Quantum State Tomography via Linear Regression Estimation

Bo Qi, Zhibo Hou, Li Li, Daoyi Dong, Guoyong Xiang & Guangcan Guo

Quantum state tomography is a standard technology for inferring the state of a quantum system through appropriate measurements and estimation. The choice of optimal measurement sets and the design of efficient state reconstruction algorithms are critical issues in quantum state tomography.

One of the essential tasks in quantum technology is to verify the integrity of a quantum state. Quantum state tomography has become a standard technology for inferring the state of a quantum system through appropriate measurements and estimation. To reconstruct a quantum state, one may first perform measurements on a collection of identically prepared copies of a quantum system (data collection) and then infer the quantum state from these measurement outcomes using appropriate estimation algorithms (data analysis). Measurement on a quantum system generally gives a probabilistic result and an individual measurement outcome only provides limited information on the state of the system, even when an ideal measurement device is used. In principle, an infinite number of measurements are required to determine a quantum state precisely. However, practical quantum state tomography consists of only finite measurements and appropriate estimation algorithms. Hence, the choice of optimal measurement sets and the design of efficient state reconstruction algorithms are two critical issues in quantum state tomography.

Many results have been presented for choosing optimal measurement sets to increase the estimation accuracy and efficiency in quantum state tomography. Several sound choices that can provide excellent performance for tomography are, for instance, tetrahedron measurement bases, cube measurement sets, and mutually unbiased bases. However, for most existing results, the optimality of a given measurement set is only verified through numerical results. There are few methods that can analytically give an estimation error bound, which is essential to evaluate the optimality of a measurement set and the appropriateness of an estimation method.

For estimation algorithms, several useful methods including maximum-likelihood estimation (MLE), Bayesian mean estimation (BME) and least-squares (LS) inversion have been proposed for quantum state reconstruction. The MLE method simply chooses the state estimate that gives the observed results with the highest probability. This method is asymptotically optimal in the sense that the estimation error can asymptotically achieve the Cramér-Rao bound. However, MLE usually involves solving a large number of nonlinear equations where their solutions are notoriously difficult to obtain and often not unique. Recently, an efficient method has been proposed for computing the maximum-likelihood quantum state from measurements with additive Gaussian noise, but this method is not general. Compared to MLE, BME can always give a unique state estimate, since it constructs a state from an integral averaging over all possible quantum states with proper weights. The high computational complexity of this method significantly limits its application. The LS inversion method can be applied when measurable quantities exist that are linearly related to all density matrix elements of the quantum state being reconstructed. However, the estimation result may be a nonphysical state and the mean squared error (MSE) bound of the estimate cannot be determined analytically.

Here, we present a new linear regression estimation (LRE) method for quantum state tomography that can identify optimal measurement sets and reconstruct a quantum state efficiently. We first convert the quantum state reconstruction into a parameter estimation problem of a linear regression model. Next, we employ an LS
algorithm to estimate the unknown parameters. The positivity of the reconstructed state can be guaranteed by an additional least-squares minimization problem. The total computational complexity is $O(d^3)$ where $d$ is the dimension of the quantum state. In order to evaluate the performance of a chosen measurement set, an MSE upper bound for all possible states to be estimated is given analytically. This MSE upper bound depends explicitly upon the involved measurement bases, and can guide us to choose the optimal measurement set. The efficiency of the method is demonstrated by examples on qubit systems.

**Results**

**Linear regression model.** We first convert the quantum state tomography problem into a parameter estimation problem of a linear regression model. Suppose the dimension of the Hilbert space $\mathcal{H}$ of the system of interest is $d$, and $\{\Omega_i\}_{i=0}^{d-1}$ is a complete basis set of orthonormal operators on the corresponding Liouville space, namely, $\text{Tr}(\Omega_i^\dagger \Omega_j) = \delta_{ij}$, where $\dagger$ denotes the Hermitian adjoint and $\delta_{ij}$ is the Kronecker function. Without loss of generality, let $\Omega_i = \Omega_i^\dagger$ and $\Omega_0 = (1/d)^{1/2}$, such that the other bases are traceless. That is $\text{Tr}(\Omega_i) = 0$, for $i = 1, 2, \ldots, d - 1$. The quantum state $\rho$ to be reconstructed may be parameterized as

$$\rho = \frac{1}{d} + \sum_{i=1}^{d-1} \Theta_i \Omega_i,$$

where $\Theta_i = \text{Tr}(\rho \Omega_i)$. Given a set of measurement bases $\{|\psi_i^{(n)}\rangle\}_{n=1}^M$, each $|\psi_i\rangle \langle \psi_i|$ can be parameterized under the bases $\{\Omega_i\}_{i=0}^{d-1}$ as

$$|\psi_i^{(n)}\rangle = \frac{1}{d} + \sum_{i=1}^{d-1} \psi_i^{(n)} \Omega_i,$$

where $\psi_i^{(n)} = \text{Tr}(|\psi_i\rangle \langle \psi_i|)$.

