Understanding Quantum Information and Computation

Fundamentals of quantum algorithms

Lesson 4: Grover's algorithm

Contents

1. Unstructured search

Unstructured search

Let $\Sigma = \{0, 1\}$ denote the binary alphabet (throughout the lesson).

Suppose we're given a function

$$f : \Sigma^n \rightarrow \Sigma$$

that we can *compute efficiently.*

Our goal is to find a *solution,* which is a binary string $x \in \Sigma^n$ for which $f(x) = 1$.

Search

Input: $f : \Sigma^n \rightarrow \Sigma$

Output: a string $x \in \Sigma^n$ satisfying $f(x) = 1$, or "no solution" if no such strings exist

This is *unstructured* search because f is arbitrary — there's *no promise* and we can't rely on it having a structure that makes finding solutions easy.

Algorithms for search

Search

Input: $f : \Sigma^n \rightarrow \Sigma$

Output: a string $x \in \Sigma^n$ satisfying $f(x) = 1$, or "no solution" if no such strings exist

Hereafter let us write

$$N = 2^n$$

By iterating through all $x \in \Sigma^n$ and evaluating f on each one, we can solve Search with N queries.

This is the best we can do with a *deterministic* algorithm.

Probabilistic algorithms offer minor improvements, but still require a number of queries linear in N.

Grover's algorithm is a *quantum algorithm* for Search requiring $O(\sqrt{N})$ queries.

Phase query gates

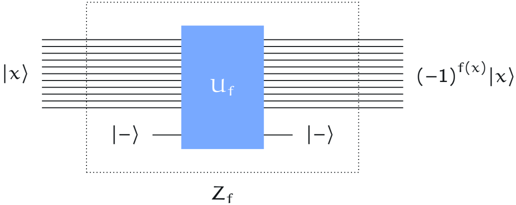
We assume that we have access to the function $f : \Sigma^n \rightarrow \Sigma$ through a query gate:

$$U_f : |a\rangle|x\rangle \mapsto |a \oplus f(x)\rangle|x\rangle \qquad \text{(for all } a \in \Sigma \text{ and } x \in \Sigma^n\text{)}$$

(We can build a circuit for U_f given a Boolean circuit for f.)

The *phase query gate* for f operates like this:

$$Z_f : |x\rangle \mapsto (-1)^{f(x)}|x\rangle \qquad \left(\text{for all } x \in \Sigma^n\right)$$



Exercise: show how to build a U_f operation using a *controlled* Z_f operation.

Phase query gates

The *phase query gate* for f operates like this:

$$Z_f : |x\rangle \mapsto (-1)^{f(x)}|x\rangle \qquad (\text{for all } x \in \Sigma^n)$$

We're also going to need a phase query gate for the n-bit OR function:

$$\mathrm{OR}(x) = \begin{cases} 0 & x = 0^n \\ 1 & x \neq 0^n \end{cases} \qquad (\text{for all } x \in \Sigma^n)$$

$$Z_{\mathrm{OR}}|x\rangle = \begin{cases} |x\rangle & x = 0^n \\ -|x\rangle & x \neq 0^n \end{cases} \qquad (\text{for all } x \in \Sigma^n)$$

2. Grover’s algorithm

Algorithm description

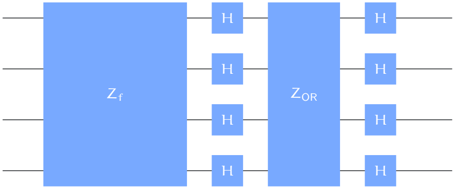
Grover's algorithm

1. *Initialize:* set n qubits to the state $H^{\otimes n}|0^n\rangle$.
2. *Iterate:* apply the *Grover operation* t times (for t to be specified later).
3. *Measure:* a standard basis measurement yields a candidate solution.

The Grover operation is defined like this:

$$G = H^{\otimes n} Z_{\mathrm{OR}} H^{\otimes n} Z_f$$

Z_f is the phase query gate for f and Z_{OR} is the phase query gate for the n-bit OR function.



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A typical way that Grover's algorithm can be applied:

1. Choose the number of iterations t (next section).
2. Run Grover's algorithm with t iterations to get a candidate solution x.
3. Check the solution. If $f(x) = 1$ then output x, otherwise either run Grover's algorithm again (possibly with a different t) or report "no solutions."

