Presented by

Man-Hong Yung

Department of Chemistry and Chemical Biology,
Harvard University

at

QIP Singapore 2011

Quantum-Quantum Metropolis Algorithm

Co-author: Alan Aspuru-Guzik

Summary of Markov-chain based Thermal state preparation

Related works	Hamiltonian	Quantum Speedup
Somma et al (PRL 2008)	Classical	Yes
Terhal and Divincenzo (PRA 2000) Temme et al (arXiv 2009)	Quantum	No
This work	Quantum	Yes

3

Basic concepts

- Master equation and Markov chain
- Metropolis method
- Markov-chain quantization (by Szegedy)

4

Basic 1: Master equation & Markov chain

$$P(x,t+1)-P(x,t)=-\sum_{x'\neq x} M(x\to x')P(x,t)+\sum_{x'\neq x} M(x'\to x)P(x',t)$$

$$\Rightarrow \quad P(x,t+1)=\sum_{x'} M(x'\to x)P(x',t)$$

Detailed balance:

$$M(x\to x')\pi(x)=M(x'\to x)\pi(x')$$

$$\pi(x):\quad \text{equilibrium distribution}$$

5 Basic 2: Metropolis method

- Prepare known distribution

$$M(x \to x') = A(x,x')z(x,x')$$

$$A(x,x') = A(x',x): \text{ symmetric function}$$

$$z(x,x') = \min\left\{1, \frac{\pi(x')}{\pi(x)}\right\}: \text{ Metropolis filter}$$

$$M(x \to x')\pi(x) = M(x' \to x)\pi(x')$$

Thermal distribution:

$$\pi(x) = e^{-\beta E(x)} / Z$$

$$z(x,x') = \min\left\{1, e^{-\beta(E(x)-E(x'))}\right\}: \text{ Metropolis filter}$$

6

Markov-chain quantization by Szegedy (1/2)

(See also the talk by J. Roland for another application)

- Define two operations (in computational basis)

$$U_X |x\rangle|0\rangle = \sum_y \sqrt{M_\beta(x,y)}\,|x\rangle|y\rangle$$

$$U_Y |0\rangle|y\rangle = \sum_x \sqrt{M_\beta(y,x)}\,|x\rangle|y\rangle$$

Connection with the Metropolis method

$$M_\beta(x \to x') = A(x,x')\, z_\beta(x,x')$$

$$A(x,x') = A(x',x):\ \text{symmetric function}$$

$$z_\beta(x,x') = \min\left\{1, e^{-\beta(E(x)-E(x'))}\right\}:\ \text{Metropolis filter}$$

Markov-chain quantization by Szegedy (2/2)

- With these two operations

$$U_X|x\rangle|0\rangle = \sum_y \sqrt{M_\beta(x,y)}|x\rangle|y\rangle$$

$$U_Y|0\rangle|y\rangle = \sum_x \sqrt{M_\beta(y,x)}|x\rangle|y\rangle$$

and one operator (modification by Somma et al)

$$W_\beta = U_X^+(2\Lambda_2 - I)(2\Lambda_1 - I)U_X$$

$$\Lambda_1 \equiv I \otimes |0\rangle\langle 0|$$

$$\Lambda_2 \equiv U_Y S \Lambda_1 S U_Y^+$$

8 Szegedy's main results

- Quadratic quantum speedup

Define an effective Hamiltonian

$$W_\beta = e^{-iH_\beta}$$

$$\Delta \geq 2\sqrt{\delta} \quad \Rightarrow \quad O\left(\frac{1}{\Delta}\right) = O\left(\frac{1}{\sqrt{\delta}}\right)$$

Δ : eigenvalue gap

δ: makov transition matrix gap

- Coherent thermal state as the eigenstate

$$\left|\psi_\beta\right\rangle = \sum_x \sqrt{e^{-\beta E(x)} / Z}\,|x\rangle|0\rangle$$

where $\quad \mathrm{W}_\beta\left|\psi_\beta\right\rangle = \left|\psi_\beta\right\rangle$

Quantum simulated annealing (QSA) with Szegedy (Somma et al)

- Use the Szegedy operator

$$\left|\psi_{\beta}\right\rangle \to O(1)\left|\psi_{\beta+\Delta}\right\rangle + \ldots$$

Phase estimation using $W_{\beta+\Delta}$

$$\left|\psi_{\beta}\right\rangle|000...0\rangle \to O(1)\left|\psi_{\beta+\Delta}\right\rangle|1\rangle + \ldots$$

Continue on and on ...

$$\left|\psi_{\beta}\right\rangle \to \left|\psi_{\beta+\Delta}\right\rangle \to \left|\psi_{\beta+2\Delta}\right\rangle + \ldots$$

