

① Grover search algorithm

② Simon's algorithm

▣ Grover search algorithm

(I) Algorithm (Review)

- Problem: Given a data set S with a labeled elements $s \in A$ we are able to check if a given $x \in A$ is the solution or not

$$f(x) = \begin{cases} 1 & x = s \\ 0 & x \neq s \end{cases}$$

our goal is to find target element x^* using the fewest queries possible.

- Classical brute-force search $|A| = N$
 - ▷ in the worst case, we must query all N possible elements
 - ▷ on average, query half of the elements
 - ▷ complexity: $O(N)$
- Grover's algorithm

▷ oracle (subroutine): we are still able to check if a given element is the solution or not

$$f(x) = \begin{cases} 1, & x = s \\ 0, & x \neq s \end{cases}$$

Quantum description:

$$\textcircled{1} \tilde{U}_f^A |\alpha\rangle = (-1)^{f(\alpha)} |\alpha\rangle = \begin{cases} -|\alpha\rangle, & \alpha = s \\ |\alpha\rangle, & \alpha \neq s \end{cases} \quad \tilde{U}_f = \mathbb{I} - 2|s\rangle\langle s|$$

$$\textcircled{2} U_f^{AB} |\alpha\rangle_A |z\rangle_B = |\alpha\rangle_A |z \oplus f(\alpha)\rangle_B$$

$$\begin{aligned} U_f(|\alpha\rangle |-\rangle) &= \frac{1}{\sqrt{2}} (U_f(|\alpha\rangle |0\rangle) - U_f(|\alpha\rangle |1\rangle)) \\ &= \frac{1}{\sqrt{2}} (|\alpha\rangle |f(\alpha)\rangle - |\alpha\rangle |1 \oplus f(\alpha)\rangle) \\ &= (\hat{U}_f |\alpha\rangle) |-\rangle \end{aligned}$$

▷ Reflection

$$|\psi\rangle = \frac{1}{\sqrt{N}} \sum_x |\alpha\rangle = H^{\otimes n} |0\rangle \otimes \dots \otimes |0\rangle$$

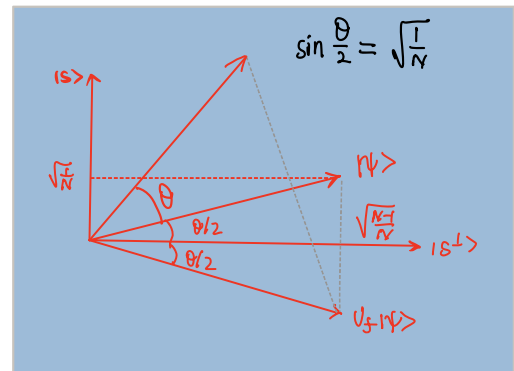
$$U_\psi = 2|\psi\rangle\langle\psi| - \mathbb{I} = H^{\otimes n} (2|0\rangle\langle 0| - \mathbb{I}) H^{\otimes n}$$

▷ Grover operation

$$G = U_\psi \tilde{U}_f$$

$$|s\rangle, |s^\perp\rangle = \frac{1}{\sqrt{N-1}} \sum_{x \neq s} |\alpha\rangle$$

$$|\psi\rangle = \frac{1}{\sqrt{N}} |s\rangle + \sqrt{\frac{N-1}{N}} |s^\perp\rangle$$



Algorithm:

- ① initial state $|\psi\rangle = H^{\otimes n} (|0\rangle \otimes \dots \otimes |0\rangle)$
- ② apply Grover iteration $G^k |\psi\rangle = |s^{(k)}\rangle \approx |s\rangle$
- ③ measure and output $s^{(k)}$

(II) Correctness

(1) Geometric analysis (Done)

