arXiv:2509.20610v2 [quant-ph] 21 Jan 2026

Optimal phase change for a generalized Grover's algorithm

Christopher Cardullo[1] and Min Kang[1]

[1]Department of Mathematics, North Carolina State University, 2108 SAS Hall, Raleigh, 27695, North Carolina, United States of America.

Contributing authors: cacardul@ncsu.com; mkang2@ncsu.edu;

Abstract

We study the generalized Grover's algorithm with an arbitrary amplitude vector to find the optimal phase change for maximizing the gain in probability for the target of each iteration. In the classic setting of Grover's algorithm with a real initial amplitude vector, we find that a phase change of π stays optimal until the probability of observing the target is quite close to 1. We provide a formula for identifying this cut-off point based on the size of the data set. When the amplitude is truly complex, we find that the optimal phase change depends non-trivially on the complexity of the amplitude vector. We provide an optimization formula to identify the required optimal phase change.

Keywords: quantum computing, generalized Grover's algorithm, optimization phase change

MSC Classification: 68Q12 , 81P68 , 68W01 , 68Q99 , 90C15

1 Introduction

Search algorithms are an important tool in mathematics, computer science, and other related areas, as they allow for a space to be searched for either one or multiple target elements that match a given criteria. Applications of this include optimization, root finding, or any problem where verification of a solution is easy but finding a solution is difficult. Two broad categories we can break search algorithms into are structured search algorithms, where we have some prior knowledge of the underlying data set, and unstructured search algorithms, where we do not. Unstructured search is of particular interest in the field of quantum computation because it shows a clear advantage

that quantum computers provide. Proved by Grover in 1996 [1], by exploiting quantum superposition and entanglement, the time required to perform an unstructured search can be brought down from $\mathcal{O}(N)$ to $\mathcal{O}(\sqrt{N})$ for a database of size N. Grover's algorithm is an example of an amplitude amplification method, and it has been shown to have the optimal complexity level a quantum unstructured search can achieve, that of $\mathcal{O}(\sqrt{N})$[2].

There are other major methods adjacent to unstructured search in quantum computation that arise from different settings, such as quantum walk search and the collision detection method. Similar to the use of random walks in classical computing, quantum random walks can be used for searching unstructured spatial data in quantum computing. A good use of this is in simulating controlled dynamics in quantum systems. Collision detection algorithms are named for their use in collision identification problems where we seek to identify the inputs that map to the same output for a non-injective function. One of the most well-known of this approach is the Brassard-Høyer-Tapp algorithm [3]. Grover's algorithm and these other unstructured search algorithms altogether leverage entanglement and superposition to achieve the speedups we see over classical algorithms.

In this paper, we focus on Grover's algorithm and its generalizations. These approaches are all types of amplitude amplification algorithms, which take an initial amplitude vector and increase the amplitude for a target state in certain ways. Since in a quantum computing setting, the probability of observing a given state is the modulus squared of its amplitude, this process will increase the probability of observing the target state. Grover's algorithm does this by utilizing Householder reflections to increase the amplitude of a target element iteratively. The system is initialized using the Hadamard gate to induce a uniform distribution on the data set to begin with. This choice is natural, considering that we do not know the underlying distribution of the data.

Grover's algorithm is the subject of much research from various points of view. Some research has focused on implementation by using distributed quantum computing [4], others have focused on limiting what the user has control over while still implementing the algorithm [5], and some have researched using partial oracles to speed up the algorithm [6]. There has also been continued interest in understanding the mathematics of Grover's algorithm. This sort of research includes comparisons of different generalizations of Grover's algorithm [7], and how the algorithm behaves when searching a database that contains multiple targets [8][9]. Another area of interest has been research into phase matching, and its implications on a multiple target search [10][11][12].

We will discuss the details of our research shortly, but to first touch upon areas adjacent to the work we did, we need to mention the studies of arbitrary initial amplitudes, and phase changes that differ from π. Both of these have been studied for different purposes. Arbitrary initial amplitudes, both pure and mixed states, have been studied to show the robustness of Grover's algorithm [13][14]. Research into phase changes that are different from π have been done to understand their effects on amplitude amplification [15] and to improve the performance of Grover's algorithm when the size of the database is small and accuracy becomes more important [16]. Other

research has also been done that considers both non-uniform initial amplitudes and phase changes that differ from π to analyze Grover's algorithm and its generalizations [9]. However, as far as we know, there have not been any results in the direction of optimizing the phase change at each iteration to maximize the probability of the target state.

Speaking to our research, we are interested in optimizing the phase change chosen at every step of the iteration based on the current amplitude vector. What we have done is to calculate the amplitude vector after any given iteration as a function of the size of the database, the previous amplitude, and the phase change chosen. This is proved in Theorem 1. We then optimize this function over the phase change using this single lever of control we have to maximize the probability of observing the target, presented in Corollary 1. We find that in the case of an initial state induced by the Hadamard gate, regular Grover's algorithm is the optimal choice for a sufficiently large database until the probability of observing the target gets close to 1. The specific region where the optimal phase change strays away from π is identified as $\mathbf{R}_2$ in Theorem 2. If the initial state is induced differently though, and the initial amplitude is complex, then the optimal phase change depends on the complexity of that initial amplitude, and it is non-trivially different from π. This relationship is shown in Figure 1, and the optimization formula is found in (8).

Having identified $\mathbf{R}_2$, we further investigate when this region is reached for Hadamard initialized states in Corollary 2. This study was motivated by the unexpected observation that the optimal phase change remained π for longer than anticipated. We therefore determine the exact threshold at which the optimal phase change drifts away from π, resolving this completely in section 4.

Lastly, we want to provide a brief description on how the rest of the paper is structured, to help the readers. In section 2, we provide necessary preliminaries on Grover's algorithm, and Long's generalization. In section 3, we derive the optimization formula for the probability of our target state given an arbitrary amplitude vector, found in (8). We discuss the relationship we find here in figures 1 and 2. In section 4 we apply this approach to the regular Grover's algorithm setting with an initialization performed by the Hadamard gate. And in section 5, we discuss the conclusion and our further research interests and directions.

2 Preliminaries

Consider the space $\mathbf{S}$ with $|\mathbf{S}| = 2^n = N$ which contains all elements we are searching over. We will assign each element in $\mathbf{S}$ a unique number between 0 and $N-1$ (ordering does not matter). Let $\tau \in \mathbf{S}$ be the target element we are searching for. Consider the standard basis for $\mathbb{C}^2$, renamed as $\mathbf{e}_1 = |0\rangle$ and $\mathbf{e}_2 = |1\rangle$. $|\cdot\rangle$ and $\langle\cdot|$ are called the Dirac Bra-Ket notation, with $|\cdot\rangle$ being a column vector and $\langle\cdot|$ being a row vector intuitively. We also can use the Dirac Bra-Ket notation in discussion of binary representation. Take for example $|5\rangle_3$, with the subscript 3 standing for the number of binary places we are working with. So we have that $|5\rangle_3 = |101\rangle_3 = |1\rangle \otimes |0\rangle \otimes |1\rangle = [0\ 0\ 0\ 0\ 1\ 0\ 0]^\top$.

