## 量子計算的數學基礎 MA5501＊

## Chapter 4．Simon＇s Algorithm

§4．1 Simon＇s Problem

§4．2 The Quantum Algorithm
§4．3 Classical Algorithms for Simon＇s Problem

## §4．1 Simon＇s Problem

Simon＇s algorithm was the first quantum algorithm to show an ex－ ponential speed－up versus the best classical algorithm in solving a specific problem．This inspired the quantum algorithms based on the quantum Fourier transform，which is used in the most famous quantum algorithm：Shor＇s factoring algorithm．


## §4．1 Simon＇s Problem

Simon＇s algorithm was the first quantum algorithm to show an ex－ ponential speed－up versus the best classical algorithm in solving a specific problem．This inspired the quantum algorithms based on the quantum Fourier transform，which is used in the most famous quantum algorithm：Shor＇s factoring algorithm．

Let $N=2^{n}$ ，and identify the set $\{0, \cdots, N-1\}$ with $\{0,1\}^{n}$ ．Let $j \oplus s$ be the $n$－bit string obtained by bitwise adding the $n$－bit strings $j$ and $s \bmod 2$ ；that is，

$$
j \oplus s=\left(\left(j_{1} \oplus s_{1}\right)\left(j_{2} \oplus s_{2}\right) \cdots\left(j_{n} \oplus s_{n}\right)\right)_{2}
$$

if

$$
j=\left(j_{1} j_{2} \cdots j_{n}\right)_{2} \quad \text { and } \quad s=\left(s_{1} s_{2} \cdots s_{n}\right)_{2} .
$$

## §4．1 Simon＇s Problem

## Simon＇s problem：

－Formulation 1：For $N=2^{n}$ ，we are given $x=\left(x_{0}, \cdots, x_{N-1}\right)$ ， with $x_{i} \in\{0,1\}^{n}$ ，with the property that there is a unique but unknown nonzero $s \in\{0,1\}^{n}$ such that $x_{i}=x_{j}$ if and only if （ $i=j$ or $i=j \oplus s$ ）．Find $s$ ．
－Formulation 2：If $f:\{0,1\}^{n} \rightarrow\{0,1\}^{n}$ is either an one－to－one or
a two－to－one function satisfying the property that there exists

Determine the class to which $f$ belongs to．
Note that the input $x=\left\{x_{0}, \cdots, x_{N-1}\right\}$ now has variables $x_{i}$ that
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Note that the input $x=\left\{x_{0}, \cdots, x_{N-1}\right\}$ now has variables $x_{i}$ that themselves are $n$－bit strings，and one query gives such a string com－ pletely $|i\rangle\left|0^{n}\right\rangle \mapsto|i\rangle\left|x_{i}\right\rangle$ ．

## §4．2 The Quantum Algorithm

Simon＇s algorithm starts in a state of $2^{n}$ zero qubits $\left|0^{n}\right\rangle\left|0^{n}\right\rangle$ and apply Hadamard transforms to the first $n$ qubits，giving

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\frac{1}{\sqrt{2^{n}}} \sum_{i \in\{0,1\}^{n}}|i\rangle\left|0^{n}\right\rangle .
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A query turns this into

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Now the algorithm measures the second $n$－qubit register in the com－
putational basis；this measurement is actually not necessary，but it facilitates analysis．
$x_{i}$ and the first register will collapse to the superposition of the two
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Now the algorithm measures the second $n$－qubit register in the com－ putational basis；this measurement is actually not necessary，but it facilitates analysis．The measurement outcome will be some value $x_{i}$ and the first register will collapse to the superposition of the two indices having that $x_{i}$－value：

$$
\frac{1}{\sqrt{2}}(|i\rangle+|i \oplus s\rangle)\left|x_{i}\right\rangle
$$

## §4．2 The Quantum Algorithm

We will now ignore the second register and apply Hadamard trans－ forms to the first $n$ qubits．Using

$$
\mathrm{H}^{\otimes n}|i\rangle=\frac{1}{\sqrt{2^{n}}} \sum_{j \in\{0,1\}^{n}}(-1)^{i \bullet j}|j\rangle,
$$

and the fact that $(i \oplus s) \bullet j=(i \bullet j) \oplus(s \bullet j)$（which is a direct consequence of $\left(i_{k} \oplus s_{k}\right) \cdot j_{k}=\left(i_{k} \cdot j_{k}\right) \oplus\left(s_{k} \cdot j_{k}\right)$ for all $\left.i_{k}, s_{k}, j_{k} \in\{0,1\}\right)$ ， we can write the resulting state as

