Grover's Search Algorithm

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Outline

- Day 1
  - Review
    - Math and Quantum Mechanics Review
  - Introduction to the Algorithm
    - Classical Search Algorithms
    - Visually Implement Grover's
- Day 2
  - Coding the Two Qubit Case
  - Coding the General Case (Three Ways)

Review

Identity Matrix

$$\mathbf{I} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

- The identity matrix shown above is for 4x4 matrices, general pattern extends to matrices of all size
  - 1's on main diagonal, 0's everywhere else

States are Vectors, Gates are Matrices

- Quantum mechanical states are represented by vectors, describe the entire system
  - One qubit states are length 2, two qubit states are length 2, n qubit states are 2^n
- Quantum computing gates are represented by **unitary** matrices
  - One qubit gates are 2x2, two qubit gates are 4x4, n qubit gates are $2^n x 2^n$
- Note that many multi-qubit gates involve one or more control qubits and one or more target qubits:
  - Fredkin Gate (one control, two targets)
  - Three-Qubit X Gate (two controls, one target)

Statevectors Are Made of Basis States

- Consider the following state vector: $|\psi\rangle = \frac{1}{2}|00\rangle + \frac{1}{2}|01\rangle + \frac{1}{2}|10\rangle + \frac{1}{2}|11\rangle$
- The amplitude of the $|00\rangle$ state is $\frac{1}{2}$
- The probability of measuring $|\psi\rangle$ and obtaining $|00\rangle$ is $|\frac{1}{2}|^2 = \frac{1}{4}$
- Consider the following state vector: $|\psi\rangle = \frac{-1}{2}|00\rangle + \frac{1}{2}|01\rangle + \frac{1}{2}|10\rangle + \frac{1}{2}|11\rangle$
- The amplitude of the $|00\rangle$ state is $\frac{-1}{2}$
- The probability of measuring $|\psi\rangle$ and obtaining $|00\rangle$ is $|\frac{-1}{2}|^2 = \frac{1}{4}$

Define Multiple Gate Result Through Matrix Multiplication

Figure 1: One Qubit Circuit with Two Gates

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

- Expected Output?
- Now show it one gate at a time.
- Now show it with a combination gate

Overlap of Wavefunctions

- For an inner product where one of the states is a statevector and the other state is a basis state, the calculation is called an overlap
  - It determines the portion of the statevector in the direction of the basis vector
- Example: Consider the following basis in Cartesian coordinates

$$|x\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad |y\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \quad |\phi\rangle = \begin{bmatrix} 3 \\ 4 \end{bmatrix}$$

- Then $\langle y|\phi\rangle = 4$ which is the overlap between $|y\rangle$ and $|\phi\rangle$

Outer Product

- An outer product takes two vectors and creates a matrix (an inner product takes two vectors and creates a scalar).
- Consider the following two vectors of length 3:

$$|x\rangle = \begin{bmatrix} x_0 \\ x_1 \\ x_2 \end{bmatrix} \quad |y\rangle = \begin{bmatrix} y_0 \\ y_1 \\ y_2 \end{bmatrix}$$

- The outer product between these two vectors, represented as $|x\rangle\langle y|$ is

$$|x\rangle\langle y| = \begin{bmatrix} x_0 y_0^* & x_0 y_1^* & x_0 y_2^* \\ x_1 y_0^* & x_1 y_1^* & x_1 y_2^* \\ x_2 y_0^* & x_2 y_1^* & x_2 y_2^* \end{bmatrix}$$

Completeness Relation

- If the states $|x_i\rangle$ form a complete basis then:

$$\sum_i |x_i\rangle\langle x_i| = \mathbb{I}$$

Projection Operator

- A useful application of the outer product is in the construction of projection operators.
- The projection operator *projects* out a specific component of a of a state related to the basis state that was used to the projection operator.
- Example: Consider the following basis in Cartesian coordinates

$$|x\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad |y\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \quad |\phi\rangle = \begin{bmatrix} 3 \\ 4 \end{bmatrix}$$

- $|y\rangle\langle y|$ is the projection operator for $|y\rangle$, so

$$|y\rangle\langle y|\phi\rangle = |y\rangle 4 = 4|y\rangle = \begin{bmatrix} 0 \\ 4 \end{bmatrix}$$