Consider the space $\mathbb{C}^{2\otimes n}$. Its basis will be $\{|x\rangle_n\}$ with $x \in \{0, 1, \ldots, N-1\}$ and written in binary format. We will consider the subspace $\mathbf{E}_n \subset \mathbb{C}^{2\otimes n}$ s.t.

$\sum_{0\leq x<N} a_x \left|x\right\rangle_n = \mathbf{a} \in \mathbf{E}_n$ if $\sum_{0\leq x<N} |a_x|^2 = 1$. In the context of quantum mechanics, our n-qubits are in $\mathbf{E}_n$, and we define a_x to be the amplitude associated with $\left|x\right\rangle_n$ and $|a_x|^2$ is the probability that upon observation, our n-qubit will collapse to $\left|x\right\rangle_n$. Consider $\mathbf{a} \in \mathbf{E}_2$. Then $\mathbf{a} = a_0 \left|00\right\rangle_2 + a_1 \left|01\right\rangle_2 + a_2 \left|10\right\rangle_2 + a_3 \left|11\right\rangle_2 = [a_0 \ a_1 \ a_2 \ a_3]^\top$. Thus we can translate an element from $\mathbf{E}_n \subset \mathbb{C}^{2\otimes n}$ to one in $\mathbb{C}^{2n}$.

The last crucial aspect of quantum computing we need to cover are gates and how we do operations on states. Firstly, we have that all gates can be represented as matrices that act on states, which as we showed just before, can be represented as column vectors in $\mathbb{C}^{2n}$. Next, there can be no information loss in the system, meaning that all gates must be reversible, and hence the matrices must be Hermitian.

Now we will have a more in-depth discussion of Grover's algorithm, and a generalized Grover's algorithm proposed by Long. Grover's algorithm is comprised of the following steps [1],

1. Use the Hadamard gate to equalize the amplitude for all qubits
2. Rotate the amplitude of the target element $\left|\tau\right\rangle$ by π radians. This process is represented by the operator $I^{\pi}_{\left|\tau\right\rangle}$. We do this using the U_f operator.
3. Apply the product of operators $FI^{\pi}_{\left|0\right\rangle}F$. F is the Fourier transform matrix, and is defined as $2^{-n/2}(-1)^{\bar{i}\cdot\bar{j}}$ with n being the number of qubits in the system, $\bar{i}\cdot\bar{j}$ being the binary dot product of i and j, and our index starting at 0. We refer to this product of operators as the operator W.

Steps 2 and 3 are repeated until $P(\left|\tau\right\rangle)$ is sufficiently large. We call this the Grover iterate, and write it as $G \equiv WU_f \otimes I_2$. It can be shown that the optimal number of iterations with the classical Grover's algorithm is $\frac{\pi}{4}\sqrt{N}$. Note, that if we were to do more than this, the probability for the target would in fact start to decrease, so it is important that we know the optimal number of times the Grover iterate is applied. In fact, Grover also showed that this search can be used with any unitary gate [17].

Building off of this work, Long generalized this by allowing for a phase change that is not strictly π [16]. His motivation for this was from the case that the database is relatively small, hence accuracy becomes most important, a phase change of π is not optimal. The way he implemented these arbitrary phase rotations is by using the following operator which generalizes classical Grover's algorithm with arbitrary phase ϕ.

$$I^{\phi}_{\left|\tau\right\rangle} = I + (e^{i\phi} - 1)\left|\tau\right\rangle\left\langle\tau\right|$$

We can see here that if $\phi = \pi$, then we get a so-called Householder reflection, which is the exact reflections used in the classical Grover's algorithm. To simplify the computation further, we reduce the iteration into 2-dimensional linear maps by adopting the approach used by Long. We condense the non-target elements into a single basis vector $\left|a\right\rangle$, observing that they all go through the same change in amplitude in each iteration. Note that it is properly normalized so that the existing computations get simpler. This new basis vector $\left|a\right\rangle$ is defined as

$$\left|a\right\rangle = \frac{1}{\sqrt{N-1}} \sum_{i\neq\tau} \left|i\right\rangle$$

This condenses our amplitude vector into a vector of $\mathbb{C}^2$, and lets us calculate the amplitudes after one iteration using the following linear map,

$$\begin{bmatrix} -e^{i\phi}(1+(e^{i\phi}-1)\sin^2\beta) & -(e^{i\phi}-1)\sin\beta\cos\beta \\ -e^{i\phi}(e^{i\phi}-1)\sin\beta\cos\beta & -e^{i\phi}+(e^{i\phi}-1)\sin^2\beta \end{bmatrix} \begin{bmatrix} Amp_{|\tau\rangle} \\ Amp_{|a\rangle} \end{bmatrix} \tag{1}$$

where ϕ is the phase rotation, and $Amp_{|\tau\rangle}$ and $Amp_{|a\rangle}$ are the amplitudes for the target element $|\tau\rangle$ and the other element $|a\rangle$ made of the non-target elements properly normalized. For further simplification in future computations, we introduce β defined as

$$\sin\beta = \frac{1}{\sqrt{N}} \qquad \cos\beta = \sqrt{\frac{N-1}{N}} \tag{2}$$

From (1), note that if the initial amplitude is known, then the amplitude and probability of observation can be calculated at any step of the iteration mathematically, which allows further optimization through classical computing.

3 Optimizing the probability of a generic step

Before fully investigating optimal phase change for generalized Grover's algorithm, let us go over optimizing phase change for the very first step when starting from the Hadamard gate. In this simple computation, we can easily identify the classical Grover's phase change arising as optimal in the first iteration. This straightforward derivation serves as motivation and a preindication of the broader task addressed in this section.

Recall the generalized Grover's updating linear map given in (1) as well as the corresponding initial vector $\mathbf{v}_0^H$ given as $\mathbf{v}_0^H = [\sin\beta\cos\beta]^\top = [\frac{1}{\sqrt{N}}\ \sqrt{\frac{N-1}{N}}]^\top$ (see (2)) from the Hadamard gate.

From (1) and (2), we acquire the probability of the target $|\tau\rangle$ as

$$P(|\tau\rangle) = |e^{i\phi}((1-e^{i\phi})\sin^2\beta - 1)\sin\beta - (e^{i\phi}-1)\cos^2\beta\sin\beta|^2$$

which simplifies to

$$P(|\tau\rangle) = \sin^2\beta|((1-e^{i\phi})\sin^2\beta - 1) + (e^{-i\phi}-1)\cos^2\beta|^2$$

.

