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Point estimation of states of finite quantum systems

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Abstract

The estimation of the density matrix of a k-level quantum system is studied when the parametrization is given by the real and imaginary part of the entries, and they are estimated by independent measurements. It is established that the properties of the estimation procedure depend very much on the invertibility of the true state. In particular, in the case of a pure state, the estimation should be constrained to ensure the positive definiteness of the estimate. An efficient constraining algorithm is proposed and it yields an asymptotically unbiased estimate. Moreover, several estimation schemes are compared for the unknown state of a qubit when one copy is measured at a time. It is shown that the average mean quadratic error matrix is the smallest if the applied observables are complementary. All the results are illustrated by computer simulations.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

The problem of inferring the state of a quantum system from measurement data is fundamental. Although this problem may be traced back to the seventies [7] the interest in such questions has been renewed in the field of quantum information theory. One side of this problem is the adequate experimental techniques, and the other side is the theory based on the adaptation of statistics to the quantum-mechanical formalism. A quantum state estimation strategy includes the selection of suitable observables, a parametrization of the state, an estimation procedure and a distance between the true and estimated density matrices. Most of the papers use maximum-likelihood (ML) or Bayesian estimation procedures with compatible parametrization and distance [4].

Most of the work in state estimation has focused on states of a qubit, pure states [6], or mixed states [1, 9, 13]. An adaptive observable selection strategy based on a Bloch vector parametrization in spherical coordinates and on a Bayesian estimation method of qubits in

mixed states is reported in [2]. The estimation procedure for pure states is simpler, partially due to the smaller number of parameters, but the procedures designed for the case of mixed state encounter difficulties if applied for a pure or nearly pure unknown state. This is partially caused by the limited amount and accuracy of measured data implying that the positivity of the reconstructed density matrix may not be ensured. In order to solve this problem, a normalization procedure for incompatible operators is proposed in [8] for using a ML approach and relative entropy as a distance.

The subject of the present paper is state estimation for a k-level quantum system. In this case the boundary of the state space is not the set of pure states but the non-invertible density matrices. The entries of the density matrix provide a natural parametrization of the state space. Based on this parametrization, the aim of this paper is to develop efficient strategies for point estimation that can handle the positivity constraint on the state estimate.

The accuracy of the estimation can be quantified by the fidelity or by the Hilbert–Schmidt distance. For larger matrices the latter seems to be easier to handle. In order to be consistent with the proposed point estimation strategy, the mean quadratic error matrix is used when different estimation schemes are compared.

2. The estimation scheme

The goal of state estimation is to determine the density operator ρ of a quantum system by measurements on n copies of the quantum system which are all prepared according to ρ [3, 4, 9]. The number n corresponds to the sample size in classical mathematical statistics. An estimation scheme means a collection of measurements and an estimate for every n. The estimate is a mapping defined on the measurement data and its values are density operators. For a reasonable scheme, we expect the estimation error to tend to 0 when n tends to infinity (i.e. we expect to have an asymptotically unbiased estimate) as a consequence of the law of large numbers.

Assume that ρ is the density matrix of our system described on the Hilbert space $\mathcal{H}$. Then the n identical copies are described by the n-fold tensor product $\mathcal{H}_n := \mathcal{H}^{n\otimes}$ and the state is $\rho_n := \rho^{n\otimes}$. When $\dim \mathcal{H} = k$, we can identify the operators of $\mathcal{H}_n$ with matrices of $k^n \times k^n$. In this paper we study measurement schemes given by self-adjoint matrices

$$\mathbf{A}(n) = (\mathbf{A}(n)_{ij})_{i,j=1}^{k}, \tag{1}$$

where $\mathbf{A}(n)_{ij} \in B(\mathcal{H}_n)$. Note that $\mathbf{A}(n)$ is determined by k^2 self-adjoint operators acting on $\mathcal{H}_n$. They are the diagonal entries $Z(n)_{ii} \equiv \mathbf{A}(n)_{ii}$ of $\mathbf{A}(n)$, moreover the off-diagonal entries are written as

$$\mathbf{A}(n)_{ij} = X(n)_{ij} + \mathrm{i}Y(n)_{ij} \qquad (i < j)$$

by means of self-adjoint $X(n)_{ij}$ and $Y(n)_{ij}$. The measurement scheme $\mathbf{A}(n)$ means that the observables $Z(n)_{ii}$, $X(n)_{ij}$ and $Y(n)_{ij}$ are measured on the r copies of the original system. Since the sum of the diagonal entries of a density matrix is 1, it is enough to measure $k-1$ diagonal entries; for example, $Z(n)_{kk}$ can be removed from the set of observables to be measured and k^2-1 observables remain. Hence $n = r(k^2-1)$.

