Could Quantum Computation Aid Path Integration?

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Computing Numerical Integrals

D. S. Abrams and C. P. Williams, quant-ph/9908083 (1999)
J. F. Traub and H. Wozniakowski, quant-ph/0109113 (1999)

Path integral: $\int \mathcal{D}x F(x)$

Integral: $\int \ldots \int dx_1 \ldots dx_n f(x_1, \ldots, x_n)$

Sum: $\dfrac{1}{M^n} \sum_{y_1=0}^{M-1} \ldots \sum_{y_n=0}^{M-1} f(y_1/M, \ldots, y_n/M)$

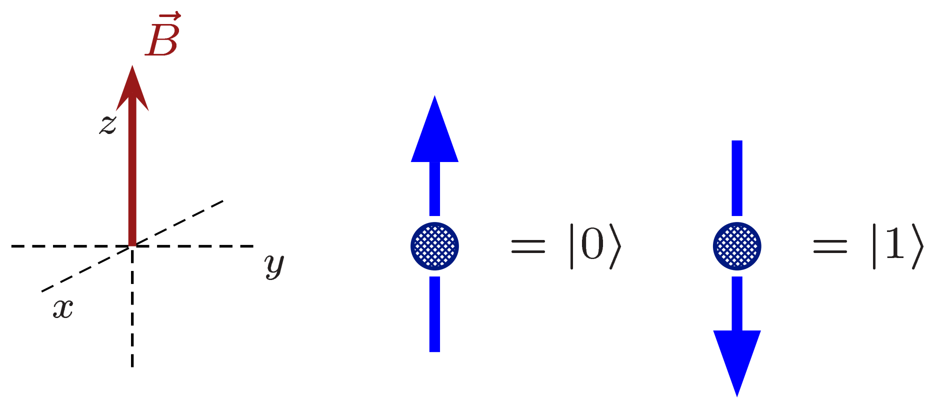
Monte Carlo $O(1/\varepsilon^2)$ for accuracy ε

Quantum $O(1/\varepsilon)$ for accuracy ε

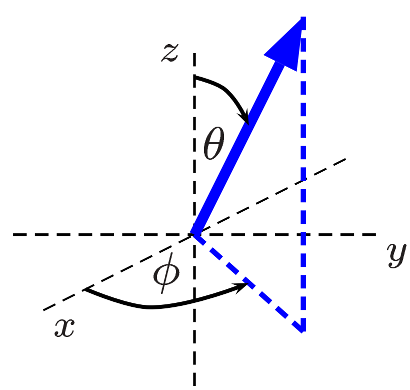
Storing Information

Information is stored as a state of a collection of distinguishable two-state quantum systems (qubits).

- Example: Spin $\frac{1}{2}$ particle in a magnetic field represents a single conventional bit via its energy eigenstates.



- Superpositions extend information representation:



$$|\psi\rangle = \cos(\theta/2) e^{-i\phi/2} |0\rangle + \sin(\theta/2) e^{+i\phi/2} |1\rangle$$

Multiple qubits

General state of an n qubit system:

- "Binary" format

$$|\Psi\rangle = \sum_{x_n=0}^{1} \dots \sum_{x_1=0}^{1} a_{x_n \dots x_1} |x_n\rangle \dots |x_1\rangle$$

  where

$$|x_n\rangle \dots |x_1\rangle := |x_n\rangle \otimes \dots \otimes |x_2\rangle \otimes |x_1\rangle \, .$$

- "Decimal" format

$$|\Psi\rangle = \sum_{x=0}^{2^n-1} a_x |x\rangle$$

  where $x_n \dots x_1$ is the binary representation of x and

$$|x\rangle := |x_n\rangle \dots |x_1\rangle \, .$$

- Computational basis:

$$|0\rangle \, , |1\rangle \, , |2\rangle \, , \dots , |2^n - 1\rangle \, .$$

Extracting Information

Information is extracted by performing a projective measurement in the computational basis.

