Quantum Metropolis Sampling
An algorithm to simulate thermal systems with a quantum computer

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Perimeter Institute for Theoretical Physics
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Outline

1. Motivation
2. Quantum simulators
3. Metropolis algorithm
4. Quantum Metropolis
What are computers used for?

From talk by F. Verstraete, from a talk by S. Aaronson, from a talk by A. Aspuru-Guzik
Motivation

What are they computing?

Inputs

- A local Hamiltonian $H = \sum_k h_k$:
  - $\|h_k\| = \mathcal{O}(1)$.
  - $h_k$ acts on a few particles, i.e. $h_k = I \otimes I \otimes A \otimes I \otimes I \otimes B \otimes I \otimes I$.

- An efficiently specifiable state $\rho$, e.g.
  - The Gibbs state $\rho_G(\beta) = \frac{1}{Z} e^{-\beta H}$.
  - The ground state of $H$, i.e. $\rho_G(\infty)$.
  - Physically relevance: thermal equilibrium at temperature $\frac{1}{\beta}$.

Output

$$\langle X(t) Y \rangle = \text{Tr}\{X e^{-iHt} Y e^{iHt} \rho_G(\beta)\} \text{ for one-body operators } X \text{ and } Y.$$
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Why is this complicated?

\[ \text{Tr}\{ X e^{-iHt} Y e^{iHt} \rho \} \]

- Matrix multiplication in vector space \( \mathcal{H} \) of dimension exponential with the number of particles.

- \( \rho \) is not specified in a useful format:
  - E.g., \( \rho \propto e^{-\beta H} \).
  - Computing its matrix elements \( \rho_{ij} \) is hard.
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Some partial solutions

- **Weakly interacting particles**: $H = H_0 + \epsilon V$.
  - Perturbation theory
  - Hartree-Fock
  - Density functional theory
  - etc.
- Weakly entangled particles/one dimension
  - Renormalization methods (NRG, DMRG, MPS, PEPES).
  - Other variational methods (Laughlin state, Moore-Read).
- Unfrustrated bosonic systems
  - Quantum Monte Carlo $e^{-\beta H} \sim (I - \epsilon H) \otimes (I - \epsilon H) \otimes \ldots$

The interesting physics appears to lie outside the scope covered by these methods.

- Standard model for elementary particle masses
- Hubbard model for superconductivity
- Coulomb force for molecular binding energies
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Simulating Physics with Computers

Richard P. Feynman

Department of Physics, California Institute of Technology, Pasadena, California 91107

Received May 7, 1981

1. INTRODUCTION

On the program it says this is a keynote speech—and I don’t know what a keynote speech is. I do not intend in any way to suggest what should be in this meeting as a keynote of the subjects or anything like that. I have my own things to say and to talk about and there’s no implication that anybody needs to talk about the same thing or anything like it. So what I want to talk about is what Mike Dertouzos suggested that nobody would talk about. I want to talk about the problem of simulating physics with computers and I mean that in a specific way which I am going to explain.
Simulating Physics with Computers

be understood very well in analyzing the situation. And I’m not happy with all the analyses that go with just the classical theory, because nature isn’t classical, dammit, and if you want to make a simulation of nature, you’d better make it quantum mechanical, and by golly it’s a wonderful problem, because it doesn’t look so easy. Thank you.

1. INTRODUCTION

On the program it says this is a keynote speech—and I don’t know with it, with quantum-mechanical rules). For example, the spin waves in a spin lattice imitating Bose-particles in the field theory. I therefore believe it’s true that with a suitable class of quantum machines you could imitate any quantum system, including the physical world. But I don’t know whether the general theory of this intersimulation of quantum systems has
Solving the dynamics

Lloyd’s idea, ’96

\[
\exp(-it \sum_k h_k) = \left[ \prod_k \exp(-ih_k/N) \right]^N + O\left(\frac{1}{N^2}\right)
\]

So we can integrate Schrödinger’s equation, solve \( \dot{\rho} = -i[H, \rho] \).

