Algorithm for Preparing Thermal Gibbs States

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Related work

This work is based on

- *Sampling from the Thermal Quantum Gibbs State and Evaluating Partition Functions with a Quantum Computer*

  with David Poulin, Phys. Rev. Lett. 103, 220502 (2009)

- *Algorithm for Preparing Thermal States – Detailed Analysis*

  with C.-F. Chiang, Proc. NATO ARW "Quantum Cryptography and Computing: Theory and Implementation, Gdansk, Poland, 9-12 September 2009

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Definitions

Let H be a Hamiltonian with spectral decomposition

$$H = \sum_{a=1}^{D} E_a |\psi_a\rangle\langle\psi_a|$$

The partition function Z_β at inverse temperature β is

$$Z_\beta := \sum_{a=1}^{D} e^{-\beta E_a}$$

The thermal state ρ_β at inverse temperature β is

$$\rho_\beta := \sum_{a=1}^{D} \frac{e^{-\beta E_a}}{Z_\beta} |\psi_a\rangle\langle\psi_a|$$

Thermalizing quantum systems

Given H, β, and ϵ, prepare a quantum state $\tilde{\rho}_\beta$ with

$$\|\rho_\beta - \tilde{\rho}_\beta\|_{\mathrm{tr}} \leq \epsilon$$

Methods

Metropolis Sampling

Quantized Metropolis Sampling

- Somma, Boixo, Barnum, and Knill, PRL 101,130504
- W. and Abeyesinghe, PRA 78, 032311

Method based on Amplitude Amplification (this presentation)

Quantum Metropolis Sampling (David Poulin's presentation)

Classical Hamiltonians

Let Ω be a set whose elements x correspond the states of some classical system

Let $E : \Omega \rightarrow [0, 1]$ denote the energy function, assigning to each state x its energy $E(x)$

Let

$$H = \sum_{x \in \Omega} E(x)|x\rangle\langle x|$$

Thermalizing such classical systems is easier because H is diagonal in the computational basis $\{|x\rangle\}_{x \in \Omega}$

Metropolis sampling

Given such classical Hamiltonian H, we can always construct a Markov chain P whose limiting distribution is equal to ρ_β

The spectral gap δ determines how fast we can approach the Boltzmann distribution

The run time scales like $1/\delta$

In general, it is not possible to determine (or bound) the spectral gap $\Rightarrow$ heuristics

There are important cases where it can be shown that the gap is large

Quantized Metropolis algorithm

Given such classical Hamiltonian H, there is a "quantized" Metropolis algorithm preparing a state $|\tilde{\varphi}_\beta\rangle$ with

$$\left\| |\varphi_\beta\rangle - |\tilde{\varphi}_\beta\rangle \right\| \leq \epsilon$$

where $|\varphi_\beta\rangle$ is a "quantized" version of the Boltzmann distribution

$$|\varphi_\beta\rangle := \sum_{x\in\Omega} \sqrt{\frac{e^{-\beta E_x}}{Z_\beta}} |x\rangle$$

The run times scales like $\sqrt{1/\delta}$

Structure of our method

Prepare the state

$$\frac{1}{\sqrt{D}} \sum_{x \in \Omega} |x\rangle \otimes |E_x\rangle \otimes |0\rangle$$

Apply a controlled rotation to obtain the state

$$|\Psi\rangle = \frac{1}{\sqrt{D}} \sum_{x \in \Omega} |x\rangle \otimes |E_x\rangle \otimes \left(\sqrt{e^{-\beta E_x}} |0\rangle + \sqrt{1 - e^{-\beta E_x}} |1\rangle \right)$$

