Could Quantum Computation Aid Path Integration?

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Computing Numerical Integrals


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

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

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

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

Quantum \( O(1/\varepsilon) \) for accuracy \( \varepsilon \)
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.

\[
\begin{align*}
\vec{B} &= |0\rangle \\
\vec{B} &= |1\rangle
\end{align*}
\]

- 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**

\[
|\Psi\rangle = \sum_{x_n=0}^{1} \cdots \sum_{x_1=0}^{1} a_{x_n \ldots x_1} |x_n\rangle \cdots |x_1\rangle
\]

where

\[
|x_n\rangle \ldots |x_1\rangle := |x_n\rangle \otimes \cdots \otimes |x_2\rangle \otimes |x_1\rangle.
\]

- **“Decimal” format**

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

where \( x_n \ldots x_1 \) is the binary representation of \( x \) and

\[
|x\rangle := |x_n\rangle \ldots |x_1\rangle.
\]

- **Computational basis:**

\[
|0\rangle, |1\rangle, |2\rangle, \ldots, |2^n - 1\rangle.
\]
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:
  \[
  |\Psi\rangle = \sum_{x=0}^{2^n-1} a_x |x\rangle \quad \rightarrow \quad \text{Prob}(x) = |a_x|^2.
  \]

- 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

<table>
<thead>
<tr>
<th>Spin for qubit ( j )</th>
<th>( x_j )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Up ((+\hbar/2))</td>
<td>0</td>
</tr>
<tr>
<td>Down ((-\hbar/2))</td>
<td>1</td>
</tr>
</tbody>
</table>
Processing Information

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

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

- 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 \( \theta \) about axis \( \hat{n} \):

\[
|\psi\rangle \quad \xrightarrow{\hat{R}_{\hat{n}}(\theta)} \quad \exp(-i\hat{n}.\vec{\sigma} \theta/2) |\psi\rangle \\
\hat{n}.\vec{\sigma} = n_x \sigma_x + n_y \sigma_y + n_z \sigma_z
\]

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

- **Two qubit controlled-NOT:**

  Control: \[|x\rangle \quad \xrightarrow{\bullet} \quad |x\rangle\]

  Target: \[|y\rangle \quad \xrightarrow{\bullet} \quad |x \oplus y\rangle\]
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:

$$\hat{H}(t) = \underbrace{\hat{H}_0}_{\text{fixed}} + \underbrace{\hat{H}_1(t)}_{\text{adjustable}}$$

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

$$\hat{H}_1(t) = B \cos(\omega t + \phi) \left( \sigma_x^{(1)} + \sigma_x^{(2)} \right)$$

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

- Generates unitary evolution operator:

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

satisfying

$$i\hbar \frac{\partial}{\partial t} \hat{U}(t, t_i) = \hat{H}(t) \hat{U}(t, t_i)$$

$$\hat{U}(t_i, t_i) = \hat{I}$$

- 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.


Example: Unstructured search

- Alice randomly chooses
  \[ s \in \{0, \ldots, N - 1\}. \]

- Bob must determine \( s \) using:
  - Unitaries independent of \( s \) and
  - An oracle supplied by Alice:
    \[ \hat{U}_s |x\rangle |y\rangle = |x\rangle |y \oplus \delta_{xs}\rangle \]
    where \[ \begin{cases} x = 0, 1, \ldots, N - 1 \\ y = 0, 1 \end{cases} \]
  - “Classical” usage:
    \[ \hat{U}_s |x\rangle |0\rangle = |x\rangle |\delta_{xs}\rangle . \]

- Classical sequential search:
  \[ \approx \frac{N}{2} \text{ oracle queries on average.} \]
Classical Search on a Quantum Computer

▶ Assume \( N = 2^L \).

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

▶ System evolution:

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

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

▶ Hadamards are optimum:

\[ \hat{V} := \hat{H} \otimes \ldots \otimes \hat{H} \]

\[ \hat{H} := \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \]

\[ \Rightarrow |V_{s0}|^2 = \frac{1}{2^L} = \frac{1}{N} \Rightarrow O(N) \text{ runs on average.} \]
Quantum Search by Amplitude Amplification

- Modified oracle for $L$ qubits

$$\hat{I}_s |x\rangle := (-1)^{\delta xs} |x\rangle$$

for $x = 0, \ldots, N - 1$.

features in

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

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

where

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

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

Applications of $\hat{Q}$ can amplify the amplitude of $|s\rangle$. 
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:
  \[ \hat{V} := \hat{H} \otimes \ldots \otimes \hat{H} \quad \Rightarrow \quad |V_{s0}| = 1/\sqrt{N} \]

$O \left( \sqrt{N} \right)$ 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 $s$,

$$|0\rangle \xrightarrow{\hat{V}} p\,|s\rangle + \sqrt{1-p^2}\,|s_{\perp}\rangle$$

where $0 \leq p \leq 1$ and $\langle s|s_{\perp}\rangle = 0$

determine $p$ with error at most $\varepsilon$ using minimum number of applications of $\hat{V}$.

- $N$ independent binary tests:

$$p \approx \frac{n_s}{N}$$

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 $\varepsilon$. 
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 $\hat{V}_j$

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

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

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

and set

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

4: Repeat steps 2 and 3.

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


- **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 \(\hat{V}\):**

\[
|0\rangle |0\ldots0\rangle \\
\downarrow
\frac{1}{\sqrt{M^d}} \sum_{y_1, \ldots, y_d = 0}^{M-1} |0\rangle |y_1, \ldots, y_d\rangle \\
\downarrow
\frac{1}{\sqrt{M^d}} \sum_{y_1, \ldots, y_d = 0}^{M-1} f(y_1, \ldots, y_d) |0\rangle |y_1, \ldots, y_d\rangle \\
+ \sum_{y_1, \ldots, y_d = 0}^{M-1} \sqrt{1 - f(y_1, \ldots, y_d)^2} |1\rangle |y_1, \ldots, y_d\rangle \\
\downarrow
T|0\rangle |0\ldots0\rangle + \text{orthogonal terms}
\]

- **Quantum probability amplitude estimation gives** \(T\) **with accuracy** \(\varepsilon\) **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:
  