Letting η denote the quantity inside the norm, we compute its real and imaginary parts

$$\begin{aligned} Re(\eta) &= \sin^2\beta(1-\cos\phi) - 1 + \cos^2\beta(\cos\phi - 1) \\ &= \cos(2\beta)\cos\phi - \cos(2\beta) - 1 \\ Im(\eta) &= -(\sin^2\beta + \cos^2\beta)\sin\phi = -\sin\phi \end{aligned}$$

Thus, the target probability becomes

$$P(|\tau\rangle) = \sin^2\beta((\cos(2\beta)\cos\phi - \cos(2\beta) - 1)^2 + \sin^2\phi)$$

Recalling that $\sin\beta = \frac{1}{\sqrt{N}}$ and $\cos\beta = \sqrt{\frac{N-1}{N}}$, we let $a = \cos(2\beta) = 1 - \frac{2}{N} \in (0,1)$ and rewrite $P(|\tau\rangle)$ accordingly.

$$P(|\tau\rangle) = \frac{1-a}{2}((a\cos\phi - a - 1)^2 + 1 - \cos^2\phi)$$

Since the dependence on ϕ is only through $\cos\phi$, by letting $u = \cos\phi \in [-1,1]$, we get the probability $P(|\tau\rangle)$ as a function of u on $[-1,1]$.

$$\begin{aligned} P(|\tau\rangle) &= \frac{1-a}{2}((a^2-1)u^2 - 2a(a+1)u + (a+1)^2 + 1) \\ &= -\frac{(a-1)^2(a+1)}{2}\left(u^2 - 2\frac{a}{a-1}u + \frac{(a+1)^2+1}{a^2-1}\right) \end{aligned}$$

This quadratic polynomial in u is maximized when $u = \frac{a}{a-1} = 1 - \frac{N}{2}$. Since maximization is done on the interval $[-1,1]$, if $N \geq 4$, which ensures $\frac{a}{a-1} = 1 - \frac{N}{2} \leq -1$, then the maximum is achieved when $u = -1$, in other words, $\phi = \pi$. This proves that in the generalized Grover's algorithm initialized with the Hadamard gate, the optimal phase change in the very first iteration is π, which is the phase used in the classical Grover's algorithm.

However, after each iteration, the amplitude vector evolves, meaning subsequent phase changes must be optimized for arbitrary complex input vectors. We now turn to this general case.

To calculate the optimal angle for the probability of our target at any step, we first need to derive a formula for the probability. Let us start with describing the amplitude of a generic state, and for this, we will be using the setup made in section 2. We remind the reader that the amplitudes satisfy the following:

1. The amplitudes are complex,
2. The sum of their modulus squared is equal to 1, i.e. $|Amp_{|\tau\rangle}|^2 + |Amp_{|a\rangle}|^2 = 1$.

Therefore, we know there exists an α and θ_1, θ_2 in $\mathbb{R}$ such that $Amp_{|\tau\rangle} = \sin(\alpha)e^{i\theta_1}$ and $Amp_{|a\rangle} = \cos(\alpha)e^{i\theta_2}$. Using this as our amplitude vector, we get

$$\begin{bmatrix} \sin\alpha\ e^{i\theta_1} \\ \cos\alpha\ e^{i\theta_2} \end{bmatrix} = e^{i\theta_2}\begin{bmatrix} \sin\alpha\ e^{i(\theta_1-\theta_2)} \\ \cos\alpha \end{bmatrix}$$

Then because the shared phase changes on both vectors do not impact the probability, we will drop $e^{i\theta_2}$, leaving us with our generic amplitude vector of the following form,

$$\mathbf{v}_m = \begin{bmatrix} \sin(\alpha)e^{i\theta} \\ \cos(\alpha) \end{bmatrix} \tag{3}$$

where $\theta = \theta_1 - \theta_2$ and $\alpha \in [0, \frac{\pi}{2}]$. From (1) note that the generalized Grover's iteration matrix is as follows:

$$\mathbf{A}^\phi = \begin{bmatrix} -e^{i\phi}(1 + (e^{i\phi}-1)\sin^2\beta) & -(e^{i\phi}-1)\sin\beta\cos\beta \\ -e^{i\phi}(e^{i\phi}-1)\sin\beta\cos\beta & -e^{i\phi} + (e^{i\phi}-1)\sin^2\beta \end{bmatrix}$$

$$= \begin{bmatrix} e^{i\phi}\left(\frac{1-e^{i\phi}}{N} - 1\right) & \frac{\sqrt{N-1}}{N}(1-e^{i\phi}) \\ \frac{\sqrt{N-1}}{N}e^{i\phi}(1-e^{i\phi}) & -\left(\frac{1}{N} + \left(1-\frac{1}{N}\right)e^{i\phi}\right) \end{bmatrix} \tag{4}$$

Theorem 1 *Suppose we carry out the generalized Grover's iteration defined in (4) with the general initial vector given by* $\mathbf{v}_m^\top = [\sin(\alpha)e^{i\theta},\ \cos(\alpha)]^\top$ *from (3), then* $P(|\tau\rangle)$*, the probability of the target vector* $|\tau\rangle$*, is given by the following function of* ϕ*,* α*, and* N*,*

$$P(|\tau\rangle) = \frac{2\sqrt{N-1}}{N}\left[\left(\frac{\sqrt{N-1}}{N}\cos(2\alpha) + \frac{1}{N}\sin(2\alpha)\cos(\phi+\theta)\right)(1-\cos\phi) - \right.$$
$$\left. - \frac{1}{2}\sin(2\alpha)\cos(\phi+\theta)\right] + \frac{\sqrt{N-1}}{N}\sin(2\alpha)\cos(\theta) + \sin^2\alpha$$

Proof To calculate the updated probability for our target element after one iteration, we find the first element of $\mathbf{A}^\phi\mathbf{v}_m$ and square the modulus, which is

$$P(|\tau\rangle) = \left|\sin\alpha\ e^{i\theta}e^{i\phi}\left(\frac{1-e^{i\phi}}{N} - 1\right) + \cos\alpha\frac{\sqrt{N-1}}{N}(1-e^{i\phi})\right|^2$$
$$= \left|\sin\alpha\ e^{i\theta}(\sin^2\beta(1-e^{i\phi}) - 1) + \cos\alpha\cos\beta\sin\beta(e^{-i\phi}-1)\right|^2$$

With further algebraic simplification, this reduces to

$$P(|\tau\rangle) = \frac{1}{4}\Big|-\sin\alpha(\cos(2\beta)+1)e^{i\theta} - \cos\alpha\sin(2\beta) + e^{i(\theta+\phi)}(\cos(2\beta)-1)\sin\alpha + \tag{5}$$
$$+ e^{-i\phi}\cos\alpha\sin(2\beta)\Big|^2$$

To organize the modulus calculation, we denote

$$\dagger = -\sin\alpha(\cos(2\beta)+1)e^{i\theta} - \cos\alpha\sin(2\beta) + e^{i(\theta+\phi)}(\cos(2\beta)-1)\sin\alpha +$$
$$+ e^{-i\phi}\cos\alpha\sin(2\beta)$$

$$Re(\dagger) = -\Big[\sin\alpha\Big\{(\cos\theta+\cos(\phi+\theta))+\cos(2\beta)(\cos\theta-\cos(\phi+\theta))\Big\}+\cos\alpha\Big\{\sin(2\beta)(1-\cos\phi)\Big\}\Big]$$

$$Im(\dagger) = -\Big[\sin\alpha\Big\{(\sin\theta+\sin(\phi+\theta))+\cos(2\beta)(\sin\theta-\sin(\phi+\theta))\Big\}+\cos\alpha\Big\{\sin(2\beta)\sin\phi\Big\}\Big]$$