- Possible outcomes:

$$x \in \{0, \ldots, 2^n - 1\}$$

- Probability of outcomes:

$$|\Psi\rangle = \sum_{x=0}^{2^n-1} a_x |x\rangle \quad \rightarrow \quad \mathrm{Prob}(x) = |a_x|^2 .$$

- The same quantum computation can result in many different outcomes, some of which may be erroneous.

- Example: Spin $\frac{1}{2}$ particles in a magnetic field:
    - For each qubit, j, measure the component of the spin along the magnetic field

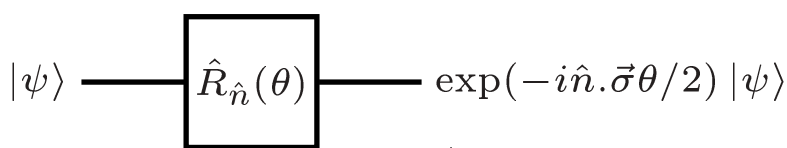
Spin for qubit j	x_j
Up $(+\hbar/2)$	0
Down $(-\hbar/2)$	1

Processing Information

Information is processed by applying a sequence of unitary transformations ("gates").

$$|\Psi_{\text{final}}\rangle = \hat{U}_n \ldots \hat{U}_1 |\Psi_{\text{initial}}\rangle \qquad \text{where} \quad \hat{U}_j^\dagger \hat{U}_j = \hat{I}$$

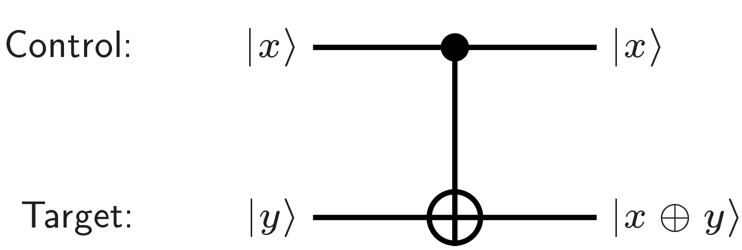
- Quantum algorithms are described via sequences of unitaries.
- $\hat{U}_j$ can be decomposed into a product of fundamental gates:
  - Single qubit rotation through angle θ about axis $\hat{n}$:



$$\hat{n}.\vec{\sigma} = n_x\sigma_x + n_y\sigma_y + n_z\sigma_z$$

$$\sigma_x := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_z := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

  - Two qubit controlled-NOT:



Gate construction

Controlling a quantum system is usually envisaged in terms of the system Hamiltonian, which must be related to unitary transformations.

- Example: Two spin $\frac{1}{2}$ particles in external magnetic fields:

$$\hat{H}(t) = \underbrace{\hat{H}_0}_{\text{fixed}} + \underbrace{H_1(t)}_{\text{adjustable}}$$

$$\hat{H}_0 = \underbrace{\omega_1 \sigma_z^{(1)} + \omega_2 \sigma_z^{(2)}}_{\text{External field along } \hat{z}} + \underbrace{J \sigma_z^{(2)} \otimes \sigma_z^{(1)}}_{\text{Internal coupling}}$$

$$\hat{H}_1(t) = \underbrace{B \cos(\omega t + \phi) \left(\sigma_x^{(1)} + \sigma_x^{(2)} \right)}_{\text{External field along } \hat{x}}$$

  where $\hat{H}_1(t)$ can be applied for arbitrary durations.

- Generates unitary evolution operator:

$$|\Psi(t_i)\rangle \to |\Psi(t)\rangle = \hat{U}(t, t_i)\, |\Psi(t_i)\rangle$$

  satisfying

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \hat{U}(t, t_i) &= \hat{H}(t) \hat{U}(t, t_i) \\ \hat{U}(t_i, t_i) &= \hat{I} \end{aligned}$$

- In practice, choose simple $\hat{H}_1(t)$ to give fundamental gates.

Amplitude Amplification

Basis for quantum algorithms (Grover's search, mean estimation, numerical integration) offering quadratic speedups.

