## QuANTUM ALGORITHMS 1:

 circuits, QFT and Grover

## Simon Apers <br> (CNRS \& IRIF, Paris)

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(simonapers.github.io/mckinsey.html)
tutorial $=$ overview $(2 h)+$ exercises $(2 h)$
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TUTORIAL 1: BASICS (21/4) quantum circuits<br>quantum Fourier transform<br>Grover search

# tutorial = overview (2h) + exercises (2h) 

TUTORIAL 1: BASICS (21/4)<br>quantum circuits<br>quantum Fourier transform<br>Grover search

## TUTORIAL 2: CHEMISTRY (28/4)

Hamiltonian simulation
energy estimation
variational quantum algorithms
tutorial $=$ overview $(2 h)+$ exercises $(2 h)$

> TUTORIAL 1: BASICS $(21 / 4)$ quantum circuits quantum Fourier transform
> Grover search

Tutorial 2: CHEMISTRY (28/4)
Hamiltonian simulation
energy estimation
variational quantum algorithms
TUTORIAL 3: OPTIMIZATION (26/5)
adiabatic algorithm
HHL
quantum walks

## CIRCUITS

## QFT

Grover

## quantum state on 1 qubit

$$
|\psi\rangle=\alpha_{0}|0\rangle+\alpha_{1}|1\rangle=\left[\begin{array}{l}
\alpha_{0} \\
\alpha_{1}
\end{array}\right]
$$

## quantum state on 1 qubit

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|\psi\rangle=\alpha_{0}|0\rangle+\alpha_{1}|1\rangle=\left[\begin{array}{l}
\alpha_{0}  \tag{_}\\
\alpha_{1}
\end{array}\right]
$$

unitary dynamics

$$
|\psi\rangle-U \quad\left|\psi^{\prime}\right\rangle=U|\psi\rangle=\left[\begin{array}{ll}
U_{00} & U_{10} \\
U_{01} & U_{11}
\end{array}\right]\left[\begin{array}{l}
\alpha_{0} \\
\alpha_{1}
\end{array}\right]
$$

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\end{array}\right]
$$

measurement

$$
|\psi\rangle=\alpha_{0}|0\rangle+\alpha_{1}|1\rangle-\infty \quad \begin{aligned}
& |0\rangle \text { with probability }\left|\alpha_{0}\right|^{2} \\
& |1\rangle \text { with probability }\left|\alpha_{1}\right|^{2}
\end{aligned}
$$

## Hadamard gate

$$
H=\frac{1}{\sqrt{2}}\left[\begin{array}{cc}
1 & 1 \\
1 & -1
\end{array}\right]
$$

## Hadamard gate

$$
H-\equiv \frac{1}{\sqrt{2}}\left[\begin{array}{cc}
1 & 1 \\
1 & -1
\end{array}\right]
$$

such that

$$
\begin{aligned}
& |0\rangle-H-\frac{1}{\sqrt{2}}(|0\rangle+|1\rangle) \\
& |1\rangle-H-\frac{1}{\sqrt{2}}(|0\rangle-|1\rangle)
\end{aligned}
$$

$X$ or NOT gate
$\square \oplus\left[\begin{array}{ll}0 & 1 \\ 1 & 0\end{array}\right]$

$$
\begin{gathered}
X \text { or NOT gate } \\
-\oplus\left[\begin{array}{ll}
0 & 1 \\
1 & 0
\end{array}\right]
\end{gathered}
$$

Z gate

$$
-Z=\left[\begin{array}{cc}
1 & 0 \\
0 & -1
\end{array}\right]
$$

$$
\begin{gathered}
X \text { or NOT gate } \\
-\neq\left[\begin{array}{ll}
0 & 1 \\
1 & 0
\end{array}\right]
\end{gathered}
$$

Z gate

$$
-Z=\left[\begin{array}{cc}
1 & 0 \\
0 & -1
\end{array}\right]
$$

phase or $T$ gate

$$
-T \equiv\left[\begin{array}{cc}
1 & 0 \\
0 & e^{i \pi / 4}
\end{array}\right]
$$

EX: what is the outcome of the following circuits?

