CS 880: Quantum Algorithms 2/23/2021

Lecture 8: Quantum Search

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Today's lecture will discuss a search algorithm. It will begin with a specification of the problem statement of search problems, then discuss Grover's Algorithm. Finally, we will discuss a generalization of our approach to the search problem and explore the possibility of error elimination.

1 Problem Statement

1.1 Search Problem

A search problem can be represented as a black-box function with the following properties:

- The function maps n qubits input to 1 qubit output such that $f : \{0,1\}^n \to \{0,1\}$.
- The function finds good items $x \in \{0,1\}^n$ such that $f(x) = 1$

In this lecture, assume that there is at least one given good item. $t = |f^{-1}(1)| > 0$ where t denotes the number of good items in the list. The overall problem can be seen as a search for good items in an unsorted list of entries. The most difficult setting is when t =1 since there is only a single good entry that the algorithm will attempt to find.

1.2 Algorithms

Consider a search for a good item in a list with N number of items, t number of good items, and b number of bad items $b = N - t$. The three types of algorithms that can solve this problem are the following:

Deterministic Algorithms

To give a deterministic answer, the algorithm will have to go through each item. In the worst-case scenario, the algorithm will have to go through all $N - t$ bad items before finding a good item. Therefore, the run-time would be $N - t$ queries.

Probabilistic Algorithms

The chance of getting a good item from queries of items at random is $p = t/N$. From the Bernoulli experiment, the expected number of items the algorithm needs to go through to hit a good item is $\Theta(N/t)$ with constant error ϵ.

Quantum Algorithms

For Quantum algorithms, we will need $\Theta(\sqrt{N/t})$ queries. The improvement over probabilistic algorithm is quadratic. Note that Θ represents the upper and lower bounds of the run-time. In contrast to a probabilistic algorithm, Quantum algorithms can be tuned to produce no error. The derivation of run-time $\Theta(\sqrt{N/t})$ will be studied more closely later in the lecture.

1.3 Applications

Although the quantum search algorithm seems useful for unsorted database search problems, it does not offer any clear advantage over classical algorithms. To utilize quantum search algorithms, quantum black-box functions must be constructed, and the entire database must be uploaded to the black-box for interference and superposition to occur. Furthermore, the database is normally sorted or can be sorted, which allows for other more efficient algorithms than a linear search, such as binary search, to complete the task.

One useful application is the satisfiability problem, where the algorithm checks each item if it satisfies a condition and assigns a Boolean output. In this case, the run time of classical algorithms will be 2^n. There are other more efficient classical algorithms known for this problem, but they all still run in time $O(2^n)$ where n is the number of variables.

2 Quantum Approach

The approach can be broken into 3 main procedures.

1. First, a uniform superposition of all possible x is created,

$$|\psi\rangle = \sum_x \alpha_x |x\rangle = \frac{1}{\sqrt{N}} \sum_x |x\rangle \tag{1}$$

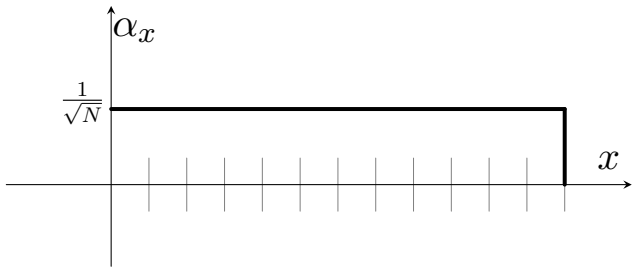


Figure 1: The initial state of the system. Each state is equally likely to be observed if a measurement is taken. We sometimes refer to this state as the *uniform distribution.*

2. From the uniform superposition, Amplify good item's weight and phase, α_{x_g}, using unitary operator U_f.

3. Measure $|\psi_{final}\rangle$ and output the observed x

The first step of the algorithm can be trivially accomplished with $\hat{H}^{\otimes n}$. The second step, however, is complex and can be broken down into two unitary procedures: Flip Good Component Around x-Axis R_{bad} and Flip Around Average $R_{average}$.