When one performs measurements with measurement set $\{|\psi_i^{(n)}\rangle\}_{n=1}^M$ on a collection of identically prepared copies of a quantum system (with state $\rho$), the probability to obtain the result of $|\psi_i\rangle \langle \psi_i|$ is

$$p_n = \text{Tr}(|\psi_i\rangle \langle \psi_i| \rho) = \frac{1}{d} + \sum_{i=1}^{d-1} \theta_i \psi_i^{(n)} \leq \frac{1}{d} + \theta \psi_i^{(n)}.$$

Assume that the total number of experiments is $N$ and $N/M$ experiments are performed on $N/M$ identically prepared copies of a quantum system for each measurement basis $|\psi_i\rangle \langle \psi_i|$. Denote the corresponding outcomes as $x_i^{(n)}, \ldots, x_{N/M}^{(n)}$, which are independent

and identically distributed. Let $e_n = p_n - p_a$. According to the central limit theorem, $e_n$ converges in distribution to a normal distribution with mean 0 and variance $p_a - p_a^2 / N/M$. Using (3), we have the linear regression equations for $n = 1, 2, \ldots, M$,

$$\hat{p}_n = \frac{1}{d} + \psi_n \Theta^\dagger + e_n,$$

where $\dagger$ denotes the matrix transpose.

Note that $\hat{p}_n, d$ and $\psi_n^{(n)}$ are all available, while $e_n$ may be considered as the observation noise whose variance is asymptotically $p_a - p_a^2 / N/M$. Hence, the problem of quantum state tomography is converted into the estimation of the unknown vector $\Theta$. Denote $Y = \left[\hat{p}_1 - \frac{1}{d}, \ldots, \hat{p}_M - \frac{1}{d}\right]$, $X = \left[\psi_1^{(1)}, \ldots, \psi_M^{(M)}\right]^\dagger$, $e = (e_1, \ldots, e_M)^\dagger$.

We can transform the linear regression equations (4) into a compact form

$$Y = X\Theta + e.$$

We define the MSE as $E\text{Tr}(\hat{\rho} - \rho)^2$, where $\hat{\rho}$ is an estimate of the quantum state $\rho$ based on the measurement outcomes and $E(\cdot)$ denotes the expectation on all possible measurement outcomes. For a fixed tomography method, $E\text{Tr}(\hat{\rho} - \rho)^2$ depends on the state $\rho$ to be reconstructed and the chosen measurement bases. From a practical viewpoint, the optimality of a chosen set of measurement bases may rely upon prior information but should not depend on any specific unknown quantum state to be reconstructed. In this paper, no prior assumption is made on the state $\rho$ to be reconstructed. Given a fixed tomography method, we use the maximum MSE for all possible states (i.e., $\sup_{\rho} E\text{Tr}(\hat{\rho} - \rho)^2$) as the index to evaluate the performance of a chosen set of measurement bases.

**Linear regression estimation.** To give an estimate with high level of accuracy and low computational complexity, we employ the LS method, where the basic idea is to find an estimate $\hat{\Theta}_{LS}$ such that

$$\hat{\Theta}_{LS} = \arg\min_{\Theta} \left(Y - X\hat{\Theta}\right)^\dagger W \left(Y - X\hat{\Theta}\right),$$

where $\hat{\Theta}$ is an estimate of $\Theta$, and $W$ is a diagonal weighting matrix. Since the objective function is quadratic, one has the LS solution as follows:

$$\hat{\Theta}_{LS} = (X^\dagger W X)^{-1} X^\dagger W Y.$$

The LS solution (7) can be calculated in a recursive way (see the Methods section). In practical experiments, the cost of time can be greatly reduced by employing a recursive reconstruction protocol since the estimate can be calculated recursively based on available data at the same time of performing measurements to acquire data.