Calculating the modulus squared of †, we get

$$|\dagger|^2 = \sin^2\alpha\left[(2\cos(\theta+\frac{\phi}{2})\cos(\frac{\phi}{2}) + 2\cos(2\beta)\sin(\theta+\frac{\phi}{2})\sin(\frac{\phi}{2})\right]^2 + \cos^2\alpha\sin^2(2\beta)(1-\cos\phi)^2 +$$
$$+ 2\sin\alpha\cos\alpha\left[(2\cos(\theta+\frac{\phi}{2})\cos(\frac{\phi}{2}) + 2\cos(2\beta)\sin(\theta+\frac{\phi}{2})\sin(\frac{\phi}{2})\right]\sin(2\beta)(1-\cos\phi) +$$
$$+ \sin^2\alpha\left[(2\sin(\theta+\frac{\phi}{2})\sin(\frac{\phi}{2}) - 2\cos(2\beta)\cos(\theta+\frac{\phi}{2})\sin(\frac{\phi}{2})\right]^2 + \cos^2\alpha\sin^2(2\beta)\sin^2\phi +$$
$$+ 2\sin\alpha\cos\alpha\left[(2\sin(\theta+\frac{\phi}{2})\sin(\frac{\phi}{2}) - 2\cos(2\beta)\cos(\theta+\frac{\phi}{2})\sin(\frac{\phi}{2})\right]\sin(2\beta)\sin\phi.$$

Grouping related terms together, we get

$$
\begin{aligned}
|\dagger|^2 = 4\sin^2\alpha\Bigg[&\Big((\cos(\theta+\tfrac{\phi}{2})\cos(\tfrac{\phi}{2})+\cos(2\beta)\sin(\theta+\tfrac{\phi}{2})\sin(\tfrac{\phi}{2})\Big)^2+\\
&+\Big((\sin(\theta+\tfrac{\phi}{2})\sin(\tfrac{\phi}{2})-\cos(2\beta)\cos(\theta+\tfrac{\phi}{2})\sin(\tfrac{\phi}{2})\Big)^2\Bigg]+\\
&+\cos^2\alpha\Big[\sin^2(2\beta)(2\sin^2\tfrac{\phi}{2})^2+\sin^2(2\beta)(2\sin(\tfrac{\phi}{2})\cos(\tfrac{\phi}{2}))^2\Big]+\\
&+4\sin\alpha\cos\alpha\Bigg\{\Big[(\cos(\theta+\tfrac{\phi}{2})\cos(\tfrac{\phi}{2})+\cos(2\beta)\sin(\theta+\tfrac{\phi}{2})\sin(\tfrac{\phi}{2})\Big]\sin(2\beta)(1-\cos\phi)+\\
&+\Big[(\sin(\theta+\tfrac{\phi}{2})\sin(\tfrac{\phi}{2})-\cos(2\beta)\cos(\theta+\tfrac{\phi}{2})\sin(\tfrac{\phi}{2})\Big]\sin(2\beta)\sin\phi\Bigg\}
\end{aligned}
$$

If we use some trigonometric identities to express this in terms of $\frac{\phi}{2}$,

$$
\begin{aligned}
|\dagger|^2 = 4\sin^2\alpha\Bigg[&\Big((\cos(\theta+\tfrac{\phi}{2})\cos(\tfrac{\phi}{2})+\cos(2\beta)\sin(\theta+\tfrac{\phi}{2})\sin(\tfrac{\phi}{2})\Big)^2+\\
&+\Big((\sin(\theta+\tfrac{\phi}{2})\sin(\tfrac{\phi}{2})-\cos(2\beta)\cos(\theta+\tfrac{\phi}{2})\sin(\tfrac{\phi}{2})\Big)^2\Bigg]+\\
&+4\cos^2\alpha\Big[\sin^2(2\beta)\sin^4\tfrac{\phi}{2}+\sin^2(2\beta)\sin^2\tfrac{\phi}{2}\cos^2\tfrac{\phi}{2}\Big]+\\
&+4\sin\alpha\cos\alpha\sin(2\beta)\Bigg\{\Big[(\cos(\theta+\tfrac{\phi}{2})\cos(\tfrac{\phi}{2})+\cos(2\beta)\sin(\theta+\tfrac{\phi}{2})\sin(\tfrac{\phi}{2})\Big](2\sin^2\tfrac{\phi}{2})+\\
&+\Big[(\sin(\theta+\tfrac{\phi}{2})\sin(\tfrac{\phi}{2})-\cos(2\beta)\cos(\theta+\tfrac{\phi}{2})\sin(\tfrac{\phi}{2})\Big]2\sin(\tfrac{\phi}{2})\cos(\tfrac{\phi}{2})\Bigg\}.
\end{aligned}
$$

Now we return to calculating the probability of our target $|\tau\rangle$.

$$P(|\tau\rangle) = \frac{1}{4}|\dagger|^2 = (\sin^2\alpha)\boldsymbol{a} + (\cos^2\alpha)\boldsymbol{b} + 2\sin\alpha\cos\alpha\Big(\sin(2\beta)\sin(\tfrac{\phi}{2})\Big)\boldsymbol{c}$$

, where the $\boldsymbol{a}$, $\boldsymbol{b}$, and $\boldsymbol{c}$ are defined as follows.

$$
\begin{aligned}
\boldsymbol{a} = &\Big\{\cos(\theta+\tfrac{\phi}{2})\cos(\tfrac{\phi}{2})+\cos(2\beta)\sin(\theta+\tfrac{\phi}{2})\sin(\tfrac{\phi}{2})\Big\}^2+\\
&+\Big\{\sin(\theta+\tfrac{\phi}{2})\cos(\tfrac{\phi}{2})-\cos(2\beta)\cos(\theta+\tfrac{\phi}{2})\sin(\tfrac{\phi}{2})\Big\}^2\\
\boldsymbol{b} = &\sin^2(2\beta)\sin^4(\tfrac{\phi}{2})+\sin^2(2\beta)\sin^2(\tfrac{\phi}{2})\cos^2(\tfrac{\phi}{2})
\end{aligned}
$$

$$
\begin{aligned}
\boldsymbol{c} = &\sin(\tfrac{\phi}{2})\Big(\cos(\theta+\tfrac{\phi}{2})\cos(\tfrac{\phi}{2})+\cos(2\beta)\sin(\theta+\tfrac{\phi}{2})\sin(\tfrac{\phi}{2})\Big)+\\
&+\cos(\tfrac{\phi}{2})\Big(\sin(\theta+\tfrac{\phi}{2})\cos(\tfrac{\phi}{2})-\cos(2\beta)\cos(\theta+\tfrac{\phi}{2})\sin(\tfrac{\phi}{2})\Big)
\end{aligned}
$$

Below we simplify these three terms ($\boldsymbol{a}$, $\boldsymbol{b}$, and $\boldsymbol{c}$) a little more.

