CS 59300 – Algorithms for Data Science

Classical and Quantum approaches

Lecture 20 (11/20)

Quantum Gibbs Sampling and Open Quantum Systems (I)

https://ruizhezhang.com/course_fall_2025.html

Outline

- Motivation
- Description of open quantum system dynamics
- Quantum simulation algorithms
- Applications

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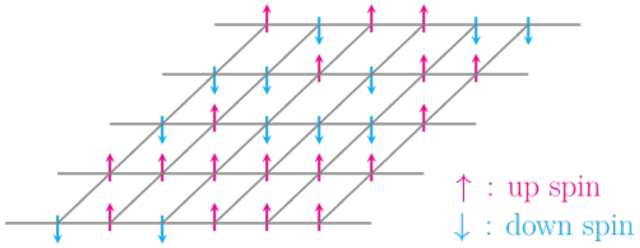
Classical Gibbs sampling: revisited

- Consider a classical spin system (e.g., the Ising model):

$$H_{\text{Ising}} = -\sum_{i\sim j} Z_i Z_j$$



- Eigenstates $\{0,1\}^n$ and eigenvalues $\{E_x\}_{x\in\{0,1\}^n}$
- The goal is to (approximately) sample from the Gibbs distribution:

$$\pi_\beta(x) = \frac{e^{-\beta E_x}}{Z_\beta}, \qquad Z_\beta = \sum_x e^{-\beta E_x}$$

The Metropolis-Hastings algorithm

Set of jump operators $\{A^a\}$ such that A^a is selected with probability $p(a)$

- Example: flip a randomly chosen spin

Let x be the current state

- Pick A^a with probability $p(a)$
- $y \leftarrow A^a$ applied to x
- Accept move with probability $\gamma_\beta(x, y) \coloneqq \min\left\{1, \exp\left(-\beta\left(E_y - E_x\right)\right)\right\}$
- If reject, stay at x

Fact. Under certain conditions, the Gibbs distribution π_β is the unique fixed point.

- Detailed balance (DBC): $e^{-\beta E_x}\gamma_\beta(x, y) = e^{-\beta E_y}\gamma_\beta(y, x)$

Quantum Gibbs sampling

- Let H be a quantum Hamiltonian with eigenstates $\{|\psi_j\rangle\}$ and eigenvalues $\{E_j\}$
- The goal is to (approximately) sample from the “quantum Gibbs distribution”:

$$\pi_\beta(|\psi_j\rangle) = \frac{e^{-\beta E_j}}{Z_\beta}$$

- Mixed state:

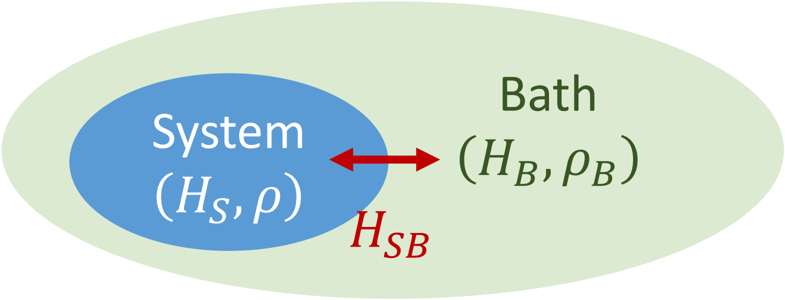
$$\rho_\beta = \sum \frac{e^{-\beta E_j}}{Z_\beta} |\psi_j\rangle\langle\psi_j| = \frac{\exp(-\beta H)}{\mathrm{tr}[\exp(-\beta H)]}$$

Gibbs state

Challenges:

1. Given $|\psi_j\rangle$ cannot calculate the energy E_j exactly
2. Rejection requires backing up after a quantum measurement

Open quantum system



System dimension: d $\ll$ Bath dimension: D

- Total Hamiltonian $H = H_S + H_B + H_{SB}$
- The whole system evolution follows the Liouville-von Neumann equation:

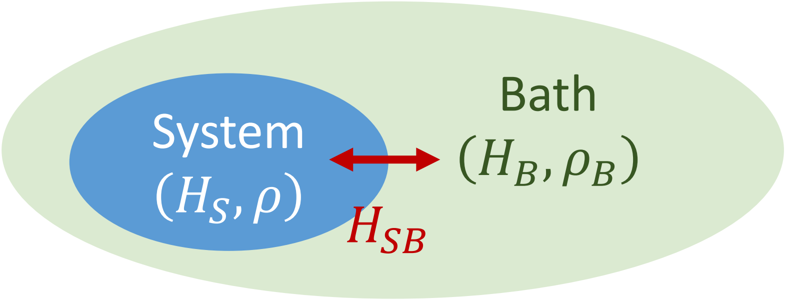
$$\frac{\mathrm{d}\rho_{SB}}{\mathrm{d}t} = -\mathbf{i}[H, \rho_{SB}]$$

- We only care the system part, i.e., $\rho = \mathrm{tr}_B[\rho_{SB}]$

Is it possible to describe the dynamics of ρ **without** simulating the bath?

i.e. a kind of **dimension reduction**

Open quantum system



System dimension: d $\ll$ Bath dimension: D

Thermalization

- If you leave a quantum system in contact with a heat bath at temperature $T = 1/\beta$, then the state $\rho(t) = \mathrm{tr}_B[\rho_{SB}(t)]$ forgets its initial condition and converges to the Gibbs state:

$$\rho_\beta = \frac{\exp(-\beta H_S)}{\mathrm{tr}[\exp(-\beta H_S)]}$$

- A physical approach to quantum Gibbs sampling:

Put the quantum spin system into a refrigerator and wait for thermalization