Introduction

Classical Linear Search

- If the data is sorted there are a variety of algorithms which have good performance
- If the data is unsorted you are left essentially with brute force
  - Average performance is $\frac{N}{2}$ searches
  - Worst case is N searches
- Computational Performance: $O(N)$

A New Way of Thinking of the Algorithm

- Standard algorithm returns the index of the wanted element
- Consider instead marking the indices corresponding to the wanted element

```
def linear_search_version_2 (my_list, element):
    length = len(my_list)
    results = np.zeros(length)
    for i in range(length):
        if my_list[i] == element:
            results[i] = 1
    return results
```

Reflections

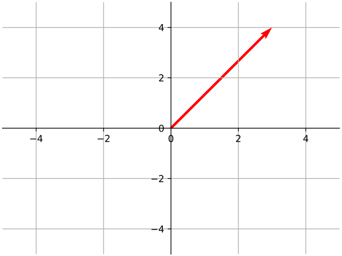


Figure 2: Reflection About the X Axis

Reflections

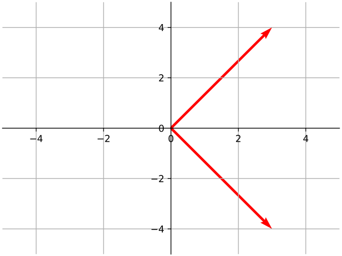


Figure 3: Reflection About the X Axis

Reflections

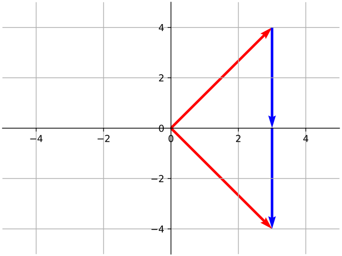


Figure 4: Reflection About the X Axis

Mathematical Representations of Reflections

$$\begin{bmatrix}3\\4\end{bmatrix} - \begin{bmatrix}0\\4\end{bmatrix} - \begin{bmatrix}0\\4\end{bmatrix} = \begin{bmatrix}3\\-4\end{bmatrix}$$

$$\begin{bmatrix}3\\4\end{bmatrix} - 2\begin{bmatrix}0\\4\end{bmatrix} = \begin{bmatrix}3\\-4\end{bmatrix}$$

- But consider the following representation:

$$|x\rangle = \begin{bmatrix}1\\0\end{bmatrix} \quad |y\rangle = \begin{bmatrix}0\\1\end{bmatrix} \quad |\phi\rangle = 3|x\rangle + 4|y\rangle$$

Mathematical Representations of Reflections

- Then we can represent the reflection as:

$$ref_x(|\phi\rangle) = |\phi\rangle - 4|y\rangle - 4|y\rangle = |\phi\rangle - 2(4|y\rangle)$$

- But remember that from our discussion of overlaps, $\langle y|\phi\rangle = 4$, so

$$ref_x(|\phi\rangle) = |\phi\rangle - 2|y\rangle\langle y|\phi\rangle = (\mathbf{I} - 2|y\rangle\langle y|)|\phi\rangle$$

- Where we are reflecting around the x-axis, so y is the other axis

Mathematical Representations of Reflections

- For a reflection in more than two-dimensional space we would need to subtract the outer products of all other basis vectors besides the axis we are rotating around:

$$ref_x(|\phi\rangle) = (\mathbf{I} - 2|y\rangle\langle y| - 2|z\rangle\langle z|)|\phi\rangle$$

- This can be tedious for many basis vectors, but remember that the identity matrix can be represented as a sum of outer products of all basis vectors. So in 3D Cartesian:

$$\begin{aligned} ref_x(|\phi\rangle) &= (\mathbf{I} - 2|y\rangle\langle y| - 2|z\rangle\langle z|)|\phi\rangle \\ &= (|x\rangle\langle x| + |y\rangle\langle y| + |z\rangle\langle z| - 2|y\rangle\langle y| - 2|z\rangle\langle z|)|\phi\rangle \\ &= (|x\rangle\langle x| - |y\rangle\langle y| - |z\rangle\langle z|)|\phi\rangle \end{aligned}$$

