Effect of Purity on Maximum Likelihood Quantum State Tomography

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***Abstract*—Maximum likelihood estimation (MLE) is the most practised method for estimating the density matrix associated with a quantum state. However, the efficiency of MLE commensurate with the purity of the given quantum state. We show the estimation of mixed quantum state is more precise than the pure quantum state using the MLE algorithm.**

I. Introduction

Quantum state tomography is a non-deterministic process of ascertaining the underlying quantum information. Measurements on ensemble of given identically prepared quantum state are made to better estimate the state [1]–[3]. Theoretically, an infinite number of measurements are required to exactly determine the given state which is not experimentally feasible [4]–[6]. However, statistical approaches help in better recovering density matrix ρ associated with a given quantum state [7], [8]. In an ideal state tomography process, the given state is projected onto some known basis multiple times to get an estimate of the state itself.

Linear inversion (LI) method is a rudimentary technique used to determine density matrix ρ by direct inversion of the observed data. Nevertheless, the density matrix is not well approximated because of experimental noise. Therefore, LI method can recover an illegitimate density matrix, having negative eigenvalues or not having unit trace. To solve this problem, maximum likelihood estimation (MLE) is used which parameterizes the invalid state to valid physical states [9], [10].

MLE is widely used in quantum state tomography [11]. Even though MLE provides a better physically valid estimate of the states, it is not equally efficient in estimation from a spectrum of maximally mixed to pure states. In a practical scenario, we are mostly dealing with mixed quantum states. In this paper, we demonstrate that the MLE accurately characterizes the mixed state in comparison with the pure states. Infidelity is used as a metric to determine the performance of MLE across purity of the given state.

II. Maxmimum Likelihood Estimation (MLE)

In this section, we formulate our experiment under MLE to study the trend of infidelity by varying purity of the quantum state. A pure qubit system is mathematically expressed as

$$|\psi\rangle = \alpha |0\rangle + \beta |1\rangle . \tag{1}$$

Any physical density matrix can be represented through spectral decomposition as

$$\rho = \sum_i \lambda_i |\psi_i\rangle \langle\psi_i| , \tag{2}$$

where $0 \leq \lambda_i \leq 1$, $\sum_i \lambda_i = 1$ are the eigenvalues and $|\psi_i\rangle$ are the corresponding eigenvectors. For a pure qubit system ρ is a 2×2 matrix represented generally as

$$\rho = |\psi\rangle \langle\psi| = \begin{bmatrix} |\alpha|^2 & \alpha\bar{\beta} \\ \bar{\alpha}\beta & |\beta|^2 \end{bmatrix} . \tag{3}$$

The probability of getting measurement outcomes is obtained by elementary projectors $\Pi_i = |\psi_i\rangle \langle\psi_i|$ through born's rule

$$p(i|\rho) = \mathrm{tr}(\Pi_i \rho) . \tag{4}$$

The elementary projector forms the POVM. These POVM should sum to identity i.e.,

$$\sum_i |\psi_i\rangle \langle\psi_i| = \mathbb{I}. \tag{5}$$

The measured data θ comprises of series of N detection events $\theta_1, \theta_2, ..., \theta_N$. Likelihood function for θ given state ρ is given as

$$\mathcal{L}(\theta|\rho) = \prod_{i=1}^{N} \mathrm{tr}(\Pi_i \rho)^{n_i} \tag{6}$$

where n_i represents the number of times the measurement bases Π_i is observed. The MLE interprets the likelihood as a function of ρ for the obtained θ and identifies the quantum state with ρ that maximizes $\mathcal{L}(\theta|\rho)$. This is basically an optimization problem for normalized negative log-likelihood function

$$\begin{aligned} &\min_{\rho \in \mathcal{B}(\mathcal{H})} \; -\sum_{i=1}^{N} n_i \log(\mathrm{tr}(\rho \Pi_i)) \\ &\text{s.t:} \qquad \rho \geq 0; \\ &\qquad\qquad \mathrm{tr}(\rho) = 1 \end{aligned} \tag{7}$$

where $\mathcal{B}(\mathcal{H})$ is the convex set of the valid quantum state. As we are going to study MLE's performance from a maximally mixed state to a pure state, we will have to come up with a unified equation in which we can change the purity of the randomly generated state and apply MLE.

