithm 2 finds an $x \in A$ in $O(\sqrt{\sqrt{N/a}})$ expected number of iterations.

\(^3\)This is reminiscent of the *exponential back-off* algorithm in some network protocols, but the rate of increment here needs more vigilance.
**Algorithm 2** Quantum search with number of solutions unknown

**Input:** $O_f$ with $f(x) = 1$ iff. $x \in A$. $\lambda = 6/5$.

**Output:** $x \in A$, a marked item.

1. Initialize $m = 1$.
2. while $m \leq \sqrt{N}$ do
3. pick uniformly random $k \leftarrow \{1, \ldots, m\}$.
4. apply $k$ times the basic Grover iteration $G$ on initial state $|h\rangle = \sum_x \frac{1}{\sqrt{N}} |x\rangle$.
5. measure and obtain $x$. If $x \in A$, output $x$ and abort. Otherwise set $m \leftarrow \lambda m$.
6. end while

**Proof.** Let $m^* = 1/\sin(2\theta_a)$ denote the critical point. Then

$$m^* = \frac{1}{2 \sin \theta_a \cos \theta_a} = \frac{1}{2 \sqrt{a/N} \sqrt{1-a/N}} = \frac{N}{2 \sqrt{(N-a)/a}} < \sqrt{N/a},$$

assuming $a \leq N/2$. Let $t = \lceil \log_\lambda m^* \rceil$ be the number of main loops in the algorithm needed to reach $m^*$. From Lemma 1, once we go beyond $m^*$, every loop will succeed with probability at least 1/4. Thus we just need to count the number of Grover iterations necessary to reach the critical point plus the number of iterations afterwards to find a solution.

- To reach the critical point, the number of iterations in the $j$th loop is bounded by $m_j = \lambda^j - 1$. Hence the total number of Grover iterations $G$ is bound by

$$\sum_{j=1}^{t} \lambda^j - 1 = \frac{\lambda^t - 1}{\lambda - 1} \leq \frac{\lambda}{\lambda - 1} m^* = 6m^*.$$

- After reaching the critical point, let $X$ be the random variable denoting the Grover iterations needed till finding a solution. Let $L$ be the random variable denoting the additional loops till a solution is found. By Lemma 1, $\Pr[L = \ell] \leq (\frac{3}{4})^{\ell-1} \cdot \frac{1}{4} \leq (\frac{3}{4})^\ell$.

$$E[X] = E LE_X[X|L = \ell] = \sum_{\ell} E[X|L = \ell] \cdot \Pr[L = \ell]$$

$$\leq \sum_{\ell} (\sum_{j=1}^{\ell} \lambda^{\ell+j}) \cdot \Pr[L = \ell] \quad \text{(each loop runs } \leq \lambda^{\ell+j} \text{ iterations)}$$

$$= \sum_{\ell} \lambda^\ell \cdot \lambda \cdot \frac{\lambda^\ell - 1}{\lambda - 1} \cdot \Pr[L = \ell]$$

$$\leq \frac{\lambda \cdot m^*}{\lambda - 1} \cdot \sum_{\ell} \Pr[L = \ell] \cdot \lambda^\ell$$

$$\leq \frac{\lambda m^*}{\lambda - 1} \cdot \sum_{\ell=1}^{\infty} (\frac{3\lambda}{4})^\ell$$

$$\leq \frac{\lambda \cdot m^*}{\lambda - 1} \cdot \frac{1}{1 - 3\lambda/4} \quad \text{(b.c. we picked } \lambda = 6/5 < 4/3)$$

$$\leq 10m^*.$$

Thus the expected total number of Grover iterations is at most $6m^* + 10m^* = O(m^*) = O(\sqrt{N/a})$. □
Remark 3. Note that any $1 < \lambda < 4/3$ would work. Another feature of these algorithms is that the solution from measuring the register after appropriate number of Grover iterations is distributed uniformly in the set of solutions. This is a key property behind some applications such as finding the minimum [DH96].

3 Quantum amplitude amplification and quantum counting

An immediate generalization leads to a general technique called amplitude amplification, first introduced in [BH97], but for page limitation, little details were provided. It was later fully specified in [BHT98b, BHMT02]. It is a quantum analogue of amplifying the success probability of a randomized algorithm classically. If we repeat independently $t$ times a randomized algorithm that succeeds with probability $p$, then the probability that it succeeds at least once is roughly boosted to $1 - (1 - p)^t \approx tp$. Therefore we need $O(1/p)$ repetitions to succeed with probability close to 1.