$$
\begin{aligned}
& \mathrm{H}^{\otimes n}\left(\frac{1}{\sqrt{2}}(|i\rangle+|i \oplus s\rangle)\right) \\
& \quad=\frac{1}{\sqrt{2^{n+1}}}\left(\sum_{j \in\{0,1\}^{n}}(-1)^{i \bullet j}|j\rangle+\sum_{j \in\{0,1\}^{n}}(-1)^{(i \oplus s) \bullet j}|j\rangle\right) \\
& \quad=\frac{1}{\sqrt{2^{n+1}}} \sum_{j \in\{0,1\}^{n}}(-1)^{i \bullet j}\left(1+(-1)^{s \bullet j}\right)|j\rangle .
\end{aligned}
$$

## §4．2 The Quantum Algorithm

Note that $|j\rangle$ has nonzero amplitude if $s \bullet j=0 \bmod 2$ ．Measuring the state gives a uniformly random element from the set $\{j \mid s \bullet j=$ $0 \bmod 2\}$ ．Accordingly，we get a linear equation

$$
s \bullet j=0 \bmod 2
$$

that gives information about $s$ ．We repeat this algorithm until we


The solutions to these equations will be $0^{n}$ and the correct $s$ ，which
we can compute efficiently by a classical algorithm（Gaussian elimi－ nation modulo 2）．This can be done by means of a classical circuit of size roughly $\mathcal{O}\left(n^{3}\right)$ ．

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Note that $|j\rangle$ has nonzero amplitude if $s \bullet j=0 \bmod 2$ ．Measuring the state gives a uniformly random element from the set $\{j \mid s \bullet j=$ 0 mod 2$\}$ ．Accordingly，we get a linear equation

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$$
\left[\begin{array}{cccc}
j_{n-1}^{(1)} & j_{n-2}^{(1)} & \cdots & j_{0}^{(1)} \\
j_{n-1}^{(2)} & j_{n-2}^{(2)} & \cdots & j_{0}^{(2)} \\
\vdots & \vdots & \ddots & \vdots \\
j_{n-1}^{(n-1)} & j_{n-2}^{(n-1)} & \cdots & j_{0}^{(n-1)}
\end{array}\right]\left[\begin{array}{c}
s_{n-1} \\
s_{n-2} \\
\vdots \\
s_{0}
\end{array}\right]=\left[\begin{array}{c}
0 \\
0 \\
\vdots \\
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Note that if the j＇s you have generated at some point span a space of size $2^{k}$ ，for some $k<n-1$ ，then the probability that your next run of the algorithm produces a $j$ that is linearly independent of the earlier ones，is $\left(2^{n}-2^{k}\right) / 2^{n} \geqslant 1 / 2$ ．Hence an expected number of $\mathcal{O}(n)$ runs of the algorithm suffices to find $n-1$ linearly independent $j$＇s． Simon＇s algorithm thus finds $s$ using an expected number of $\mathcal{O}(n)$ $x_{i}$－queries and polynomially many other operations．


Figure 1：Quantum circuit for Simon＇s algorithm

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## §4．2 The Quantum Algorithm

## Example

Let $f$ be a periodic function of 2 qubits given by

$$
f\left(x_{1}, x_{2}\right)=\left(x_{1} \oplus x_{2}, x_{1} \oplus x_{2}\right) \quad \forall x_{1}, x_{2} \in\{0,1\}
$$

The quantum circuit to solve the problem is：


Figure 2：Quantum circuit for Simon＇s algorithm in this example

## §4．2 The Quantum Algorithm

## Example（Cont＇d）

To check the four CNOT operations indeed provide the oracle $U_{f}$ ， we note that by writing $|x\rangle=\left|x_{1} x_{2}\right\rangle$ and $|y\rangle=\left|y_{1}\right\rangle\left|y_{2}\right\rangle$ ，we have

