Quantum Search as Simulation

Algorithm design:

1. Guess Hamiltonian H, depending on solution x and initial state $|\psi\rangle$, so that:

   System evolving according to H will change from $|\psi\rangle$ to $|x\rangle$ after some prescribed time.

2. Simulate H using a quantum circuit.

Algorithm starts in state $|\psi\rangle$.

We wish to evolve to state $|x\rangle$.

Which Hamiltonian?

Try:

$$H = |x\rangle\langle x| + |\psi\rangle\langle\psi|$$

or

$$H = |x\rangle\langle\psi| + |\psi\rangle\langle x|.$$

Choose

$$H = |x\rangle\langle x| + |\psi\rangle\langle\psi|.$$

After time t,

evolution is:

$$|\psi\rangle \longrightarrow e^{-iHt}|\psi\rangle$$

Can we find t such that,

$$|x\rangle = e^{-iHt}|\psi\rangle \; ?$$

Restrict analysis to 2-D space spanned by, $|x\rangle$ and $|\psi\rangle$.

Use Gram-Schmidt to find $|y\rangle$, such that $|x\rangle, |y\rangle$ form an orthonormal basis for space spanned by $|x\rangle$ and $|\psi\rangle$.

Therefore,

$$|\psi\rangle = \alpha|x\rangle + \beta|y\rangle,$$

where $\alpha^2 + \beta^2 = 1$ (we choose α and β real and non-negative)

In the $|x\rangle, |y\rangle$ basis,

Remember: $H = |x\rangle\langle x| + |\psi\rangle\langle\psi|$

$$H = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} \alpha^2 & \alpha\beta \\ \alpha\beta & \beta^2 \end{bmatrix} = \begin{bmatrix} 1+\alpha^2 & \alpha\beta \\ \alpha\beta & 1-\alpha^2 \end{bmatrix}$$

$$= I + \alpha(\beta X + \alpha Z)$$

$$\Rightarrow \quad e^{-iHt}|\psi\rangle = e^{-it}\left[\cos(\alpha t)|\psi\rangle - i\sin(\alpha t)(\beta X + \alpha Z)|\psi\rangle\right]$$

but $(\beta X + \alpha Z)|\psi\rangle = |x\rangle$,

$$\Rightarrow$$

$$|\psi\rangle \xrightarrow{H} \cos(\alpha t)|\psi\rangle - i\sin(\alpha t)|x\rangle$$

Observe at $t = \pi/2\alpha$ yields $|x\rangle$ with prob. $= 1$.

Remember: $|\psi\rangle \xrightarrow{H} \cos(\alpha t)|\psi\rangle - i\sin(\alpha t)|$

choose $t = \frac{\pi}{2\alpha}$

But ....

t depends on α, the component of $|\psi\rangle$ in the $|x\rangle$ direction...

...but we are trying to find x.

... so choose α to be the same for all $|x\rangle$,

i.e., choose

$$|\psi\rangle = \frac{\sum_x |x\rangle}{\sqrt{N}}$$

Remember: $|\psi\rangle \xrightarrow{H} \cos(\alpha t)|\psi\rangle - i\sin(\alpha t)|$

$t = \frac{\pi}{2\alpha}$

$|\psi\rangle = \frac{\sum_x |x\rangle}{\sqrt{N}}$

... therefore

$\alpha = \frac{1}{\sqrt{N}}$ for all x,

$t = \pi\frac{\sqrt{N}}{2}$, (independent on value of x)

In summary:

Given, $H = |x\rangle\langle x| + |\psi\rangle\langle\psi|$, where $|\psi\rangle = \frac{\sum_x |x\rangle}{\sqrt{N}}$

then, H rotates $|\psi\rangle$ to $|x\rangle$ after time $t = \frac{\pi}{2}\sqrt{N}$.

Quantum Circuit for H?