Mathematical Representations of Reflections

- Now add and subtract by the outer product of the axis we are rotating around:

$$ref_x = (|x\rangle\langle x| + |x\rangle\langle x| - |x\rangle\langle x| - |y\rangle\langle y| - |z\rangle\langle z|)|\phi\rangle$$
$$= (2|x\rangle\langle x| - (|x\rangle\langle x| + |y\rangle\langle y| + |z\rangle\langle z|)|\phi\rangle$$
$$= (2|x\rangle\langle x| - \mathbf{I})|\phi\rangle$$

- Generalization: To rotate a statevector $|\phi\rangle$ around any axis k:

$$ref_k(|\phi\rangle) = (2|k\rangle\langle k| - \mathbf{I})|\phi\rangle$$

Parts of Grover's Algorithm

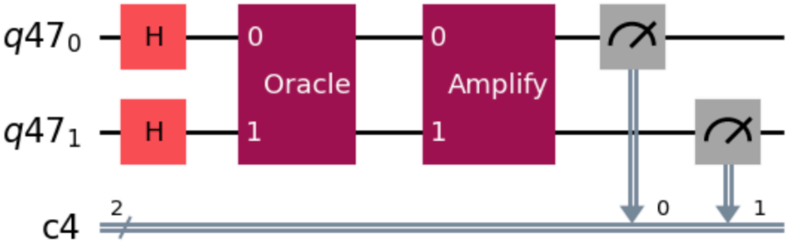


Figure 5: Grover's Algorithm

Hadamard Gates

- First step is to apply a Hadamard gate to every qubit, creating a superposition of every possible state

$$H^{\otimes n}|0^n\rangle = \frac{1}{\sqrt{N}} \sum_{x \in \{0,1\}^n} |x\rangle = |\phi\rangle$$

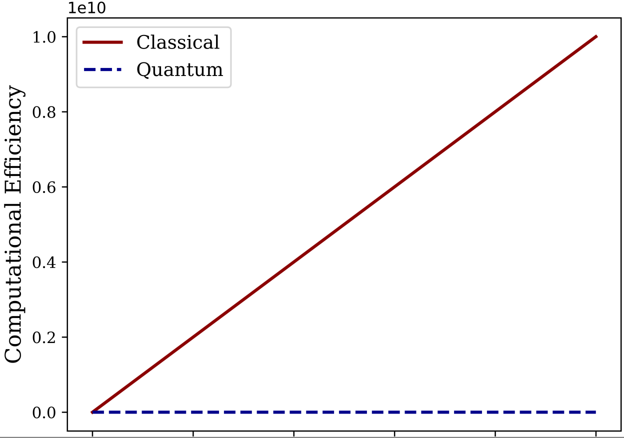
Oracle

- The goal of the algorithm is to flip the sign on the amplitude of the desired state(s)
  - Grover's can be used to find more than one desired solution at a time
- The oracle should flip the sign of the amplitude for all desired states but leave all other amplitudes unchanged

Amplification Algorithm (Diffusion Algorithm)

- A negative amplitude gives the same probability as a positive amplitude, so we need another step in the algorithm
- The amplification algorithm (amplitude amplification algorithm or diffusion algorithm) increase the amplitude on the marked states but decreases the amplitude on the unmarked states
- **NOTE** the oracle and amplification algorithm may have to be applied more than once to achieve significant separation in amplitudes between the marked and unmarked states.

$O(N)$ vs. $O(\sqrt{N})$ Run Times



Visual Walkthrough

- In the next few slides we will visually walkthrough what Grover's algorithm is doing as it processes a system.
- The basic steps are to negate the amplitude of the desired state (oracle) and then reflect the entire state around the mean amplitude (amplification)

