Precision-Guaranteed Quantum Tomography

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Quantum state tomography is currently the standard tool for verifying that a state prepared in the lab is close to an ideal target state, but up to now there have been no rigorous methods for evaluating the precision of the state preparation in tomographic experiments. We propose a new estimator for quantum state tomography, and prove that the (always physical) estimates will be close to the true prepared state with a high probability. We derive an explicit formula for evaluating how high the probability is for an arbitrary finite-dimensional system and explicitly give the one- and two-qubit cases as examples. This formula applies for any informationally complete sets of measurements, arbitrary finite number of data sets, and general loss functions including the infidelity, the Hilbert-Schmidt, and the trace distances. Using the formula, we can evaluate not only the difference between the estimated and prepared states, but also the difference between the prepared and target states. This is the first result directly applicable to the problem of evaluating the precision of estimation and preparation in quantum tomographic experiments.

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The development of science has always been supported by the development of precise and accurate techniques of measurement and control. Measurement outcomes are affected by statistical and systematic noise, and evaluating the measurement precision under these errors is a fundamental aspect of those techniques. In physics, now more than ever, high-precision experiments are required for testing whether a theoretical model is suitable for describing nature. A popular figure of merit for this precision is the standard deviation, but, in more demanding experiments, a different figure of merit, called a confidence level, is also used. For example, in the search for the standard model Higgs boson, the ATLAS group at the LHC reported an experimental result that narrowed the range of the possible Higgs boson mass at the 95% confidence level [1]. This shows the confidence level to be a compelling benchmark for justifying whether an experimental result is reliable or not.

Quantum information is another field where highly precise measurement and control are necessary. It has been shown theoretically that by using "quantumness," we can perform more efficient computations [2] and more secure cryptography [3] compared to existing protocols. In the practical implementation of these new protocols, highly precise preparation and control of specific quantum states are required. Quantum tomography is a standard tool in current quantum information experiments for verifying a successful realization of states and operations [4]. Let us consider the case of state preparation, where ρ_* denotes a target state that we are trying to prepare in the lab. In real experiments, the true prepared state ρ does not coincide with ρ_* because of imperfections. We wish to evaluate the precision of this preparation, that is, the difference between ρ_* and ρ—however, we do not know ρ. Instead, we perform quantum state tomography; let ρ_N^{est} denote an estimate of the state made from N sets of data obtained in a tomographic experiment. To date, the best we have been able to do is to evaluate the difference between ρ_* and ρ_N^{est} (see Fig. 1), but even if the difference is small, it does not guarantee that the prepared state ρ is close to the target state ρ_*, because ρ_N^{est} is given probabilistically and can deviate from ρ when N is finite. In this context, we refer to the difference between ρ_N^{est} and ρ as the precision of the estimation.

There are many proposals for evaluating the precision of estimation [5–7] and preparation [8,9]. An approach using confidence regions is one currently popular example. Unlike standard quantum tomography, in this approach the estimate is not a point but a region in state space. In Refs. [5,6], confidence region estimators for quantum state estimation were proposed, and the region's volume was analyzed. The confidence level can be used for evaluating the precision of region estimates, but these cannot be directly applied for evaluating the precision of point

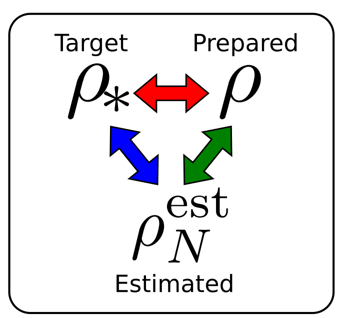

FIG. 1 (color online). Three-way relationship: ρ_* is a target state we want to prepare, ρ is the true prepared state, and ρ_N^{est} is an estimate made from N tomographic data sets.

estimates. In Ref. [7], two state estimators were proposed that use random sampling of Pauli measurements. Called compressed sensing, the authors proved that the estimates are close to the true state with high probability. However, the formulae derived for evaluating the difference between the estimates and the true state include indeterminate coefficients, and the value of the difference cannot be calculated. Therefore, the compressed sensing results are not directly applicable to the evaluation of the estimation precision of tomographic experiments. In Refs. [8,9], a method for estimating the difference between ρ_* and ρ as evaluated by the fidelity was proposed. Called direct fidelity estimation, it avoids point estimates altogether, and by performing random Pauli measurements it allows the precision of state preparation to be evaluated. However, the method is not capable of evaluating the estimation precision of point estimates. Thus, this remains a crucial problem in the current theory of quantum tomography.