How do we specify the initial conditions \( \rho_G(\beta) \)?
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\[ \exp(-it \sum_k h_k) = \left[ \prod_k \exp(-ih_k/N) \right]^N + \mathcal{O}(\frac{1}{N^2}) \]

\[ e^{-iHt} = U \]

\# of gates = poly(n, t, \varepsilon)

So we can integrate Schrödinger’s equation, solve \( \dot{\rho} = -i[H, \rho] \).

How do we specify the initial conditions \( \rho_G(\beta) \)?
Simulate evolution of "system+bath" and Metropolis-like.
- Conditions for thermalization not reproduced (poorly understood).
- Use adiabatic evolution $H(t) = (1 - t/T)H_0 + t/TH_{hard}$
  - Must avoid quantum phase transition.
  - Limited to ground state.
- Use Grover-like algorithm to search ground state.
  - Slow.
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How is this problem solved for classical systems?

Use Markov Chain Monte Carlo to sample from \( p_G(x) = \frac{1}{Z} e^{-\beta E(x)} \)

The Metropolis algorithm

1. Start from a random configuration \( x \) of energy \( E(x) \).
2. Generate a new configuration \( y \) by changing \( x \) at a few locations.
3. Accept / reject new configuration with \( w_{xy} = \min\{1, e^{\beta(E(x) - E(y))}\} \):
   - Accept \( x \leftarrow y \) with probability \( w_{xy} \).
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Equation of State Calculations by Fast Computing Machines

Nicholas Metropolis, Arianna W. Rosenbluth, Marshall N. Rosenbluth, and Augusta H. Teller,
Los Alamos Scientific Laboratory, Los Alamos, New Mexico

AND

Edward Teller,* Department of Physics, University of Chicago, Chicago, Illinois

(Received March 6, 1953)
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Markov chain

\[ x_0 \xrightarrow{P(x_1|x_0)} x_1 \xrightarrow{P(x_2|x_1)} x_2 \ldots x_{n-1} \xrightarrow{P(x_n|x_{n-1})} x_n \]

Detailed balance condition

The distribution \( p_G(x) = \frac{1}{Z} e^{-\beta H(x)} \) obeys the condition

\[ p_G(x) P(y|x) = p_G(y) P(x|y) \]

so it is the fixed point of the Markov chain \( P(x|y) \).

Convergence rate

The convergence rate is given by the inverse spectral gap \( \Delta^{-1} \) of the stochastic matrix \( P(x|y) \): \( n \in O(\Delta^{-1}) \).

\( \Delta^{-1} \) appears to scale polynomially for problems of interest.
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\[
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x_0 & \xrightarrow{P(x_1|x_0)} x_1 \xrightarrow{P(x_2|x_1)} x_2 \ldots x_{n-1} \xrightarrow{P(x_n|x_{n-1})} x_n \sim \frac{1}{\mathcal{Z}} e^{-\beta H(x_n)}
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### Detailed balance condition

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Can’t we do the same with quantum systems?

Objective

CPTP map $\mathcal{E}$ such that $\mathcal{E}^n(\rho_0) \to \frac{1}{Z} e^{-\beta H}$ for large enough $n$.

Straightforward generalization of Metropolis

1. Start from a random energy eigenstate $\psi_i$ of energy $E_i$.
2. Generate a new "nearby" energy eigenstate $\psi_j$ of energy $E_j$.
3. Accept / reject new configuration with $w_{ij} = \min\{1, e^{\beta(E_i - E_j)}\}$:
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Use quantum phase estimation.
Problems

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- Use quantum phase estimation.
The ability to simulate the dynamics generated by $H$ can be used to construct an efficient circuit to (approximately) measure the energy:

$$\sum_i \alpha_i |\psi_i\rangle \cdot e^{-iHr} \cdot \sum_i \alpha_i |\psi_i\rangle \otimes |E_i\rangle$$

- Can use to prepare a random energy eigenstate.
- Can use to measure the energy of a given eigenstate.
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- We don’t know what the energy eigenstates $\psi_i$ are.
  - Use quantum phase estimation.
- How do we jump to a "nearby" energy eigenstate?