Step 1: Starting Point for Two Qubits

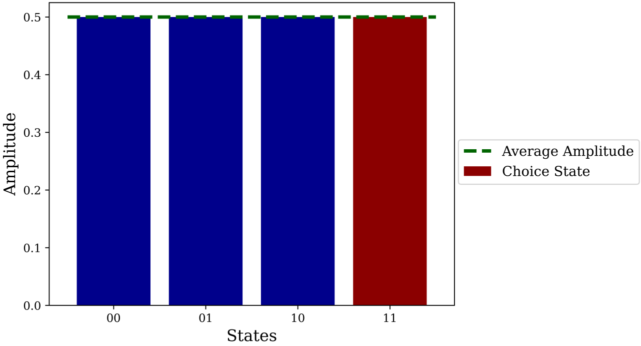


Figure 7: Grover's Algorithm Visualization Step 1

Step 2: Negate Amplitude of Desired State

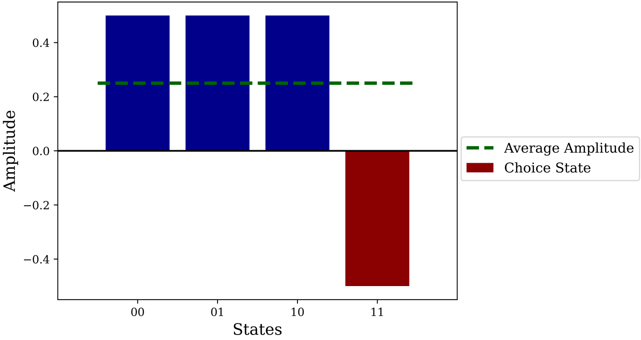


Figure 8: Grover's Algorithm Visualization Step 2

Step 3: Reflect Around Mean Amplitude

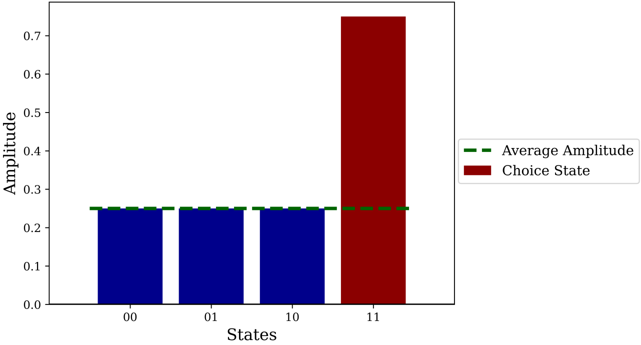


Figure 9: Grover's Algorithm Visualization Step 3

Step 4: Negate Amplitude of Desired State

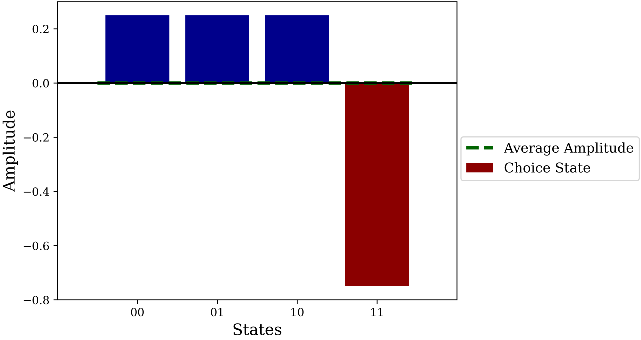


Figure 10: Grover's Algorithm Visualization Step 4

Step 5: Reflect Around Mean Amplitude

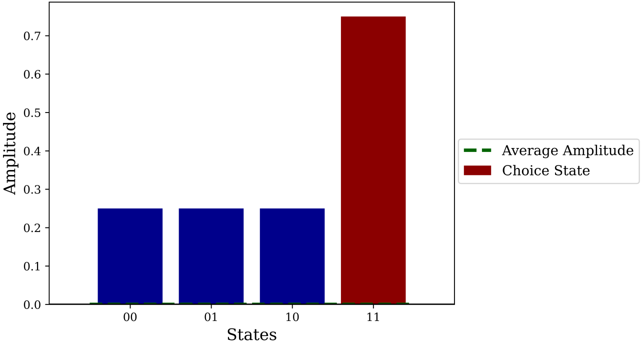
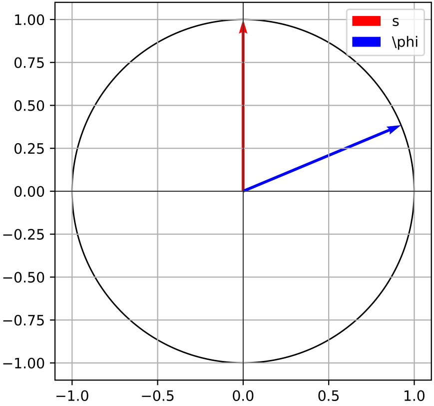
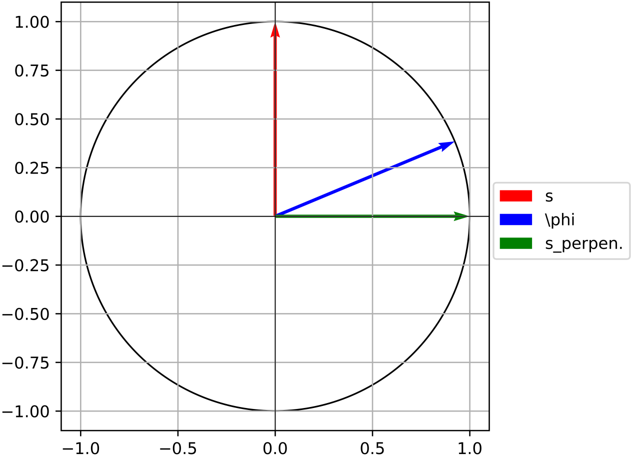