$$
\begin{aligned}
\boldsymbol{a} = \; & \cos^2(\theta+\frac{\phi}{2})\cos^2\frac{\phi}{2} + \cos^2(2\beta)\sin^2(\theta+\frac{\phi}{2})\sin^2\frac{\phi}{2} + \\
& + \sin^2(\theta+\frac{\phi}{2})\cos^2\frac{\phi}{2} + \cos^2(2\beta)\cos^2(\theta+\frac{\phi}{2})\sin^2\frac{\phi}{2} + \\
& + 2\cos(\theta+\frac{\phi}{2})\cos(\frac{\phi}{2})\cos(2\beta)\sin(\theta+\frac{\phi}{2})\sin(\frac{\phi}{2}) - \\
& - 2\sin(\theta+\frac{\phi}{2})\cos(\frac{\phi}{2})\cos(2\beta)\cos(\theta+\frac{\phi}{2})\sin(\frac{\phi}{2}) \\
= \; & \cos^2\frac{\phi}{2} + \cos^2(2\beta)\sin^2\frac{\phi}{2} \\
= \; & \cos^2\frac{\phi}{2} + (1-\sin^2(2\beta))\sin^2\frac{\phi}{2} \\
= \; & 1 - \sin^2(2\beta)\sin^2(\frac{\phi}{2}) \\
\boldsymbol{b} = \; & \sin^2(2\beta)\sin^2(\frac{\phi}{2})
\end{aligned}
$$

$$
\begin{aligned}
\boldsymbol{c} &= \cos(\theta+\frac{\phi}{2})\sin(\frac{\phi}{2})\cos(\frac{\phi}{2})(1-\cos(2\beta)) + \sin(\theta+\frac{\phi}{2})(\cos(2\beta)\sin^2(\frac{\phi}{2}) + \cos^2(\frac{\phi}{2})) \\
&= \cos(\theta+\frac{\phi}{2})\sin(\frac{\phi}{2})\cos(\frac{\phi}{2})(1-\cos(2\beta)) + \sin(\theta+\frac{\phi}{2})(\sin^2(\frac{\phi}{2})\cos(2\beta) + (1-\sin^2(\frac{\phi}{2})) \\
&= \cos(\theta+\frac{\phi}{2})\sin(\frac{\phi}{2})\cos(\frac{\phi}{2})(1-\cos(2\beta)) + \sin(\theta+\frac{\phi}{2})(-\sin^2(\frac{\phi}{2})(1-\cos(2\beta)) + 1) \\
&= (1-\cos(2\beta))\sin(\frac{\phi}{2})\Big[\cos(\theta+\frac{\phi}{2})\cos(\frac{\phi}{2}) - \sin(\theta+\frac{\phi}{2})\sin(\frac{\phi}{2})\Big] + \sin(\theta+\frac{\phi}{2}) \\
&= \cos(\theta+\phi)\sin(\frac{\phi}{2})(1-\cos(2\beta)) + \sin(\theta+\frac{\phi}{2})
\end{aligned}
$$

Putting these all together, our target probability becomes

$$
\begin{aligned}
P(|\tau\rangle) = \; & \sin^2\alpha\Big[1-\sin^2(2\beta)\sin^2(\frac{\phi}{2})\Big] + \cos^2\alpha\sin^2(2\beta)\sin^2(\frac{\phi}{2}) + \\
& + 2\sin\alpha\cos\alpha\sin(2\beta)\sin(\frac{\phi}{2})\Big[\cos(\theta+\phi)\sin(\frac{\phi}{2})(1-\cos(2\beta)) + \sin(\theta+\frac{\phi}{2})\Big] \\
= \; & \sin^2\alpha + \sin^2(2\beta)\cos(2\alpha)\sin^2(\frac{\phi}{2}) + \sin(2\alpha)\sin(2\beta)\Big[2\cos(\phi+\theta)\sin^2(\frac{\phi}{2})\sin^2\beta + \\
& + \sin(\frac{\phi}{2}+\theta)\sin(\frac{\phi}{2})\Big]
\end{aligned}
$$

which reduces to

$$
\begin{aligned}
P(|\tau\rangle) = \; & \sin^2\alpha + \sin^2(2\beta)\cos(2\alpha)\left(\frac{1-\cos\phi}{2}\right) + \\
& + \sin(2\alpha)\sin(2\beta)\Big[\cos(\phi+\theta)(1-\cos\phi)\sin^2\beta - \frac{1}{2}\cos(\phi+\theta) + \frac{1}{2}\cos\theta\Big]
\end{aligned} \tag{6}
$$

We then use (2) to incorporate $\sin\beta = \frac{1}{\sqrt{N}}$ and $\sin(2\beta) = \frac{2\sqrt{N-1}}{N}$. Substituting these values into (6),

$$P(|\tau\rangle) = \frac{2\sqrt{N-1}}{N}\left[\left(\frac{\sqrt{N-1}}{N}\cos(2\alpha) + \sin(2\alpha)\frac{1}{N}\cos(\phi+\theta)\right)(1-\cos\phi) - \right.$$
$$\left. - \frac{1}{2}\sin(2\alpha)\cos(\phi+\theta)\right] + \frac{\sqrt{N-1}}{N}\sin(2\alpha)\cos(\theta) + \sin^2\alpha \tag{7}$$

This completes the proof. □

Now we can address our goal to find the optimal phase to maximize $P(|\tau\rangle)$, the probability of the target vector $|\tau\rangle$ in the following Corollary.

Corollary 1 For the one-step iteration of the generalized Grover's algorithm in equation (4) with the general initial vector $\mathbf{v}_m^\top = [\sin(\alpha)e^{i\theta},\ \cos(\alpha)]^\top$, the optimal phase change for the target probability $P(|\tau\rangle)$ is given as follows

$$argmax_{\phi\in[-\pi,\pi]}\left(\frac{\sqrt{N-1}}{N}\cos(2\alpha) + \frac{1}{N}\sin(2\alpha)\cos(\phi+\theta)\right)(1-\cos(\phi)) - \frac{1}{2}\sin(2\alpha)\cos(\phi+\theta). \tag{8}$$

This optimal phase change is identified in Figure 1.

Proof The statement of (8) can be seen directly by examination of equation (7). Recall that α and θ are from the amplitude vector $\mathbf{v}_m$ before update.

To visualize this computationally, we utilize the optimization and global optimization toolboxes of MATLAB. Because α and θ are values that come from the description of the original amplitude vector, we create a grid of 100 values of α and of θ ranging over $[0, \pi/2]$ and $[-\pi, \pi]$ respectively.

We use a Golden-section search (fminbnd) due to its speed when doing many examples. To account for the fact that this might give us local maximums, we utilized the global optimization toolbox to run interior-point methods for randomly selected starting points to find our global maximum, or at least provide a better optimization than the golden-section search. What we found is that the differences between these two searches were negligible as seen in Figure 1.

□

Remark 1 As can be seen in Figure 1, the optimal ϕ is in fact related to the value of θ found in (3), the amplitude vector. This relationship roughly is

$$\begin{cases} \phi \approx -\pi - \theta, & \theta < 0 \\ \phi \approx \pi - \theta, & \theta > 0 \end{cases} \tag{9}$$

This generalization does not hold when α is an extreme value, either being too close to 0 (corresponding to an amplitude close to 0 for our target), or too close to $\pi/2$ (corresponding to an amplitude close to 1 for our target). In these cases, the optimal ϕ cannot be estimated in the same way, and does require use of an optimization algorithm to find.