10 Summary of the key point …

- To construct

$$W_\beta = U_X^+ \left(2\Lambda_2 - I\right)\left(2\Lambda_1 - I\right) U_X$$

$$\Lambda_1 \equiv I \otimes |0\rangle\langle 0|$$

$$\Lambda_2 \equiv U_Y S \Lambda_1 S U_Y^+$$

$$U_X |x\rangle|0\rangle = \sum_y \sqrt{M_\beta(x,y)}\,|x\rangle|y\rangle$$

$$U_Y |0\rangle|y\rangle = \sum_x \sqrt{M_\beta(y,x)}\,|x\rangle|y\rangle$$

11 Quantum-Classical Metropolis algorithm
(unpublished, see my notes on QIP website)

- Implementation of the acceptance and rejection

$$M_\beta(x \to x') = A(x,x') z_\beta(x,x')$$

Previously:

$$U_X |x\rangle|0\rangle = \sum_y \sqrt{M_\beta(x,y)}\,|x\rangle|y\rangle$$

$A(x,x') = A(x',x)$: symmetric function

$z_\beta(x,x') = \min\left\{1, e^{-\beta(E(x)-E(x'))}\right\}$: Metropolis filter

Now, break it into several steps:

$$\begin{aligned}
|x\rangle|x\rangle|0\rangle &\to \sum_y \sqrt{A(x,y)}\,|x\rangle|y\rangle|0\rangle \\
&\to \sum_y \sqrt{A(x,y)}\,|x\rangle|y\rangle\left(\sqrt{z_\beta(x,y)}\,|0\rangle + \sqrt{1-z_\beta(x,y)}\,|1\rangle\right) \\
&\to \sum_y \left(\sqrt{A(x,y) z_\beta(x,y)}\,|y\rangle|x\rangle|0\rangle + \sqrt{A(x,y)\left(1-z_\beta(x,y)\right)}\,|x\rangle|y\rangle|1\rangle\right)
\end{aligned}$$

Quantum Metropolis algorithm with Szegedy

- Goal: prepare thermal states of quantum Hamiltonians
- Method:
  1. Construct the corresponding Szegedy operator (with Metropolis filter)
  2. Quantum simulated Annealing

The Challenges

- Direct translate from the classical case doesn’t work
  - Can’t duplicate quantum states (no cloning)
  - Solution: use a special basis

- Don’t know eigenvalues
  - Solution: phase estimation
    - Need to deal with degeneracy (precision)

14 The working basis for QQMA

- Maximally entangled basis:

$$\frac{1}{\sqrt{N}}\sum_x |x\rangle|x\rangle = \frac{1}{\sqrt{N}}\sum_i |\phi_i\rangle|\tilde{\phi}_i\rangle$$

$$|\phi_i\rangle = \sum_x \langle\phi_i|x\rangle|x\rangle \quad \& \quad |\tilde{\phi}_i\rangle = \sum_x \langle x|\phi_i\rangle|x\rangle$$

$$H|\phi_i\rangle = E_i|\phi_i\rangle$$

$$H^*|\tilde{\phi}_i\rangle = E_i|\tilde{\phi}_i\rangle$$

From QCMA to QQMA

Quantum-Classical Metropolis:

$$|x\rangle|x\rangle|0\rangle \xrightarrow{U_X} \sum_y \sqrt{A(x,y)}\,|x\rangle|y\rangle|0\rangle$$

$$\rightarrow \sum_y \sqrt{A(x,y)}\,|x\rangle|y\rangle\left(\sqrt{z(x,y)}\,|0\rangle + \sqrt{1-z(x,y)}\,|1\rangle\right)$$

$$\rightarrow \sum_y \left(\sqrt{A(x,y)z(x,y)}\,|y\rangle|x\rangle|0\rangle + \sqrt{A(x,y)\left(1-z(x,y)\right)}\,|x\rangle|y\rangle|1\rangle\right)$$

Quantum-Quantum Metropolis:

$$z_{ij}(x,x') = \min\left\{1, e^{-\beta\left(E_i - E_j\right)}\right\}: \text{ Metropolis filter}$$

$$|\phi_i\rangle|\tilde{\phi}_i\rangle|0\rangle \xrightarrow{U_X} \sum_j \sqrt{A_{ij}}\,|\phi_i\rangle|\phi_j\rangle|0\rangle$$

$$|\tilde{\phi}_i\rangle \equiv \sum_j \sqrt{A_{ij}}\,|\phi_j\rangle$$

$$\rightarrow \sum_j \sqrt{A_{ij}}\,|\phi_i\rangle|\phi_j\rangle\left(\sqrt{z_{ij}}\,|0\rangle + \sqrt{1-z_{ij}}\,|1\rangle\right)$$

$$\rightarrow \sum_j \left(\sqrt{A_{ij}z_{ij}}\,|\phi_j\rangle|\phi_i\rangle|0\rangle + \sqrt{A_{ij}\left(1-z_{ij}\right)}\,|\phi_i\rangle|\phi_j\rangle|0\rangle\right)$$

16

The END

- More on arXiv: 1011.1468