Flip Good Component Around x-Axis: R_{bad}

The goal of this R_{bad} operator is to flip and switch the sign of good items x and leave bad items invariant such that

$$|\psi\rangle = R_{bad} |x\rangle = (-1)^{f(x)} |x\rangle \tag{2}$$

Thus, the operator R_{bad} produces a sign change if and only if x_i is a good item or $f(x_i) = 1$. The resulting amplitudes are shown in figure 2. .

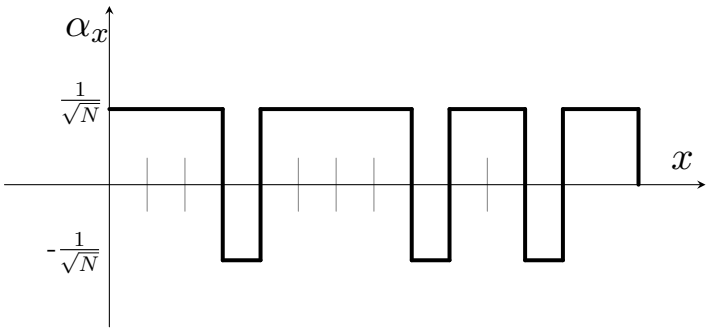


Figure 2: The state of the system after a phase kick on all states where $f(x) = 1$. In this example, there were three states affected, which were reflected across the x-axis.

This operator is unitary as the norm of the state is conserved. In the physical implementation, the operator is utilizing the phase kickback (discussed in lecture 7.)

Flip Around Average: $R_{average}$

This operator $R_{average}$ flips the plot of amplitude around its mean. Applying $R_{average}$ to figure 3 and assuming that t is small compared to N, the mean will be slightly below $\frac{1}{\sqrt{N}}$. The operator will flip the good state around the mean and will result to around $\frac{3}{\sqrt{N}}$ and the bad state will also flip around the mean and drop slightly below the mean as shown in figure 3.

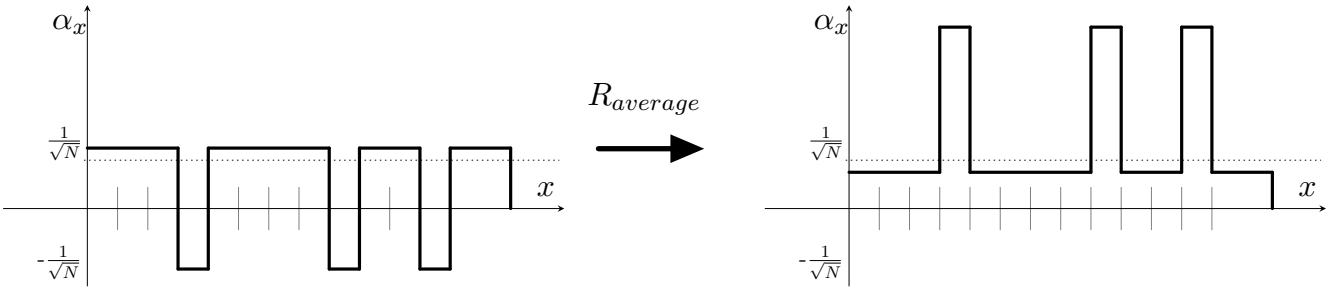


Figure 3: The state of the system after being reflected across the average, which is indicated by a dotted line. Note that the states where $f(x) = 1$ are now more probable if a measurement is taken.