(2) Algebraic analysis

• key observation: During the computation, all states are in the plane spanned

by $|S\rangle$ and $|S^\perp\rangle$

• Matrix form

$$\triangleright |S\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad |S^\perp\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\triangleright \hat{U}_\xi |S\rangle = -|S\rangle \quad \hat{U}_\xi |S^\perp\rangle = |S^\perp\rangle$$

$$\hat{U}_\xi = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\begin{aligned} \triangleright U_\psi |S\rangle &= 2|\psi\rangle\langle\psi|S\rangle - |S\rangle \\ &= 2|\psi\rangle\langle\psi|S\rangle - |S\rangle \\ &= 2\sqrt{\frac{1}{N}} \left(\frac{1}{\sqrt{N}} |S\rangle + \sqrt{\frac{N-1}{N}} |S^\perp\rangle \right) - |S\rangle \\ &= 2\frac{1}{N} |S\rangle + \frac{2\sqrt{N-1}}{N} |S^\perp\rangle - |S\rangle \\ &= \frac{2-N}{N} |S\rangle + \frac{2\sqrt{N-1}}{N} |S^\perp\rangle \end{aligned}$$

$$\begin{aligned} U_\psi |S^\perp\rangle &= 2|\psi\rangle\langle\psi|S^\perp\rangle - |S^\perp\rangle \\ &= 2\sqrt{\frac{N-1}{N}} |\psi\rangle - |S^\perp\rangle \\ &= 2\sqrt{\frac{N-1}{N}} \left(\frac{1}{\sqrt{N}} |S\rangle + \sqrt{\frac{N-1}{N}} |S^\perp\rangle \right) - |S^\perp\rangle \\ &= \frac{2\sqrt{N-1}}{N} |S\rangle + \left(\frac{2(N-1)}{N} - 1 \right) |S^\perp\rangle \\ &= \frac{2\sqrt{N-1}}{N} |S\rangle + \frac{N-2}{N} |S^\perp\rangle \end{aligned}$$

$$U_\psi = \begin{pmatrix} \frac{N-2}{N} & \frac{2\sqrt{N-1}}{N} \\ \frac{2\sqrt{N-1}}{N} & \frac{2-N}{N} \end{pmatrix}$$

$$\triangleright G = U_\psi \hat{U}_\xi = \begin{pmatrix} \frac{N-2}{N} & -\frac{2\sqrt{N-1}}{N} \\ \frac{2\sqrt{N-1}}{N} & \frac{N-2}{N} \end{pmatrix}$$

$$\text{Set } \sin\theta = \frac{2\sqrt{N-1}}{N}$$

$$G = \begin{pmatrix} \cos \alpha & -\sin \alpha \\ \sin \alpha & \cos \alpha \end{pmatrix} \quad \text{rotation matrix}$$

$$\begin{aligned} \text{Notice that } \sin \theta &= \sin 2 \times \frac{\theta}{2} \\ &= 2 \sin \frac{\theta}{2} \cos \frac{\theta}{2} \\ &= 2 \sqrt{\frac{1}{N}} \cdot \sqrt{\frac{N-1}{N}} \end{aligned}$$

coincides with the one we give before.

$$\begin{aligned} \triangleright \text{Initial state is } |\psi\rangle &= \sqrt{\frac{1}{N}} |s\rangle + \sqrt{\frac{N-1}{N}} |s^\perp\rangle \\ &= \sin \frac{\theta}{2} |s\rangle + \cos \frac{\theta}{2} |s^\perp\rangle \end{aligned}$$

$$G^k = \begin{pmatrix} \cos k\theta & -\sin k\theta \\ \sin k\theta & \cos k\theta \end{pmatrix}$$

$$|\text{output}\rangle = G^k |\psi\rangle$$

$$= G^k \begin{pmatrix} \cos \frac{\theta}{2} \\ \sin \frac{\theta}{2} \end{pmatrix}$$

$$= \begin{pmatrix} \cos k\theta & -\sin k\theta \\ \sin k\theta & \cos k\theta \end{pmatrix} \begin{pmatrix} \cos \frac{\theta}{2} \\ \sin \frac{\theta}{2} \end{pmatrix}$$

$$= \begin{pmatrix} \cos k\theta \cos \frac{\theta}{2} - \sin k\theta \sin \frac{\theta}{2} \\ \sin k\theta \cos \frac{\theta}{2} + \cos k\theta \sin \frac{\theta}{2} \end{pmatrix}$$

$$= \begin{pmatrix} \cos(k\theta + \frac{\theta}{2}) \rightsquigarrow s^\perp \\ \sin(k\theta + \frac{\theta}{2}) \rightsquigarrow s \end{pmatrix}$$

