### Grover's algorithm

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16, Nov., 2021

# Searching problem

#### Searching problem:

$$f: \{1, 2, ..., N\} \rightarrow \{0, 1\}$$

Find  $x \in \{1, 2, ..., N\}$  satisfying f(x) = 1.

How many times, do we have to evaluate f(x)?

Obviously, O(N).

### Quantum searching problem

Unitary oracle

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

Find  $x \in \{1, 2, ..., N\}$  satisfying f(x) = 1.

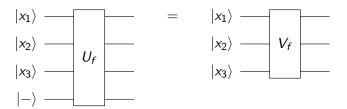
How many times, do we have to evaluate  $U_f$ ?

 $O(\sqrt{N})$  by Grover's algorithm.

#### Unitary matrix for Grover's algorithm

#### Another unitary

$$V_f|x\rangle=(-1)^{f(x)}|x\rangle$$
.



$$|x\rangle |-\rangle \longmapsto U_f |x\rangle |-\rangle = (-1)^{f(x)} |x\rangle |-\rangle.$$

#### Grover's algorithm

$$|\psi\rangle := \frac{1}{\sqrt{N}} \sum_{x=1}^{N} |x\rangle$$

$$V_f = I - 2 \sum_{x=1}^{N} |x\rangle \langle x|$$

$$W := I - 2 |\psi\rangle \langle \psi|$$
.

Then,  $G := -WV_f$  is called the Grover's operator.

The Grover's algorithm just measures  $G^k | \psi \rangle$  by the computational basis  $\{|x\rangle\}_x$  for some appropriately chosen k.

#### The two dimensional subspace

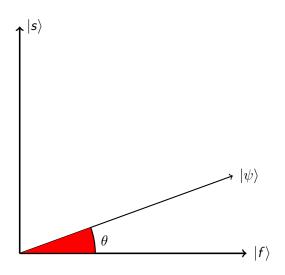
$$|s\rangle := \frac{1}{\sqrt{M}} \sum_{x:f(x)=1} |x\rangle$$

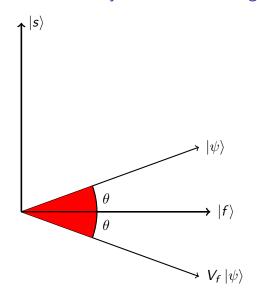
$$|f\rangle := \frac{1}{\sqrt{N-M}} \sum_{x:f(x)=0} |x\rangle.$$

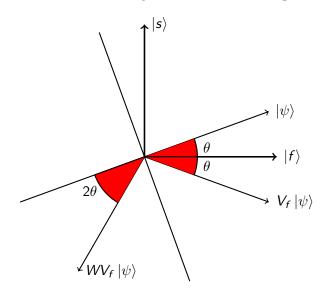
Then,

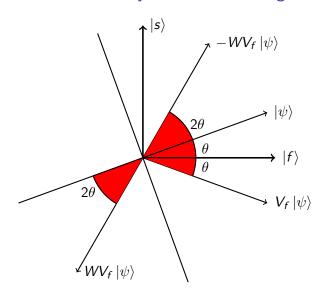
$$|\psi\rangle = \frac{1}{\sqrt{N}} \sum_{x=1}^{N} |x\rangle = \sqrt{\frac{M}{N}} |s\rangle + \sqrt{\frac{N-M}{N}} |f\rangle$$
$$= \sin\theta |s\rangle + \cos\theta |f\rangle$$

where 
$$\theta = \arcsin \sqrt{\frac{M}{N}}$$
.









$$(-WV_f)^k |\psi\rangle = \sin((2k+1)\theta)|s\rangle + \cos((2k+1)\theta)|f\rangle$$

The probability of success is  $\sin^2((2k+1)\theta)$ .