Solutions and non-solutions

We'll refer to the n qubits being used for Grover's algorithm as a register Q.

We're interested in what happens when Q is initialized to the state $H^{\otimes n}|0^n\rangle$ and the Grover operation G is performed iteratively.

$$G = H^{\otimes n} Z_{\mathrm{OR}} H^{\otimes n} Z_f$$

These are the sets of non-solutions and solutions:

$$A_0 = \{x \in \Sigma^n : f(x) = 0\}$$
$$A_1 = \{x \in \Sigma^n : f(x) = 1\}$$

We will be interested in *uniform superpositions* over these sets:

$$|A_0\rangle = \frac{1}{\sqrt{|A_0|}} \sum_{x \in A_0} |x\rangle$$
$$|A_1\rangle = \frac{1}{\sqrt{|A_1|}} \sum_{x \in A_1} |x\rangle$$

Analysis: basic idea

$$A_0 = \{x \in \Sigma^n : f(x) = 0\} \qquad A_1 = \{x \in \Sigma^n : f(x) = 1\}$$

$$|A_0\rangle = \frac{1}{\sqrt{|A_0|}} \sum_{x \in A_0} |x\rangle \qquad |A_1\rangle = \frac{1}{\sqrt{|A_1|}} \sum_{x \in A_1} |x\rangle$$

The register Q is first initialized to this state:

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

This state is contained in the subspace spanned by $|A_0\rangle$ and $|A_1\rangle$:

$$|u\rangle = \sqrt{\frac{|A_0|}{N}}|A_0\rangle + \sqrt{\frac{|A_1|}{N}}|A_1\rangle$$

The state of Q *remains in this subspace* after every application of the Grover operation G.

Action of the Grover operation

We can better understand the Grover operation by splitting it into two parts:

$$G = \left(H^{\otimes n} Z_{\mathrm{OR}} H^{\otimes n}\right)\left(Z_f\right)$$

1. Recall that Z_f is defined like this:

   $$Z_f|x\rangle = (-1)^{f(x)}|x\rangle \qquad \left(\text{for all } x \in \Sigma^n\right)$$

   Its action on $|A_0\rangle$ and $|A_1\rangle$ is simple:

   $$\begin{aligned} Z_f|A_0\rangle &= |A_0\rangle \\ Z_f|A_1\rangle &= -|A_1\rangle \end{aligned}$$

Action of the Grover operation

We can better understand the Grover operation by splitting it into two parts:

$$G = \left(H^{\otimes n} Z_{\mathrm{OR}} H^{\otimes n}\right)\left(Z_f\right)$$

2. The operation Z_{OR} is defined like this:

$$Z_{\mathrm{OR}}\vert x\rangle = \begin{cases} \vert x\rangle & x = 0^n \\ -\vert x\rangle & x \neq 0^n \end{cases} \qquad \text{(for all } x \in \Sigma^n\text{)}$$

Here's an alternative way to express Z_{OR}:

$$Z_{\mathrm{OR}} = 2\vert 0^n\rangle\langle 0^n\vert - \mathbb{1}$$

Using this expression, we can write $H^{\otimes n} Z_{\mathrm{OR}} H^{\otimes n}$ like this:

$$H^{\otimes n} Z_{\mathrm{OR}} H^{\otimes n} = H^{\otimes n}\left(2\vert 0^n\rangle\langle 0^n\vert - \mathbb{1}\right)H^{\otimes n} = 2\vert u\rangle\langle u\vert - \mathbb{1}$$

Action of the Grover operation

$$Z_f|A_0\rangle = |A_0\rangle$$
$$Z_f|A_1\rangle = -|A_1\rangle$$

$$|u\rangle = \sqrt{\frac{|A_0|}{N}}|A_0\rangle + \sqrt{\frac{|A_1|}{N}}|A_1\rangle$$

$$\begin{aligned}
G|A_0\rangle &= \left(2|u\rangle\langle u| - \mathbb{1}\right)Z_f|A_0\rangle \\
&= \left(2|u\rangle\langle u| - \mathbb{1}\right)|A_0\rangle \\
&= 2\sqrt{\frac{|A_0|}{N}}|u\rangle - |A_0\rangle \\
&= 2\sqrt{\frac{|A_0|}{N}}\left(\sqrt{\frac{|A_0|}{N}}|A_0\rangle + \sqrt{\frac{|A_1|}{N}}|A_1\rangle\right) - |A_0\rangle \\
&= \frac{|A_0| - |A_1|}{N}|A_0\rangle + \frac{2\sqrt{|A_0| \cdot |A_1|}}{N}|A_1\rangle
\end{aligned}$$

