

# CS 506 : Intro to Quantum Computing

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## 1 Grover's Search Algorithm

Suppose we need to find an element in an unstructured database of  $N$  elements. We are given a black-box query function

$$f : \{0, 1, \dots, N-1\} \rightarrow \{0, 1\},$$

The goal is to find the unique  $x^*$  such that

$$f(x^*) = 1.$$

Classically (non-quantum), deterministic algorithms need  $N$  queries and randomized algorithms require  $\Omega(N)$  queries to find  $x^*$  with a success probability  $\geq 2/3$ .

Grover's Search Algorithm is a quantum algorithm that solves this unstructured search problem using only  $O(\sqrt{N})$  queries and  $O(\sqrt{N} \log N)$  1-qubit and 2-qubit gates with a success probability  $\geq 2/3$ .

### 1.1 Example: Database Search

Consider an array  $A[0], \dots, A[N-1]$ , and a query  $q$ . The task is to find  $x^*$  such that  $A[x^*] = q$ .

We define the function as:

$$f(x) = \begin{cases} 1 & \text{if } A[x] = q, \\ 0 & \text{otherwise.} \end{cases}$$

Function  $f(x)$ : if  $A[x] = q$  then return 1 else return 0

Classically, searching requires  $N$  comparisons, whereas Grover's algorithm finds  $x^*$  in approximately  $O(\sqrt{N})$  queries.

## 1.2 Example: Satisfiability

We are given  $n$  variables  $x_1, \dots, x_n$  and  $m$  clauses, where each clause is an OR of literals.  
Goal: Find an assignment  $x^* = (x_1^*, \dots, x_n^*)$  such that each clause is True(1).

Example:

- $n = 3, m = 4$
- Variables:  $x_1, x_2, x_3$
- Clauses:

$$C_1 = \bar{x}_1 \vee x_2$$

$$C_2 = x_1 \vee x_2 \vee \bar{x}_3$$

$$C_3 = \bar{x}_2 \vee x_3$$

$$C_4 = \bar{x}_1 \vee x_3$$

Where  $f(x_1 x_2 x_3) = 1$  if all clauses are satisfied, else 0.

For example: for  $f(101)$  it returns 0.

The search space is defined by  $f : \{0, 1, \dots, 2^n - 1\} \rightarrow \{0, 1\}$  and  $N = 2^n$ .

Grover's algorithm solves this problem by using  $O(\sqrt{N}) = O(\sqrt{2^n}) = O(2^{n/2})$  queries to  $f$ .

Classical algorithms take exponential time  $O(2^n)$  to solve the satisfiability problem.

Grover's algorithm solves it faster in  $O(2^{n/2})$  but still in exponential time although there is a quadratic speedup.

**Grover's search algorithm does not solve NP-complete problems in polynomial time!**

## 2 Key Components of Grover's Search Algorithm

### 2.1 Oracle Gate

The oracle gate in Grover's algorithm is the  $U_f$  gate.

It marks the correct solution by inverting its amplitude.

$$U_f : |x\rangle|y\rangle = |x\rangle|y \oplus f(x)\rangle$$

$$U_f : |x\rangle \left( \frac{|0\rangle - |1\rangle}{\sqrt{2}} \right) = (-1)^{f(x)} |x\rangle \left( \frac{|0\rangle - |1\rangle}{\sqrt{2}} \right)$$

When  $x = x^*$ ,  $(-1)^{f(x^*)} = (-1)^1 = -1$

When  $x \neq x^*$ ,  $(-1)^{f(x)} = (-1)^0 = +1$

## 2.2 Diffusion Operator

After the oracle gate ( $U_f$  gate), we use the diffusion operator to increase the amplitude of  $x^*$  while reducing the others.

## 3 Amplitude Amplification

Given a set of vectors  $|X_1\rangle, |X_2\rangle, \dots, |X_N\rangle$  in  $\mathbb{R}^d$  and a target vector  $|Y\rangle$  in  $\mathbb{R}^d$ ,  $\varepsilon$  we want to find  $|X_i\rangle$  such that  $\langle X_i|Y\rangle \geq \varepsilon$

### 3.1 Assumptions

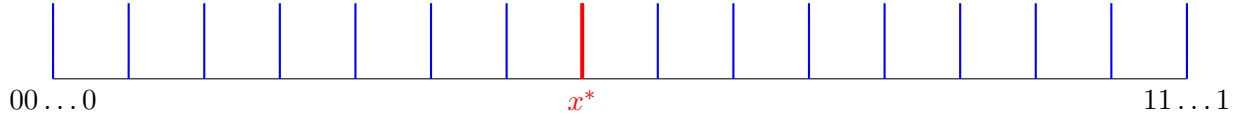
- $N$  is a power of 2 and  $n = \log_2 N$ .
- There is a unique  $x^*$  such that  $f(x^*) = 1$

### 3.2 Initial State

We begin with a uniform superposition where all states have equal amplitudes.