Quantum amplitude amplification takes a (classical or quantum) subroutine $U$ that succeeds with probability $p$ (or amplitude of magnitude $\sqrt{p}$), and boosts the success probability close to 1 within $O(1/\sqrt{p})$ invocations of the original subroutine. Hence this offers a generic quadratic speedup.

The procedure is similar to Grover’s algorithm by composing two reflections that effectively moves towards the “good” state. For instance, consider a unitary operation $U$ and $\chi : \{0,1\}^n \to \{0,1\}$. Then $\chi$ induces a partition on $\{0,1\}^n$: call $A := \{x \in \{0,1\}^n : \chi(x) = 1\}$ the “good” subspace with size $a = |A|$, and $B := \{x \in \{0,1\}^n : \chi(x) = 0\}$ the “bad” subspace. Let $|A\rangle = \frac{1}{\sqrt{|A|}} \sum_{x \in A} |x\rangle$ and $|B\rangle = \frac{1}{\sqrt{|B|}} \sum_{x \in B} |x\rangle$. Suppose $|\psi\rangle := U|0^n\rangle = \sqrt{|A|} |A\rangle + \sqrt{1 - p} |B\rangle$. Then define

$$G := R_A R_B \text{ with } R_A := -U Z_0 U^* \quad \& \quad R_B := Z_{\chi},$$

where

$$Z_0 |x\rangle := \begin{cases} -|x\rangle & \text{if } x = 0^n \\ |x\rangle & \text{if } x \neq 0^n \end{cases} \quad \& \quad Z_{\chi} |x\rangle := (-1)^{\chi(x)} |x\rangle,$$

are as before. We can see that $R_A$ is a reflection about $|\psi\rangle = U|0\rangle$, and $R_B$ is reflection about $|B\rangle$ in the plane defined by $\{ |A\rangle, |B\rangle \}$, and repeated application of $G$ on $|\psi\rangle$ will amplify the amplitude on $|A\rangle$.

Remark 4. If $p$ is unknown, similar idea as in Algorithm 2 can be adapted here. Details can be found in [BHMT02]. There they also described, when $p$ is known, two approaches that amplify the success probability to exactly one, but there is technicality about implementing some unitary exactly and one needs to be careful about the quantum gate set to work with.

Recently, an oblivious quantum amplitude amplification technique has been developed [BCC+14, Wat09], which is applicable to a unitary with an arbitrary and unknown input state $|\psi\rangle$ (rather than just $|0\rangle$).

3.1 Quantum counting & amplitude estimation

Consider the same setup as in Grover’s search problem, can we find out how many marked items are there? Namely given $O_f$, can we compute $|A| = |f^{-1}(1)|$? This is the quantum counting problem, and it can be solved by considering a slightly more general problem, amplitude estimation.

Again, consider a unitary operation $U$, and $\chi : \{0,1\}^n \to \{0,1\}$. Then $\chi$ induces a partition on $\{0,1\}^n$: call $A := \{x \in \{0,1\}^n : \chi(x) = 1\}$ the “good” subspace with size $a = |A|$, and $B := \{x \in \{0,1\}^n : \chi(x) = 0\}$ the “bad” subspace. Let $|A\rangle = \frac{1}{\sqrt{a}} \sum_{x \in A} |a\rangle$ and $|B\rangle = \frac{1}{\sqrt{N-a}} \sum_{x \in B} |x\rangle$. 


We will compare two states.

4.1 Standard lower bound proof

Let \( |\psi \rangle = U |0 \rangle = \sqrt{\alpha} |A \rangle + \sqrt{1 - \alpha} |B \rangle \). Estimate \( \alpha \), i.e., compute \( \hat{\alpha} \) such that \( |\alpha - \hat{\alpha}| \leq \epsilon \).

Quantum counting is then a special case of amplitude estimation. Let \( U = H^{\otimes n} \). Then \( |h \rangle = \frac{1}{\sqrt{n}} \sum_x |x \rangle = \sqrt{\frac{1}{N}} |A \rangle + \sqrt{\frac{N-a}{N}} |B \rangle \). Thus \( \alpha = a/N \) and a fine estimation of \( \alpha \) also gives a good approximation of \( \alpha \text{- the number of marked elements. This immediately gives an alternative approach to searching without knowing the number of solutions: one just starts off approximating the number of solutions, and proceeds using the approximate number to decide the proper number of Grover iterations.} \)

So how do we solve amplitude estimation? Kitaev’s phase estimation technique turns out to be the bomb. The key is to observe that the operator

\[
G := -AZ_0A^*Z_X
\]

has eigenvectors

\[
|\psi_\pm \rangle := \frac{1}{\sqrt{2}} \left( \frac{1}{\sqrt{\alpha}} |\psi_A \rangle \pm \frac{i}{\sqrt{1 - \alpha}} |\psi_B \rangle \right),
\]

with eigenvalues \( \lambda_\pm = e^{\pm 2i\alpha} \), where \( \sin^2(\theta_\alpha) = \alpha \). (Exercise: verify this.) Note that \( |\psi_\pm \rangle \) form an eigen-basis.