To show $R_{average}$ is unitary, we first show it is linear. To understand how $R_{average}$ might be implemented, we note that reflecting around the average is equivalent to subtracting the average, reflecting across the x-axis, and then adding the average back. In formal notation, we can describe $R_{average}$ as

$$R_{average}\,|\psi\rangle = -\left(|\psi\rangle - AVG\,(\alpha_x)\sum|x\rangle\right) + AVG(\alpha_x)\sum|x\rangle \tag{3}$$

where

$$AVG(\alpha_x) = \frac{1}{N} \sum \alpha_x. \tag{4}$$

This is clearly linear in a_x, as $AVG(\alpha_x)$ is simply a linear combination of the a_x's and all of the operators are linear.

We complete this proof by showing that all the eigenvalues of $R_{average}$ are a magnitude of 1, a condition required of unitary matrices. First, consider what happens when we apply $R_{average}$ to the initial state shown in figure 1. Nothing will happen, as the reflection across the average transforms this state to itself. Thus, the uniform distribution is an eigenvector with an eigenvalue of 1.

Now consider the case shown in figure 4. On the left, we have a system where the average is zero, and after applying $R_{average}$, we have the system mirrored across the x-axis. Thus, this state is another eigenvector and the eigenvalue is -1. All the eigenvectors orthogonal to the uniform distribution will be states that $R_{average}$ reflects across the x-axis. Therefore, all eigenvalues are either 1 or -1, as we can consider $R_{average}$ to be a reflection across the $\sum_x |x\rangle$axis.

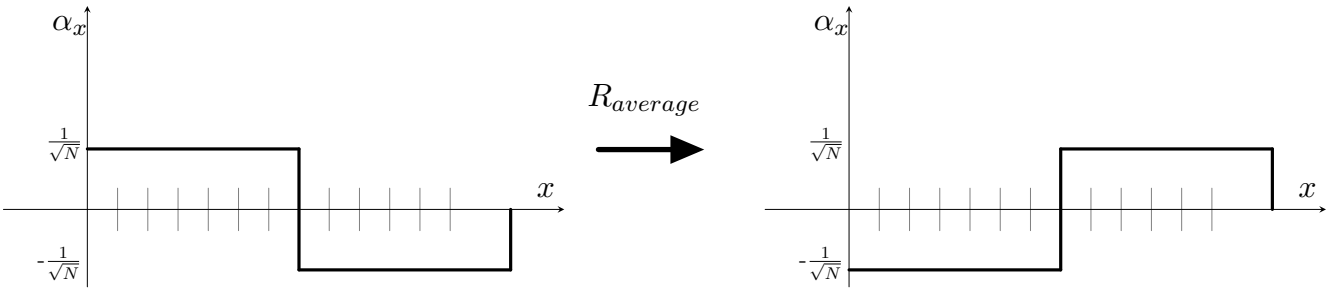


Figure 4: The state of the system before applying $R_{average}$ is on the left, and the system afterwards is on the right. As the average is zero, the system is merely reflected across the x-axis.

Repeatedly applying R_{bad} and $R_{average}$, good states' amplitudes can be amplified after each iteration. However, applying too many iterations can lead to an increase in the error which will be discussed in the next section.

The physical implementation of this gate is done in three steps as follows

1. Bring the average axis (dash-line) to the zero-axis by applying $H^{\otimes n}$.
2. Flip phase of all components around the zero-axis: $R_{|0^n\rangle}$
3. Bring the average axis back from the zero-axis by undoing step: $(H^{\otimes n})^{-1} = H^{\otimes n}$

In summary, the Flip Around Average: $R_{average} = H^{\otimes n} R_{|0^n\rangle} H^{\otimes n}$