Here, we give a solution to this problem. We propose a new point estimator for quantum state tomography in finite-dimensional systems, and prove that the estimated states are within a distance δ of the prepared state with high probability. We derive an explicit formula for the confidence level, evaluating how high that probability is. This formula applies for any informationally complete set of measurements, for an arbitrary finite amount of data, and for general loss functions including the infidelity, the Hilbert-Schmidt, and the trace distances. Importantly, for a given experimental setup we can calculate the value of the formula without knowing the true prepared state, and so the formula can also be used to evaluate the precision of state preparation. To our knowledge this is the first result directly applicable to evaluating the precisions of both estimation and preparation in quantum tomography. We demonstrate the technique for examples of one- and two-qubit state tomography.

Preliminaries.—We consider a finite $d(<\infty)$ dimensional quantum system, with Hilbert space $\mathcal{H}$. A state of the system is described by a density matrix, which is a positive-semidefinite and trace-one matrix, the space of which we denote by $\mathcal{S}(\mathcal{H})$. Let $\rho \in \mathcal{S}(\mathcal{H})$ denote the density matrix describing the true prepared state. It is unknown, and we make no further assumptions on ρ. Suppose that N identical copies of the unknown true state, $\rho^{\otimes N}$, are available, and we can perform a measurement on each copy. Our aim is to estimate ρ from measurement results. Let $\boldsymbol{\lambda} = (\lambda_1, \ldots, \lambda_{d^2-1})$ denote a set of Hermitian matrices satisfying (i) (tracelessness) $\mathrm{Tr}[\lambda_\alpha] = 0$ and (ii) (orthogonality) $\mathrm{Tr}[\lambda_\alpha \lambda_\beta] = 2\delta_{\alpha\beta}$. Using this set, a density matrix can be parametrized as [10,11]

$$\rho(\boldsymbol{s}) = \frac{1}{d} I + \frac{1}{2} \boldsymbol{s} \cdot \boldsymbol{\lambda}, \quad (1)$$

where I is the identity matrix and $\boldsymbol{s}$ is a vector in $\mathbb{R}^{d^2-1}$. The matrix and vector are uniquely related as $s_\alpha = \mathrm{Tr}[\rho \lambda_\alpha]$. Positive semidefiniteness of ρ requires constraints on the parameter space. Let S denote the set of parameters corresponding to density matrices; S is a convex subset of $\mathbb{R}^{d^2-1}$. Estimation of ρ is equivalent to that of $\boldsymbol{s} \in S$.

The statistics of a quantum measurement are described by a positive operator-valued measure (POVM), which is a set of positive-semidefinite matrices that sum to the identity. In the standard setting of quantum tomography, we choose a combination of measurements. Let $\vec{\boldsymbol{\Pi}} = \{\boldsymbol{\Pi}^{(j)}\}_{j=1}^{J}$ denote a finite set of POVMs. Suppose that for estimating ρ we independently perform a measurement described by a POVM $\boldsymbol{\Pi}^{(j)} = \{\Pi_m^{(j)}\}_{m=1}^{M^{(j)}}$ a number $n^{(j)}$ of times $(j = 1, \ldots, J)$. The total number of measurement trials is $\sum_{j=1}^{J} n^{(j)} = N$. Let us define $r^{(j)} := N/n^{(j)}$. Elements of the POVM can also be parametrized as

