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

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

with

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

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:

$$\hat{\rho} = \operatorname{argmin}_{\vec{\rho}} ||A\vec{\rho} - \hat{p}|| \tag{5}$$

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

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

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

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

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

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Markov chain Monte Carlo methods

Context: We are working in the Bayesian framework:

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

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

They build a Markov chain of samples ν_1, ν_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

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

The Metropolis-Hastings algorithm

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

Given a first sample $\nu^{(0)}$:

for
$$t = 1 \rightarrow T$$

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

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

Illustration of the Metropolis-Hastings algorithm

Prob-estimator

Introduced in [MA17], it uses Metropolis-Hastings to ,

Bibliography

[MA17] The Tien Mai and Pierre Alquier. "Pseudo-Bayesian quantum tomography with rank-adaptation". In: Journal of Statistical Planning and Inference 184 (May 2017), pp. 62–76. ISSN: 0378-3758. DOI: 10.1016/j.jspi.2016.11.003. URL: http://dx.doi.org/10.1016/j.jspi.2016.11.003.