Kitaev’s phase estimation (PE) algorithm computes an approximation of the eigenvalue. Namely

\[
\text{Input: } (U, |\phi \rangle \text{ with } U |\phi \rangle = e^{i\theta} |\phi \rangle) \rightarrow \text{PE} \rightarrow \tilde{\theta} \approx \theta .
\]

Therefore if we can prepare any one of \( |\psi_\pm \rangle \) and send it in PE algorithm with \( G \), we will be able to approximate \( \theta = \theta_0 \) and hence \( \alpha \). But how to prepare \( |\psi_\pm \rangle \)?

Well, we don’t have to. The trick is to note that \( U |0 \rangle = |\psi \rangle = \frac{1}{\sqrt{2}} (e^{i\theta_0} |\psi_+ \rangle - e^{-i\theta_0} |\psi_- \rangle) \) can be spanned under the eigenvectors. Therefore if we send \( |\psi \rangle \) and \( G \) in the PE algorithm, the effect will be as if measuring \( |\psi \rangle \) under the eigenbasis and then estimating the eigenvalue (phase) of the eigenvector corresponding to the measurement outcome. Be it \( \psi_+ \) or \( \psi_- \), we get approximation of \( \alpha \) either way. Read more details in [BHMT02].

4 Optimality of Grover’s algorithm: an average-case lower bound

We discuss optimality of Grover’s algorithm, i.e., hardness of solving the search problem in this section. Read [BBBV97] for more details such as the hybrid argument.

Let \( O_r \) define an instance of Grover’s search problem where \( O_r(x) = 1 \text{ iff. } x = r \). Given quantum access to \( O_r \), an arbitrary \( k \)-query quantum algorithm can be described as

\[
U_k(O \otimes I_A)U_{k-1} \ldots U_1(O \otimes I_A)U_0 |0^n \rangle |0^{m-n} \rangle_A ,
\]

where \( A \) is a register (work space) of \( m - n \) auxiliary qubits, and \( U_j \) are arbitrary unitary operations on \( m \) qubits. In what follows, we abuse notation and write \( O_r \) to represent \( O_r \otimes I_A \) with some implicit auxiliary system.

4.1 Standard lower bound proof

We will compare two states

\[
|\psi^{(k)}_r \rangle := U_kO_rU_{k-1} \ldots U_1O_rU_0 |0^n \rangle \\
|\phi^{(k)} \rangle := U_k IU_{k-1} \ldots U_1 IU_0 |0^m \rangle
\]
Identity operator $I$ can be viewed as a unitary oracle implementing the constant-0 function, i.e., $f(x) = 0$ for all $x \in \{0,1\}^n$.

**Lemma 6.** Let $N = 2^n$. $\exists r \in \{0,1\}^n$ such that $\| \psi_r^{(k)} \rangle - \| \phi^{(k)} \rangle \| \leq 2k/\sqrt{N}$.

These immediately give hardness of the unstructured search problem (and hence optimality of Grover’s algorithm).

**Theorem 7.** Any algorithm needs $\Omega(\sqrt{N})$ queries to $O_r$ in order to find $r$ with constant probability.

**Proof.** For an arbitrary $k$-query algorithm $A$, it needs to be able to distinguish $\| \psi_r^{(k)} \rangle$ from $\| \phi^{(k)} \rangle$ (this will made more precise in the next section). Therefore $\| \| \psi_r^{(k)} \rangle - \| \phi^{(k)} \rangle \|$ has to be bigger than some constant, which implies that $k$ needs to be at least $\Omega(\sqrt{N})$.

Now let’s prove Lemma 6 by the elegant hybrid argument.

