Master's thesis: Numerical comparison of MCMC methods for Quantum Tomography

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Problem: quantum state reconstruction

Goal: We want to reconstitute a quantum state

Unfortunately, there are some challenges:

- Quantum systems are inherently probabilistic
- A measurement can ony be made once
- We can only measure the position or momentum, but not both

Quantum Tomography

Quantum tomography provides a solution to this problem.

Key steps:

1. Replicate the initial state of the system multiple times
2. Measure each clone once
3. Calculate the empirical probabilities
4. Estimate the quantum state with any appropriate method

Quantum Tomography: mathematical description (1)

The Born rule states that

$$p(m) = \mathrm{tr}(\rho P_m) \tag{1}$$

with

- P_m the projector matrix associated to the eigenvalue m of an *observable* O
- $p(m)$ the probability of occurence of m
- ρ the *density matrix* representing the quantum state
  - positive semi-definite
  - Hermitian ($\rho = \rho^\dagger$)
  - trace(ρ) $= 1$

Quantum Tomography: mathematical description (2)

If we flatten the matrices

$$A = \begin{bmatrix} \vec{P}_1 \\ \vec{P}_2 \\ \vec{P}_3 \\ \vdots \end{bmatrix} \qquad \vec{\rho} = \begin{bmatrix} \rho_{11} \\ \rho_{12} \\ \rho_{13} \\ \vdots \end{bmatrix} \tag{2}$$

then we can estimate ρ by solving the resulting system of equations

$$A\vec{\rho} = \hat{p} \tag{3}$$

Existing methods

- Direct methods:
$$\hat{\rho} = (A^T A)^{-1} A^T \hat{p} \tag{4}$$
- Optimization-based methods:
$$\hat{\rho} = \text{argmin}_{\vec{\rho}} ||A\vec{\rho} - \hat{p}|| \tag{5}$$
- Pauli basis expansion:
$$\hat{\rho} = \sum_{b \in \{I,x,y,z\}^n} \rho_b \sigma_b \tag{6}$$
- Bayesian methods, and in particular MCMC methods
$$\hat{\rho} = \frac{1}{N} \sum_{i=1}^{N} \nu_i \quad \text{with } \nu_i \sim \pi(\nu|\mathbf{D}) \tag{7}$$

Existing methods: our focus in this thesis

- Direct methods:

$$\hat{\rho} = (A^T A)^{-1} A^T \hat{p} \tag{8}$$

- Optimization-based methods:

$$\hat{\rho} = \text{argmin}_{\vec{\rho}} ||A\vec{\rho} - \hat{p}|| \tag{9}$$

- Pauli basis expansion:

$$\hat{\rho} = \sum_{b \in \{I,x,y,z\}^n} \rho_b \sigma_b \tag{10}$$

- Bayesian methods, and in particular MCMC methods

$$\hat{\rho} = \frac{1}{N} \sum_{i=1}^{N} \nu_i \quad \text{with } \nu_i \sim \pi(\nu|\mathbf{D}) \tag{11}$$

Markov chain Monte Carlo methods

Context: We are working in the Bayesian framework:

$$\pi(\nu|\mathbf{D}) \propto \mathcal{L}(\mathbf{D}|\nu)\pi(\nu) \tag{12}$$

Markov chain Monte Carlo (MCMC) methods allow us to *sample* from $\pi(\nu|\mathbf{D})$.

They build a Markov chain of samples $\nu_1, \nu_2, \ldots$ where at equilibrium

$$f(x) = \pi(\nu|\mathbf{D}) \tag{13}$$

with $f(x)$ the equilibrium distribution of the Markov chain.

Then, the density matrix is approximated as

$$\hat{\rho} = \frac{1}{N}\sum_{i=1}^{N}\nu_i \quad \text{with } \nu_i \sim \pi(\nu|\mathbf{D}) \tag{14}$$

The Metropolis-Hastings algorithm

The Metropolis-Hastings algorithm is one of the most common MCMC algorithms.

Given a first sample $\nu^{(0)}$ and until $t = T$:

1. Generate a candidate $\nu^* \sim q(\nu|\nu^{(t-1)})$
2. Set $\nu^{(t)} = \begin{cases} \nu^* & \text{with prob. } \alpha(\nu^*, \nu^{(t-1)}) \\ \nu^{(t-1)} & \text{with prob. } 1 - \alpha(\nu^*, \nu^{(t-1)}) \end{cases}$

with

$$\alpha(\nu^*, \nu^{(t-1)}) = \frac{\pi(\nu^*|\mathbf{D})q(\nu^{(t-1)}|\nu^*)}{\pi(\nu^{(t-1)}|\mathbf{D})q(\nu^*|\nu^{(t-1)})} \tag{15}$$

Prob-estimator

Introduced in MA17, it uses Metropolis-Hastings to ,