Note that if $p_a = 1$, we have already reconstructed the state as $|\psi_i\rangle \langle \psi_i|$, if $p_a = 0$, we should choose the following measurement basis from the orthogonal complementary space of $|\psi_i\rangle \langle \psi_i|$. Hence, in general the smaller the variance of $e_n$ is, the more the information can be extracted by $|\psi_i\rangle \langle \psi_i|$. Therefore, the corresponding weight of the $n$-th regression equation should be bigger. It can be verified that if all $p_n$ are known, the LS solution $\hat{\Theta}_{LS}$ satisfying $\hat{\Theta}_{LS} = \arg\min_{\Theta} \left(Y - X\hat{\Theta}\right)^\dagger V \left(Y - X\hat{\Theta}\right)$ is asymptotically the minimum variance unbiased estimator of $\Theta$, where $V$ is the inverse of $\text{diag}(p_1 - p_1^2, \ldots, p_M - p_M^2)$. Hence, an appropriate choice of $W$ is the inverse of $\text{diag}(p_1 - p_1^2, \ldots, p_M - p_M^2)$.

However, for simplicity we consider the case where $W = I$, and the corresponding LS solution is

$$\hat{\Theta}_{LS} = (X^\dagger X)^{-1} X^\dagger Y = (X^\dagger X)^{-1} \sum_{n=1}^M \psi_n^{(n)} \left(\hat{p}_n - \frac{1}{d}\right),$$

where $X^\dagger X = \sum_{n=1}^M \psi_n^{(n)} \psi_n^{(n)^\dagger}$.

If the measurement bases $\{|\psi_i\rangle \langle \psi_i|\}_{n=1}^M$ are informationally complete or overcomplete, $X^\dagger X$ is invertible. Using (5), (8) and the statistical property of the observation noise $\{e_n\}_{n=1}^M$ (independent and asymptotically Gaussian), the estimate $\hat{\Theta}_{LS}$ has the following properties for a fixed set of chosen measurement bases:
reconstruction algorithms, this task is computationally intensive. We will discuss this problem in other work.

Optimality of measurement bases. One of the advantages of LRE is that the MSE upper bound can be given analytically as \( \frac{M}{N} \text{Tr} \left( \sum_{n=1}^{M} \psi^{(n)} \psi^{(n)} \right)^{-1} \), which is dependant explicitly upon the measurement bases. Note that if the PLRE \( \hat{\mu} \) is a physical state, then the MSE upper bound is asymptotically tight for the evaluation of the performance of a fixed set of measurement bases. Hence, to choose an optimal set \( \left\{ \psi^{(n)} \right\}_{n=1}^{M} \), one can solve the following optimization problem:

\[
\begin{align*}
\text{Minimize} & \quad \text{Tr} \left( \sum_{n=1}^{M} \psi^{(n)} \psi^{(n)} \right)^{-1} \\
\text{s.t.} & \quad \psi^{(n)} = \frac{d-1}{d}, \text{ for } n = 1, \cdots, M.
\end{align*}
\]

The optimization problem can be solved in an off-line way by employing appropriate algorithms though it may be computationally intensive. We will discuss this problem in other work.

With the help of the analytical MSE upper bound, we can ascertain which one is optimal among the available measurement sets. This is demonstrated when we prove the optimality of several typical sets of measurement bases for 2-qubit systems.

For 2-qubit systems, it is convenient to chose \( \Omega = \frac{1}{\sqrt{2}} \sigma_{1} \otimes \sigma_{2} \), where \( i = 4l + m, l, m = 0, 1, 2, 3 ; \sigma_{i} = I_{2 \times 2}, \sigma_{1} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_{2} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_{3} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \).

If the form of the measurement bases is not restricted, the minimum of the MSE upper bound \( \frac{M}{N} \text{Tr} \left( X^{\dagger} X \right)^{-1} \) for all possible measurement bases is \( \frac{75}{N} \). This minimum can be reached by using the

---

**Figure 1**| The run time and MSE of LRE and MLE for random \( n \)-qubit pure states mixed with the identity. The measurement bases are from the \( n \)-qubit cube measurement set and the resource is \( N = 3 \times 4 \). The simulated measurement results for every basis \( \langle \psi \rangle \langle \psi \rangle^{\dagger} \) are generated from a binomial distribution with probability \( p_{s} = \text{Tr}(\psi^{\dagger} \psi) / p \) and trials \( N / M \). LRE is much more efficient than MLE with a small amount of accuracy sacrificed since the maximum MSE could reach 2 for the worst estimate. All timings were performed in MATLAB on the computer with 4 cores of 3 GHz Intel i5-2320 CPUs.
mutually unbiased measurement bases. While as in many practical experiments, if only local measurements can be performed, the minimum of the MSE upper bound \( \frac{M}{4N} \text{Tr}(X^\dagger X)^{-1} \) is \( \frac{99}{N} \). This minimum can be reached by using the 2-qubit cube or tetrahedron measurement set.