$$
|0\rangle-H-\infty
$$



$$
|0\rangle-H-Z-H
$$

quantum states on $n$ qubits $\left(N=2^{n}\right)$ :

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basis state $\left(z \in\{0,1\}^{n}\right)$

$$
|z\rangle=\left|z_{1}\right\rangle \otimes \cdots \otimes\left|z_{n}\right\rangle=\left|z_{1} \ldots z_{n}\right\rangle \quad \begin{gathered}
- \\
\quad \\
\left|z_{1}\right\rangle \\
\vdots \\
\left|z_{n}\right\rangle
\end{gathered}
$$

## quantum states on $n$ qubits $\left(N=2^{n}\right)$ :

basis state $\left(z \in\{0,1\}^{n}\right)$

$$
\left.|z\rangle=\left|z_{1}\right\rangle \otimes \cdots \otimes\left|z_{n}\right\rangle=\left|z_{1} \ldots z_{n}\right\rangle \quad \begin{gathered}
\text { - }
\end{gathered} \right\rvert\, \begin{gathered}
\left|z_{1}\right\rangle \\
\vdots \\
\left|z_{n}\right\rangle
\end{gathered}
$$

## superposition

$$
|\psi\rangle=\sum_{z \in\{0,1\}^{n}} \alpha_{z}|z\rangle=\left[\begin{array}{c}
\alpha_{0} \\
\alpha_{1} \\
\vdots \\
\alpha_{N-1}
\end{array}\right]
$$

## unitary dynamics



## unitary dynamics


measurement

$$
|\psi\rangle=\sum_{z \in\{0,1\}^{n}} \alpha_{z}|z\rangle \xlongequal[|c|]{\frac{\mid x}{\mid x}}|z\rangle \text { with probability }\left|\alpha_{z}\right|^{2}
$$

controlled unitary


## controlled unitary



## such that



CNOT


## CNOT



CCNOT or Toffoli


## EX:

fill in:

what is the outcome of the following circuits?


## universality:

any unitary operation can be approximated with

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such that

$$
O|z\rangle|0\rangle=|z\rangle|f(z)\rangle
$$

and
$O\left(\sum_{z} \alpha_{z}|z\rangle|0\rangle\right)=\sum_{z} \alpha_{z}|z\rangle|f(z)\rangle$

## quantum oracle/RAM query (for function $f$ )


such that

$$
\begin{gathered}
O|z\rangle|0\rangle=|z\rangle|f(z)\rangle \\
\text { and } \\
O\left(\sum_{z} \alpha_{z}|z\rangle|0\rangle\right)=\sum_{z} \alpha_{z}|z\rangle|f(z)\rangle
\end{gathered}
$$

EX: which function does CNOT evaluate?

## CIRCUITS

## QFT

## Grover

discrete Fourier transform $F_{N}: \mathbb{C}^{N} \rightarrow \mathbb{C}^{N}$

$$
F_{N}=\frac{1}{\sqrt{N}}\left[\begin{array}{cccc}
1 & 1 & \ldots & 1 \\
1 & \omega_{N} & \ldots & \omega_{N}^{N-1} \\
\vdots & \vdots & \ddots & \vdots \\
1 & \omega_{N}^{N-1} & \ldots & \omega_{N}^{(N-1)(N-1)}
\end{array}\right], \quad \omega_{N}=e^{i 2 \pi / N}
$$

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1 & \omega_{N}^{N-1} & \ldots & \omega_{N}^{(N-1)(N-1)}
\end{array}\right], \quad \omega_{N}=e^{i 2 \pi / N}
$$

Fourier modes

$$
F_{N}|k\rangle=|\tilde{k}\rangle=\frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} \omega_{N}^{j k}|j\rangle
$$

! $F_{N}$ unitary matrix on $n=\log (N)$ qubits

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lemma: can implement $F_{N}$ using $O\left(n^{2}\right)$ 2-qubit gates

application 1: quantum phase estimation (Kitaev '95)

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given: circuit $] U$, state $|\phi\rangle \bar{\square}$
promise:

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given: circuit $] U$, state $|\phi\rangle=\bar{\square}$
promise:

goal: find $\theta$

Kitaev '95:
$\varepsilon$-approximation of $\theta$ with $O(1 / \varepsilon)$ calls to $U$ and 1 copy of $|\phi\rangle$