$$\Pi_m^{(j)} = a_{m,0}^{(j)} I + \boldsymbol{a}_m^{(j)} \cdot \boldsymbol{\lambda}, \quad (2)$$

where $a_{m,0}^{(j)} = \mathrm{Tr}[\Pi_m^{(j)}]/d$, and $a_{m,\beta}^{(j)} = \mathrm{Tr}[\Pi_m^{(j)} \lambda_\beta]/2$. When we perform the measurement on a system in state ρ, the probability that we observe an outcome m is given by

$$p(m|\boldsymbol{\Pi}^{(j)}, \rho) = \mathrm{Tr}[\Pi_m^{(j)} \rho] = a_{m,0}^{(j)} + \boldsymbol{a}_m^{(j)} \cdot \boldsymbol{s}. \quad (3)$$

A set of POVMs $\vec{\boldsymbol{\Pi}}$ is called informationally complete (IC) if it spans the vector space of Hermitian matrices on $\mathcal{H}$ [12]. Such a set allows for the reconstruction of an arbitrary quantum state, and we will assume that our $\vec{\boldsymbol{\Pi}}$ is always IC.

Let $n_m^{(j)}$ denote the number of appearances of outcome m in the data from the $n^{(j)}$ measurement trials of $\boldsymbol{\Pi}^{(j)}$ $(m = 1, \ldots, M^{(j)})$; then $f_m^{(j)} := n_m^{(j)}/n^{(j)}$ is the relative frequency. A map from a data set to the space of interest—in this case, the space of quantum states—is called an estimator, and an estimation result is called an estimate. One of the simplest is a linear estimator, ρ^{L} [13], defined as a matrix σ satisfying

$$f_m^{(j)} = p(m|\boldsymbol{\Pi}^{(j)}, \sigma), \qquad j = 1, \ldots, J, \qquad m = 1, \ldots, M^{(j)}. \quad (4)$$

The idea is to use the relative frequencies instead of the unknown true probability distributions. This might seem natural, but there are two problems. The first problem is that when $\vec{\boldsymbol{\Pi}}$ is over complete, Eq. (4) might have no solutions; i.e., we happen to obtain a data set from which we cannot calculate the estimate. The second problem is that even if there exists a solution, it can be unphysical, i.e., lie outside of $\mathcal{S}(\mathcal{H})$. For these two reasons linear estimators are rarely used today. The current standard is a maximum-likelihood (ML) estimator, which is defined as the point in $\mathcal{S}(\mathcal{H})$ maximizing the likelihood function [14]. By definition, such estimates are always physical. The asymptotic $(N \sim \infty)$ behavior of the confidence level of a ML estimator is analyzed in Ref. [15], but there have been no such results for finite data sets.

A loss function is a measure for evaluating the difference between two states. We analyze the following three loss functions:

$$\Delta^{\mathrm{HS}}(\rho', \rho) := \frac{1}{\sqrt{2}} \mathrm{Tr}[(\rho' - \rho)^2]^{1/2}, \quad (5)$$

$$\Delta^{\mathrm{T}}(\rho', \rho) := \frac{1}{2} \mathrm{Tr}[|\rho' - \rho|], \quad (6)$$

$$\Delta^{\mathrm{IF}}(\rho', \rho) := 1 - \mathrm{Tr}\left[\sqrt{\sqrt{\rho'}\rho\sqrt{\rho'}}\right]^2, \quad (7)$$

called the Hilbert-Schmidt (HS) distance, the trace distance (T), and the infidelity (IF), respectively. The trace distance and the infidelity are most often used.