Figure 11: Grover's Algorithm Visualization Step 5

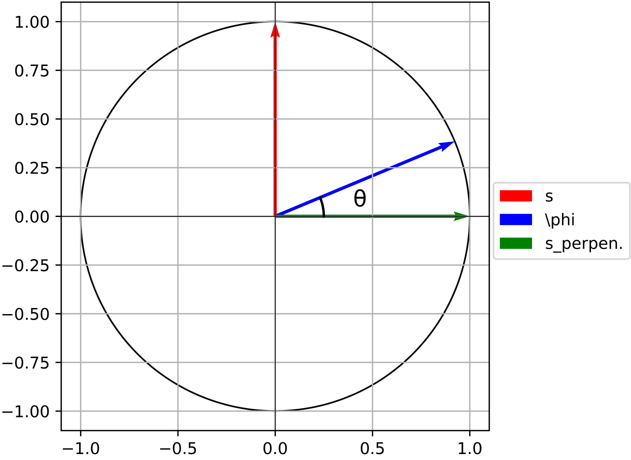
How Many Times To Run ⟶ Grover's Circle



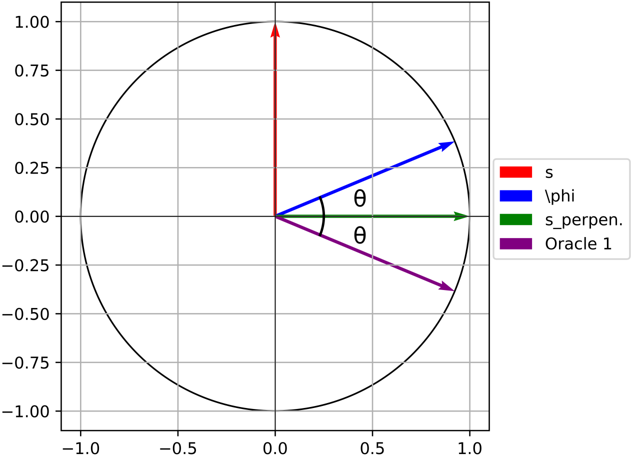
Add $|s^{\perp}\rangle$, a state which is perpendicular to $|s\rangle$



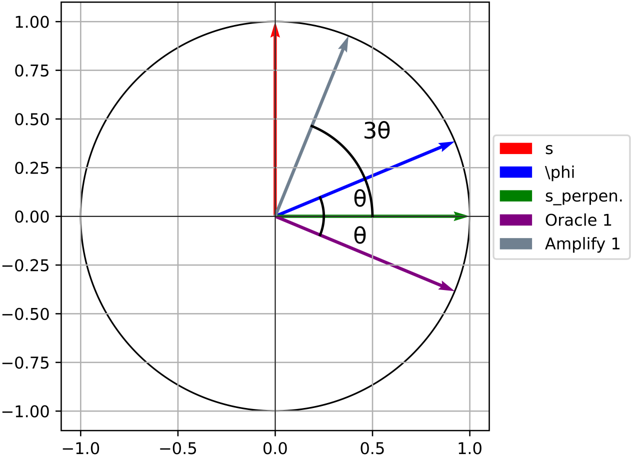
Note the angle θ



Negate the component of $|\phi\rangle$ that comes from $|s\rangle$ (Oracle)



Reflect around the original value of $|\phi\rangle$ (Amplification)