Importance of local moves

- If classical configurations $x$ and $y$ differ only at a few positions, then $E(x) \approx E(y)$ for any local Hamiltonian $H$. 

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$E$ $C_x^y$

David Poulin (Sherbrooke)
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- If classical configurations $x$ and $y$ differ only at a few positions, then $E(x) \approx E(y)$ for any local Hamiltonian $H$.

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Use QPE to prepare an initial random energy eigenstate $\psi_i$.

Apply a local random unitary transformation $C$:

$$C : |\psi_i\rangle \rightarrow \sum_j c_j^i |\psi_j\rangle \quad E_i \sim E_j$$

Use QPE to collapse onto a new energy eigenstate $\psi_j$ and learn the associated energy $E_j$:

$$QPE : \sum_j c_j^i |\psi_j\rangle \rightarrow \sum_j c_j^i |\psi_j\rangle \otimes |E_j\rangle \xrightarrow{|c_j^i|^2} |\psi_j\rangle \otimes |E_j\rangle$$

Compute $w_{ij} = min\{1, e^{\beta(E_i - E_j)}\}$

- With probability $w_{ij}$, go to step 2.
- With probability $1 - w_{ij}$, return computer to state $\psi_i$ and go to step 2.
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Quantum Metropolis

Not quite there yet...

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Coherent Metropolis move

We combine steps 3&4 coherently \((E_j \text{ is known})\):

\[
\sum_j c_j^i |\psi_j\rangle \otimes |E_j\rangle \rightarrow \sum_j c_j^i |\psi_j\rangle \otimes |E_j\rangle \otimes (\sqrt{w_{ij}}|0\rangle + \sqrt{1-w_{ij}}|1\rangle)
\]

Measure last qubit:
- If the outcome is 0, measure the "energy register" to learn \(E_j\) and return to step 2.
- If the outcome is 1, go back to state \(\psi_i\).

This is already better because only one bit of information was learned–accept/reject–so less damage was made to the state.

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**Goal**

Starting from $Q^\perp|\psi\rangle$, go back to $|\psi\rangle$.

**Solution**

Iterate $\mathcal{P}$ and $\mathcal{Q}$ measurements until outcome $P$ is obtained.

| $|\psi\rangle$ | $= (Q + Q^\perp)|\psi\rangle$ | $= \sqrt{q}|\phi_Q\rangle + \sqrt{1-q}|\phi_Q^\perp\rangle$ |
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Repeat $m$ times, probability of failure is $\sim p^{-m}$.

We can reject the update $\rightarrow$ quantum Metropolis step $\mathcal{E}$. 
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David Poulin (Sherbrooke)
Quantum Metropolis

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Asymptotic properties

Quantum detailed balance

The following condition is satisfied

\[ \sqrt{\rho_m \rho_n} \langle \psi_i | \mathcal{E}(|\psi_m\rangle\langle\psi_n|) | \psi_j \rangle = \sqrt{\rho_i \rho_j} \langle \psi_m | \mathcal{E}(|\psi_i\rangle\langle\psi_j|) | \psi_n \rangle. \]

Hence \( \rho_G = \sum_j p_j |\psi_j\rangle\langle\psi_j| \) is the fixed point, \( p_j \propto e^{-\beta E_j} \).

Gap

Like in the classical setting, the rate at which this stochastic process converges to its stationary state (the Gibbs distribution) is given by the inverse gap of \( \mathcal{E} \) (viewed as a linear operator).

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The model

\[ H = \sum_k \sigma_k^x \sigma_{k+1}^x + \sigma_k^y \sigma_{k+1}^y + g \sigma_k^z \]

The local moves

\[ C_k = \left( \bigotimes_{j=1}^{k-1} \sigma_j^z \right) \sigma_k^x \]
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