# Generalized Grover Search Algorithm for Arbitrary Initial Amplitude Distribution

David Biron,[1] Ofer Biham,[1] Eli Biham,[2] Markus Grassl,[3] Daniel A. Lidar[4]

[1]Racah Institute of Physics, The Hebrew University, Jerusalem 91904, Israel
[2]Computer Science Department, Technion, Haifa 32000, Israel
[3]Institut für Algorithmen und Kognitive Systeme, Universität Karlsruhe, Am Fasanengarten 5, D–76128 Karlsruhe, Germany
[4]Department of Chemistry, University of California, Berkeley, CA 94720, USA

**Abstract.** Grover's algorithm for quantum searching of a database is generalized to deal with arbitrary initial amplitude distributions. First order linear difference equations are found for the time evolution of the amplitudes of the $r$ marked and $N-r$ unmarked states. These equations are solved *exactly*. An expression for the optimal measurement time $T \sim O(\sqrt{N/r})$ is derived which is shown to depend only on the initial average amplitudes of the marked and unmarked states. A bound on the probability of measuring a marked state is derived, which depends only on the standard deviation of the initial amplitude distributions of the marked or unmarked states.
**Keywords:** Quantum searching, Grover's algorithm, exact solution.

## 1 Introduction

The power of Quantum Computation (QC) was most dramatically demonstrated in the algorithms of Shor, for the polynomial time solution of the factorization problem [1], and of Grover [2, 3], for a search which can find a marked element in an unsorted database of size $N$, in $O(\sqrt{N})$ steps (compared to $O(N)$ steps on a classical computer). The importance of Grover's result stems from the fact that it proves the enhanced power of quantum computers compared to classical ones for a whole class of problems, for which the bound on the efficiency of classical algorithms is known. This is unlike the case of Shor's algorithm, since in spite of the fact that no efficient classical algorithm for the factorization problem is known, there is no proof that such an algorithm does not exist.

A large number of related results followed Grover's original paper [2]. Among these, the efficiency of Grover's algorithm was analyzed and compared to the theoretical efficiency limit of quantum computers for such benchmark search problems as introduced (before Grover's result [2]) by Bennett et al. [4]. The algorithm was recently shown to be optimal, i.e., to satisfy the theoretical limit [5]. Further developments include the use of Grover's algorithm or slightly modified versions of it as the essential step in algorithms that solve a variety of other problems such as quantum search for the median [6] and the minimum [7] in a set of $N$ items, as well as the collision problem [8]. It was also shown that other search problems which classically require $\log_2 N$ evaluations (*queries*) of

a black–box function, can be reduced to a single query using Grover's approach [9, 10]. Finally, it was shown that a simple closed formula describes the time evolution of the amplitudes of the generalized problem, which includes several marked states [11]. As this work is directly relevant to ours, we briefly summarize some of its pertinent results.

Let $k(t)$ $[l(t)]$ denote the amplitude of the *marked* [*unmarked*] states in the database, $r$ the number of marked states, and $\omega = 2\arcsin(\sqrt{r/N})$. It was shown by Boyer et al. [11] that after $t$ steps of the algorithm, the marked states' amplitude increases as: $k(t) = \sin[\omega(t+1/2)]/\sqrt{r}$, while at the same time that of the unmarked states decreases as: $l(t) = \cos[\omega(t+1/2)]/\sqrt{N-r}$. Since $N$ is large, the optimal time to measure and complete the calculation is thus after $T = O(\sqrt{N/r})$ time steps, when $k(t)$ is maximal. This analysis relies on the fact that the initial amplitude distribution is *uniform*. However, in a variety of interesting cases it would be desirable to apply Grover's algorithm to a *non*-uniform initial distribution. Generically, this could arise in situations where the search is used as a subroutine in a larger quantum computation, and the input to the algorithm can thus not be controlled. Another example would be cases where the given initial distribution over the elements is intrinsically non-uniform.