Structure of our method

Measure in the basis $|0\rangle$, $|1\rangle$

If we obtain $|0\rangle \Rightarrow$ the post-measurement state is

$$\frac{|\Pi_0|\Psi\rangle}{\|\Pi_0|\Psi\rangle\|} = \sum_{x\in\Omega} \sqrt{\frac{e^{-\beta E_x}}{Z_\beta}} |x\rangle \otimes |E_x\rangle \otimes |0\rangle$$

where $\Pi_0 = I \otimes |0\rangle\langle 0|$

Using amplitude amplification, we can achieve an expected run time

$$\frac{1}{\|\Pi_0|\Psi\rangle\|} = \sqrt{\frac{D}{Z_\beta}}$$

Generalization to quantum Hamiltonians

Let H be an arbitrary quantum Hamiltonian with spectral decomposition

$$H = \sum_{a=1}^{D} E_a |\psi_a\rangle\langle\psi_a| \qquad E_a \in [0, 1/2]$$

There are two difficulties:

- we cannot change between the computational basis $|a\rangle$ and the eigenvector basis $|\psi_a\rangle$ of H
- we do not know the energies E_a

Both difficulties can be overcome with quantum phase estimation
$\Rightarrow$ we can extend the previous method to quantum Hamiltonians

Error sources

Given H, β, and ϵ, our quantum algorithm prepares $\tilde{\rho}_\beta$

$$\|\rho_\beta - \tilde{\rho}_\beta\|_{\mathrm{tr}} \leq \epsilon$$

The errors come from two sources:

$$\|\rho_\beta - \tilde{\rho}_\beta\|_{\mathrm{tr}} \leq \|\rho - \rho_{\mathrm{sim}}\|_{\mathrm{tr}} + \|\rho_{\mathrm{sim}} - \rho_{\mathrm{fail}}\|_{\mathrm{tr}}$$

- ρ_{sim} due to imperfect simulation of $\exp(2\pi i H)$
- $\tilde{\rho}_\beta = \rho_{\mathrm{fail}}$ due to nonzero failure probability and limited precision of quantum phase estimation

Imperfect simulation of Hamiltonians

Assume that H is sparse and let $U = \exp(2\pi i H)$

Using techniques for simulating Hamiltonian time evolutions, we can implement $U_{\rm sim}$ with

$$\|U - U_{\rm sim}\| \leq \epsilon_{\rm sim}$$

The cost scales like

$$\mathrm{poly}(\log D, 1/\epsilon_{\rm sim}, s)$$

where s indicates the sparseness of H

Technical results

Matrix logarithm is Lipschitz continuous:

$$\|U - U_{\rm sim}\| \leq \epsilon_{\rm sim}$$

$\Rightarrow$ there is a Hamiltonian $H_{\rm sim}$ with

$$\|H - H_{\rm sim}\| \leq O(\epsilon_{\rm sim})$$

Thermal states are Hölder continuous:

$$\|H - H_{\rm sim}\| \leq O(\epsilon_{\rm sim})$$

$\Rightarrow$ the corresponding thermal states satisfy

$$\|\rho - \rho_{\rm sim}\|_{\rm tr} \leq O(\sqrt{\beta\epsilon_{\rm sim}})$$

Structure of our method

Start with the maximally entangled state

$$|\Phi\rangle := \frac{1}{\sqrt{D}} \sum_{a=1}^{D} |a\rangle \otimes |a\rangle$$

Run phase estimation of $U_{\rm sim}$ on first part of $|\Phi\rangle$ and record eigenphase in the energy register

Apply the controlled rotation $R = \sum_E |E\rangle\langle E| \otimes R_E$

$$R_E = \begin{pmatrix} \sqrt{e^{-\beta E}} & -\sqrt{1-e^{-\beta E}} \\ \sqrt{1-e^{-\beta E}} & \sqrt{e^{-\beta E}} \end{pmatrix}$$

Use amplitude amplification to increase overlap with $|0\rangle$ component

Invariance of maximally entangled state

Let

$$|\Phi\rangle := \frac{1}{\sqrt{D}} \sum_{a=1}^{D} |a\rangle \otimes |a\rangle$$

$$V := \sum_{a=1}^{D} |\psi_a\rangle\langle a|$$

Due to invariance of $|\Phi\rangle$ under $V \otimes \bar{V}$, we have

$$|\Phi\rangle = \frac{1}{\sqrt{D}} \sum_{a=1}^{D} |\psi_a\rangle \otimes |\bar{\psi}_a\rangle$$