Action of the Grover operation

$$Z_f|A_0\rangle = |A_0\rangle$$
$$Z_f|A_1\rangle = -|A_1\rangle$$

$$|u\rangle = \sqrt{\frac{|A_0|}{N}}|A_0\rangle + \sqrt{\frac{|A_1|}{N}}|A_1\rangle$$

$$G|A_0\rangle = \frac{|A_0| - |A_1|}{N}|A_0\rangle + \frac{2\sqrt{|A_0|\cdot|A_1|}}{N}|A_1\rangle$$

$$\begin{aligned}
G|A_1\rangle &= \big(2|u\rangle\langle u| - \mathbb{1}\big)Z_f|A_1\rangle \\
&= \big(\mathbb{1} - 2|u\rangle\langle u|\big)|A_1\rangle \\
&= |A_1\rangle - 2\sqrt{\frac{|A_1|}{N}}|u\rangle \\
&= |A_1\rangle - 2\sqrt{\frac{|A_0|}{N}}\left(\sqrt{\frac{|A_0|}{N}}|A_0\rangle + \sqrt{\frac{|A_1|}{N}}|A_1\rangle\right) \\
&= -\frac{2\sqrt{|A_0|\cdot|A_1|}}{N}|A_0\rangle + \frac{|A_0| - |A_1|}{N}|A_1\rangle
\end{aligned}$$

Action of the Grover operation

$$Z_f|A_0\rangle = |A_0\rangle$$
$$Z_f|A_1\rangle = -|A_1\rangle$$

$$|u\rangle = \sqrt{\frac{|A_0|}{N}}|A_0\rangle + \sqrt{\frac{|A_1|}{N}}|A_1\rangle$$

$$G|A_0\rangle = \frac{|A_0| - |A_1|}{N}|A_0\rangle + \frac{2\sqrt{|A_0| \cdot |A_1|}}{N}|A_1\rangle$$

$$G|A_1\rangle = -\frac{2\sqrt{|A_0| \cdot |A_1|}}{N}|A_0\rangle + \frac{|A_0| - |A_1|}{N}|A_1\rangle$$

The action of G on $\text{span}\{|A_0\rangle, |A_1\rangle\}$ can be described by a 2×2 matrix:

$$M = \begin{array}{cc} \begin{pmatrix} \frac{|A_0|-|A_1|}{N} & -\frac{2\sqrt{|A_0|\cdot|A_1|}}{N} \\ \frac{2\sqrt{|A_0|\cdot|A_1|}}{N} & \frac{|A_0|-|A_1|}{N} \end{pmatrix} & \begin{array}{c} |A_0\rangle \\ |A_1\rangle \end{array} \\ \begin{array}{cc} \quad|A_0\rangle & \qquad\qquad |A_1\rangle \end{array} & \end{array}$$

Rotation by an angle

The action of G on $\mathrm{span}\{|\mathcal{A}_0\rangle, |\mathcal{A}_1\rangle\}$ can be described by a 2×2 matrix:

$$M = \begin{pmatrix} \frac{|\mathcal{A}_0|-|\mathcal{A}_1|}{N} & -\frac{2\sqrt{|\mathcal{A}_0|\cdot|\mathcal{A}_1|}}{N} \\ \frac{2\sqrt{|\mathcal{A}_0|\cdot|\mathcal{A}_1|}}{N} & \frac{|\mathcal{A}_0|-|\mathcal{A}_1|}{N} \end{pmatrix} = \begin{pmatrix} \sqrt{\frac{|\mathcal{A}_0|}{N}} & -\sqrt{\frac{|\mathcal{A}_1|}{N}} \\ \sqrt{\frac{|\mathcal{A}_1|}{N}} & \sqrt{\frac{|\mathcal{A}_0|}{N}} \end{pmatrix}^2$$

This is a *rotation* matrix.