Results.—Instead of ML, we propose a new estimator ρ^{ENM}, where ENM is extended norm minimization. To define it, we first introduce an intermediate estimator ρ^{LLS}, a linear least squares (LLS) estimator [16]. Let us define $\boldsymbol{p}(\sigma)$ and $\boldsymbol{f}_N$ as vectors with (j, m)th element $p(m|\boldsymbol{\Pi}^{(j)}, \sigma)$ and $f_m^{(j)}$, respectively. Define ρ^{LLS} as

$$\rho_N^{\mathrm{LLS}} := \underset{\substack{\sigma;\sigma=\sigma^\dagger,\\ \mathrm{Tr}[\sigma]=1}}{\mathrm{argmin}} \|\boldsymbol{p}(\sigma) - \boldsymbol{f}_N\|_2. \quad (8)$$

The range of the minimization is restricted by the Hermiticity and trace-one conditions, but positive semidefiniteness ($\sigma \geq 0$) is not required. Therefore, the estimates can be unphysical. Let us define $\boldsymbol{a}_0$ as a vector with (j, m)th element $a_{m,0}^{(j)}$ and A as a matrix with $[(j, m), \alpha]$th element $a_{m,\alpha}^{(j)}$ ($\alpha = 1, \ldots, d^2 - 1$). When $\vec{\boldsymbol{\Pi}}$ is IC, A is full rank and the left-inverse matrix $A_{\mathrm{L}}^{-1} = (A^T A)^{-1} A^T$ exists. Then the minimization in Eq. (8) has an analytic solution, and the LLS estimate of the Bloch vector, $\boldsymbol{s}_N^{\mathrm{LLS}}$, is given as

$$\boldsymbol{s}_N^{\mathrm{LLS}} = A_{\mathrm{L}}^{-1}(\boldsymbol{f}_N - \boldsymbol{a}_0). \quad (9)$$

The LLS estimate of a density matrix is calculated $\rho_N^{\mathrm{LLS}} = \rho(\boldsymbol{s}_N^{\mathrm{LLS}})$. Using ρ^{LLS}, we define the new estimator ρ^{ENM} as

$$\rho_N^{\mathrm{ENM}} := \underset{\rho' \in \mathcal{S}(\mathcal{H})}{\mathrm{argmin}} \|\rho' - \rho_N^{\mathrm{LLS}}\|_2. \quad (10)$$

We call ρ^{ENM} an extended norm-minimization estimator [17]. Again, the estimates are always physical by definition.

The following theorem establishes that the ENM estimates are close to the true prepared state with high probability.

Theorem 1 (confidence level of ENM estimator).—Suppose that $\vec{\boldsymbol{\Pi}}$ is IC. Then for the arbitrary true density matrix $\rho \in \mathcal{S}(\mathcal{H})$, the set of positive integers $n^{(j)}$ satisfying $\sum_{j=1}^J n^{(j)} = N$, and the positive number δ,

$$\Delta(\rho_N^{\mathrm{ENM}}, \rho) \leq \delta \quad (11)$$

holds with probability at least

$$\mathrm{C.L.} := 1\text{–}2 \sum_{\alpha=1}^{d^2-1} \exp\left[-\frac{b}{c_\alpha} \delta^2 N\right], \quad (12)$$

where b is determined by our choice of the loss function as

$$b := \begin{cases} 8/(d^2 - 1) & \text{if } \Delta = \Delta^{\mathrm{HS}} \\ 16/d(d^2 - 1) & \text{if } \Delta = \Delta^{\mathrm{T}} \\ 4/d(d^2 - 1) & \text{if } \Delta = \Delta^{\mathrm{IF}} \end{cases}, \quad (13)$$

and c_α are determined by our choice of the measurement setting as

$$c_\alpha := \sum_{j=1}^J r^{(j)} \{\max_m [A_{\mathrm{L}}^{-1}]_{\alpha,(j,m)} - \min_m [A_{\mathrm{L}}^{-1}]_{\alpha,(j,m)}\}^2. \quad (14)$$

We call C.L. in Eq. (12) the confidence level of ρ^{ENM} at the (user-specified) error threshold δ.