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

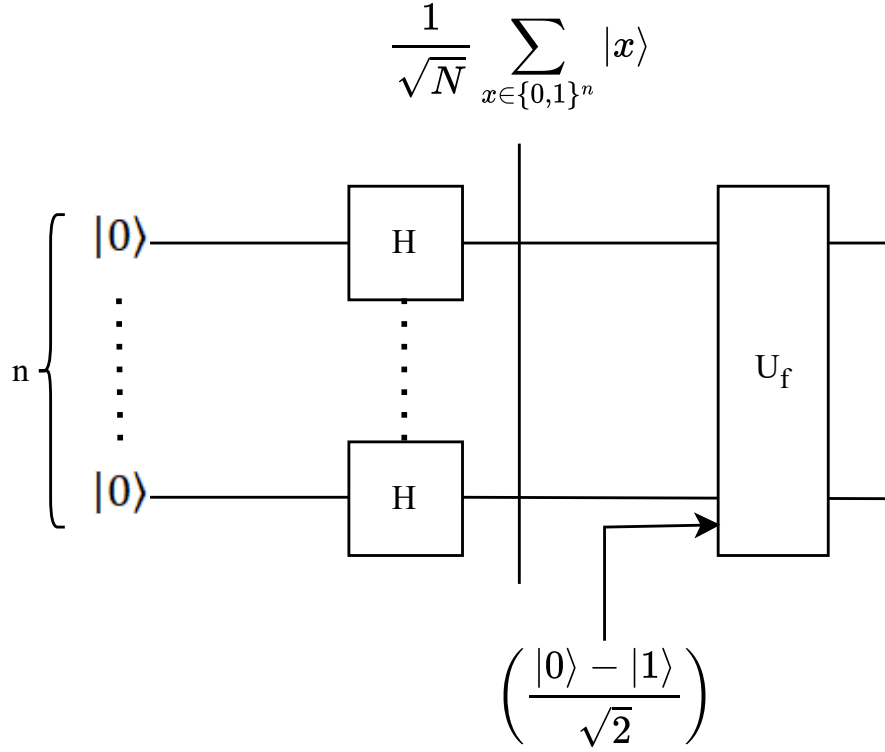
The probability of finding the solution  $x^*$  is  $\frac{1}{N}$ .



### 3.3 Applying the Oracle Gate ( $U_f$ )

The first step is to use the oracle gate or  $U_f$  gate on the initial state  $\frac{1}{\sqrt{N}} \sum_{x \in \{0,1\}^n} |x\rangle$ .

$$U_f \left( \frac{1}{\sqrt{N}} \sum_{x \in \{0,1\}^n} |x\rangle \right) = \frac{1}{\sqrt{N}} \sum_{x \in \{0,1\}^n} (-1)^{f(x)} |x\rangle$$



Mathematically, this operation translates to:

$$\begin{aligned}
U_f \left( \frac{1}{\sqrt{N}} \sum_{x \in \{0,1\}^n} |x\rangle \right) &= \frac{1}{\sqrt{N}} \sum_{x \in \{0,1\}^n} (-1)^{f(x)} |x\rangle \\
&= \frac{1}{\sqrt{N}} \sum_{x=0}^{N-1} (-1)^{f(x)} |x\rangle \\
&= \frac{1}{\sqrt{N}} \left[ (-1)^{f(x^*)} |x^*\rangle + \sum_{x \neq x^*} (-1)^{f(x)} |x\rangle \right] \\
&= \frac{1}{\sqrt{N}} \left[ (-1)^1 |x^*\rangle + \sum_{x \neq x^*} (-1)^0 |x\rangle \right] \\
&= \frac{1}{\sqrt{N}} \left[ -|x^*\rangle + \sum_{x \neq x^*} |x\rangle \right] \\
&= -\frac{1}{\sqrt{N}} |x^*\rangle + \frac{1}{\sqrt{N}} \sum_{x \neq x^*} |x\rangle
\end{aligned}$$