L. K. Grover, Proc 30th ACM STOC, 53-62 (1998)

G. Brassard, P. Hoyer, M. Mosca, and A. Tapp, quant-ph/0005055 (2000)

Example: Unstructured search

- Alice randomly chooses

$$s \in \{0, \dots N-1\}.$$

- Bob must determine s using:
  - Unitaries independent of s and
  - An oracle supplied by Alice:

$$\boxed{\hat{U}_s \left|x\right\rangle \left|y\right\rangle = \left|x\right\rangle \left|y \oplus \delta_{xs}\right\rangle} \quad \text{where} \quad \left\{ \begin{array}{l} x = 0, 1, \dots, N-1 \\ y = 0, 1 \end{array} \right.$$

  - "Classical" usage:

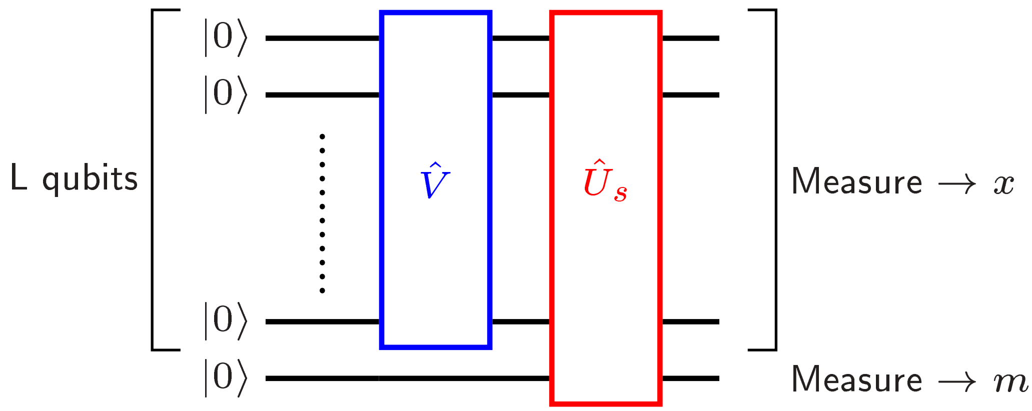
$$\hat{U}_s \left|x\right\rangle \left|0\right\rangle = \left|x\right\rangle \left|\delta_{xs}\right\rangle .$$

- Classical sequential search:

$$\boxed{\approx \frac{N}{2} \quad \text{oracle queries on average.}}$$

Classical Search on a Quantum Computer

- Assume $N = 2^L$.



$$V_{s0} := \langle s| \hat{V} |0\rangle \neq 0$$

- System evolution:

$$|0\rangle\,|0\rangle \rightarrow \sum_{x=0}^{N-1} V_{x0}\,|x\rangle\,|0\rangle \rightarrow \sum_{x=0}^{N-1} V_{x0}\,|x\rangle\,|\delta_{xs}\rangle$$

$$\mathrm{Prob}(m=1) = |V_{s0}|^2 \Rightarrow \boxed{O\left(\frac{1}{|V_{s0}|^2}\right) \text{ runs on average.}}$$

- Hadamards are optimum:

$$\hat{V} := \hat{H} \otimes \ldots \otimes \hat{H} \qquad \hat{H} := \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

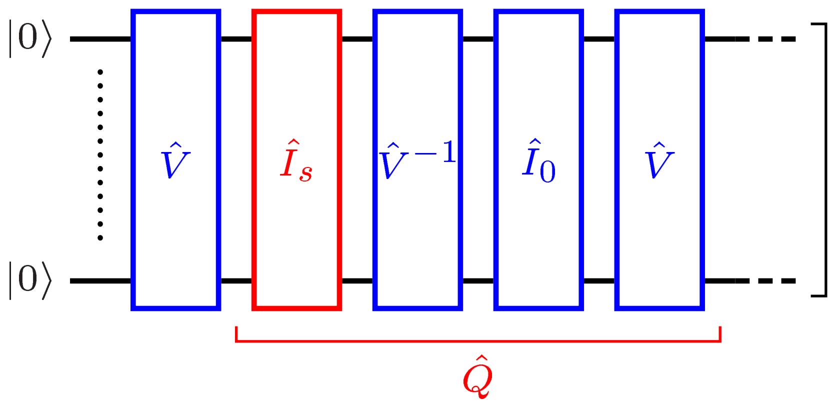
$$\Rightarrow |V_{s0}|^2 = \frac{1}{2^L} = \frac{1}{N} \Rightarrow \boxed{O(N) \text{ runs on average.}}$$