> CNOT $_{2,4}$ CNOT $_{2,3}$ CNOT $_{1,4}$ CNOT $_{1,3}|x\rangle|y\rangle$
> $=$ CNOT $_{2,4}$ CNOT $_{2,3}$ CNOT $_{1,4}$ CNOT $_{1,3}\left|x_{1}\right\rangle\left|x_{2}\right\rangle\left|y_{1}\right\rangle\left|y_{2}\right\rangle$
> $=\mathbf{C N O T}_{2,4} \mathbf{C N O T}_{2,3}$ CNOT $_{1,4}\left|x_{1}\right\rangle\left|x_{2}\right\rangle\left|x_{1} \oplus y_{1}\right\rangle\left|y_{2}\right\rangle$
> $=$ CNOT $_{2,4}$ CNOT $_{2,3}\left|x_{1}\right\rangle\left|x_{2}\right\rangle\left|x_{1} \oplus y_{1}\right\rangle\left|x_{1} \oplus y_{2}\right\rangle$
> $=\mathbf{C N O T}_{2,4}\left|x_{1}\right\rangle\left|x_{2}\right\rangle\left|x_{1} \oplus x_{2} \oplus y_{1}\right\rangle\left|x_{1} \oplus y_{2}\right\rangle$
> $=\left|x_{1}\right\rangle\left|x_{2}\right\rangle\left|x_{1} \oplus x_{2} \oplus y_{1}\right\rangle\left|x_{1} \oplus x_{2} \oplus y_{2}\right\rangle=|x\rangle|y \oplus f(x)\rangle$
> $=Q_{f}|x\rangle|y\rangle$.

## §4．3 Classical Algorithms for Simon＇s Problem

## §4．3．1 Upper bound

Let us first sketch a classical randomized algorithm that solves Si － mon＇s problem using $\mathcal{O}\left(\sqrt{2^{n}}\right)$ queries．Our algorithm will make $T$ randomly chosen distinct queries $i_{1}, \cdots, i_{T}$ ，for some $T$ to be de－ termined later．If there is a collision among those queries（that is， $x_{i_{k}}=x_{i_{\ell}}$ for some $k \neq \ell$ ），then we are done，because then we know $i_{k}=i_{\ell} \bmod s$ ，equivalently $s=i_{k} \oplus i_{\ell}$ ．
that we are likely to see a collision in case $s \neq 0^{n}$（there will not be
any collisions if $\left.s=0^{n}\right)$ ？
in our secuence that could be a collision，and the probability for a
fixed pair to form a collision is $1 / 2^{n-1}$ ；thus the expected number
of collisions in our sequence will be roughly $T^{2} / 2^{n}$ ．If we choose $T=\sqrt{2^{n}}$ ，we expect to have roughly 1 collision in our sequence． which is good enough to find $s$ ．

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## §4．3 Classical Algorithms for Simon＇s Problem

Of course，an expected value of 1 collision does not mean that we will have at least one collision with high probability，but a slightly more involved calculation shows the latter statement as well．

## §4．3 Classical Algorithms for Simon＇s Problem

## §4．3．2 Lower bound

Simon proved that any classical randomized algorithm that finds $s$ with high probability needs to make $\Omega\left(\sqrt{2^{n}}\right)$ queries，so the above classical algorithm is essentially optimal．
bounded－error algorithms（let us stress again that this does not prove an exponential separation in the usual circuit model，because we are counting queries rather than ordinary operations here）．Simon＇s algorithm inspired Shor to his factoring algorithm
$\square$ Given

Promise：there exists $s \in\{0,1\}^{n}$ such that

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We prove a lower bound for the decision version of Simon＇s problem：
Given：input $x=\left(x_{0}, \cdots, x_{N-1}\right)$ ，where $N=2^{n}$ and $x_{i} \in\{0,1\}^{n}$ ．
Promise：there exists $s \in\{0,1\}^{n}$ such that $x_{i}=x_{j}$ if and only if

$$
(i=j \text { or } i=j \oplus s)
$$

Task：decide whether $s=0^{n}$ ．

## §4．3 Classical Algorithms for Simon＇s Problem

Consider the input distribution $\mu$ that is defined as follows．With probability $1 / 2, x$ is a uniformly random permutation of $\{0,1\}^{n}$ ；this corresponds to the case $s=0^{n}$ ．With probability $1 / 2$ ，we pick a nonzero string $s$ at random，and for each pair $(i ; i \oplus s)$ ，we pick a unique value for $x_{i}=x_{i \oplus s}$ at random．If there exists a randomized $T$－query algorithm that achieves success probability $\geqslant 2 / 3$ under this input distribution $\mu$ ，then there also is deterministic $T$－query algo－ rithm that achieves success probability $\geqslant 2 / 3$ under $\mu$（because the behavior of the randomized algorithm is an average over a number of deterministic algorithms）．Now consider a deterministic algorithm with error $\leqslant 1 / 3$ under $\mu$ ，that makes $T$ queries to $x$ ．We want to show that $T=\Omega\left(\sqrt{2^{n}}\right)$

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## §4．3 Classical Algorithms for Simon＇s Problem