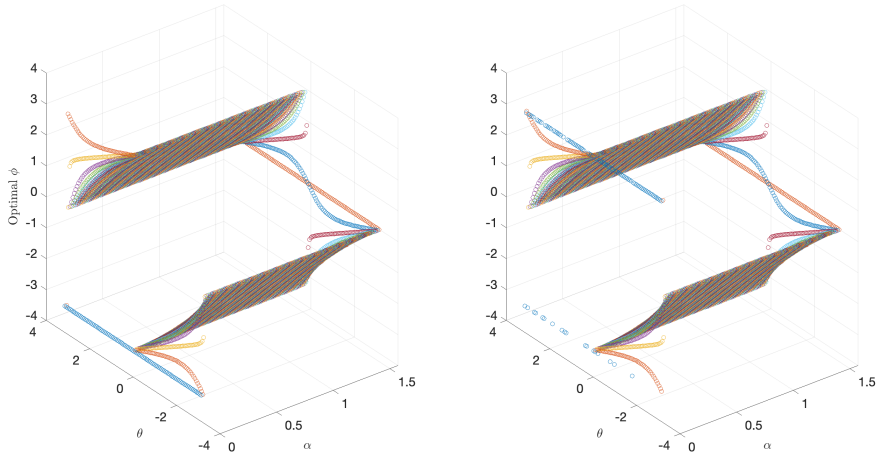


Fig. 1 Comparison of optimal phase change found by local search (left) and global search (right) for $N = 2^{10}$

It is important to note that the relationship described in (9) is a rough estimate. While it is a good approximate, the global search does differ, and the difference is shown in Figure 2 where we compare the optimal phase identified in Corollary 1 with

$$\phi = \begin{cases} -\pi - \theta, & \theta < 0 \\ \pi - \theta, & \theta > 0 \end{cases} \tag{10}$$

Remark 2 By using the optimal ϕ as the phase change rather than π, we find a range of improvement in the probability increase provided by one iteration. This improvement depends on the amplitude vector's α and θ values. This comparison results in Figure 3.

As can be seen in Figure 3, when θ is close to 0, there is little improvement over the probability attained by Grover's algorithm. However, as θ moves away from 0, the improvement provided by the optimized phase change increases, with the bigger improvements as θ gets closer to π. This agrees with the relationship seen in Figure 1 and also observed in (9), since they suggest an optimal phase change would be close to $\phi = 0$ when θ gets close to π, while Grover's algorithm would be using a phase change of $\phi = \pi$.

In the next section, we try to use this framework to understand the optimality of classical Grover's algorithm in much more precise terms, and determine when the optimal phase change strays away from π, the phase from classical Grover's algorithm.

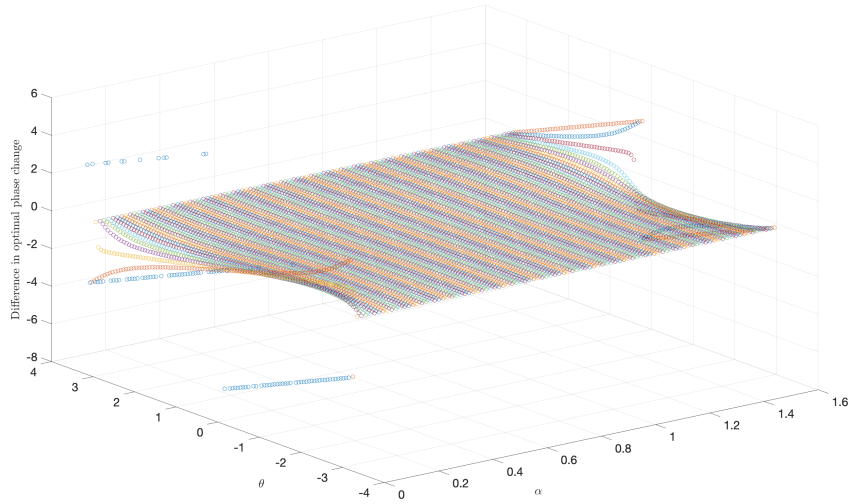


Fig. 2 Difference between phase change determined by (10) and optimal phase change found by global search for $N = 2^{10}$

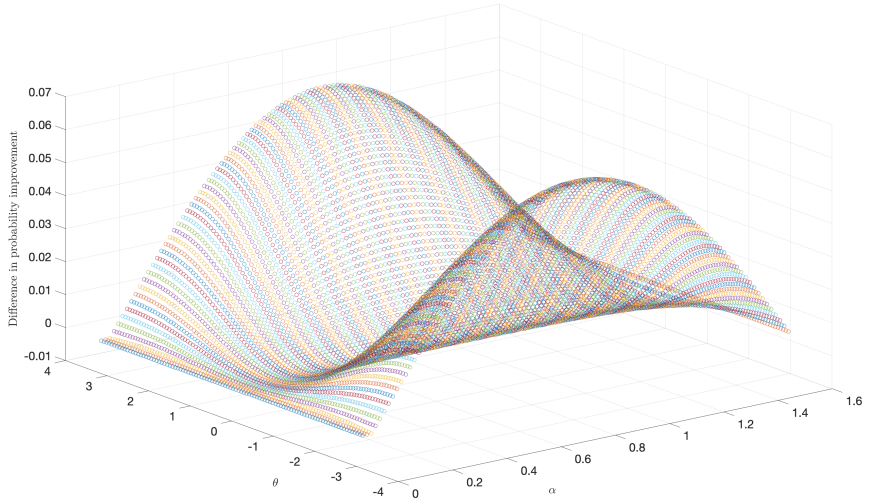


Fig. 3 Difference in probability improvement from one iteration between the optimal phase change, and π for $N = 2^{10}$

4 Optimizing when initializing with the Hadamard gate

Adopting the Hadamard gate at the beginning is part of the standard procedure when using Grover's algorithm since it initializes all states with the same amplitude, mimicking the lack of underlying structure in the database (or potentially, our lack of understanding information about it). This leaves us with an initial amplitude vector based on $|\tau\rangle$ and $|a\rangle$

$$\mathbf{v}_0 = \begin{bmatrix} \frac{1}{\sqrt{N}} \\ \sqrt{\frac{N-1}{N}} \end{bmatrix} = \mathbf{v}_0^H \tag{11}$$

As can be seen in (11), the vector is completely real, i.e. $\mathbf{v}_0 \in \mathbb{R}^2$, hence our $\theta = 0$, when compared to the general amplitude vector (3). Recall that $|v_1|^2 + |v_2|^2 = 1$ for $\mathbf{v} = [v_1 \ v_2]^\top$. Let us first consider a general but real amplitude vector. First of all, note the Hadamard gate, which is how most of the unstructured search algorithms begin in general, is real, and we want to first explore how and when the vector derails from real, while updated with the optimal phase change.