**Proof of Lemma 6.** Introduce two sequences of intermediate states:

\[
\begin{align*}
|\psi_r^{(0)}\rangle &= U_0 |0^m\rangle, & |\phi^{(0)}\rangle &= U_0 |0^m\rangle \\
|\psi_r^{(1)}\rangle &= U_1 O_r |\psi_r^{(0)}\rangle, & |\phi^{(1)}\rangle &= U_1 I |\phi^{(0)}\rangle \\
|\psi_r^{(j+1)}\rangle &= U_{j+1} O_r |\psi_r^{(j)}\rangle, & |\phi^{(j+1)}\rangle &= U_{j+1} I |\phi^{(j)}\rangle \\
|\psi_r^{(k)}\rangle &= U_k O_r |\psi_r^{(k-1)}\rangle, & |\phi^{(k)}\rangle &= U_k I |\phi^{(k-1)}\rangle
\end{align*}
\]

Define:

\[
D_r := \| |\psi_r^{(j)}\rangle - |\phi^{(j)}\rangle \|, \quad E_r := \| O_r |\phi^{(j)}\rangle - |\phi^{(j)}\rangle \|.
\]

Let $\Pi_r = |r\rangle \langle r|$ be the projection on the basis $|r\rangle$ (more precisely $\Pi_r = |r\rangle \langle r| \otimes I_A$ is identity on the remaining working space).

**Claim 8.** For $j = 0, \ldots, k-1$, $D_r^{j+1} \leq D_r^j + E_r^j$, and $E_r^j \leq 2 \| \Pi_r |\phi^{(j)}\rangle \|$.

**Proof of Claim 8.**

\[
\begin{align*}
D_r^{j+1} &= \| |\psi_r^{(j+1)}\rangle - |\phi^{(j+1)}\rangle \| \\
&= \| U_{j+1} O_r |\psi_r^{(j)}\rangle - U_{j+1} I |\phi^{(j)}\rangle \| \\
&= \| U_{j+1} O_r |\psi_r^{(j)}\rangle - U_{j+1} O_r |\phi^{(j)}\rangle + U_{j+1} O_r |\phi^{(j)}\rangle - U_{j+1} O_r |\phi^{(j)}\rangle \| \\
&\leq \| U_{j+1} O_r (|\psi_r^{(j)}\rangle - |\phi^{(j)}\rangle) \| + \| U_{j+1} O_r (|\phi^{(j)}\rangle - |\phi^{(j)}\rangle) \| \text{ triangle-inequality} \\
&= \| |\psi_r^{(j)}\rangle - |\phi^{(j)}\rangle \| + \| O_r |\phi^{(j)}\rangle - |\phi^{(j)}\rangle \| \quad \text{unitary preserves norm} \\
&= D_r^j + E_r^j.
\end{align*}
\]
For the second part, note that
\[ O_r \phi^{(j)} \]  
\[ = O_r (\Pi_r + (I - \Pi_r)) \phi^{(j-1)} \]
\[ = O_r \Pi_r \phi^{(j-1)} + (I - \Pi_r) \phi^{(j-1)} \] (Note: \( O_r (I - \Pi_r) = I - \Pi_r \));
\[ |\phi^{(j-1)}\rangle = \Pi_r |\phi^{(j-1)}\rangle + (I - \Pi_r) |\phi^{(j-1)}\rangle. \]

Therefore
\[ E_r^j = \| O_r \Pi_r |\phi^{(j-1)}\rangle - \Pi_r |\phi^{(j-1)}\rangle \| \leq \| O_r \Pi_r |\phi^{(j-1)}\rangle \| + \| \Pi_r |\phi^{(j-1)}\rangle \| = 2 \| \Pi_r |\phi^{(j-1)}\rangle \|. \]

Back to proving the Lemma, we have
\[ \| \psi_r^{(k)} \rangle - \| \phi(k) \rangle \| = D_r^k \leq E_r^{k-1} + \ldots + E_r^0 = \sum_{j=0}^{k-1} E_r^j. \]

**Claim 9.** \( \sum_{r \in \{0,1\}^n} D_r^k \leq 2k \sqrt{N} \).

**Proof of Claim 9.**
\[
\sum_{r \in \{0,1\}^n} D_r^k = \sum_r \sum_j E_r^j = \sum_j \sum_r E_r^j \\
\leq \sum_j \sqrt{N} \sum_r (E_r^j)^2 \quad \text{(Cauchy-Schwarz)}
\]
\[
\leq 2 \sqrt{N} \sum_j \sum_r \| \Pi_r |\phi^{(j-1)}\rangle \|^2 = 2 \sqrt{N} \sum_{j=0}^{k-1} \| \phi^{(j-1)} \|^2 \\
= 2 \sqrt{N} \sum_{j=0}^{k-1} 1 = 2k \sqrt{N}. \]

Therefore there must be at least one \( r^* \) such that \( D_{r^*}^k \leq 2k / \sqrt{N} \), because otherwise the \( \sum_r D_r^k > N \cdot 2k / \sqrt{N} = 2k \sqrt{N} \). 