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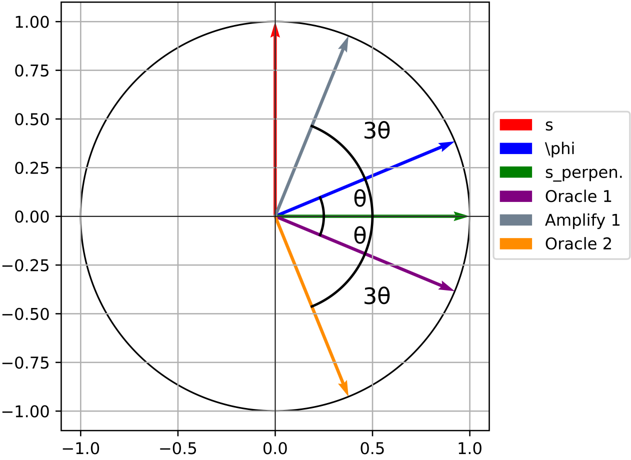

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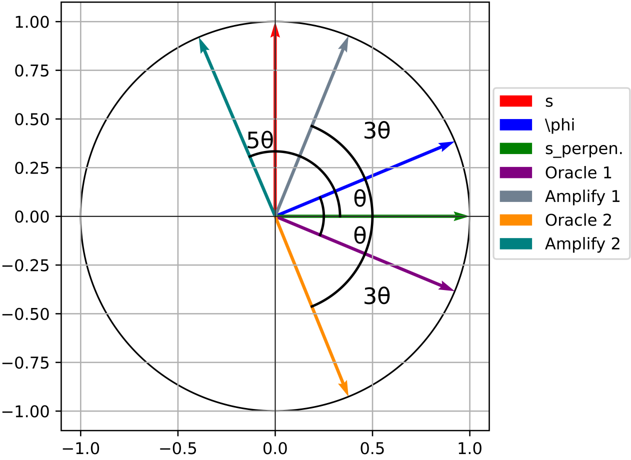

How Many Times To Run $\longrightarrow$ Grover's Circle

- Now some trigonometry

$$sin\theta = \frac{1/\sqrt{N}}{1} \longrightarrow \langle s|\phi\rangle = \frac{1}{\sqrt{N}},\ |\langle\phi|\phi\rangle|^2 = 1$$

$$\theta = arcsin(\frac{1}{\sqrt{N}}) \approx \frac{1}{\sqrt{N}}$$

$$(2t+1)\theta = \frac{\pi}{2} \longrightarrow t = \frac{\pi}{4}\sqrt{N} - \frac{1}{2}$$

How Many Times To Run $\longrightarrow$ Grover's Circle

- In general the algorithm will run $\frac{\pi}{4}\sqrt{\frac{N}{M}}$ times where there are N items in the search space and the algorithm is looking for M different items.
  - Typically this equation is "floored" to avoid overshooting

Programming Grover's Algorithm

Two Qubit Case

- Let's consider a two-qubit Grover's algorithm
  - The "good state" is $|11\rangle$
  - The other states are the "bad states"

What Could the Oracle Be?

- General form: $U_s = \mathbf{I} - |s\rangle\langle s|$
- What gate or combination of a gates would turn $|11\rangle \longrightarrow -|11\rangle$ but leave all other states unchanged?
  - Controlled Z!

What Could the Amplification Be?

$$U_d = 2|\phi\rangle\langle\phi| - \mathbf{I}$$

- Remember this step is a rotation around the mean amplitude
- But since $|\phi\rangle$ is a superposition of all possible states:

$$H^{\otimes n}(2|0\rangle\langle 0| - \mathbf{I})H^{\otimes n}$$

- Very similar implementation as the Oracle, same gates will be involved

Amplification Algorithm

1. Hadamard to all qubits
2. NOT to all qubits
3. Multi-controlled-Z where all top qubits are the control and the bottom qubit is the target
4. NOT to all qubits
5. Hadamard to all qubits

General Case

- The amplification algorithm will remain the same, but what could be a general form for the oracle?
- It must have a multi-controlled-Z gate, only other change is to add leading and post NOT gates if the digit is a zero

1. For any digit in the marked string that is a 0, apply a NOT gate to the corresponding qubit.
2. Multi-controlled-Z where all top qubits are the control and the bottom qubit is the target
3. For any digit in the marked string that is a 0, apply a NOT gate to the corresponding qubit.

- **To Qiskit!**