Theorem 2 *Consider a general but real initial vector* $\boldsymbol{v}^\top = [\sin(\alpha),\ \cos(\alpha)]^\top$ *to start the generalized Grover's iteration given in* (4)*. Then the optimal phase change for the target probability* $P(|\tau\rangle)$ *behaves differently depending on the region* α *belongs to of three different regions* $\{\boldsymbol{R}_i\}_{1\leq i\leq 3}$*. More precisely,*

$$argmax P(|\tau\rangle)_{\phi\in[-\pi,\pi]} = \begin{cases} \pi,\ \alpha \in \boldsymbol{R}_1 \\ \cos^{-1}(\frac{1}{4}(-N+2-2\sqrt{N-1}\cot(2\alpha)),\ \alpha \in \boldsymbol{R}_2 \\ 0,\ \alpha \in \boldsymbol{R}_3 \end{cases}$$

,

where

$$\begin{cases} \boldsymbol{R}_1 = \left(0, \frac{1}{2}\cot^{-1}\left(\frac{-N+6}{2\sqrt{N-1}}\right)\right] \\ \boldsymbol{R}_2 = \left(\frac{1}{2}\cot^{-1}\left(\frac{-N+6}{2\sqrt{N-1}}\right), \frac{1}{2}\cot^{-1}\left(\frac{-N-2}{2\sqrt{N-1}}\right)\right) \\ \boldsymbol{R}_3 = \left[\frac{1}{2}\cot^{-1}\left(\frac{-N-2}{2\sqrt{N-1}}\right), \frac{\pi}{2}\right) \end{cases}$$

Proof Consider a general but real initial vector

$$\mathbf{v} = \begin{bmatrix} \sin\alpha \\ \cos\alpha \end{bmatrix}.$$

We then apply Grover's iterate matrix (4) to this general but real amplitude vector. Then the updated amplitude vector is

$$\begin{bmatrix} e^{i\phi}\left(\frac{1-e^{i\phi}}{N} - 1\right)\sin\alpha + \frac{\sqrt{N-1}}{N}(1-e^{i\phi})\cos\alpha \\ \frac{\sqrt{N-1}}{N}e^{i\phi}(1-e^{i\phi})\sin\alpha - \frac{1}{N}(1+(N-1)e^{i\phi})\cos\alpha \end{bmatrix} \tag{12}$$

Now we look at the real and imaginary parts of each coordinate in (12). Note that the imaginary parts for both are multiplied by either $\sin\phi$ or $\sin(2\phi)$. Therefore, if $\phi = \pi$, as in the classical Grover's algorithm, the imaginary part becomes 0. This means that if the amplitude vector is real, and a Grover iterate matrix with a phase change of π (i.e. classical Grover's iterate) is applied to it, the resulting amplitude vector will remain real. Hence if the system is initialized with a Hadamard gate, giving us the real initial amplitude vector (11), the amplitude vector will remain real throughout all of the iterations.

With this in mind, we return to our amplitude vector after one iteration (12). We can calculate the resulting probability of observing our target

$$P(|\tau\rangle) = \left| e^{i\phi}\left(\frac{1-e^{i\phi}}{N} - 1\right)\sin\alpha + \frac{\sqrt{N-1}}{N}(1-e^{i\phi})\cos\alpha \right|^2$$

Substituting in our notation with β in (2) and factoring out $-e^{i\phi}$ from the amplitude, we get

$$P(|\tau\rangle) = \left|((e^{i\phi}-1)\sin^2\beta + 1)\sin\alpha + \sin\beta\cos\beta(1-e^{-i\phi})\cos\alpha\right|^2. \tag{13}$$

To calculate the probability, we break down the transformed amplitude as follows.

$$\begin{aligned} \xi &= ((e^{i\phi}-1)\sin^2\beta + 1)\sin\alpha + \sin\beta\cos\beta(1-e^{-i\phi})\cos\alpha \\ Re(\xi) &= A\cos\phi + B \\ Im(\xi) &= C\sin\phi \end{aligned}$$

, where

$$\begin{aligned} A &= \sin^2\beta\sin\alpha - \sin\beta\cos\beta\cos\alpha \\ B &= \sin\alpha\cos^2\beta + \cos\alpha\sin\beta\cos\beta \\ C &= \sin^2\beta\sin\alpha + \sin\beta\cos\beta\cos\alpha \end{aligned}$$

We can then rewrite the probability (13) as

$$P(|\tau\rangle) = (A^2 - C^2)\cos^2\phi + 2AB\cos\phi + B^2 + C^2$$

To simplify our notation, let us define a and b as follows.

$$\begin{aligned} a = C^2 - A^2 = {} & \sin^4\beta\sin^2\alpha + \sin^2\beta\cos^2\beta\cos^2\alpha + 2\sin^3\beta\sin\alpha\cos\alpha\cos\beta - \\ & - \sin^4\beta\sin^2\alpha - \sin^2\beta\cos^2\beta\cos^2\alpha + 2\sin^3\beta\sin\alpha\cos\alpha\cos\beta \\ = {} & 4\sin^2\beta(\sin\beta\cos\beta)(\sin\alpha\cos\alpha) \\ = {} & \sin^2\beta\sin(2\beta)\sin(2\alpha) \\ b = -2AB = {} & -2\sin\beta\cos\beta(\sin\beta\sin\alpha - \cos\beta\cos\alpha)(\sin\alpha\cos\beta + \cos\alpha\sin\beta) \\ = {} & \sin(2\beta)\cos(\alpha+\beta)\sin(\alpha+\beta) \\ = {} & \frac{1}{2}\sin(2\beta)\sin(2\alpha+2\beta) \end{aligned}$$

Note that $a \geq 0$ since $\alpha \in [0, \frac{\pi}{2}]$. Letting $u = \cos\phi$, $P(|\tau\rangle)$ becomes a quadratic polynomial in u which is concave down.

$$\begin{aligned} P(|\tau\rangle) &= -a\,u^2 - b\,u + B^2 + C^2 \\ &= -a\left(u + \frac{b}{2a}\right)^2 + \textit{constant} \end{aligned}$$

Note that if $|\frac{b}{2a}| \geq 1$, then the optimality for maximization is acquired at the boundary, that is when $u = -1$ or $u = 1$, meaning ϕ is π or 0. Hence, we now determine when we achieve the condition $|\frac{b}{2a}| < 1$ since this is when the optimal ϕ maximizing $P(|\tau\rangle)$ differs from π or 0. Recall that $\sin\beta = \frac{1}{\sqrt{N}}$, $\sin(2\beta) = \frac{2\sqrt{N-1}}{N}$, and see that $\cos(2\beta) = \frac{N-2}{N}$.

$$\frac{b}{2a} = \frac{\frac{1}{2}\sin(2\beta)\sin(2\alpha+2\beta)}{2\sin^2\beta\sin(2\beta)\sin(2\alpha)}$$

By utilizing the angle addition identity, this turns into

$$\begin{aligned}\frac{b}{2a} &= \frac{N}{4}\left(\frac{\sin(2\alpha)\cos(2\beta)+\cos(2\alpha)\sin(2\beta)}{\sin(2\alpha)}\right)\\ &= \frac{N}{4}(\cos(2\beta)+\cot(2\alpha)\sin(2\beta))\end{aligned}$$

.