First consider the case $s=0^{n}$ ．We can assume the algorithm never queries the same point twice．Then the $T$ outcomes of the queries are $T$ distinct $n$－bit strings，and each sequence of $T$ strings is equally likely．
> the indices $i_{1}, \cdots, i_{T}$（this sequence depends on $x$ ）and gets outputs Call a sequence of queries $i_{1}, \cdots, i_{T}$ good if it shows a collision（that is，$x_{i,}=x_{i_{0}}$ ，for some $k \neq \ell$ ），and bad otherwise．If the sequence of queries of the algorithm is good，then we can find $s$ ，since $i_{k} \oplus i_{\ell}=s$ ．On the other hand，if the sequence is bad，then each sequence of $T$ distinct outcomes is equally likely－just as in the $s=0^{n}$ case！We will now show that the probability of the bad case is very close to 1 for small $T$ ．

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First consider the case $s=0^{n}$ ．We can assume the algorithm never queries the same point twice．Then the $T$ outcomes of the queries are $T$ distinct $n$－bit strings，and each sequence of $T$ strings is equally likely．Now consider the case $s \neq 0^{n}$ ．Suppose the algorithm queries the indices $i_{1}, \cdots, i_{T}$（this sequence depends on $x$ ）and gets outputs $x_{i_{1}}, \cdots, x_{i_{T}}$ ．Call a sequence of queries $i_{1}, \cdots, i_{T}$ good if it shows a collision（that is，$x_{i_{k}}=x_{i_{\ell}}$ for some $k \neq \ell$ ），and bad otherwise．If the sequence of queries of the algorithm is good，then we can find $s$ ，since $i_{k} \oplus i_{\ell}=s$ ．On the other hand，if the sequence is bad，then each sequence of $T$ distinct outcomes is equally likely－just as in the $s=0^{n}$ case！

## §4．3 Classical Algorithms for Simon＇s Problem

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## §4．3 Classical Algorithms for Simon＇s Problem

If $i_{1}, \cdots, i_{k-1}$ is bad，then we have excluded at most $C_{2}^{k-1}$ possible values of $s$（namely all values $i_{j} \oplus i_{j^{\prime}}$ for all distinct $j, j^{\prime} \in[k-1]$ ），and all other values of $s$ are equally likely．The probability that the next
query $i_{k}$ makes the sequence good，is the probability that $x_{i_{k}}=x_{i_{j}}$ for some $j<k$ ，equivalently，that the set $S=\left\{i_{k} \oplus i_{j} \mid j<k\right\}$ happens to contain the string $s$ ．However，$S$ has only $k-1$ members，while there are $2^{n}-1-C_{2}^{k-1}$ equally likely remaining possibilities for $s$ ． This means that the probability that the sequence is still bad after query $i_{k}$ is made，is very close to 1 ．In formulas：
here we used the fact that $(1-a)(1-b) \geqslant 1-(a+b)$ if $a, b \geqslant 0$ ．

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$$
\begin{gathered}
\operatorname{Pr}\left[i_{1}, \cdots, i_{T} \text { is bad }\right]=\prod_{k=2}^{T} \operatorname{Pr}\left[i_{1}, \cdots, i_{k} \text { is bad } \mid i_{1}, \cdots i_{k-1} \text { is bad }\right] \\
\quad=\prod_{k=2}^{T}\left(1-\frac{k-1}{2^{n}-1-C_{2}^{k-1}}\right) \geqslant 1-\sum_{k=2}^{T} \frac{k-1}{2^{n}-1-C_{2}^{k-1}}
\end{gathered}
$$

here we used the fact that $(1-a)(1-b) \geqslant 1-(a+b)$ if $a, b \geqslant 0$ ．

## §4．3 Classical Algorithms for Simon＇s Problem

Note that $2^{n}-1-C_{2}^{k-1} \approx 2^{n}$ as long as $k \ll \sqrt{2^{n}}$ and $\sum_{k=2}^{T}(k-1)=$ $\frac{T(T-1)}{2} \approx T^{2} / 2$ ．Hence we can approximate the last term in the formula by $1-T^{2} / 2^{n+1}$ if $k \ll \sqrt{2^{n}}$ ．
with probability nearly 1 （probability taken over the distribution $\mu$ ） the algorithm＇s sequence of queries is bad．If it gets a bad sequence， it cannot＂see＂the difference between the $s=0^{n}$ case and the $s \neq 0^{n}$ case，since both cases result in a uniformly random sequence of $T$ distinct $n$－bit strings as answers to the $T$ queries．This shows that $T$ has to be $\sqrt{2^{n}}$ in order to enable the algorithm to get a good sequence of queries with high probability．

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[^0]:    We prove a lower bound for $t$
    Given
    nromise：