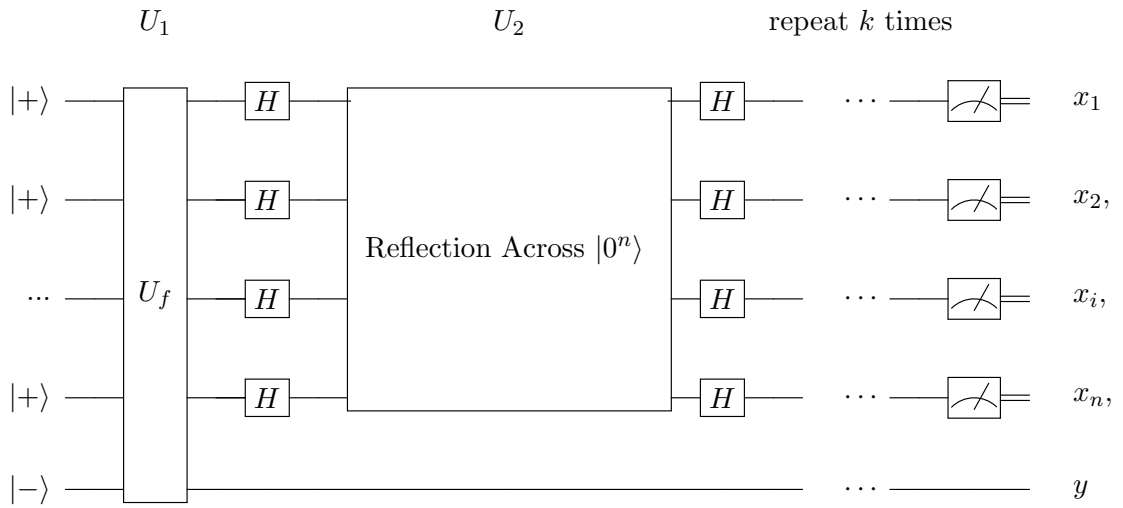
3 Quantum Algorithm

By repeatably applying R_{bad} and $R_{average}$, the amplitudes of good states can be amplified after each iteration. However, the mean of the states will slightly decrease each time R_{bad} and $R_{average}$ is applied. As soon as the mean reaches a negative value, applying more iterations of R_{bad} and $R_{average}$ will increase the error. Therefore, the number of iteration k is critical and must be carefully

determined. Note that both R_{bad} and $R_{average}$ are unitary operators which can be represented as rotations of states. Repeatably applying unitary operators will be a cyclic behavior.

3.1 Quantum Circuit

At this point, we will construct the quantum circuit that implements Grover's algorithm. We can repeat the combination of R_{bad} and $R_{average}$ as many times as desired. The full circuit is shown below.



There are alternative ways to implement U, but this is adequate for our purposes.

3.2 Two-Dimensional State Representation

We now seek to determine the optimal value of k, where k is the number of applications of U. Consider that the amplitude α_x of $|x\rangle$ at any point in time depends only whether $f(x) = 0$ or $f(x) = 1$. Since $\alpha_x^{(i)}$ only depends on $f(x)$, we can describe the system state after i iterations of U as

$$|\psi^{(i)}\rangle = \beta_i \frac{1}{\sqrt{N-t}} \sum_{x:f(x)=0} |x\rangle + \gamma_i \frac{1}{\sqrt{t}} \sum_{x:f(x)=1} |x\rangle\,, \tag{5}$$

where β_i and γ_i are reals and are constrained by

$$\beta_i^2 + \gamma_i^2 = 1. \tag{6}$$

We can thus describe the system as a two-dimensional system with parameters β and γ, where (β, γ) lie on the unit circle, as shown in figure 5. Here we plot β on the B axis and γ on the C axis.

We can also describe the state with trigonometric function:

$$|\psi^{(i)}\rangle = \frac{\cos(\theta_0)}{\sqrt{N-t}} \sum_{x:f(x)=0} |x\rangle + \frac{\sin(\theta_0)}{\sqrt{t}} \sum_{x:f(x)=1} |x\rangle \tag{7}$$

where we describe the initial value of θ as $\sin(\theta_0) = \gamma_0 = \sqrt{\frac{t}{N}}$.