Correspondance between energy levels and eigenphases

Recall that $U = \exp(2\pi i H)$

We have

$$(U \otimes I_D)|\psi_a\rangle \otimes |\bar{\psi}_a\rangle = e^{2\pi i E_a}|\psi_a\rangle \otimes |\bar{\psi}_a\rangle$$

$$(U \otimes I_D)|\Phi\rangle = \frac{1}{\sqrt{D}} \sum_{a=1}^{D} e^{2\pi i E_a}|\psi_a\rangle \otimes |\bar{\psi}_a\rangle$$

The energy levels E_a of H correspond bijectively to the eigenphases E_a of U

$\Rightarrow$ Apply quantum phase estimation to approximate the energy levels

Intuition – perfect quantum phase estimation

If perfect quantum phase estimation were possible (infinite precion and zero probability of failure), we could prepare the state

$$|\Psi\rangle = \frac{1}{\sqrt{D}} \sum_{a=1}^{D} |\psi_a\rangle \otimes |\bar{\psi}_a\rangle \otimes |E_a\rangle \otimes \left(\sqrt{e^{-\beta E_a}}|0\rangle + \sqrt{1 - e^{-\beta E_a}}|1\rangle \right)$$

$\Rightarrow$ Using amplitude amplification just as in the case of classical Hamiltonians, we could obtain a purification of the thermal state

Imperfect quantum phase estimation

We use quantum phase estimation that invokes the controlled $U_{\rm sim}$ operation

$$O((1/\epsilon_{\rm prec})\log(1/\epsilon_{\rm fail}))\text{ times}$$

$\Rightarrow$ We transform $|\Phi\rangle$ to the state

$$\frac{1}{\sqrt{D}}\sum_{a=1}^{D}|\psi_a\rangle\otimes|\bar{\psi}_a\rangle\otimes\left(c_a^-|E_a^-\rangle+c_a^+|E_a^+\rangle\right)+|\xi\rangle$$

- $E_a^+ - E_a \leq \epsilon_{\rm prec}, \quad E_a - E_a^- \leq \epsilon_{\rm prec}$
- $|c_a^+|^2+|c_a^-|^2 \geq 1-\epsilon_{\rm fail}$
- $\||\xi\rangle\|^2 \leq \epsilon_{\rm fail}$

Controlled rotation

After quantum phase estimation, we apply the rotation controlled by the value in the energy register to prepare the state $|\tilde{\Psi}\rangle$

$$\frac{1}{\sqrt{D}}\sum_{a=1}^{D}|\psi_a\rangle\otimes|\bar{\psi}_a\rangle\otimes c_a^{\pm}|E_a^{\pm}\rangle\otimes\left(\sqrt{e^{-\beta E_a^{\pm}}}|0\rangle+\sqrt{1-e^{-\beta E_a^{\pm}}}|1\rangle\right)+|\tilde{\xi}\rangle$$

Amplitude amplification

We apply amplitude amplification to obtain

$$|\tilde{\beta}\rangle := \frac{\Pi_0|\tilde{\Psi}\rangle}{\|\Pi_0|\tilde{\Psi}\rangle\|}$$

The required number of iterations is

$$1/\|\Pi_0|\tilde{\Psi}\rangle\|$$

The desired approximate thermal state is

$$\tilde{\rho}_\beta = \mathrm{Tr}_{\bar{A}}(|\tilde{\beta}\rangle\langle\tilde{\beta}|)$$

where we trace out over the ancilla, the energy register and the register holding $|\bar{\psi}_a\rangle$

Error analysis

The approximate thermal state $\tilde{\rho}_\beta$ is close to the perfect ρ_β provided that simulation and phase estimation are accurate enough

Given H, β, and ϵ, our quantum algorithm makes it possible to prepare $\tilde{\rho}_\beta$

$$\|\rho_\beta - \tilde{\rho}_\beta\|_{\mathrm{tr}} \leq \epsilon$$

The expected run time is

$$\sqrt{\frac{D}{Z_\beta}} \cdot \frac{\beta}{\epsilon} \cdot \left(\log \frac{1}{\epsilon} + \beta\right)$$