Fig. 2 shows the dependant relationships of the MSEs for Werner states on \( q \) (varying from 0 to 1) and different number of copies \( N \) using the cube measurement bases. The fact that the MSE of PLRE is larger than that of LRE demonstrates that the process of pulling \( \mu \) back to a physical state further reduces the estimation error.

**Discussion**

In the LRE method, data collection is achieved by performing measurements on quantum systems with given measurement bases. This process can also be accomplished by considering the evolution of quantum systems with fewer measurement bases. For example, suppose only one observable \( s \) is given, and the system evolves according to a unitary group \( \{U_t\} \). At a given time \( t \),

\[
\langle s_t \rangle = \text{Tr}(U^\dagger(t) \sigma U(t) \rho) = \text{Tr}(s_t \rho).
\]

Suppose one measures the observable \( s \) at time \( t(=1, \cdots, M) \) on \( m \) identically prepared copies of a quantum system. Denote the obtained outcomes as \( s_1^t, \cdots, s_m^t \), and their algebraic average as \( \bar{s}_t = \frac{1}{m} \sum_{i=1}^{m} s_i^t \). Note that \( \sigma_1, \cdots, \sigma_m \) are independent and identically distributed. According to the central limit theorem, \( \bar{s}_t \) converges in distribution to a normal distribution with mean 0 and variance \( \frac{1}{m} \sum_{i=1}^{m} \langle s_i^2 \rangle - \langle s_i \rangle^2 \). We have the following linear regression equations

\[
\bar{s}_t = \text{Tr}(s_t \rho) + e_t, \quad t = 1, \cdots, M,
\]

which are similar to (4). Hence, we can use the proposed LRE method to accomplish quantum state tomography.

The LRE method can also be extended to reconstruct quantum states with a prior information or states of open quantum systems. Actually, LRE can be applied whenever there are measurable quantities that are linearly related to all density matrix elements of the quantum system under consideration.

In conclusion, an efficient state reconstruction algorithm of linear regression estimation has been presented for quantum state tomography. The computational complexity of LRE is \( O(d^4) \), which is much lower than that of MLE and BME. We have analytically provided an MSE upper bound for all possible states to be estimated, which explicitly depends upon the used measurement bases. This analytical upper bound can assist to identify optimal measurement sets. The LRE method has potential for wide applications in real experiments.
**Methods**

The recursive LS algorithm. For \( n = 1, \ldots, M \), define \( \Theta_n \) as

\[
\Theta_n = \arg\min_\Theta \sum_{i=1}^{n} W_i \left( \beta_i - 1 - Y_i^0 \Theta \right)^2, 
\]

where \( W_i \) is the \( i \)-th element of the diagonal of \( W \) and \( \Theta \) is an estimate of \( \Theta \). Hence, the LS solution \( \Theta_{LS} \) is equal to \( \Theta_M \). From (7), we have

\[
\Theta_n = \left( \sum_{i=1}^{n} W_i Y_i^0 Y_i^0 \right)^{-1} \sum_{i=1}^{n} Y_i^0 W_i \left( \beta_i - 1 - Y_i^0 \right). 
\]

Define

\[
Q_n = \left( \sum_{i=1}^{n} W_i Y_i^0 Y_i^0 \right)^{-1}, \quad a_n = \frac{1}{W_n + \psi_n^0 \phi_n^0} Q_{n-1}. 
\]

Using the matrix inversion formula (see, e.g., page 19 of [ref])

\[
(A - BCD)^{-1} = A^{-1} + A^{-1} B(C^{-1} - DA^{-1} B)^{-1} DA^{-1}, 
\]

we have

\[
Q_n = Q_{n-1} - a_n Q_{n-1} \psi_n^0 \phi_n^0 \psi_n^0 Q_{n-1}. 
\]

From (14), (15) and (16), the recursive form of \( \Theta_n \) can be obtained as

\[
\Theta_n = \Theta_{n-1} + a_n (Q_{n-1} \psi_n^0 \phi_n^0) \left( \beta_n - 1 - Y_n^0 \Theta_{n-1} \right). 
\]

Note that \( Q_n \) is not always invertible, especially when \( n \) is small. In order to apply the recursive algorithm in this case, one may choose the initial value in (16) \( Q_1 \) being a given positive matrix, while \( \Theta_0 \) being a given vector. From (16) and the matrix inverse formula, one has

\[
Q_n = \left( \sum_{i=1}^{n} W_i Y_i^0 Y_i^0 + Q_{n-1} \right)^{-1}. 
\]

Hence, the recursive LS algorithm can still be applied. Although the solution obtained from (17) may be slightly different from the solution obtained using (14), this does not affect the asymptotic properties of the LS solution.