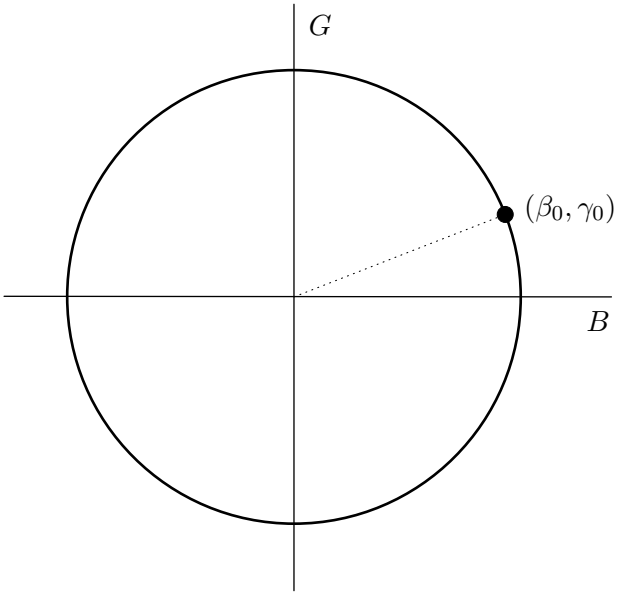


Figure 5: β and γ can be mapped on a unit circle, with β on the B axis and γ on the G axis.

3.3 Analysis

Given some point (β,γ) on this unit circle, what will the effect of the U_1 and U_2 operators be on this point? Since U_1 is a phase kick, it transforms (β,γ) by

$$(\beta, \gamma) \rightarrow (\beta, -\gamma) \tag{8}$$

which is simply a reflection across the B-axis. U_2 reflects the point across the line defined by the origin and the point (β_0,γ_0). Taken together, these two reflections form a rotation of $2\theta_0$. That is, every application of U rotates the point $2\theta_0$ counterclockwise. It follows that after i iterations,

$$\begin{aligned} \theta_i &= (2i+1)\theta_0, \\ \beta_i &= \cos(\theta_i), \\ \gamma_i &= \sin(\theta_i). \end{aligned}$$

From looking at the unit circle, it should be clear that the best time to make a measurement is when (β,γ) is on or very close to the C-axis, as that is when the amplitudes of the valid states are highest. It follows that the ideal value of k would satisfy

$$(2k+1)\theta_0 = \frac{\pi}{2} \tag{9}$$

which leads to

$$k = \frac{1}{2}\left(\frac{\pi}{2\theta_0} - 1\right). \tag{10}$$

This may not be an integer, so we simply choose the closest integer value. We now claim that if we choose a k such that

$$k = \left\lceil \frac{1}{2}\left(\frac{\pi}{2\theta_0} - 1\right) \right\rfloor \tag{11}$$

then

$$\text{Prob}\left[\text{observe } x \in f^{-1}(1)\right] \geq \frac{1}{2}. \tag{12}$$

We know this as k must bring us with the top quarter of the unit circle, as shown in figure 6.

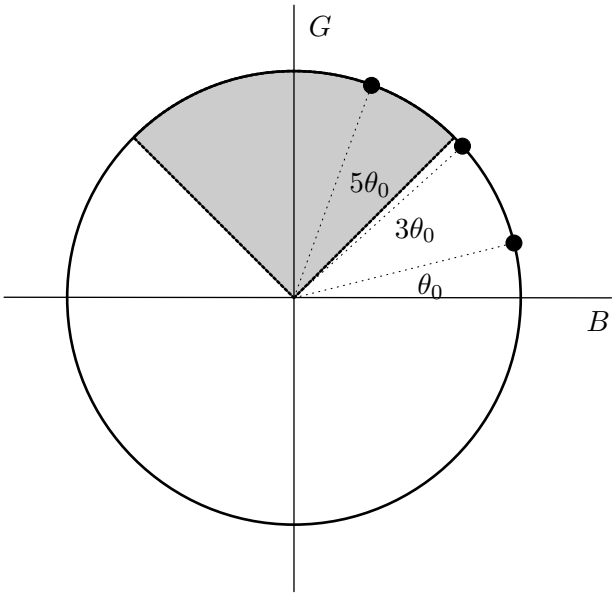


Figure 6: Here is an example where we have applied U three times, which brings us into the shaded part the of unit circle. Each application of U rotates us by $2\theta_0$, and there is no value of $\theta_0 < \pi/2$ that will allow us to completely jump over the shaded area when applying U. Measurements taken in the shaded region have probability a $\geq 1/2$ of observing a valid state.