$$\begin{pmatrix} \sqrt{\frac{|\mathcal{A}_0|}{N}} & -\sqrt{\frac{|\mathcal{A}_1|}{N}} \\ \sqrt{\frac{|\mathcal{A}_1|}{N}} & \sqrt{\frac{|\mathcal{A}_0|}{N}} \end{pmatrix} = \begin{pmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{pmatrix} \qquad \theta = \sin^{-1}\left(\sqrt{\frac{|\mathcal{A}_1|}{N}}\right)$$

$$M = \begin{pmatrix} \cos(2\theta) & -\sin(2\theta) \\ \sin(2\theta) & \cos(2\theta) \end{pmatrix}$$

Rotation by an angle

$$M = \begin{pmatrix} \cos(2\theta) & -\sin(2\theta) \\ \sin(2\theta) & \cos(2\theta) \end{pmatrix} \qquad \theta = \sin^{-1}\left(\sqrt{\frac{|A_1|}{N}}\right)$$

After the initialization step, this is the state of the register Q:

$$|u\rangle = \sqrt{\frac{|A_0|}{N}}|A_0\rangle + \sqrt{\frac{|A_1|}{N}}|A_1\rangle = \cos(\theta)|A_0\rangle + \sin(\theta)|A_1\rangle$$

Each time the Grover operation G is performed, the state of Q is rotated by an angle 2θ:

$$\begin{aligned} |u\rangle &= \cos(\theta)|A_0\rangle + \sin(\theta)|A_1\rangle \\ G|u\rangle &= \cos(3\theta)|A_0\rangle + \sin(3\theta)|A_1\rangle \\ G^2|u\rangle &= \cos(5\theta)|A_0\rangle + \sin(5\theta)|A_1\rangle \\ &\vdots \\ G^t|u\rangle &= \cos((2t+1)\theta)|A_0\rangle + \sin((2t+1)\theta)|A_1\rangle \end{aligned}$$

Geometric picture

Main idea

The operation $G = H^{\otimes n} Z_{OR} H^{\otimes n} Z_f$ is a composition of *two reflections:*

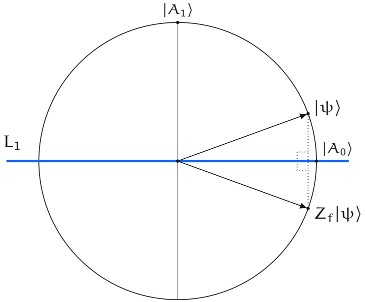
$$Z_f \quad \text{and} \quad H^{\otimes n} Z_{OR} H^{\otimes n}$$

Composing two reflections yields a *rotation.*

1. Recall that Z_f has this action on the 2-dimensional space spanned by $|A_0\rangle$ and $|A_1\rangle$:

$$Z_f|A_0\rangle = |A_0\rangle$$
$$Z_f|A_1\rangle = -|A_1\rangle$$

This is a *reflection* about the line L_1 parallel to $|A_0\rangle$.



Geometric picture

Main idea

The operation $G = H^{\otimes n} Z_{OR} H^{\otimes n} Z_f$ is a composition of *two reflections:*

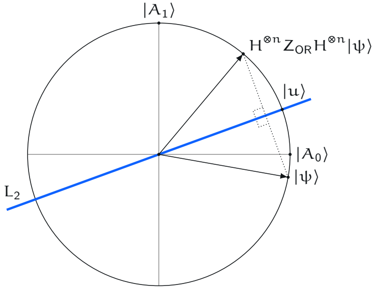
$$Z_f \quad \text{and} \quad H^{\otimes n} Z_{OR} H^{\otimes n}$$

Composing two reflections yields a *rotation.*

2. The operation $H^{\otimes n} Z_{OR} H^{\otimes n}$ can be expressed like this:

$$H^{\otimes n} Z_{OR} H^{\otimes n} = 2|u\rangle\langle u| - \mathbb{1}$$

Again this is a *reflection,* this time about the line L_2 parallel to $|u\rangle$.



Geometric picture

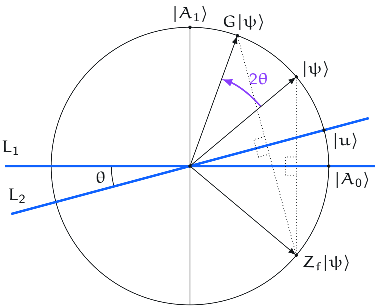
Main idea

The operation $G = H^{\otimes n} Z_{OR} H^{\otimes n} Z_f$ is a composition of *two reflections:*

$$Z_f \quad \text{and} \quad H^{\otimes n} Z_{OR} H^{\otimes n}$$

Composing two reflections yields a *rotation.*

When we compose two reflections, we obtain a *rotation* by twice the angle between the lines of reflection.