**The minimum of the MSE upper bound.** The MSE upper bound of 2-qubit states is

\[
\frac{M}{4N} \text{Tr}(X^* X)^{-1} = \frac{M}{4N} \text{Tr} \left( \sum_{\sigma=0}^{M} \psi_\sigma^0 \phi_\sigma^0 \right)^{-1}. 
\]

Minimizing this MSE upper bound is equivalent to minimizing \( \text{Tr}(X^* X)^{-1} \). Denote the eigenvalues of \( X^* X \) as \( \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_M \). Since for all possible measurement bases, we have \( \psi_{\sigma_1}^0 = 1, \sum_{\sigma=0}^{M} \psi_\sigma^0 \phi_\sigma^0 = 1 \) for \( n = 1, \ldots, M \), the problem is converted to the following conditional extremum problem:

\[
\text{Minimize } \sum_{i=1}^{M} \frac{1}{\lambda_i}, \\
\text{s.t. } \sum_{i=1}^{M} \lambda_i = 3. 
\]

It can be proven that \( \sum_{i=1}^{M} \frac{1}{\lambda_i} \) reaches its minimum \( \frac{300}{M} \) when \( \lambda_1 = \cdots = \lambda_{15} = M/40 \).

Hence, the minimum of the MSE upper bound \( M/4N \text{Tr}(X^* X)^{-1} \) for all possible measurement bases is \( 75/4N \). It can be verified that this minimum MSE upper bound can be reached by using the mutually unbiased measurement bases.

If only local measurements can be performed, i.e., \( \psi_{\sigma_1} = \psi_{\sigma_2}^* \otimes \psi_{\sigma_3}^* \), \( n = 1, \cdots, M \), where \( \psi_{\sigma_1}^0 \) and \( \psi_{\sigma_2}^0 \) can be parameterized as \( \psi_{\sigma_1}^0 = \psi_{\sigma_1}^{(m)} \otimes \psi_{\sigma_2}^{(m)} \). When \( i = 4 \) and \( m \), we have \( \psi_{\sigma_1}^{(m)} = \psi_{\sigma_1}^{(m_1)} \times \psi_{\sigma_2}^{(m_2)} \), where \( i = 4 \) and \( m \).

Due to additional constraints \( \psi_{\sigma_1}^{(m)} = \frac{1}{\sqrt{2}} \sum_{k} \psi_{\sigma_1}^{(k)} \), \( k = 1, 2 \), and \( n = 1, \cdots, M \), the problem of minimizing the MSE upper bound can be converted to the following problem:

\[
\text{Minimize } \sum_{i=1}^{M} \frac{1}{\lambda_i}, \\
\text{s.t. } (i) \sum_{i=1}^{M} \lambda_i \geq \frac{4}{M}, (ii) \sum_{i=1}^{6} \lambda_i \geq \frac{1}{2} M, \\
(\text{iii}) \sum_{i=1}^{3} \lambda_i \geq \frac{3}{4} M. 
\]
30. Horn, R. A. & Johnson, C. R. Matrix Analysis (Cambridge University Press, Cambridge, 1985).

Acknowledgments
The authors would like to thank Lei Guo, Huangjun Zhu and Chuanfeng Li for helpful discussion. The work in USTC is supported by National Fundamental Research Program (Grants No. 2011CB00200 and No. 2011CB9211200), National Natural Science Foundation of China (Grants No. 61108009 and No. 61222504), Anhui Provincial Natural Science Foundation (No. 1208085QA08). B.Q. acknowledges the support of National Natural Science Foundation of China (Grants No. 61004049, No. 61227902, No. 61374092 and No. 61134008). D.D. is supported by the Australian Research Council (DP130101658).

Author contributions
B.Q., L.L. and D.D. developed the scheme based on linear regression model, Z.-B.H., G.-Y.X. and G.-C.G. performed the numerical simulations. All authors discussed the results and contributed to the writing of the paper. G.-Y.X. supervise the project.

Additional information
Competing financial interests: The authors declare no competing financial interests.
How to cite this article: Qi, B. et al. Quantum State Tomography via Linear Regression Estimation. Sci. Rep. 3, 3496; DOI:10.1038/srep03496 (2013).