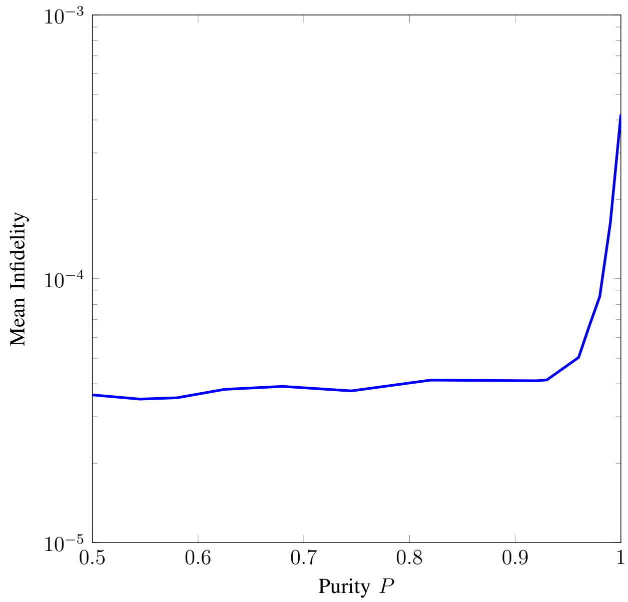

Fig. 1. We obtain 100 randomly generated mixed states according to Haar measure. Mean infidelity of (11) for all states against the purity P is shown. We use 10^3 copies for each measurement operators. We can clearly see that estimation of state is not well approximated with MLE as we move away from maximally mixed state.

III. Numerical Simulation

In this section, we will obtain the numerical results of quantum state (11) using MLE algorithm. For this purpose, we use a standard figure of merit to measure the efficiency of MLE. Infidelity is widely used as a figure of merit for the accuracy of given algorithm. The infidelity of an estimated quantum state $\hat{\rho}$ from MLE to true state ρ is given by

$$1 - F(\rho, \hat{\rho}) = 1 - \operatorname{tr}\sqrt{\sqrt{\rho}\hat{\rho}\sqrt{\rho}}. \tag{8}$$

We use the eigenvectors of the Pauli operators as basis measurements which are given as

$$|H\rangle = \begin{bmatrix}1\\0\end{bmatrix}, \quad |V\rangle = \begin{bmatrix}0\\1\end{bmatrix}, \quad |D\rangle = \begin{bmatrix}\frac{1}{\sqrt{2}}\\\frac{1}{\sqrt{2}}\end{bmatrix},$$
$$|A\rangle = \begin{bmatrix}\frac{1}{\sqrt{2}}\\-\frac{1}{\sqrt{2}}\end{bmatrix}, |R\rangle = \begin{bmatrix}\frac{1}{\sqrt{2}}\\\frac{\iota}{\sqrt{2}}\end{bmatrix}, |L\rangle = \begin{bmatrix}\frac{1}{\sqrt{2}}\\-\frac{\iota}{\sqrt{2}}\end{bmatrix}.$$

These bases are called cubic measurements. The Pauli operators for the single-qubit system is defined as

$$\sigma_x = \begin{bmatrix}0 & 1\\1 & 0\end{bmatrix}, \quad \sigma_y = \begin{bmatrix}0 & -\iota\\\iota & 0\end{bmatrix}, \quad \sigma_z = \begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}. \tag{9}$$

A maximally mixed state ρ_{mm} is represented as

$$\rho_{mm} = \frac{\mathbb{I}}{2} = \begin{bmatrix}0.5 & 0\\0 & 0.5\end{bmatrix}. \tag{10}$$

For our simulation, we make a single equation to incorporate impurity as a variable λ and generate density matrices ranging from maximally mixed to pure state

$$\rho = \lambda|\psi_1\rangle\langle\psi_1| + (1-\lambda)|\psi_2\rangle\langle\psi_2|, \tag{11}$$

where $0.5 \leq \lambda \leq 1$ and $|\psi_1\rangle, |\psi_2\rangle$ are eigenvectors of a randomly generated mixed state ρ_{mix}. We get maximally mixed state ρ_{mm} when $\lambda = 0.5$, and pure state when $\lambda = 1$.

We generate randomly 100 mixed qubits ρ_{mix} according to Haar measure. We perform eigenvalue decomposition and use its eigenvectors $|\psi_1\rangle, |\psi_2\rangle$ in (11) with λ varying from 0.5 to 1. We then estimate the given unknown quantum state using MLE by performing measurements on Pauli basis. An average infidelity of estimated quantum state through MLE is plotted as a function of purity P in Fig. 1, where purity P is given by

$$P = \lambda^2 + (1-\lambda)^2 \tag{12}$$

From Fig. 1, we can clearly see that the infidelity is increasing when we move away from maximally mixed state to pure state which shows that we require more copies for pure state to achieve the same precision as with the mixed state. More the state is mixed, less is the infidelity of measurement under MLE.

IV. Conclusion

To conclude, MLE gives better fidelity for maximally mixed state as compared to pure states. A diminishing performance of MLE can be observed when moving from maximally mixed states to pure state .The reason being that a pure state has more quantumness as compared to a mixed state.

Acknowledgment

This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (No. 2019R1A2C2007037).

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