① After k iteration, the probability of observing the target element s is

$$\begin{aligned} \text{Pr}(\text{output} = s) &= |\langle s | \text{output} \rangle|^2 \\ &= \left[\sin(k\theta + \frac{\theta}{2}) \right]^2 \end{aligned}$$

② For $N \gg 1$, $\sin \frac{\theta}{2} = \sqrt{\frac{1}{N}} \ll 1$, $\frac{\theta}{2} \approx \sqrt{\frac{1}{N}}$
 if the angular error ε is at most $\sqrt{\frac{1}{N}}$, we see that

$$k\theta + \frac{\theta}{2} \geq \frac{\pi}{2} - \frac{\theta}{2}$$

$$\Leftrightarrow (2k+2) \frac{\theta}{2} \geq \frac{\pi}{2}$$

$$2k+2 \geq \frac{\pi}{\theta} \approx \frac{\pi \sqrt{N}}{\sqrt{1/N}} = \pi \sqrt{N}$$

$$k \geq \frac{\pi \sqrt{N} - 2}{2}$$

$$k^* := \left\lceil \frac{\pi \sqrt{N} - 2}{2} \right\rceil + 1$$

★ complexity: $\mathcal{O}(\sqrt{N})$.

(III) More than one solution case

data set N

solution set $1 \leq M < N$

$$|S\rangle = \frac{1}{\sqrt{M}} \sum_{x: \text{sol}} |x\rangle$$

$$|S^\perp\rangle = \frac{1}{\sqrt{N-M}} \sum_{x: \text{not sol}} |x\rangle$$

$$|N\rangle = H^{\otimes N} |0\rangle^{\otimes N} = \sqrt{\frac{M}{N}} |S\rangle + \sqrt{\frac{N-M}{N}} |S^\perp\rangle$$

$$\sin \frac{\theta}{2} = \sqrt{\frac{M}{N}}$$

$$M \ll N \Rightarrow \text{complexity } \mathcal{O}(\sqrt{N/M})$$

(IV) Grover search is optimal

Theorem: Any quantum algorithm that can realize the search with success probability $P_n(\text{succ}) > \frac{1}{2}$ must call the oracle $\Omega(\sqrt{N})$ times.
 $\Omega(\sqrt{N/M})$

Proof. ① General k -call quantum algorithm output state

$$|\text{out}^{(k)}\rangle = U_k \tilde{U}_f U_{k-1} \tilde{U}_f \dots U_1 \tilde{U}_f |\psi\rangle$$

where $|\psi\rangle$ is initial state, U_1, \dots, U_k are unitaries, \tilde{U}_f is oracle operation.

$$\text{Pr}(\text{succ}) = |\langle s | \text{out}^{(k)} \rangle|^2, \quad |s\rangle \text{ is solution state.}$$

② Suppose $\text{Pr}(\text{succ}) > 1/2$, viz., $|\langle s | \text{out}^{(k)} \rangle|^2 > 1/2$, we have

$$\| |\text{out}^{(k)}\rangle - |s\rangle \|^2 = 2 - 2|\langle s | \text{out}^{(k)} \rangle| \leq 2 - \sqrt{2}$$

Take average over all possible solution elements

$$\sum_k = \sum_s \| |\text{out}_s^{(k)}\rangle - |s\rangle \|^2 \leq (2 - \sqrt{2}) N.$$

③ Denote $|\phi^{(k)}\rangle = U_k \dots U_1 |\psi\rangle$

$$\mathcal{D}_k = \sum_s \| |\text{out}_s^{(k)}\rangle - |\phi^{(k)}\rangle \|^2$$

Claim: $\mathcal{D}_k \leq 4k^2$

proof: Mathematical induction. (Exercise)