3. Choosing the number of iterations

Setting the target

Consider any quantum state of this form:

$$\alpha|A_0\rangle + \beta|A_1\rangle$$

Measuring yields a solution $x \in A_1$ with probability $|\beta|^2$.

$$\alpha|A_0\rangle + \beta|A_1\rangle = \frac{\alpha}{\sqrt{|A_0|}} \sum_{x \in A_0} |x\rangle + \frac{\beta}{\sqrt{|A_1|}} \sum_{x \in A_1} |x\rangle$$

$$p(x) = \begin{cases} \frac{|\alpha|^2}{|A_0|} & x \in A_0 \\ \frac{|\beta|^2}{|A_1|} & x \in A_1 \end{cases}$$

$$\Pr(\text{outcome is in } A_1) = \sum_{x \in A_1} p(x) = |\beta|^2$$

Setting the target

Consider any quantum state of this form:

$$\alpha|A_0\rangle + \beta|A_1\rangle$$

Measuring yields a solution $x \in A_1$ with probability $|\beta|^2$.

The state of Q after t iterations in Grover's algorithm:

$$\cos\big((2t+1)\theta\big)|A_0\rangle + \sin\big((2t+1)\theta\big)|A_1\rangle \qquad \theta = \sin^{-1}\left(\sqrt{\frac{|A_1|}{N}}\right)$$

Measuring after t iterations gives an outcome $x \in A_1$ with probability

$$\sin^2\big((2t+1)\theta\big)$$

We wish to maximize this probability — so we may view that $|A_1\rangle$ is our *target state.*

Setting the target

The state of Q after t iterations in Grover's algorithm:

$$\cos\big((2t+1)\theta\big)|A_0\rangle + \sin\big((2t+1)\theta\big)|A_1\rangle \qquad \theta = \sin^{-1}\left(\sqrt{\frac{|A_1|}{N}}\right)$$

Measuring after t iterations gives an outcome $x \in A_1$ with probability

$$\sin^2\big((2t+1)\theta\big)$$

To make this probability close to 1 and minimize t, we will aim for

$$(2t+1)\theta \approx \frac{\pi}{2} \qquad \Longleftrightarrow \qquad t \approx \frac{\pi}{4\theta} - \frac{1}{2} \quad \xrightarrow{\text{closest integer}} \quad t = \left\lfloor \frac{\pi}{4\theta} \right\rfloor$$

Important considerations:

- t must be an integer
- θ depends on the number of solutions $s = |A_1|$

Unique search

$$(2t+1)\theta \approx \frac{\pi}{2} \qquad \Leftarrow \qquad t = \left\lfloor \frac{\pi}{4\theta} \right\rfloor$$

Unique search

Input:	$f : \Sigma^n \to \Sigma$
Promise:	There is exactly one string $z \in \Sigma^n$ for which $f(z) = 1$, with $f(x) = 0$ for all strings $x \neq z$
Output:	The string z

For Unique search we have $s = |A_1| = 1$ and therefore

$$\theta = \sin^{-1}\left(\sqrt{\frac{1}{N}}\right) \approx \sqrt{\frac{1}{N}}$$

Substituting $\theta \approx 1/\sqrt{N}$ into our expression for t gives

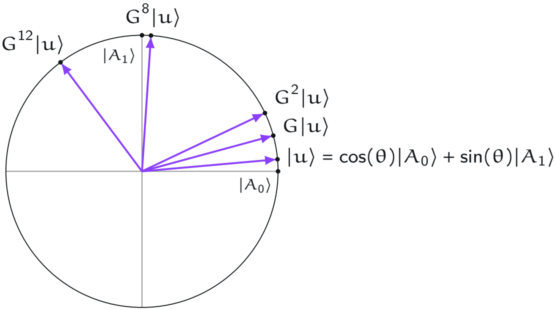
$$t \approx \left\lfloor \frac{\pi}{4}\sqrt{N} \right\rfloor \qquad \leftarrow O(\sqrt{N}) \text{ queries}$$