Remember:

$$H = |x\rangle\langle x| + |\psi\rangle\langle\psi|$$

Solution:

Simulate $H_1 = |x\rangle\langle x|$

and $H_2 = |\psi\rangle\langle\psi|$

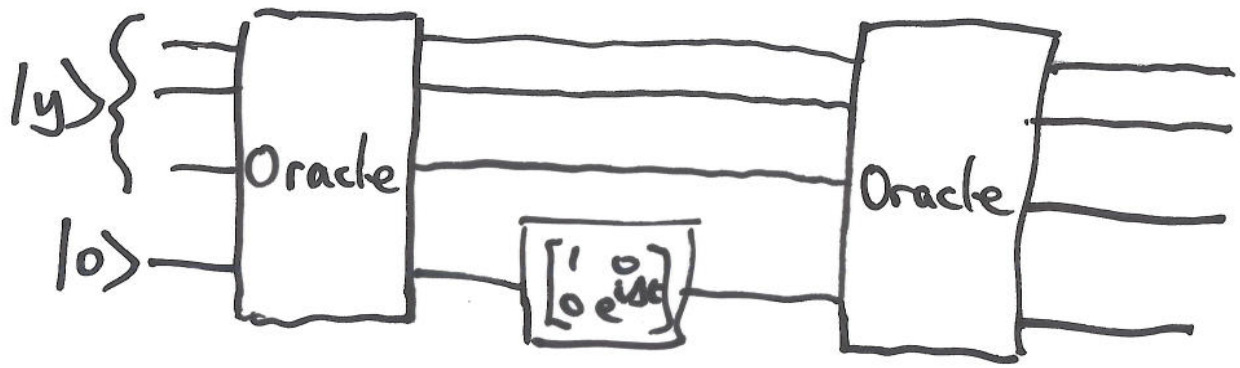
for short increments Δt.

... so ...

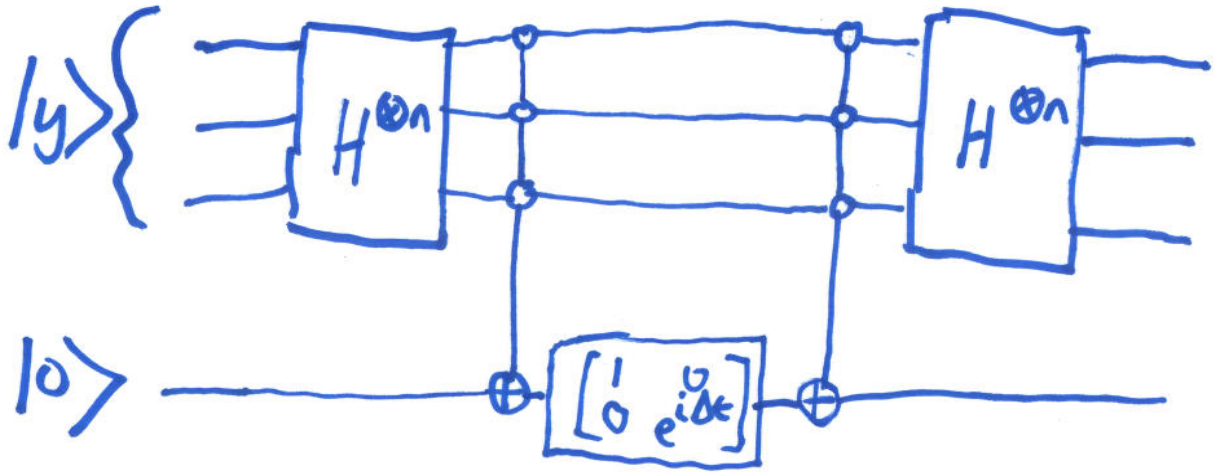
Simulate $e^{-i|x\rangle\langle x|\Delta t}$ and $e^{-i|\psi\rangle\langle\psi|\Delta t}$

where $|\psi\rangle = \frac{\sum_x |x\rangle}{\sqrt{N}}$.

$e^{-i|x\rangle\langle x|\Delta t}$:



$e^{-i|\psi\rangle\langle\psi|\Delta t}$:



Accuracy?

If simulation step of length Δt is accurate to $O(\Delta t^2)$

.. then..

total steps required $= \frac{t}{\Delta t} = \Theta\left(\frac{\sqrt{N}}{\Delta t}\right)$

$\Rightarrow$ cumulative error $= O(\Delta t^2 \times \sqrt{N}/\Delta t)$

$= O(\Delta t \sqrt{N})$

$\Rightarrow$ we require error $= O(1)$

$\Rightarrow \Delta t = \Theta\left(\frac{1}{\sqrt{N}}\right)$

$\Rightarrow$ #oracle calls scales as $O(N)$

.... no better than classical.

... so more accurate simulation required..