▷ $k=0$, true

▷ suppose k case true

$$\mathcal{D}_{k+1} = \sum_s \| |\text{out}_s^{(k+1)}\rangle - |\phi^{(k+1)}\rangle \|^2$$

$$= \sum_s \| U_k \tilde{U}_f U_{k-1} \tilde{U}_f \dots \tilde{U}_f |\psi\rangle - U_k \dots U_1 |\psi\rangle \|^2$$

$$= \sum_s \| U_k [\tilde{U}_f U_{k-1} \dots \tilde{U}_f |\psi\rangle - U_{k-1} \dots U_1 |\psi\rangle] \|^2$$

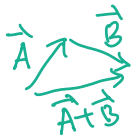
$$= \sum_s \| \tilde{U}_f |\text{out}_s^{(k-1)}\rangle - |\phi^{(k-1)}\rangle \|^2$$

$$= \sum_s \| \tilde{U}_f |\text{out}_s^{(k-1)}\rangle - \tilde{U}_f |\phi^{(k-1)}\rangle + \tilde{U}_f |\phi^{(k-1)}\rangle - |\phi^{(k-1)}\rangle \|^2$$

$$= \sum_s \| \underbrace{\tilde{U}_f (|\text{out}_s^{(k-1)}\rangle - |\phi^{(k-1)}\rangle)}_A + \underbrace{(\tilde{U}_f - I) |\phi^{(k-1)}\rangle}_B \|^2$$

$$\leq \sum_s \| A \|^2 + 2 \| A \| \| B \| + \| B \|^2$$

$$\text{Notice } B = (\tilde{U}_f - I) |\phi^{(k-1)}\rangle$$



$$\begin{aligned} & \| \vec{A} + \vec{B} \|^2 \\ & \leq \| \vec{A} \|^2 + \| \vec{B} \|^2 \\ & \quad + 2 \| \vec{A} \| \cdot \| \vec{B} \| \end{aligned}$$

$$= -2 |S\rangle \langle S| \phi^{(k-1)}\rangle$$

$$D_{k+1} \leq D_k + 2 \|A\| \|B\| + \sum_S 4 |\langle S| \phi^{(k-1)}\rangle|^2$$

$$= D_k + 2 \|A\| \|B\| + 4$$

$$2 \|A\| \|B\| = 4 \left\| \sum_S (|out_S^{k-1}\rangle - |\phi^{(k-1)}\rangle) \cdot |S\rangle \langle \phi^{(k-1)}| \right\|$$

$$= 4 a_S \cdot b_S$$

$$\sum_S a_S \cdot b_S \leq \left(\sum_S a_S^2 \right)^{1/2} \left(\sum_S b_S^2 \right)^{1/2}$$

$$= \sqrt{D_k} \cdot 1$$

$$D_{k+1} \leq D_k + 4\sqrt{D_k} + 4$$

$$\leq 4k^2 + 4\sqrt{4k^2} + 4$$

$$= 4k^2 + 8k + 4 = 4(k+1)^2$$

$$\textcircled{4}. \quad D_k = \sum_S \left\| |out_S^k\rangle - |\phi^k\rangle \right\|^2$$

$$= \sum_S \left\| \underbrace{|out_S^k\rangle}_{J_S} - \underbrace{|\phi^k\rangle}_{K_S} \right\|^2$$

$$\geq \sum_S J_S^2 - 2|J_S| |K_S| + K_S^2$$

$$= E_k + \underbrace{\sum_S \left\| |\phi^k\rangle - |S\rangle \right\|^2}_{F_k} - \sum_S 2 |J_S| \cdot |K_S|$$

$$\sum_S 2 |J_S| \cdot |K_S| \leq 2 \left(\sum_S |J_S|^2 \right)^{1/2} \left(\sum_S |K_S|^2 \right)^{1/2}$$

$$\leq 2 \sqrt{E_k F_k}$$

$$D_k \geq E_k + F_k - 2\sqrt{E_k F_k}$$

$$= \left(\sqrt{F_k} - \sqrt{E_k} \right)^2$$

Using the fact that for N basis $|S\rangle$ and a $|\Psi\rangle$

$$\sum_S \left\| |S\rangle - |\Psi\rangle \right\|^2 \geq 2N - 2\sqrt{N}$$

we see $F_k \geq 2N - 2\sqrt{N}$

\textcircled{5} Now using \textcircled{3} and \textcircled{4} we have

$$D_k \geq \left(\sqrt{F_k} - \sqrt{E_k} \right)^2$$

$$\geq M \cdot \sqrt{N} \quad M \text{ is a constant.}$$

Simon's algorithm

(I) Simon's problem \equiv Hidden subgroup problem.