Unique search

Example: $N = 128$

$$\theta = \sin^{-1}\left(\frac{1}{\sqrt{N}}\right) = 0.0885\cdots$$

$$t = \left\lfloor \frac{\pi}{4\theta} \right\rfloor = 8$$



Unique search

$$\theta = \sin^{-1}\left(\sqrt{\frac{1}{N}}\right) \qquad t = \left\lfloor \frac{\pi}{4\theta} \right\rfloor$$

Measuring after t iterations gives the (unique) outcome $x \in A_1$ with probability

$$p(N,1) = \sin^2\big((2t+1)\theta\big)$$

Success probabilities for Unique search

N	$p(N,1)$
2	.5
4	1.0
8	.9453125
16	.9613190
32	.9991823
64	.9965857

N	$p(N,1)$
128	.9956199
256	.9999470
512	.9994480
1024	.9994612
2048	.9999968
4096	.9999453

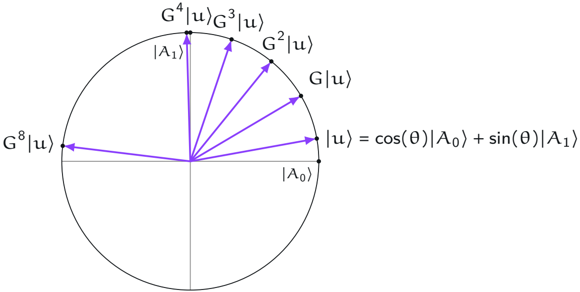
It can be proved analytically that $p(N,1) \geq 1 - 1/N$.

Multiple solutions

Example: $N = 128$, $s = 4$

$$\theta = \sin^{-1}\left(\sqrt{\frac{s}{N}}\right) = 0.1777\cdots$$

$$t = \left\lfloor \frac{\pi}{4\theta} \right\rfloor = 4$$



Multiple solutions

$$\theta = \sin^{-1}\left(\sqrt{\frac{s}{N}}\right) \qquad t = \left\lfloor \frac{\pi}{4\theta} \right\rfloor$$

For every $s \in \{1, \ldots, N\}$, the probability $p(N, s)$ to find a solution satisfies

$$p(N, s) \geq \max\left\{1 - \frac{s}{N}, \frac{s}{N}\right\}$$

Number of queries

$$\theta = \sin^{-1}\left(\sqrt{\frac{s}{N}}\right) \qquad t = \left\lfloor \frac{\pi}{4\theta} \right\rfloor$$

Each iteration of Grover's algorithm requires 1 query (or evaluations of f). How does the number of queries t depend on N and s?

$$\sin^{-1}(x) \geq x \qquad (\text{for every } x \in [0,1])$$

$$\theta = \sin^{-1}\left(\sqrt{\frac{s}{N}}\right) \geq \sqrt{\frac{s}{N}}$$

$$t \leq \frac{\pi}{4\theta} \leq \frac{\pi}{4}\sqrt{\frac{N}{s}}$$

$$t = O\left(\sqrt{\frac{N}{s}}\right)$$

Unknown number of solutions

What do we do if we don't know the number of solutions in advance?

A simple approach

Choose the number of iterations $t \in \{1, \ldots, \lfloor \pi\sqrt{N}/4 \rfloor\}$ *uniformly at random.*

- The probability to find a solution (if one exists) will be at least 40%.
  (Repeat several times to boost success probability.)
- The number of queries (or evaluations of f) is $O(\sqrt{N})$.

A more sophisticated approach

1. Set $T = 1$.
2. Run Grover's algorithm with $t \in \{1, \ldots, T\}$ chosen uniformly at random.
3. If a solution is found, output it and stop.
   Otherwise, increase T and return to step 2 (or report "no solution").

- The rate of increase of T must be carefully balanced: slower rates require more queries, higher rates decrease success probability. $T \leftarrow \lceil \frac{5}{4} T \rceil$ works.
- If the number of solutions is $s \geq 1$, then the number of queries (or evaluations of f) required is $O(\sqrt{N/s})$. If there are no solutions, $O(\sqrt{N})$ queries are required.

4. Concluding remarks

Concluding remarks

- Grover's algorithm is *asymptotically optimal.*
- Grover's algorithm is *broadly applicable.*
- The technique used in Grover's algorithm can be *generalized.*