In this paper we generalize Grover's algorithm to the case in which the initial amplitudes are either real or complex and follow *any arbitrary distribution*. The time evolution of the amplitudes is solved *exactly* for general initial conditions, and the efficiency of the algorithm is evaluated. It is found that for generic initial conditions, the search algorithm still requires $O(\sqrt{N/r})$ steps, with only a constant factor compared to the case of a uniform initial distribution [3].

The paper is organized as follows. In Sec. 2 we define the modified Grover algorithm and derive difference equations for the time evolution of the amplitudes in it. We solve these equations exactly in Sec. 3, and analyze the results in Sec. 4. A summary and conclusions are presented in Sec. 5.

## 2 The Recursion Equations

### 2.1 The Generalized Algorithm

Our modified algorithm is essentially Grover's original algorithm, but without the initialization step. It thus consists of the following stages:

1. Use any initial distribution of marked and unmarked states, e.g., the final state of any other quantum algorithm (do *not* initialize the system to the uniform distribution).
2. Repeat the following steps $T$ times [an expression for $T$ is given in Eq. (24)]:
   - **A.** Rotate the marked states by a phase of $\pi$ radians.
   - **B.** Rotate all states by $\pi$ radians around the average amplitude of *all* states. This is done by applying the "inversion about average" operator, represented by the following unitary matrix:

$$D_{i,j} = \begin{cases} \frac{2}{N} & \text{if } i \neq j \\ \frac{2}{N} - 1 & \text{if } i = j \end{cases}$$

3. Measure the resulting state.

### 2.2 The Dynamics

We will now analyze the time evolution of the amplitudes in the modified algorithm with a total of $N$ states. Let the marked amplitudes at time $t$ be denoted by $k_i(t)$, $i = 1, \ldots, r$ and the unmarked amplitudes by $l_i(t)$, $i = r+1, \ldots, N$, where the initial distribution at $t = 0$ is arbitrary. Without loss of generality we assume that the number of marked states satisfies $1 \leq r \leq N/2$. We denote the averages and variances of the amplitudes by:

$$\text{marked: } \bar{k}(t) = \frac{1}{r}\sum_{j=1}^{r} k_j(t) \qquad \sigma_k^2(t) = \frac{1}{r}\sum_{j=1}^{r} |k_j(t) - \bar{k}(t)|^2 \tag{1}$$

$$\text{unmarked: } \bar{l}(t) = \frac{1}{N-r}\sum_{j=r+1}^{N} l_j(t) \qquad \sigma_l^2(t) = \frac{1}{N-r}\sum_{j=r+1}^{N} |l_j(t) - \bar{l}(t)|^2 \tag{2}$$

The key observation is that the entire dynamics dictated by Grover's algorithm can be described in full by the time-dependence of the *averages*. (The variances are defined above for convenience, as they are used later in a different context – see Section 4.3.) Formally, let:

$$C(t) = -\frac{2}{N}\left[\sum_{j=1}^{r} k_j(t) - \sum_{j=r+1}^{N} l_j(t)\right] = \frac{2}{N}\left[(N-r)\bar{l}(t) - r\bar{k}(t)\right] . \tag{3}$$

$C(t)$ is thus the weighted average over the marked and unmarked states, with the minus sign accounting for the $\pi$ phase difference between them during the algorithm iterations. The following theorem then shows that all states evolve equally:

**Theorem 1.** *The time evolution of all amplitudes (of both marked and unmarked states) is independent of the state index, and satisfies:*

$$k_i(t+1) = C(t) + k_i(t) \qquad i = 1, \ldots, r \tag{4}$$

$$l_i(t+1) = C(t) - l_i(t) \qquad i = r+1, \ldots, N \tag{5}$$

*Proof.* – This follows directly from the algorithm. Consider any marked state $k_i(t)$; this state is flipped to $k_i'(t) = -k_i(t)$, so that the marked average becomes $\bar{k}'(t) = \frac{1}{r}\sum_{j=1}^{r} k_j'(t) = -\bar{k}(t)$. The unmarked states, on the other hand, do not flip, so that the total average after the flip is: $x(t) = \frac{1}{N}[r\,\bar{k}'(t) + (N-r)\,\bar{l}(t)] = C(t)/2$. "Inversion about average" is by definition: $k_i'(t) \to 2x(t) - k_i'(t)$ and