▷ Given a periodic function $f: \{0,1\}^n \rightarrow \{0,1\}^n$,
find the period s of the function such that
 $f(x \oplus s) = f(x)$,
where addition is bit-wise and modulo 2.

▷ $f(x) = f(y)$ if and only if $x \oplus y \in \{0^n, s\}$.

▷ $x \oplus s = y \Leftrightarrow x = y \oplus s \Leftrightarrow s = x \oplus y$

• Example. $n=3, s=110$

x	$x \oplus s$
000	110
001	111
\vdots	\vdots

(II) Classical solution.

① Input pair x, y , check if $f(x) = f(y)$

② If $f(x) = f(y)$, $s = x \oplus y$.

Complexity $\mathcal{O}(2^{n-1} + 1) = \mathcal{O}(\sqrt{N} + 1)$

↑ brute-force check

(III) Simon's algorithm.

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

- Hadamard gate $H^{\otimes n}$

$$|0 \dots 0\rangle \rightarrow |+\dots+\rangle |0 \dots 0\rangle$$

Recall $H|x\rangle = \frac{1}{\sqrt{2}}(|0\rangle + (-1)^x|1\rangle) = \frac{1}{\sqrt{2}} \sum_z (-1)^{x \cdot z} |z\rangle$

$$H^{\otimes n} |x_1 \dots x_n\rangle = \frac{1}{\sqrt{2^n}} \sum_z (-1)^{z \cdot x} |z_1 \dots z_n\rangle$$

- Algorithm:

① initial state $|0 \dots 0\rangle_A |0 \dots 0\rangle_B$

② Apply $H^{\otimes n}_A$ $\frac{1}{\sqrt{2^n}} \sum_x |x\rangle |0 \dots 0\rangle$

③ Apply oracle $\frac{1}{\sqrt{2^n}} \sum_x |x\rangle |f(x)\rangle$

④ Apply $H^{\otimes n}_A$ $\frac{1}{\sqrt{2^n}} \sum_x \frac{1}{\sqrt{2^n}} \sum_z (-1)^{x \cdot z} |z\rangle |f(x)\rangle$

⑤ if $x' = x'' \oplus s$, $f(x') = f(x'' \oplus s) = q$

by measuring $|q\rangle$ over B part, we obtain

$$\frac{1}{\sqrt{2}} \frac{1}{\sqrt{2^n}} \sum_z [(-1)^{x' \cdot z} + (-1)^{x'' \cdot z}] |z\rangle |q\rangle$$

- ⑥ Now measure A part

$$(-1)^{x' \cdot z} + (-1)^{x'' \cdot z} = \begin{cases} \pm 2 & x' \cdot z = x'' \cdot z \\ 0 & x' \cdot z \neq x'' \cdot z \end{cases}$$

determine z such that

$$x' \cdot z = x'' \cdot z$$

This is equivalent to

$$(x' \oplus x'') \cdot z = 0$$

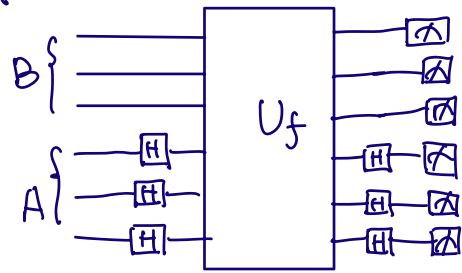
$$\Leftrightarrow s \cdot z = 0$$

$$s_1 z_1 \oplus \dots \oplus s_n z_n = 0$$

We obtain one equation.

- ⑦ Repeat $O(n)$ times, we obtain n equations, from which we can solve s .

Circuit:



Complexity $\Theta(n) = \Theta(\log N)$