... assume simulation step of length Δt is accurate to $O(\Delta t^3)$

... then,

$O(N^{\frac{3}{4}})$ calls required...

... better than classical...

In general..

more accurate simulation

leads to

a reduction in #oracle calls.

Assume simulation step achieves accuracy $O(\Delta t^r)$.

Then,

$$\#\text{oracle calls required} = O(N^{5/2(r-1)})$$

$\therefore$ as $r \to$ large,

$$\#\text{oracle calls required} \to O(N^{\frac{1}{2}}).$$

... a more explicit analysis ...

Let,

$$U(\Delta t) = e^{-i|\psi\rangle\langle\psi|\Delta t}\, e^{-i|x\rangle\langle x|\Delta t}$$

In the basis $|x\rangle, |y\rangle$,

$$|x\rangle\langle x| = (I + Z)/2 = (I + \hat{z}\cdot\vec{\sigma})/2, \quad \text{where } \hat{z} = (0,0,1)$$

$$|\psi\rangle\langle\psi| = (I + \vec{\psi}\cdot\vec{\sigma})/2, \quad \text{where } \vec{\psi} = (2\alpha\beta, 0, (\alpha^2 - \beta^2))$$

$$\Rightarrow$$

$$U(\Delta t) = \left(\cos^2\left(\frac{\Delta t}{2}\right) - \sin^2\left(\frac{\Delta t}{2}\right)\vec{\psi}\cdot\hat{z}\right) I$$

$$- 2i\sin\left(\frac{\Delta t}{2}\right)\left(\cos\left(\frac{\Delta t}{2}\right)\frac{\vec{\psi}+\hat{z}}{2} + \sin\left(\frac{\Delta t}{2}\right)\frac{\vec{\psi}\times\hat{z}}{2}\right)\cdot\vec{\sigma}$$

Remember:

$$U(\Delta t) = \left(\cos^2\left(\frac{\Delta t}{2}\right) - \sin^2\left(\frac{\Delta t}{2}\right)\vec{\psi}\cdot\hat{\jmath}\right)I - 2i\sin\left(\frac{\Delta t}{2}\right)\left(\cos\left(\frac{\Delta t}{2}\right)\frac{\vec{\psi}+\hat{\jmath}}{2} + \sin\left(\frac{\Delta t}{2}\right)\frac{\vec{\psi}\times\hat{\jmath}}{2}\right)\cdot\vec{\sigma}$$

Therefore...

$U(\Delta t)$ is a rotation on the Bloch sphere about $\vec{r}$, where,

$$\vec{r} = \cos\left(\frac{\Delta t}{2}\right)\frac{\vec{\psi}+\hat{\jmath}}{2} + \sin\left(\frac{\Delta t}{2}\right)\frac{\vec{\psi}\times\hat{\jmath}}{2}$$

through an angle Θ, where

$$\cos\left(\frac{\Theta}{2}\right) = \cos^2\left(\frac{\Delta t}{2}\right) - \sin^2\left(\frac{\Delta t}{2}\right)\vec{\psi}\cdot\hat{\jmath}$$

$$\Rightarrow \cos\left(\frac{\Theta}{2}\right) = 1 - \frac{2}{N}\sin^2\left(\frac{\Delta t}{2}\right)$$

Remember: $$U(\Delta t) = \left(\cos^2\left(\frac{\Delta t}{2}\right) - \sin^2\left(\frac{\Delta t}{2}\right)\vec{\psi}\cdot\hat{\vec{s}}\right) I$$
$$- 2i\sin\left(\frac{\Delta t}{2}\right)\left(\cos\left(\frac{\Delta t}{2}\right)\vec{\psi}\frac{+\hat{\vec{s}}}{2} + \sin\left(\frac{\Delta t}{2}\right)\vec{\psi}\frac{\times\hat{\vec{s}}}{2}\right)\cdot\vec{\sigma}$$

... in summary...

$U(\Delta t)$ rotates $|\psi\rangle\langle\psi|$ about $\vec{r}$ axis, through angle θ.

Terminate iterations of $U(\Delta t)$ when $|\psi\rangle\langle\psi|$ rotated near to $|x\rangle\langle x|$.

Remember: $\theta : \cos\left(\frac{\theta}{2}\right) = 1 - \frac{2}{N}\sin^2\left(\frac{\Delta t}{2}\right)$.