$l_i(t) \to 2x(t) - l_i(t)$. Therefore in total: $k_i(t) \to C(t) + k_i(t)$ and $l_i(t) \to C(t) - l_i(t)$. □

From this it follows by averaging that:

**Corollary 2.** *The average marked and unmarked amplitudes obey first order linear coupled difference equations:*

$$\bar{k}(t+1) = C(t) + \bar{k}(t) \tag{6}$$

$$\bar{l}(t+1) = C(t) - \bar{l}(t). \tag{7}$$

These equations can be solved for $\bar{k}(t)$ and $\bar{l}(t)$, and along with the initial distribution this yield the exact solution for the dynamics of all amplitudes by using Eqs. (4) and (5).

## 3 Solution of the Recursion Equations

The recursion formulae can be solved by a standard diagonalization method for arbitrary complex initial conditions. Let:

$$\mathbf{v}(t) = \left(\bar{k}(t), \bar{l}(t)\right),$$

and define:

$$a \equiv \frac{N-2r}{N}, \qquad b \equiv \frac{2(N-r)}{N}, \qquad c \equiv \frac{2r}{N}.$$

The recursion equations (6) and (7) can be written as:

$$\mathbf{v}(t+1) = \mathsf{A} \cdot \mathbf{v}(t), \qquad \mathsf{A} = \begin{pmatrix} a & b \\ -c & a \end{pmatrix}.$$

Diagonalization of $\mathsf{A}$ yields a solution for $\mathbf{v}(t)$, as follows. Let $\mathsf{S}$ be the diagonalizing matrix:

$$\mathsf{A}^D \equiv \mathsf{S}^{-1}\mathsf{A}\mathsf{S} = \begin{pmatrix} \lambda_- & 0 \\ 0 & \lambda_+ \end{pmatrix}, \qquad \lambda_\pm = \gamma\, e^{\pm i\omega}.$$

Then $\mathbf{w}(t) = \mathsf{S}^{-1} \cdot \mathbf{v}(t)$ satisfies:

$$\mathbf{w}(t+1) = \mathsf{A}^D \cdot \mathbf{w}(t),$$

with solution:

$$\mathbf{w}(t) = \left((\lambda_-)^t\, w_-(0), (\lambda_+)^t\, w_+(0)\right)$$

where $\mathbf{w}(0) = (w_-(0), w_+(0))$. This yields $\bar{k}(t)$ and $\bar{l}(t)$ from $\mathbf{v}(t) = \mathsf{S} \cdot \mathbf{w}(t)$. Diagonalizing $\mathsf{A}$ one finds:

$$\gamma = a^2 + bc = 1 \tag{8}$$

$$\cos\omega = a = 1 - 2\frac{r}{N}, \tag{9}$$

which is identical to the frequency found by Boyer et al. [11] The eigenvectors of $\mathsf{A}$ are the columns of $\mathsf{S}$:

$$\mathsf{S} = \begin{pmatrix} i\sqrt{\frac{N}{r}-1} & -i\sqrt{\frac{N}{r}-1} \\ 1 & 1 \end{pmatrix}, \quad \mathsf{S}^{-1} = \begin{pmatrix} -\frac{i}{2}\sqrt{\frac{r}{N-r}} & \frac{1}{2} \\ \frac{i}{2}\sqrt{\frac{r}{N-r}} & \frac{1}{2} \end{pmatrix}.$$