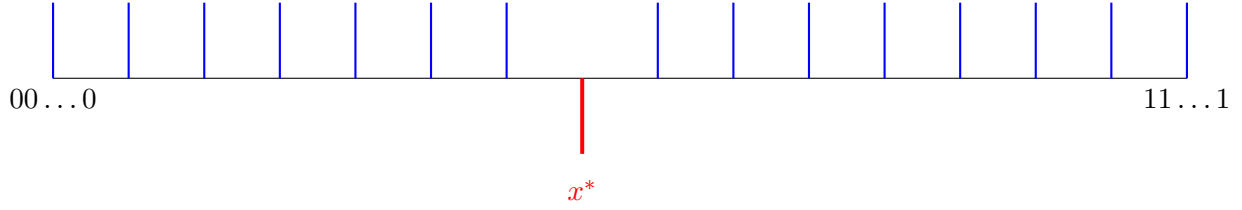
- For the solution  $x^*$ :  $f(x^*) = 1 \Rightarrow (-1)^{f(x^*)} = (-1)^1 = -1$
- For all other  $x \neq x^*$ :  $f(x) = 0 \Rightarrow (-1)^{f(x)} = (-1)^0 = +1$

This phase flip marks the solution  $x^*$  with a negative amplitude while preserving the positive amplitudes of all other states.

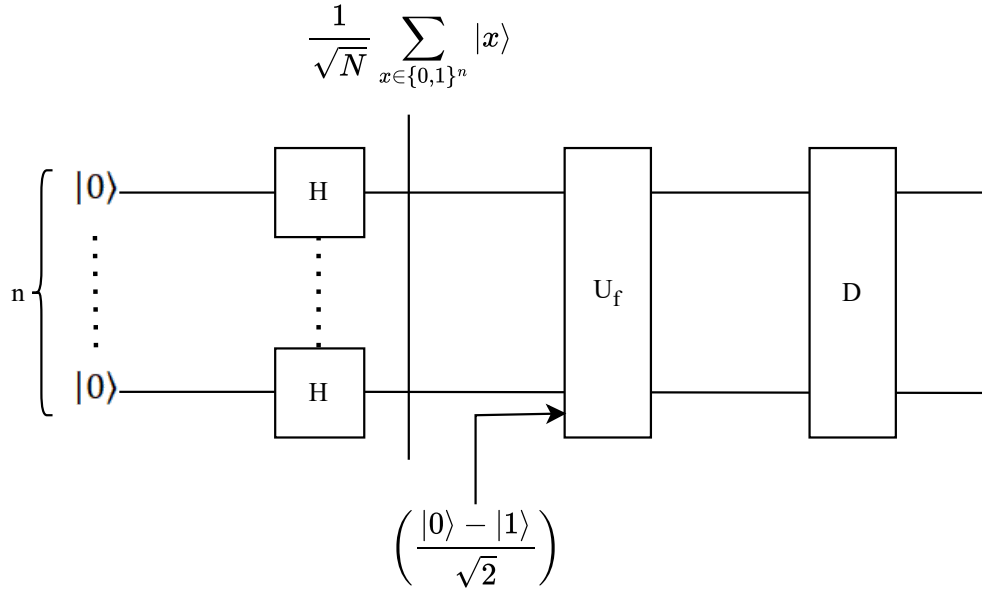
After applying the oracle ( $U_f$ ) gate:

$$\alpha_{x^*} = -\frac{1}{\sqrt{N}} \quad (\text{amplitude of the solution } x^*)$$

$$\alpha_x = +\frac{1}{\sqrt{N}} \quad \text{for all } x \neq x^* \quad (\text{amplitude of the other states})$$



### 3.4 Amplitude Amplification using the Diffusion Operator



Let  $\mu$  be the average of all  $\alpha_{x^*}$ s.

Then,

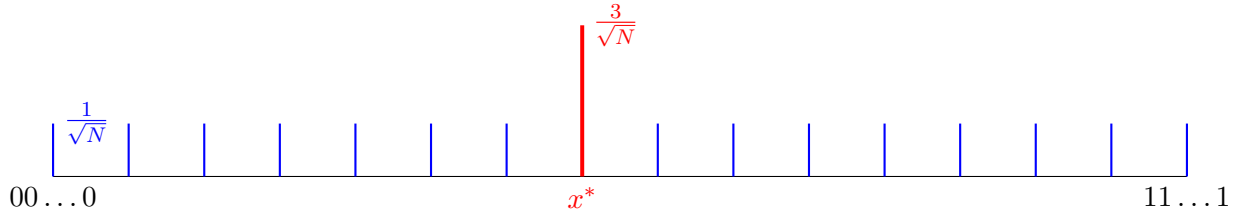
$$\mu = \frac{\frac{-1}{\sqrt{N}} + \frac{N-1}{\sqrt{N}}}{N} = \frac{N-2}{N\sqrt{N}} \approx \frac{1}{\sqrt{N}}$$

Suppose we design a quantum circuit such that  $\alpha_x$  becomes  $2\mu - \alpha_x$  for all  $x$ .