The advantage of being in the shaded area is that, in terms of absolute value, the amplitudes of the valid states exceed the amplitudes of the invalid states, thus giving us a probability $\geq 1/2$ when taking a measurement.

We can now show that

$$k = \mathcal{O}\left(\sqrt{\frac{N}{t}}\right) \tag{13}$$

4 Generalization

In the previous section, we consider a the search problem with uniform superposition of states and worked out Grover's algorithm. In this section, we will a generalize search problem to a superposition of state $|\psi\rangle$ which is not necessary uniform. The starting state $|\psi\rangle$ have the following properties:

- the state can be written as superposition $|\psi\rangle = A|0^n\rangle = \sum_x \alpha_x |x\rangle$
- good item 'x' has a positive weight. $|\psi\rangle = A|0^n\rangle$ has weight $p_x > 0$ where$f(x) = 1$
- the weight is the given magnitude of the coefficent of each state. $p = \sum_{x:f(x)=1} |\alpha_x|^2$

In the previous section, we considered a special case of this generalization where $A = H^{\otimes b}$.

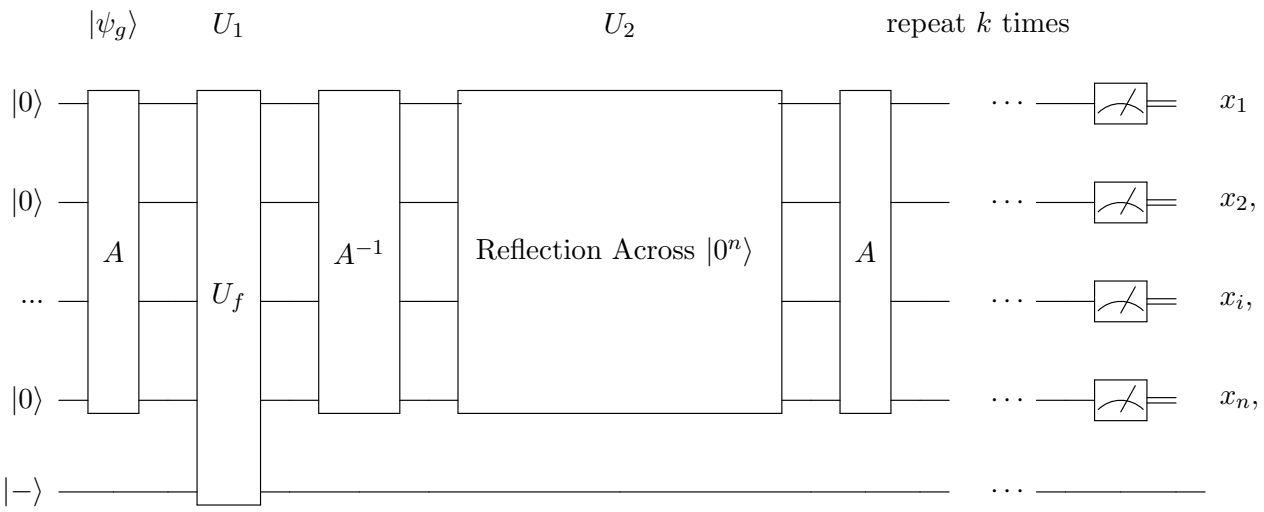
4.1 Algorithm

For the algorithm construction, we will start with the initial state and apply k-iterations of R_{bad} and $R_{average}$.