Using this:

$$\begin{pmatrix} w_-(0) \\ w_+(0) \end{pmatrix} = \mathbf{w}(0) = \mathsf{S}^{-1} \cdot \mathbf{v}(0) = \begin{pmatrix} -\frac{i}{2}\sqrt{\frac{r}{N-r}}\bar{k}(0) + \frac{1}{2}\bar{l}(0) \\ \frac{i}{2}\sqrt{\frac{r}{N-r}}\bar{k}(0) + \frac{1}{2}\bar{l}(0) \end{pmatrix},$$

so that:

$$\mathbf{v}(t) = \mathsf{S} \cdot \begin{pmatrix} \left(-\frac{i}{2}\sqrt{\frac{r}{N-r}}\bar{k}(0) + \frac{1}{2}\bar{l}(0)\right) e^{-i\omega t} \\ \left(\frac{i}{2}\sqrt{\frac{r}{N-r}}\bar{k}(0) + \frac{1}{2}\bar{l}(0)\right) e^{i\omega t} \end{pmatrix}.$$

This yields finally, after some straightforward algebra:

$$\bar{k}(t) = \bar{k}(0)\cos\omega t + \bar{l}(0)\sqrt{\frac{N-r}{r}}\,\sin\omega t \tag{10}$$

$$\bar{l}(t) = \bar{l}(0)\cos\omega t - \bar{k}(0)\sqrt{\frac{r}{N-r}}\sin\omega t. \tag{11}$$

Together with Eqs. (4) and (5) this provides the complete exact solution to the dynamics of the amplitudes in the generalized Grover algorithm, for arbitrary initial conditions.

## 4 Analysis

Next we derive several properties of the amplitudes.

### 4.1 Phase Difference

The averaged amplitudes can be expressed concisely as follows (even when $\bar{k}(0)$ and $\bar{l}(0)$ are complex):

$$\bar{k}(t) = \alpha\sin(\omega t + \phi) \tag{12}$$

$$\bar{l}(t) = \beta\cos(\omega t + \phi) \tag{13}$$

where

$$\tan\phi = \frac{\bar{k}(0)}{\bar{l}(0)}\sqrt{\frac{r}{N-r}}\,; \qquad \alpha^2 = \bar{k}(0)^2 + \bar{l}(0)^2\frac{N-r}{r}\,;$$

$$\beta^2 = \bar{l}(0)^2 + \bar{k}(0)^2\frac{r}{N-r} \tag{14}$$

which shows that there is a $\pi/2$ phase difference between the marked and unmarked amplitudes: when the average marked amplitude is maximal, the average unmarked amplitude is minimal, and *vice versa*.

### 4.2 Constant Variance

Subtracting Eq. (4) from Eq. (6), and subtracting Eq. (5) from Eq. (7), one finds:

$$k_i(t+1) - \bar{k}(t+1) = k_i(t) - \bar{k}(t) \tag{15}$$
$$l_i(t+1) - \bar{l}(t+1) = -[l_i(t) - \bar{l}(t)]. \tag{16}$$

This means that:

$$\Delta k_i \equiv k_i(t) - \bar{k}(t) \quad \text{and} \quad \Delta l_i \equiv (-1)^t [l_i(t) - \bar{l}(t)], \tag{17}$$

are *constants of motion* (time-independent). It follows immediately from the definition that the variances $\sigma_k^2$ and $\sigma_l^2$ (cf. Eqs. (eq:marked) and (eq:unmarked)) too, are both time-independent.

This allows us to simplify the expression for the time dependence of the amplitudes:

$$k_i(t) = \bar{k}(t) + \Delta k_i \tag{18}$$
$$l_i(t) = \bar{l}(t) + (-1)^t \Delta l_i, \tag{19}$$

where $\Delta k_i$ and $\Delta l_i$ are evaluated at $t = 0$.