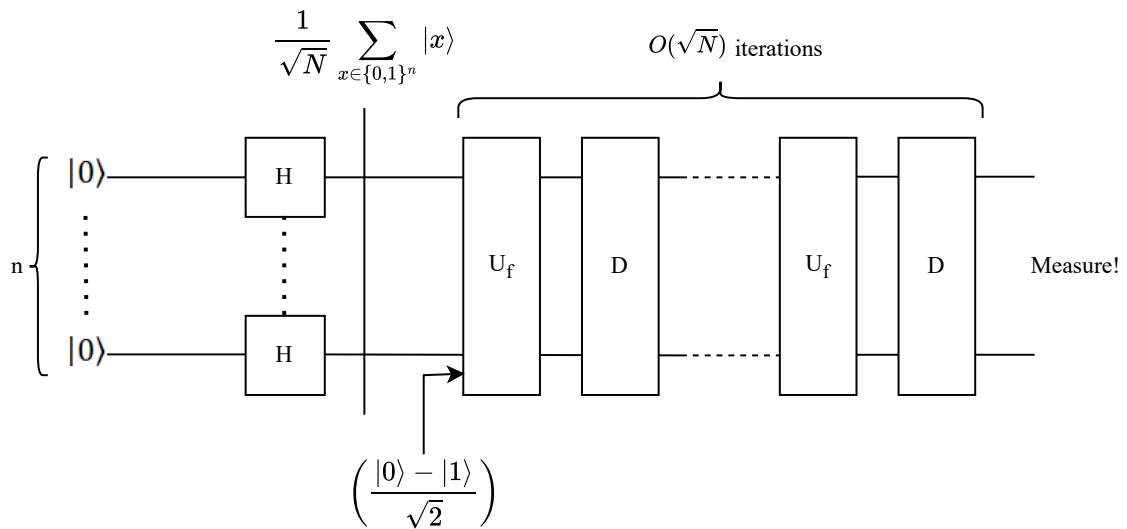
$$D \left( \sum_{x \in \{0,1\}^n} \alpha_x |x\rangle \right) = \sum_{x \in \{0,1\}^n} (2\mu - \alpha_x) |x\rangle$$

When  $x = x^*$ ,  $\alpha_{x^*}$  becomes  $2\mu - \alpha_{x^*} \approx \frac{2}{\sqrt{N}} - \left(-\frac{1}{\sqrt{N}}\right) = \frac{3}{\sqrt{N}}$

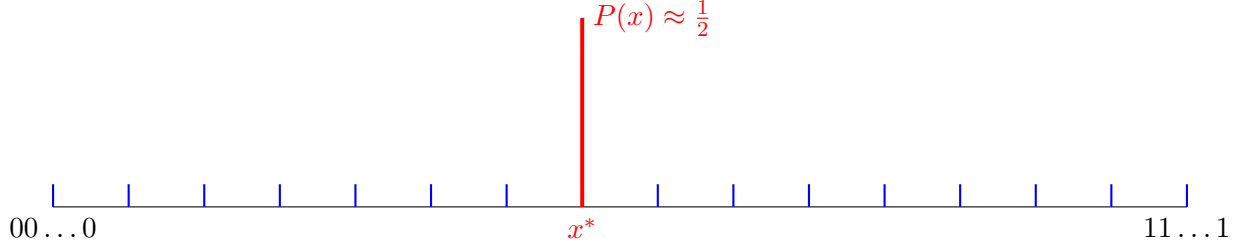
When  $x \neq x^*$ ,  $\alpha_x$  becomes  $2\mu - \alpha_x \approx \frac{2}{\sqrt{N}} - \frac{1}{\sqrt{N}} = \frac{1}{\sqrt{N}}$



### 3.5 Multiple Iterations of Amplitude Amplification



We repeat the oracle ( $U_f$ ) and diffusion operator combination multiple times until the probability of finding  $x^*$  becomes  $\frac{1}{2}$  (after roughly  $\frac{\sqrt{N}}{4}$  iterations). Then we stop!



Why do we stop when the amplitude of  $x^*$  becomes half?

- If we continue iterating beyond this point, the amplitude  $\alpha_{x^*}$  becomes very large.
- The average amplitude becomes negative.

$$\mu = \frac{-\alpha_{x^*} + \sum_{x \neq x^*} \alpha_x}{N} < 0$$

- This happens when  $\alpha_{x^*} > \sum_{x \neq x^*} \alpha_x$
- When the average  $\mu$  becomes negative, it works against our efforts.  $2\mu$  is negative and  $\alpha_{x^*}$  is very large. So the result,  $2\mu - \alpha_{x^*}$  decreases, reducing the amplitude of  $x^*$ .
- Therefore the probability of finding  $x^*$  decreases instead of increasing!