Choose k satisfying

$$(2k+1)\theta \approx \frac{\pi}{2} \iff k \approx \frac{\pi}{4\theta}$$

Here, 
$$\sin\theta = \sqrt{\frac{M}{N}} \iff \theta \approx \sqrt{\frac{M}{N}}$$
. Hence,  $k \approx \frac{\pi}{4} \sqrt{\frac{N}{M}}$ .

[Grover 1996]

#### Grover's algorithm

[Boyer, Brassard, Høyer, and Tapp 1998]

- 1 Initialize m=1 and set  $\lambda=8/7$ .
- 2 Choose an integer j uniformly from 0, 1, ..., m.
- **3** Apply Grover's algorithm with j iterations.
- 4 If solution is not found, set  $m \leftarrow \min(\lambda m, \sqrt{N})$  and go back to setp 2.

This algorithm solves the "OR problem" with  $O(\sqrt{N/M})$  query for  $U_f$ .

#### Applications of Grover's algorithm

- $O^*(2^{n/2})$  algorithm for SAT.
- $O^*(2^{n/3})$  algorithm for the subset sum [Brassard et al. 1997].
- $O(1.728^n)$  algorithm for the travelling salesman problem [Ambainis et al. 2019].
- O(1.914<sup>n</sup>) algorithm for the graph coloring problem [Shimizu and Mori 2020].

#### Optimality of Grover's search

Let  $V_x := I - 2|x\rangle \langle x|$ .

$$|\psi_x^i\rangle := (U_k V_x U_{k-1} V_x \cdots U_{i+1} V_x)(U_i U_{i-1} \cdots U_1) |\psi_0\rangle$$

$$|\psi_x^0\rangle = U_k V_x U_{k-1} V_x \cdots V_x U_1 V_x |\psi_0\rangle$$
  

$$|\psi_x^k\rangle = U_k U_{k-1} \cdots U_1 |\psi_0\rangle$$

For any "distance" function D for  $\{|a\rangle\in\mathbb{C}^N\mid \langle a|a\rangle=1\}$ ,

$$\frac{1}{N}\sum D\left(\left|x\right\rangle,\left|\neq x\right\rangle\right)$$

$$\leq \frac{1}{N}\sum_{\mathbf{x}}\left(D\left(\left|\mathbf{x}\right\rangle,\left|\psi_{\mathbf{x}}^{0}\right\rangle\right) + \sum_{i=0}^{k-1}D\left(\left|\psi_{\mathbf{x}}^{i}\right\rangle,\left|\psi_{\mathbf{x}}^{i+1}\right\rangle\right) + D\left(\left|\psi_{\mathbf{x}}^{k}\right\rangle,\left|\neq\mathbf{x}\right\rangle\right)\right).$$

#### "Distance" function

Let

$$D(|a\rangle, |b\rangle) := \arccos |\langle a|b\rangle|.$$

For any normalized  $|a\rangle$ ,  $|b\rangle$ ,  $|c\rangle$ ,

$$\begin{bmatrix} 1 & \langle a|b\rangle & \langle a|c\rangle \\ \langle b|a\rangle & 1 & \langle b|c\rangle \\ \langle c|a\rangle & \langle c|b\rangle & 1 \end{bmatrix} \succeq 0.$$

The determinant of this matrix is

$$\begin{split} &1 + \langle a|b\rangle\,\langle b|c\rangle\,\langle c|a\rangle + \langle a|c\rangle\,\langle b|a\rangle\,\langle c|b\rangle \\ &- \langle b|c\rangle\,\langle c|b\rangle - \langle a|c\rangle\,\langle c|a\rangle - \langle a|b\rangle\,\langle b|a\rangle \geq 0. \end{split}$$