The generalized $R_{average}$, however, must be adapted to our generalized case. In general, we must transform from the initial state $|\psi_g\rangle = A|0^n\rangle$ to $|0^n\rangle$, and therefore will apply A^{-1}. Then apply phase flip $R_{|0^n\rangle}$ and transform back to initial basis by applying A.

$$R_{average} = AR_{|0^n\rangle}A^{-1} \tag{14}$$

The quantum circuit for this general case is given in



If $A = H^{\otimes n}$, the circuit is identical to circuit in section 3.1.

4.2 Analysis

To determine the optimum k iterations, we must consider the initialization angle θ_0. We know that the probablity of measuring a good item in $|\psi_p\rangle$ is p. Therefore,

$$\sin(\theta_0) = \sqrt{p} \tag{15}$$

Following the derivation in section 3.3, the optimum iteration $k = \frac{1}{2}(\frac{\pi}{2\theta_0} - 1) = O(\frac{1}{\sqrt{p}})$.

4.3 Error Elimination

To eliminate all errors after applying k iterations of U rotation, the final state must be positioned exactly at $\frac{\pi}{2}$. The idea is to slightly manipulate the angle $\theta_0 \to \theta_0'$ such that after $k \in \mathbb{Z}$ iterations, the final state landed exactly at $\frac{\pi}{2}$. This can be achieved by manipulating the probability of measuring a good item $p \to p'$ by implementing reduction using additional ancilla qubit, creating new good states in the qubit state $|1\rangle$.

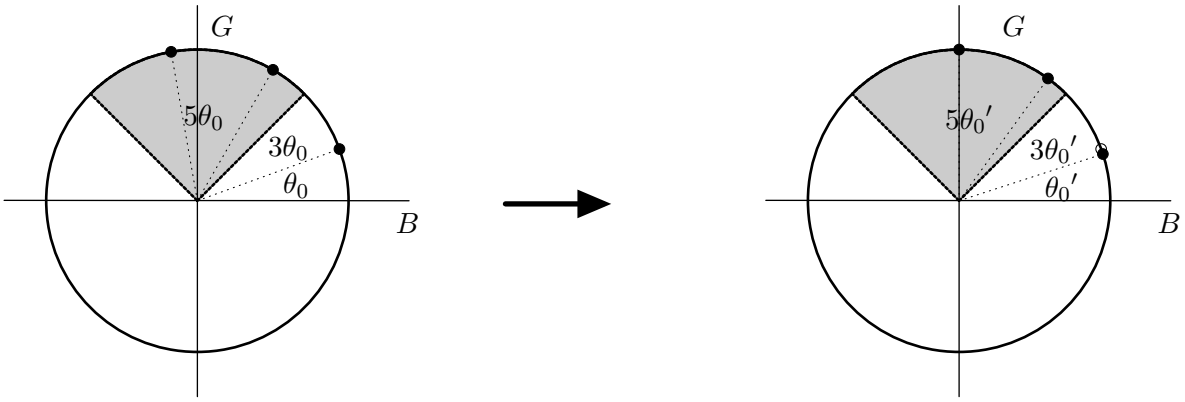


Figure 7: The left figure shows the starting state, $\theta_0 = \sqrt{p}$, and the state after first iteration and second iterations. Note that the final state is not exactly at the ideal stopping point of $\frac{\pi}{2}$. In the right figure, by slightly decreasing $\theta_0 \to \theta_0'$, the final state is exactly at $\frac{\pi}{2}$.

5 Exercise: Error Elimination

As mentioned above, the error can be eliminated by doing the following:

- Reduce starting probability p to p' where rotating p' to $\frac{\pi}{2}$ corresponds to an integral k*
- Implement reduction using additional ancilla qubit
- Create additional good states with $|1\rangle$ qubit

Exercise: To work out a way to eliminate error using the three ideas above.