(details in exercises)

## application 2: quantum period finding

given: oracle

$$
\begin{aligned}
& |z\rangle-O-|z\rangle \\
& |w\rangle-\square
\end{aligned} \quad \begin{aligned}
& |w \oplus f(z)\rangle
\end{aligned} \quad \text { with } f: \mathbb{N} \rightarrow[N]
$$

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given: oracle

promise: period $r$ s.t. $f(a)=f(b)$ iff $a=b(\bmod r)$

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given: oracle

promise: period $r$ s.t. $f(a)=f(b)$ iff $a=b(\bmod r)$ goal: find $r$

## Shor '94:

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1. factoring and discrete log reduce to period finding

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2. quantum algorithm with polylog(N) calls to $O$


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## QFT

## Grover

problem: unstructured search

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given: oracle access to $f:[N] \rightarrow\{0,1\}$
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## problem: unstructured search

$$
\text { given: oracle access to } f:[N] \rightarrow\{0,1\}
$$

promise: unique $x$ s.t. $f(x)=1$
goal: find $x$
Grover '96:
$O(\sqrt{N})$ quantum queries vs $O(N)$ classical queries

## reflection 1: phase oracle

$$
|x\rangle-O-(-1)^{f(x)}|x\rangle
$$

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$$
|x\rangle-O-(-1)^{f(x)}|x\rangle
$$

reflection 2: around $|\pi\rangle:=\frac{1}{\sqrt{N}} \sum_{y \in[N]}|y\rangle$

$$
\begin{array}{r}
|\pi\rangle-\sqrt[R_{\pi}]{ }-|\pi\rangle \\
|\pi\rangle \perp|\phi\rangle-\sqrt[R_{\pi}]{-}-|\phi\rangle
\end{array}
$$

## reflection 1: phase oracle

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|x\rangle-O-(-1)^{f(x)}|x\rangle
$$

reflection 2: around $|\pi\rangle:=\frac{1}{\sqrt{N}} \sum_{y \in[N]}|y\rangle$

$$
\begin{gathered}
|\pi\rangle-\sqrt[R_{\pi}]{ }-|\pi\rangle \\
|\pi\rangle \perp|\phi\rangle-\sqrt[R_{\pi}]{ }-|\phi\rangle \\
\text { s.t. } \\
-\sqrt{R_{\pi}}-\equiv 2|\pi\rangle\langle\pi|-I
\end{gathered}
$$

Grover operator
$\boxed{G} \equiv-R_{\pi}-O$

## Grover operator

$$
-G=-R_{\pi}-O
$$

rewriting $|\pi\rangle=\sin \theta|x\rangle+\cos \theta\left|\pi^{\prime}\right\rangle$ we get


Grover's algorithm

$$
\left|0^{n}\right\rangle-H_{N}-\underbrace{\sqrt{G} \cdots-\sqrt{G}}_{k} \sqrt{\infty}
$$

## Grover's algorithm

$$
\begin{gathered}
\left|0^{n}\right\rangle-\underbrace{H_{N}}_{k}-\underbrace{\sqrt[G]{G}-\sqrt[G]{\boldsymbol{\alpha}}}_{k} \\
G^{k}|\pi\rangle=\sin ((1+2 k) \theta)|x\rangle+\cos ((1+2 k) \theta)\left|\pi^{\prime}\right\rangle
\end{gathered}
$$

## Grover's algorithm

$$
\begin{gathered}
\left|0^{n}\right\rangle-H_{N}-\underbrace{G-\cdots-\sqrt[G]{\infty}}_{k} \\
G^{k}|\pi\rangle=\sin ((1+2 k) \theta)|x\rangle+\cos ((1+2 k) \theta)\left|\pi^{\prime}\right\rangle
\end{gathered}
$$

finds $x$ with constant probability after $k \in O(\sqrt{N})$ iterations
matching $\Omega(\sqrt{N})$ lower bound

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for $M$ marked elements:
complexity $\Theta(\sqrt{N / M})$

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for $M$ marked elements:
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generalizations:

- amplitude amplification
- quantum mean estimation