#### The triangle inequality

$$\begin{aligned} 1 + \langle a|b\rangle \langle b|c\rangle \langle c|a\rangle + \langle a|c\rangle \langle b|a\rangle \langle c|b\rangle \\ - |\langle b|c\rangle|^2 - |\langle a|c\rangle|^2 - |\langle a|b\rangle|^2 &\geq 0 \\ \Longrightarrow \quad 1 + |\langle a|b\rangle \langle b|c\rangle \langle c|a\rangle + |\langle a|c\rangle \langle b|a\rangle \langle c|b\rangle + \\ - |\langle b|c\rangle|^2 - |\langle a|c\rangle|^2 - |\langle a|b\rangle|^2 &\geq 0 \\ \Longleftrightarrow \quad 1 + \cos(\theta_{ab})\cos(\theta_{bc})z + z\cos(\theta_{ab})\cos(\theta_{bc}) \\ - \cos^2(\theta_{bc}) - z^2 - \cos^2(\theta_{ab}) &\geq 0 \\ \Longleftrightarrow \quad z^2 - 2\cos(\theta_{ab})\cos(\theta_{bc})z \\ + \cos^2(\theta_{bc}) + \cos^2(\theta_{ab}) - 1 &\leq 0 \\ \Longleftrightarrow \quad (z - \cos(\theta_{ab})\cos(\theta_{bc}))^2 - \cos^2(\theta_{ab})\cos^2(\theta_{bc}) \\ + \cos^2(\theta_{bc}) + \cos^2(\theta_{ab}) - 1 &\leq 0 \\ \Longleftrightarrow \quad (z - \cos(\theta_{ab})\cos(\theta_{bc}))^2 &\leq (1 - \cos^2(\theta_{ab})) (1 - \cos^2(\theta_{bc})) \end{aligned}$$

#### The triangle inequality

$$(z - \cos(\theta_{ab})\cos(\theta_{bc}))^{2} \leq \sin^{2}(\theta_{ab})\sin^{2}(\theta_{bc})$$

$$\Rightarrow z \geq \cos(\theta_{ab})\cos(\theta_{bc}) - \sin(\theta_{ab})\sin(\theta_{bc})$$

$$\Leftrightarrow z \geq \cos(\theta_{ab} + \theta_{bc})$$

$$\Leftrightarrow \arccos(|\langle c|a\rangle|) \leq \theta_{ab} + \theta_{bc} \quad \text{arccos is decreasing for } [-1, +1]$$

$$\Leftrightarrow \theta_{ca} \leq \theta_{ab} + \theta_{bc}$$

### Symmetrization

Let  $P_{\sigma}$  be a permutation matrix satisfying  $P_{\sigma}|x\rangle = |\sigma(x)\rangle$  for a permutation  $\sigma$  on  $\{1, 2, ..., N\}$ .

#### Symmetrization of algorithm U:

- **1** Choose a permutation  $\sigma$  with uniform probability.
- 2 Run  $U_{\sigma}$  that is U in which all  $V_x$  is replaced by  $P_{\sigma}V_xP_{\sigma}^{\dagger}$ . Note that  $P_{\sigma}V_xP_{\sigma}^{\dagger}=V_{\sigma(x)}$
- 3 Measure the state  $U_{\sigma} | \psi_0 \rangle$ , and obtain an outcome y. Output  $\sigma^{-1}(y)$ .

Let  $p_{\text{succ}}(x)$  be the probability of success of the algorithm U if the oracle is  $V_x$ .

Then, the probability of success of the modified algorithm  $U_{\sigma}$  is  $p_{\text{succ}}(\sigma(x))$ . The probability of success of the symmetrized algorithm is  $\frac{1}{N!}\sum_{\sigma}p_{\text{succ}}(\sigma(x))=\frac{1}{N}\sum_{z}p_{\text{succ}}(z)$  regardless of the choice of the oracle  $V_{x}$ .