Quantum Search by Amplitude Amplification

- Modified oracle for L qubits

$$\hat{I}_s \left|x\right\rangle := (-1)^{\delta_{xs}} \left|x\right\rangle \qquad \text{for } x = 0, \ldots, N-1.$$

features in



Repetitions of $\hat{Q}$ followed by measurement.

$$\hat{I}_0 \left|x\right\rangle := (-1)^{\delta_{x0}} \left|x\right\rangle$$

- After m applications of $\hat{Q}$:

$$\left|\Psi\right\rangle = \cos\left(\theta(2m+1)/4\right) \left|s_\perp\right\rangle + \sin\left(\theta(2m+1)/4\right) \left|s\right\rangle$$

where

$$\theta := 2 \arccos\left(1 - 2\left|V_{s0}\right|^2\right)$$

$$\left|s_\perp\right\rangle := \frac{1}{\sqrt{1 - \left|V_{s0}\right|^2}} \left(\hat{V}\left|0\right\rangle - V_{s0}\left|s\right\rangle\right)$$

Applications of $\hat{Q}$ can amplify the amplitude of $\left|s\right\rangle$.

Amplifying Small Success Probabilities

- For $|V_{s0}| \ll 1$:

$$\theta \approx 4\,|V_{s0}|$$

- Initially

$$|\Psi\rangle \approx |s_\perp\rangle$$

- Each application of $\hat{Q}$ "rotates" through $\theta/2 \approx 2\,|V_{s0}|$ towards $|s\rangle$. After about

$$\frac{\pi/2}{2\,|V_{s0}|} = \frac{\pi}{4\,|V_{s0}|}$$

applications of $\hat{Q}$, measurement yields s with probability at least $1 - |V_{s0}|^2$.

Using amplitude amplification s can be determined with near certainty with just $O\left(\frac{1}{|V_{s0}|}\right)$ oracle queries.

- For searching use:

$$\hat{V} := \hat{H} \otimes \ldots \otimes \hat{H} \qquad \Rightarrow |V_{s0}| = 1/\sqrt{N}$$

$O\left(\sqrt{N}\right)$ oracle queries on average to determine s.

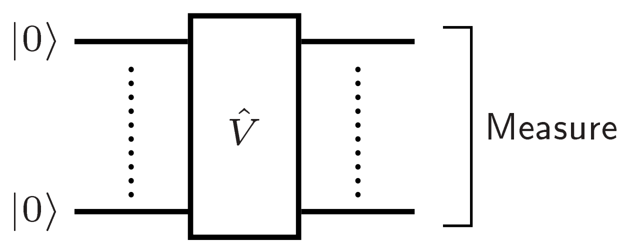
Estimating Probability Amplitudes

Amplitude amplification also speeds up estimation of probability amplitudes.

- For a unitary operation $\hat{V}$ such that, for some s,

$$|0\rangle \xrightarrow{\hat{V}} p\,|s\rangle + \sqrt{1-p^2}\,|s_\perp\rangle \qquad \text{where} \qquad \begin{array}{l} 0 \le p \le 1 \\ \langle s|s_\perp\rangle = 0 \end{array}$$

  determine p with error at most ε using minimum number of applications of $\hat{V}$.
- N independent binary tests:



$$p \approx n_s/N$$

where n_s is the number of times measurement returns s.

$O(1/\varepsilon^2)$ applications of $\hat{V}$ needed to estimate p to accuracy ε.

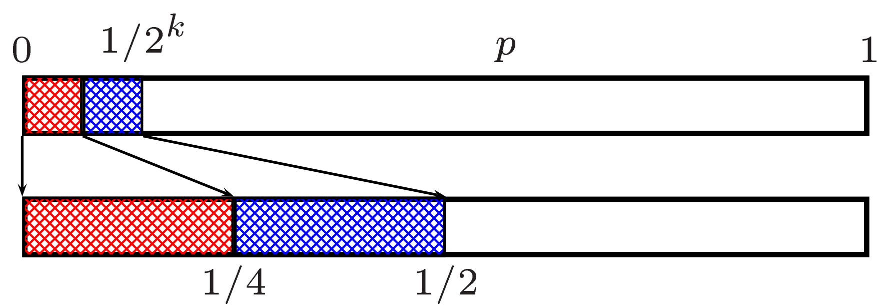
Quantum Assistance

Small fixed number of binary tests, N_0, required to determine p to accuracy $\varepsilon = \frac{1}{4}$.