We sketch the proof in two steps, with the details shown in the Supplemental Material [18]. First, we consider the Hilbert-Schmidt distance case and analyze the probability that we obtain estimates deviating from the true density matrix by more than the error threshold δ. We call this probability the estimation error probability with respect to $\Delta = \Delta^{\mathrm{HS}}$ at the error threshold δ. By using known results in convex analysis, we prove that the estimation error probability of ρ^{ENM} is smaller than that of ρ^{LLS}. Second, we derive an upper bound on the estimation error probability of ρ^{LLS}. In the derivation, we reduce the analysis of the probability for multiparameter estimation to that of one-parameter estimation and derive a ρ-independent upper bound on the probability with the Hoeffding's tail inequality [19]. The result of the first step ensures that this is also an upper bound on that of ρ^{ENM}. The confidence level for Δ^{HS} is given by one minus the upper bound of the estimation error probability. The confidence levels of Δ^{T} and Δ^{IF} are derived by combining that of Δ^{HS} with inequalities between these loss functions.

Analysis.—The most important point in Theorem 1 is that Eq. (12) is independent of the true state ρ. Therefore, we can use it to evaluate $\Delta(\rho_*, \rho)$ without knowing ρ. Suppose that we choose a loss function Δ satisfying the triangle inequality. Then, by Theorem 1, we have

$$\Delta(\rho_*, \rho) \leq \Delta(\rho_*, \rho_N^{\mathrm{ENM}}) + \Delta(\rho_N^{\mathrm{ENM}}, \rho) \quad (15)$$

$$\leq \Delta(\rho_*, \rho_N^{\mathrm{ENM}}) + \delta, \quad (16)$$

where Eq. (16) holds at the confidence level in Eq. (12). Thus, we can calculate the value of the rhs of Eq. (16) without knowing ρ. In tomographic experiments, the infidelity, [or the fidelity $F(\rho', \rho) := 1 - \Delta^{\mathrm{IF}}(\rho', \rho)$], is a popular loss function. It does not satisfy the triangle inequality, but it is related to the trace distance by $\Delta^{\mathrm{IF}}(\rho', \rho) \leq 2\Delta^{\mathrm{T}}(\rho', \rho)$ [20]. Thus, we obtain

$$\Delta^{\mathrm{IF}}(\rho_*, \rho) \leq 2\{\Delta^{\mathrm{T}}(\rho_*, \rho_N^{\mathrm{ENM}}) + \delta\}, \quad (17)$$

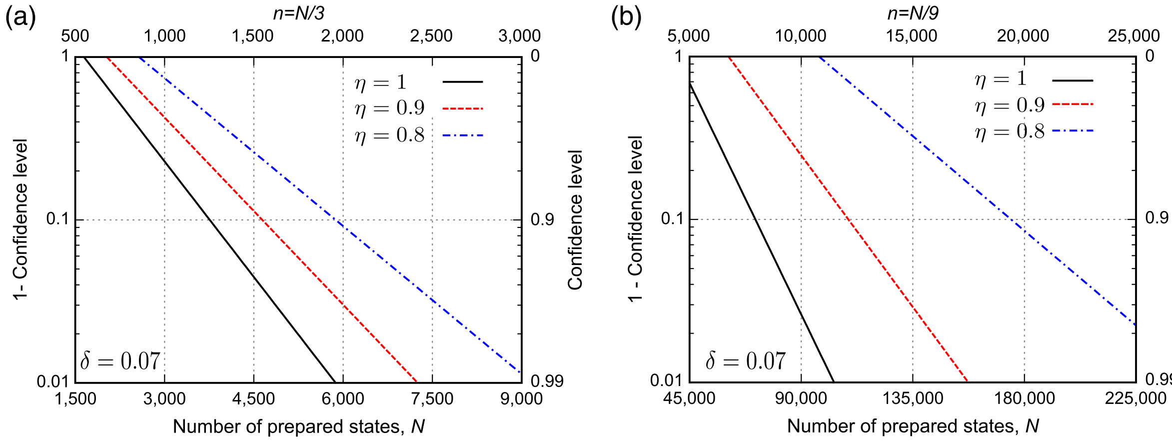

FIG. 2 (color online). Confidence level of ρ^{ENM} for the error threshold $\delta = 0.07$ in quantum state tomography: (a) is the one-qubit ($k = 1$) case and (b) is for two qubits ($k = 2$). The line styles are fixed as follows: solid (black) line for detection efficiency $\eta = 1$, dashed (red) line for $\eta = 0.9$, dot-dashed (blue) line for $\eta = 0.8$.

$$F(\rho_*, \rho) \geq 1–2\{\Delta^{\mathrm{T}}(\rho_*, \rho_N^{\mathrm{ENM}}) + \delta\}, \tag{18}$$

where Eqs. (17) and (18) hold at C.L. for Δ^{T}.