#### **Inequalities**

$$\begin{split} &\frac{\pi}{2} = \frac{1}{N} \sum_{x} D\left(\left|x\right\rangle, \left|\neq x\right\rangle\right) \\ &\leq \frac{1}{N} \sum_{x} \left(D\left(\left|x\right\rangle, \left|\psi_{x}^{0}\right\rangle\right) + \sum_{i=0}^{k-1} D\left(\left|\psi_{x}^{i}\right\rangle, \left|\psi_{x}^{i+1}\right\rangle\right) + D\left(\left|\psi_{x}^{k}\right\rangle, \left|\neq x\right\rangle\right)\right). \\ &\frac{1}{N} \sum_{x} D\left(\left|x\right\rangle, \left|\psi_{x}^{0}\right\rangle\right) = \frac{1}{N} \sum_{x} \arccos\left(\left|\left\langle x\right|\psi_{x}^{0}\right\rangle\right|\right) = \arccos\left(\sqrt{p_{\text{succ}}}\right). \end{split}$$

 $\frac{1}{N}\sum D\left(\left|\psi_{x}^{k}\right\rangle ,\left|\neq x\right\rangle \right)=\frac{1}{N}\sum \arccos\left(\left|\left\langle \psi_{x}^{k}\right|\neq x\right\rangle \right|\right)=\arccos\left(\sqrt{1-\frac{1}{N}}\right).$ 

#### **Inequalities**

$$\begin{split} \frac{1}{N} \sum_{x} D\left(\left|\psi_{x}^{i}\right\rangle, \left|\psi_{x}^{i+1}\right\rangle\right) &= \frac{1}{N} \sum_{x} \arccos\left(\left|\left\langle\psi_{x}^{i}\right|\psi_{x}^{i+1}\right\rangle\right|\right) \\ &= \frac{1}{N} \sum_{x} \arccos\left(\left|\left\langle\varphi\right| V_{x} \left|\varphi\right\rangle\right|\right) \leq \arccos\left(\frac{1}{N} \sum_{x} \left|\left\langle\varphi\right| V_{x} \left|\varphi\right\rangle\right|\right) \\ &\leq \arccos\left(\left|\frac{1}{N} \sum_{x} \left\langle\varphi\right| V_{x} \left|\varphi\right\rangle\right|\right) = \arccos\left(\left|\left\langle\varphi\right| \left(1 - \frac{2}{N}\right) I \left|\varphi\right\rangle\right|\right) \\ &= \arccos\left(1 - \frac{2}{N}\right) \end{split}$$

## Put everything together

$$\frac{\pi}{2} = \frac{1}{N} \sum_{x} D\left(|x\rangle, | \neq x\rangle\right)$$

$$\leq \frac{1}{N} \sum_{x} \left(D\left(|x\rangle, |\psi_{x}^{0}\rangle\right) + \sum_{i=0}^{k-1} D\left(|\psi_{x}^{i}\rangle, |\psi_{x}^{i+1}\rangle\right) + D\left(|\psi_{x}^{k}\rangle, | \neq x\rangle\right)\right)$$

$$\leq \arccos\left(\sqrt{p_{\text{succ}}}\right) + k \arccos\left(1 - \frac{2}{N}\right) + \arccos\left(\sqrt{1 - \frac{1}{N}}\right)$$
Since  $\theta = \arccos\left(\sqrt{\frac{N-1}{N}}\right)$ ,
$$\frac{\pi}{2} \leq \arccos\left(\sqrt{p_{\text{succ}}}\right) + 2k\theta + \theta$$

$$\iff \cos\left(\frac{\pi}{2} - (2k+1)\theta\right) \geq \sqrt{p_{\text{succ}}} \quad \text{if } (2k+1)\theta \leq \frac{\pi}{2}$$

$$\iff \sin^{2}\left((2k+1)\theta\right) > p_{\text{succ}}.$$

#### Summary

- Grover's search solves the quantum searching problem in time  $O(\sqrt{N})$ .
- Grover's search is exactly optimal if M = 1 [Zalka 1999].
- For general *M*, Grover's search is asymptotically optimal [Ito and Mori 2021].

#### Assignments

**1** Show two distinct eigenvalues and corresponding eigenvectors of the Grover operator  $-WV_f$ .