**4.2 Stronger lower bound: average-case hardness**

Note that the above proof actually holds for the decision version: for some \( r \), distinguishing \( O_r \) from constant-0 function is hard. Namely, deciding if an oracle contains a marked item is already hard, which of course implies that finding a solution is at least as hard. In fact, we can further observe something stronger. Let us introduce some more basic notions to make a formal statement.

Recall the trace distance \( \text{td}(\rho, \sigma) := \frac{1}{2} \| \rho - \sigma \|_1 = \frac{1}{2} \text{Tr}(\sqrt{(\rho - \sigma)^*(\rho - \sigma)}) \), where \( \text{Tr}(\cdot) \) computes the trace of a matrix. For two pure states \( |\psi\rangle \) and \( |\phi\rangle \), it is easy to verify that
\[
\text{td}(|\psi\rangle, |\phi\rangle) = \sqrt{1 - |\langle \psi | \phi \rangle|^2} \leq \| |\psi\rangle - |\phi\rangle \|. \]

Consider two oracles \( O \) and \( O' \). Let \( A^{O}(\cdot) \) denote an algorithm \( A \) that makes queries to \( O \) and finally output one bit. We define the distinguishing advantage of an algorithm \( A \) trying to tell apart \( O \) and \( O' \):
\[
\text{Adv}^{O,O'}_A := |\Pr[A^{O}(\cdot) = 1] - \Pr[A^{O'}(\cdot) = 1]|.
\]
We will be interested in distinguishing the oracle \( O \) and identity \( I \) (i.e., constant-0 function).

Consider the process that a random \( r \) is chosen, and then \( O \) is given to an algorithm \( A \). The goal is to find \( r \), the marked element. We show that this is hard.

**Theorem 10.** For any \( k \)-query algorithm \( A \),

\[
\text{Adv}^{O,I}_A := \left| \Pr_{r \leftarrow \{0,1\}^n}[A^O(\cdot) = 1] - \Pr[A^I(\cdot) = 1] \right| \leq 2k/\sqrt{N}.
\]

Therefore one needs at least \( \Omega(\sqrt{N}) \) queries to find the marked element.

This theorem is strong in a couple of aspects.

- It holds for a random Grover oracle, not just in the worst-case. This theorem also explicitly refers to the decision version of unstructured search problem. It follows that, for a uniformly random chosen \( r \), finding \( r \) is as hard as the worst case.

- We bound the success probability of any algorithm with certain number of queries. This is most relevant in the cryptographic setting, since even a small (e.g., inverse polynomial) winning probability matters. Usually in the literature, one only cares about the hardness for solving the problem with constant probability.

Exercise: prove the classical lower bound for solving this average-case (under uniform distribution) search problem.

**Proof.** Let \( p_r := \Pr[A^O(\cdot) = 1] \) and \( q := \Pr[A^I(\cdot) = 1] \). By Holevo-Helstrom theorem [Hel67, Hol72], we know that

\[
\text{Adv}^{O,I}_A = |\Pr[A^O(\cdot) = 1] - \Pr[A^I(\cdot) = 1]| \leq \text{td}\left( |\psi^{(k)}_r\rangle, |\phi^{(k)}\rangle \right)
\]

Therefore we have that

\[
\text{Adv}^{O,I}_A = \left| \sum_r p_r \cdot \frac{1}{N} - q \right| \leq \frac{1}{N} \sum_r |p_r - q|
\]

\[
\leq \frac{1}{N} \sum_r |p_r - q| \leq \frac{1}{N} \sum_r \text{td}\left( |\psi^{(k)}_r\rangle, |\phi^{(k)}\rangle \right) \quad \text{(Eqn. 2)}
\]

\[
\leq \frac{1}{N} \sum_r \| |\psi^{(k)}_r\rangle - |\phi^{(k)}\rangle \| \quad \text{(Eqn. 1)}
\]

\[
= \frac{1}{N} \sum_r D^k_r \leq \frac{2k}{\sqrt{N}} \quad \text{(Claim 9)}.
\]

Exercise: can you extend everything here to the case of multiple solutions?

\footnote{C.f. Theorem 3.4. of https://cs.uwaterloo.ca/~watrous/TQI/TQI.3.pdf, and set \( \lambda = 1/2 \).}
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