Grover's Algorithm: 3-Qubit Step-by-Step Derivation

1 Setup

For a 3-qubit system, we have $N = 2^3 = 8$ items.

- **Target state ($|w\rangle$):** We assume the target is $|111\rangle$.

- **Initial Amplitude (a):** The system starts in a uniform superposition, so every state has an amplitude of $\frac{1}{\sqrt{8}} \approx 0.354$.

- **Initial State ($|\psi_0\rangle$):**

$$|\psi_0\rangle = \sum_{x \in \{0,1\}^3} \frac{1}{\sqrt{8}} |x\rangle = \left[\frac{1}{\sqrt{8}}, \frac{1}{\sqrt{8}}, \dots, \frac{1}{\sqrt{8}} \right] \tag{1}$$

- **Initial Probability of measuring $|w\rangle$:**

$$P(w) = \left| \frac{1}{\sqrt{8}} \right|^2 = \frac{1}{8} = 12.5\% \tag{2}$$

2 Run 1: First Iteration

2.1 Step 1: The Oracle

The Oracle flips the sign of the target amplitude ($|w\rangle$).

$$|\psi_{\text{oracle}}\rangle = \left[\frac{1}{\sqrt{8}}, \dots, -\frac{\mathbf{1}}{\sqrt{\mathbf{8}}}, \dots \right] \tag{3}$$

- Non-winners ($x \neq w$): $\frac{1}{\sqrt{8}} \approx 0.354$

- Winner (w): $-\frac{1}{\sqrt{8}} \approx -0.354$

2.2 Step 2: The Diffuser (Inversion about the Mean)

We calculate the mean (μ) of all amplitudes in $|\psi_{\text{oracle}}\rangle$:

$$\mu = \frac{1}{N} \sum_i \alpha_i = \frac{1}{8} \left(7 \times \frac{1}{\sqrt{8}} + 1 \times \frac{-1}{\sqrt{8}} \right) = \frac{1}{8} \left(\frac{6}{\sqrt{8}} \right) = \frac{3}{4\sqrt{8}} \approx 0.265 \tag{4}$$

Now, we apply the operation $2\mu - \alpha_i$ to each amplitude:

- **For Non-winners (x):**

$$2(0.265) - 0.354 = 0.530 - 0.354 = \mathbf{0.177} \approx \frac{1}{4\sqrt{2}} \tag{5}$$

- **For Winner (w):**

$$2(0.265) - (-0.354) = 0.530 + 0.354 = \mathbf{0.884} \approx \frac{5}{4\sqrt{2}} \tag{6}$$

State after Run 1 ($|\psi_1\rangle$):

$$|\psi_1\rangle = [0.177, \dots, \mathbf{0.884}, \dots] \tag{7}$$

The probability of measuring the target is now $|0.884|^2 = \mathbf{78.1\%}$.

3 Run 2: Second Iteration

3.1 Step 1: The Oracle

We flip the sign of the winner $|w\rangle$ again.

- Non-winners: 0.177

- Winner: $-\mathbf{0.884}$

3.2 Step 2: The Diffuser

Calculate the new mean (μ):

$$\mu = \frac{1}{8}\left(7 \times 0.177 + 1 \times (-0.884)\right) = \frac{1}{8}(1.239 - 0.884) = \frac{0.355}{8} \approx \mathbf{0.044} \tag{8}$$

Note: The mean drops significantly because the large negative amplitude of the winner pulls it down.
Apply $2\mu - \alpha_i$:

- **For Non-winners (x):**

$$2(0.044) - 0.177 = 0.088 - 0.177 = -\mathbf{0.088} \tag{9}$$

- **For Winner (w):**

$$2(0.044) - (-0.884) = 0.088 + 0.884 = \mathbf{0.972} \tag{10}$$

State after Run 2 ($|\psi_2\rangle$):

$$|\psi_2\rangle = [-0.088, \ldots, \mathbf{0.972}, \ldots] \tag{11}$$

The probability of measuring the target is now $|0.972|^2 = \mathbf{94.5\%}$.

4 Conclusion and Summary

For $N = 8$, the optimal number of iterations is 2. If we were to run a 3rd iteration, the state would "over-rotate," and the probability would drop to approximately 33%.

Iteration	Probability of Finding Target ($|w\rangle$)
0 (Start)	12.5%
1	78.1%
2 (Optimal)	**94.5%**
3 (Over-rotated)	33.0%

Table 1: Probability improvement per iteration for 3 qubits.