... so don't choose Δt small...

... instead choose $\Delta t = \pi$

$\Rightarrow \theta \approx \frac{4}{\sqrt{N}}$ for large N and #oracle calls is $O(\sqrt{N})$.

By choosing $\Delta t = \pi$,

$$e^{-i\pi|\psi\rangle\langle\psi|} = I - 2|\psi\rangle\langle\psi|$$

$$e^{-i\pi|x\rangle\langle x|} = I - 2|x\rangle\langle x|$$

.... original Grover iteration recovered.

.... quantum search re-derived using concepts from quantum simulation....

Possible Algorithm strategy:

1. Specify problem - desired input and output.
2. Guess Hamiltonian to solve problem,
   ... verify it works
3. Simulate Hamiltonian (somehow).
4. Analyze resource costs.

constrained design.

a) Hamiltonian guessed - quantum circuit not designed.

b) Simulation step enforced.

Quantum Counting

Determine #solutions, M,
to an N item search problem.

(e.g. determine weight of a Boolean function).

Classically - $\Theta(N)$ queries

Quantum - Combine Grover iteration with phase estimation.

Classical Statistics

Sample uniformly and independently the search space k times.

Let $X_j = 1$ if jth oracle call revealed solution.

Estimate of #solutions is

$$S = N \times \sum_j \frac{X_j}{k}$$

Standard deviation $\Delta S = \sqrt{M(N-M)/k}$

We require $k = \mathcal{R}(N)$ in order to estimate M correctly to within accuracy $\sqrt{M}$ with prob. $\geq 3/4$.

Any classical counting algorithm with prob. $\geq \frac{3}{4}$ of estimating M correctly to within $c\sqrt{M}$, must make

$$\Omega(N)$$ oracle calls.

Quantum Counting:

Use phase estimation to estimate eigenvalues of Grover iteration,

... enables us to determine #solutions.

Let Grover iteration occur in space spanned by $|\alpha\rangle$ and $|\beta\rangle$.

Let θ be angle of Grover rotation.

Let eigenvectors of Grover iteration be $|a\rangle$ and $|b\rangle$.

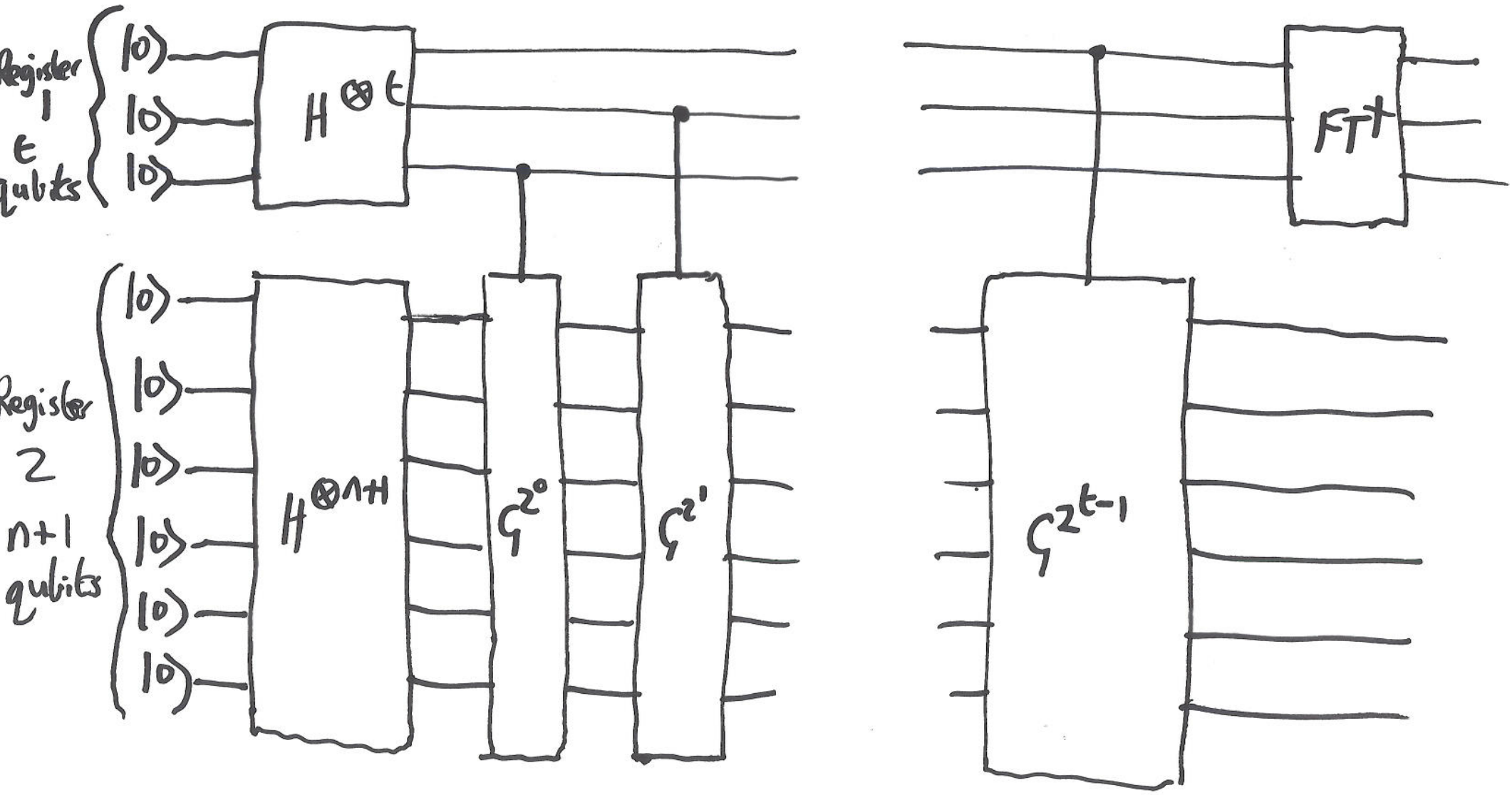
In $|\alpha\rangle, |\beta\rangle$ basis,