Again recalling how β is defined, we can simplify $\frac{b}{2a}$ further as

$$\begin{aligned}&= \frac{N}{4}\left(\frac{N-2}{N}+\frac{2\sqrt{N-1}}{N}\cot(2\alpha)\right)\\ &= \frac{1}{4}(N-2+2\sqrt{N-1}\cot(2\alpha))\end{aligned}$$

Returning to the inequality $|\frac{b}{2a}| < 1$, the equivalent inequality becomes

$$-4 < N-2+2\sqrt{N-1}\cot(2\alpha) < 4$$

This is equivalent to the following condition for the angle α

$$\frac{1}{2}\cot^{-1}\left(\frac{-N+6}{2\sqrt{N-1}}\right) < \alpha < \frac{1}{2}\cot^{-1}\left(\frac{-N-2}{2\sqrt{N-1}}\right) \tag{14}$$

This leads us to consider the following three regions $\{\mathbf{R}_i\}_{i\leq 3}$ for α,

$$\begin{cases}\mathbf{R}_1 = \left(0, \frac{1}{2}\cot^{-1}\left(\frac{-N+6}{2\sqrt{N-1}}\right)\right]\\ \mathbf{R}_2 = \left(\frac{1}{2}\cot^{-1}\left(\frac{-N+6}{2\sqrt{N-1}}\right), \frac{1}{2}\cot^{-1}\left(\frac{-N-2}{2\sqrt{N-1}}\right)\right)\\ \mathbf{R}_3 = \left[\frac{1}{2}\cot^{-1}\left(\frac{-N-2}{2\sqrt{N-1}}\right), \frac{\pi}{2}\right)\end{cases} \tag{15}$$

Note that if $\alpha \in \mathbf{R}_1$, then $\cot(2\alpha) \geq \frac{-N+6}{2\sqrt{N-1}}$, hence $\frac{1}{4}(N-2+2\sqrt{N-1}\cot(2\alpha)) \geq 1$. This means $\frac{-b}{2a} \leq -1$, hence $P(|\tau\rangle)$ is maximized when $u = -1$, which corresponds to $\phi = \pi$. This implies that in the region $\mathbf{R}_1$, classical Grover's algorithm is optimal. But once $\alpha \in \mathbf{R}_2$, then $P(|\tau\rangle)$ is maximized by a non-trivial phase change $\phi_{max}(\alpha)$, and we will identify this $\phi_{max}(\alpha)$ $(= argmax\ P(|\tau\rangle))$ more precisely below (see (16)). Finally, when $\alpha \in \mathbf{R}_3$, then $\cot(2\alpha) \leq \frac{-N-2}{2\sqrt{N-1}}$, hence $\frac{1}{4}(N-2+2\sqrt{N-1}\cot(2\alpha)) \leq -1$. This means $\frac{-b}{2a} \geq 1$, hence $P(|\tau\rangle)$ is maximized when $u = 1$, which corresponds to $\phi = 0$. This means no rotation should occur once ϕ comes into this region.

Now let us identify the precise optimal phase change necessary in case $\alpha \in \mathbf{R}_2$. Recall that if $\alpha \in \mathbf{R}_2$, then $\phi_{max}(\alpha)$ is such that

$$\cos(\phi_{max}(\alpha)) = \frac{-b}{2a} = \frac{1}{4}(-N+2-2\sqrt{N-1}\cot(2\alpha)).$$

Since $\alpha \in [0, \frac{\pi}{2}]$,

$$\phi_{max}(\alpha) = \cos^{-1}(\frac{1}{4}(-N + 2 - 2\sqrt{N-1}\cot(2\alpha)) \tag{16}$$

□

Corollary 2 Suppose we begin the generalized Grover's iteration from the Hadamard vector $(\mathbf{v}_0^H)^\top = \left[\frac{1}{\sqrt{N}}, \sqrt{\frac{N-1}{N}}\right]^\top$, and continue to use the optimal phase change at each step to maximize the target probability $P(|\tau\rangle)$. Then the classical Grover's algorithm stays optimal until the target probability $P(|\tau\rangle)$ reaches the threshold $P_r(N) = \frac{1}{2}\left(1 + \frac{N-6}{\sqrt{N^2-8N+32}}\right)$.

Proof Recall that starting from a Hadamard initial condition, of which $\theta = 0$, the optimal phase change for generalized Grover's algorithm stays π (i.e. classical Grover's algorithm) until α reaches $\frac{1}{2}\cot^{-1}(\frac{-N+6}{2\sqrt{N-1}})$. In other words, the first non-trivial optimal phase differing from that of classical Grover's begins with $\alpha_0 \equiv \frac{1}{2}\cot^{-1}(\frac{-N+6}{2\sqrt{N-1}})$. Noting that the target probability is $\sin^2\alpha_0$, this shows that the optimal phase change stays with classical Grover's algorithm till the target probability reaches $P(|\tau\rangle) = \left[\sin(\frac{1}{2}\cot^{-1}(\frac{-N+6}{2\sqrt{N-1}}))\right]^2$. We then see that

$$P(|\tau\rangle) = \sin^2\left(\frac{1}{2}\cot^{-1}\left(\frac{-N+6}{2\sqrt{N-1}}\right)\right) = \frac{1}{2}\left(1 + \frac{N-6}{\sqrt{N^2-8N+32}}\right)$$

□

Remark 3 Note that the threshold $P_r(N) = \frac{1}{2}\left(1 + \frac{N-6}{\sqrt{N^2-8N+32}}\right)$ converges to 1 as $N \to \infty$. One can see that that $P_r(N)$ converges to 1 in the order of $1/N$. This shows that the classical Grover's algorithm stays optimal till $P(|\tau\rangle)$ gets close to 1 as N grows large.

5 Conclusion & Further Research

We have found that in the setting of generalized Grover's algorithm allowing a general phase change at each step of iteration, with a sufficiently large database, and an initialization set as the Hadamard gate, the optimal phase change stays π for the vast majority of the iterations. The optimal phase change differs from π as $P(|\tau\rangle)$ gets quite close to 1. We also identify this threshold when the optimal phase change strays away from π as a function of N, the size of the data space (16). However, if the initial amplitude vector is complex, and we know how to describe it, then the optimal phase change depends non-trivially on the complexity of the target state's amplitude and it can be found by solving the equation (8) at each iteration.

Moving forward there are a few areas of research we plan to investigate further. The first is identifying scenarios in which initializing with a non-Hadamard gate could become more beneficial for possible speed-up, and if those lead to amplitude vectors that are complex. If this occurs, then a generalized Grover's algorithm with a phase change that differs from π and that non-trivially depends on the complexity of the amplitude vector would outperform $\phi = \pi$ (The phase change used in the classical

Grover's iterate) as seen in Figure 3. A non-Hadamard initial gate would imply that there is some underlying knowledge of the data set that we can take advantage of so as to choose a specific class of probability distributions in the beginning, rather than a uniform one (as in Hadamard's gate).

The second is identifying if there is an improvement to be made if the algorithm is fully generalized in the sense that $\phi \neq \psi$ in $I^{\phi}_{|\tau\rangle}$ and $I^{\psi}_{|0\rangle}$. As mentioned previously, there has been much research in this area, but we wish to approach it from a similar perspective as this paper. We wish to see if there is any speedup or optimization to be made if considering the optimal phases at every step of the algorithm, as well as considering a fully generalized initial amplitude vector.

The third is better understanding of quantum random walks. Justified by numerous applications, classical random walks are an area of interest to us, and naturally we wish to understand their quantum counterparts, both as tools to search spatial data, and as stochastic objects in and of themselves. We look forward to pursue the above research directions to understand both unstructured and structured search algorithms arising in quantum computation.

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