Consider a k-qubit system and suppose that we make the three Pauli measurements with detection efficiency η on each qubit. There are 3^k different tensor products of Pauli matrices ($J = 3^k$), and suppose that we observe each equally $n := N/3^k$ times. When we choose $\Delta = \Delta^{\mathrm{T}}$, we have

$$\mathrm{C.L.}(k) = 1–2\sum_{l=0}^{k-1} 3^{k-l}\binom{k}{l}\exp\left[-\frac{2}{2^{2k}-1}\frac{\eta^{2(k-l)}}{3^{k-l}}\delta^2 N\right]. \tag{19}$$

The details of this derivation are explained in the Supplemental Material [18]. Figure 2 shows plots of Eq. (19) for the one-qubit ($k = 1$) and two-qubit ($k = 2$) cases in Figs. 2(a) and 2(b), respectively. The error threshold is $\delta = 0.07$ and detection efficiency is $\eta = 1, 0.9, 0.8$. Both panels indicate that smaller detection efficiency requires a larger number of prepared states. The plots tell us the value of N sufficient for guaranteeing a fixed confidence level. For example, if we want to guarantee 99% confidence level for $\delta = 0.07$ in one-qubit state tomography with $\eta = 0.9$, Fig. 2(a) indicates that $N = 7500$.

In Ref. [21], an efficient ML estimator algorithm is proposed for quantum state tomography using an IC set of projective measurements with Gaussian noise whose variance is known, and numerical results for k-qubit ($k = 1, \ldots, 9$) state tomography indicate that the computational cost would be significantly lower than that of standard ML algorithms. In general, a ML estimator is different from the ENM estimator, but, in the setting considered in [21], the ML estimator is a specific case of an ENM estimator, which is defined for general IC measurements. Despite this generality, we find that their efficient algorithm can be modified and used for our ENM estimates [22]. Additionally, Theorem 1 shows that the ENM estimator can be used without assuming projective measurements or Gaussian noise.

It is natural to ask if instead of performing two sequential optimizations as in the ENM case one performs a single constrained optimization. This is well known in classical statistics and was applied to a quantum estimation problem in Ref. [23]. Define a constrained least squares (CLS) estimator

$$\rho_N^{\mathrm{CLS}} := \operatorname*{argmin}_{\rho' \in \mathcal{S}(\mathcal{H})} \|\boldsymbol{p}(\rho') - \boldsymbol{f}_N\|_2, \tag{20}$$

which always exists and is always physical. Using nearly the same proof as in Theorem 1, we can derive a confidence level for ρ^{CLS}. The result is equivalent or smaller than Eq. (12)—the details and a comparison to ρ^{ENM} are shown in the Supplemental Material [18]. Although in some cases the confidence levels coincide, in order to calculate CLS estimates we need to solve the quadratic optimization problem under inequality constraints, which the ENM case avoids.

Summary.—We considered quantum state tomography in arbitrary finite dimensional systems, proposing a new point estimator and deriving an explicit formula evaluating the precision of estimation for an arbitrary finite number of measurement trials. We applied the idea using, as an example, k-qubit state tomography with detection errors, and showed plots for the one- and two-qubit cases. We also show how the formula can be used for evaluating the precision of state preparation. To the best of our knowledge, this is the first result that makes it possible to evaluate the precision of estimation and preparation without knowing the prepared state, and we hope it finds application in the analysis of experimental data.

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