$$G = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}.$$

Therefore,

eigenvalues of Grover iteration are $e^{i\theta}$ and $e^{i(2\pi-\theta)}$.

Quantum Counting Circuit



Circuit...

... estimates θ to m bits, with success prob. $\geq 1-\epsilon$.

Register 1: $t = m + \lceil \log(2 + \frac{1}{2\epsilon}) \rceil$ qubits

Register 2: $n+1$ qubits

... initialised to $\sum_x |x\rangle$ by Hadamard transform

... a superposition of eigenstates $|a\rangle$ and $|b\rangle$.

... So circuit estimates θ or $2\pi - \theta$ to within $|\Delta\theta| \leq 2^{-m}$ with prob $\geq 1-\epsilon$.

Accuracy?

Using estimate for θ and $\sin^2\left(\frac{\theta}{2}\right) = \frac{M}{2N}$

one obtains estimate for # solutions $= M$.

Error in estimate, ΔM, satisfies:

$$\frac{|\Delta M|}{2N} = \left|\sin\left(\frac{\theta+\Delta\theta}{2}\right) + \sin\left(\frac{\theta}{2}\right)\right| \left|\sin\left(\frac{\theta+\Delta\theta}{2}\right) - \sin\left(\frac{\theta}{2}\right)\right|$$

$$< \left(2\sin\left(\frac{\theta}{2}\right) + \frac{|\Delta\theta|}{2}\right)\frac{|\Delta\theta|}{2}$$

$$< \left(\sqrt{2MN} + \frac{N}{2^{m+1}}\right)2^{-m}$$

e.g. with $m = \lceil \frac{n}{2} \rceil + 1$, $\varepsilon = \frac{1}{6}$, then $t = \lceil \frac{n}{2} \rceil + 3$, so

$O(\sqrt{N})$ iterations required, where $|\Delta M| < \sqrt{\frac{M}{2}} + \frac{1}{4}$.

Classical requires $O(N)$ calls.

In particular,

algorithm determines whether solution even exists.

i.e.

$M = 0$ or $M \neq 0$?

If $M = 0$ then $|\Delta M| < \frac{1}{4}$

$\Rightarrow$ zero estimated with prob. $\geq \frac{5}{6}$

If $M \neq 0$,

$\Rightarrow$ non-zero estimated with prob. $\geq \frac{5}{6}$.

Find a Solution to Search when M is unknown

Use quantum counting to estimate Θ and M.

Then,

apply quantum search,

repeating iteration R times,

where R is determined using Θ and M.