Refine accuracy by replacing most of the repeated binary tests with amplitude amplification using

$$\hat{Q} := \hat{V}\hat{I}_0\hat{V}^{-1}\hat{I}_s.$$

- For $p \leq 1/2^k$ amplify to improve estimate



using $O(1/2^{k+1})$ applications of $\hat{Q}$ and N_0 binary tests to find p with accuracy $1/2^{k+1}$.

General Probability Amplitude Estimation

For any $0 \leq p \leq 1$ proceed iteratively to determine binary representation:

$$p = \frac{1}{2}\,p_1 + \frac{1}{4}\,p_2 + \ldots + \frac{1}{2^k}\,p_k + \ldots$$

1: For moderate j obtain

$$E = \frac{1}{2}\,p_1 + \frac{1}{4}\,p_2 + \ldots + \frac{1}{2^j}\,p_j$$

using N_j applications of $\hat{V}$ (accuracy $1/2^j$).

2: Let $p' := p - E$ so that $0 \leq p' \leq 1/2^j$ and assume existence of $\hat{V}_j$

$$|0\rangle \overset{\hat{V}_j}{\rightarrow} p'\,|s\rangle + \sqrt{1 - p'^2}\,|s_\perp\rangle\,.$$

3: Use amplitude amplification to get accuracy $1/2^{j+1}$

$$\rightsquigarrow p_{j+1} \qquad \text{after } O(1/2^{j+1}) \text{ applications of } \hat{Q}$$

and set

$$E \to E + \frac{1}{2^{j+1}}\,p_{j+1}$$

4: Repeat steps 2 and 3.

$O((\log\varepsilon)/\varepsilon)$ applications of $\hat{Q}$ needed to determine p with accuracy ε.

Quantum Summation

L. K. Grover, Proc 30th ACM STOC, 53-62 (1998)

D. S. Abrams and C. P. Williams, quant-ph/9908083 (1999)

- Compute

$$T := \frac{1}{M^d} \sum_{y_1,\ldots,y_d=0}^{M-1} f(y_1,\ldots,y_d)$$

where $0 \leq f(y_1,\ldots,y_d) \leq 1$.

- Compose $\hat{V}$:

$$|0\rangle\,|0\ldots0\rangle$$

$$\downarrow$$

$$\frac{1}{\sqrt{M^d}} \sum_{y_1,\ldots,y_d=0}^{M-1} |0\rangle\,|y_1,\ldots,y_d\rangle$$

$$\downarrow$$

$$\frac{1}{\sqrt{M^d}} \sum_{y_1,\ldots,y_d=0}^{M-1} f(y_1,\ldots,y_d)\,|0\rangle\,|y_1,\ldots,y_d\rangle + \sum_{y_1,\ldots,y_d=0}^{M-1} \sqrt{1-f(y_1,\ldots,y_d)^2}\,|1\rangle\,|y_1,\ldots,y_d\rangle$$

$$\downarrow$$

$$T\underbrace{|0\rangle\,|0\ldots0\rangle}_{|s\rangle} + \text{orthogonal terms}$$

- Quantum probability amplitude estimation gives T with accuracy ε with $O(1/\varepsilon)$ applications of $\hat{V}$.

Summary

- Amplitude amplification provides quadratic speed up in numerical integration.
- Alternative schemes exist involving quantum counting.
- Experiments still distant: NMR leads with 7 qubits.
- References:

J. F. Traub and H. Wozniakowski, quant-ph/0109113 (1999)

D. S. Abrams and C. P. Williams, quant-ph/9908083 (1999)

L. K. Grover, Proc 30th ACM STOC, 53-62 (1998)

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