### 4.3 Maximal Probability of Success and Optimal Number of Iterations

The probability that a marked state will be obtained in the measurement at time $t$ at the end of the process is $P(t) = \sum_{j=1}^{r} |k_j(t)|^2$. A bound on this quantity can be derived as follows. Since all the operators used are unitary, the amplitudes satisfy the normalization condition:

$$\sum_{i=1}^{r} |k_i(t)|^2 + \sum_{i=r+1}^{N} |l_i(t)|^2 = 1 \tag{20}$$

at all times. Using $\overline{(y - \bar{y})^2} = \overline{y^2} - \bar{y}^2$ ($y$ is a random variable), we find from Eq. (2):

$$\sum_{i=r+1}^{N} |l_i(t)|^2 = (N-r)\sigma_l^2 + |\sum_{i=r+1}^{N} l_i(t)|^2/(N-r).$$

Let:

$$P_{\max} = 1 - (N-r)\sigma_l^2, \tag{21}$$

a time-*independent* quantity. Note that in the case of uniform initial distribution of amplitudes $\sigma_l^2 = 0$ and $P_{\max} = 1$. Now, $P(t) = P_{\max} - (N-r)|\bar{l}(t)|^2$, so that:

$$P(t) \leq P_{\max} \tag{22}$$

is the required bound. Using the exact solution, we can show that the $P_{\max}$ bound is in fact tight. For, from Eq. (13) it follows that $\bar{l}(T) = 0$ when:

$$\omega T + \phi = (j + 1/2)\pi\,, \quad j = 0, 1, 2, ... \tag{23}$$

At these times the bound is reached so that times $T$ satisfying Eq. (23) are optimal for measurement. Note that this conclusion holds only if $\bar{k}(0)/\bar{l}(0)$ is *real*. When $\bar{k}(0)/\bar{l}(0)$ is complex, the bound is generally not reached since $\bar{l}(t)$ may never vanish. Collecting our results:

**Theorem 3.** *Given arbitrary initial distributions of $r$ marked and $N-r$ unmarked states, with known averages $\bar{k}(0)$ and $\bar{l}(0)$ respectively, $\bar{k}(0)/\bar{l}(0)$ real, the optimal measurement times are after:*

$$T = \frac{(j + 1/2)\pi - \arctan\left[\frac{\bar{k}(0)}{\bar{l}(0)}\sqrt{\frac{r}{N-r}}\right]}{\arccos\left(1 - 2\frac{r}{N}\right)}\,, \quad j = 0, 1, 2, ... \tag{24}$$

*steps, when the probability of obtaining a marked state is $P_{\max}$ as given by Eq. (21).*

An important conclusion is that to determine the optimal measurement times, all one needs to know are the average initial amplitudes and the number of marked states. The more difficult case when these are unavailable will be considered in a separate publication [12]. The expansion of Eq. (24) in $r/N \ll 1$ (at $j = 0$) yields:

$$T = -\frac{1}{2}\frac{\bar{k}(0)}{\bar{l}(0)} + \frac{\pi}{4}\sqrt{N/r} - \frac{\pi}{24}\sqrt{r/N} + O(r/N), \tag{25}$$

confirming that Grover's algorithm converges in $O(\sqrt{N/r})$ steps for arbitrary distributions. The advantage of an initial amplitude distribution with a relatively high average of the marked states is manifested in the constant offset $-\frac{1}{2}\frac{\bar{k}(0)}{\bar{l}(0)}$, which may significantly reduce the required number of steps.

## 5 Summary and Conclusions

In this work we generalized Grover's quantum search algorithm to apply for initial input distributions which are non-uniform. In fact, it was shown that by simply omitting the first step of Grover's original algorithm, wherein a uniform superposition is created over all elements in the database, a more general algorithm results which applies to *arbitrary* initial distributions. To analyze the algorithm, we found that the time evolution of the amplitudes of the marked and unmarked states can be described by first-order linear difference equations with some special properties. The most important of these is that all amplitudes

essentially evolve uniformly, with the dynamics being determined completely by the average amplitudes. This observation allowed us to find an exact solution for the time-evolution of the amplitudes. An important conclusion from this solution is that generically the generalized algorithm also has a $O(\sqrt{N/r})$ running time, thus being more powerful than any classical algorithm designed to solve the same task.

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