The above construction is in an analogy to the classical estimation setting in mathematical statistics if the observables are regarded as matrix-valued random variables that carry information about the unknown parameters of the density matrix ρ through the measured values obtained by measuring the observables on the system. Because of their properties, density matrices of a k-level system can be described by k^2-1 parameters, thus one needs at least k^2-1 observables to estimate their parameters. The measurement of each observable is repeated r times, therefore one needs $n = r(k^2-1)$ measurements for the estimation.

Example 1. Let $k = 2$ and let us construct the observables in such a way that they act on the n identical copies

$$S_n(\sigma_i) = \frac{1}{n}(\sigma_i \otimes I_2 \otimes \cdots \otimes I_2 + I_2 \otimes \sigma_i \otimes I_2 \otimes \cdots \otimes I_2 + \cdots + I_2 \otimes I_2 \otimes \cdots \otimes \sigma_i)$$
$$S_n(\sigma_i) \in B(\mathcal{H}_n),$$

where $1 \leqslant i \leqslant 3$, σ_i are the Pauli matrices and I_2 is the identity matrix, all of them are 2×2 complex matrices. One term in the bracket corresponds to a measurement when one applies the observable σ_i to a particular instance from the set of n identical copies and leaves the rest unchanged. Set

$$\mathbf{A}(n) = \frac{1}{2}\begin{bmatrix} I_n + S_n(\sigma_3) & S_n(\sigma_1) - \mathrm{i}S_n(\sigma_2) \\ S_n(\sigma_1) + \mathrm{i}S_n(\sigma_2) & I_n - S_n(\sigma_3) \end{bmatrix}, \tag{2}$$

where I_n denotes the identity on $\mathcal{H}_n$.

We may have a better understanding of this estimation scheme if the n-fold product is considered to be embedded into the infinite product. This means that the unit matrices I_n are identified, and we write simply I. Then elements of $\mathbf{A}(n)$ are in one huge algebra and the limit $n \to \infty$ is more visible. If

$$\rho = \begin{bmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{bmatrix},$$

then the law of large numbers guarantees that

$$\mathbf{A}(n)_{ij} \to \rho_{ij} I.$$

Therefore, the error is going to 0 when n goes to ∞ for any reasonable definition of the error.

The entries of the matrix (2) do not commute, therefore there is no joint Kolmogorovian model for them and the observables cannot be measured simultaneously. We modify this matrix, in order to use standard probabilistic tools.

On the infinite tensor product $M_k \otimes M_k \otimes \cdots$ we introduce the right shift γ:

$$\gamma(H_1 \otimes H_2 \otimes \cdots H_n \otimes I_k \otimes I_k \cdots) = I_k \otimes H_1 \otimes H_2 \otimes \cdots H_n \otimes I_k \otimes I_k \cdots.$$

Now we set

$$\hat{\mathbf{A}}(n) = \frac{1}{2}\begin{bmatrix} I + S_r(\sigma_3) & \gamma^r(S_r(\sigma_1)) - \mathrm{i}\gamma^{2r}(S_r(\sigma_2)) \\ \gamma^r(S_r(\sigma_1)) + \mathrm{i}\gamma^{2r}(S_r(\sigma_2)) & I - S_r(\sigma_3) \end{bmatrix}. \tag{3}$$

The operators $S_r(\sigma_3)$, $\gamma^r(S_r(\sigma_1))$ and $\gamma^{2r}(S_r(\sigma_2))$ commute. They may be regarded as classical random variables, one can speak about their joint distribution, variance etc.

The simplest case is when $r = 1$, i.e. one measurement of each $k^2 - 1 = 3$ observables is performed. This way the total number of measurements is 3, and $\hat{\mathbf{A}}(3)$ turns to be

$$\hat{\mathbf{A}}(3) = \frac{1}{2}\begin{bmatrix} I_3 + \sigma_3 \otimes I \otimes I & I \otimes \sigma_1 \otimes I - \mathrm{i}(I \otimes I \otimes \sigma_2) \\ I \otimes \sigma_1 \otimes I + \mathrm{i}(I \otimes I \otimes \sigma_2) & I_3 - \sigma_3 \otimes I \otimes I \end{bmatrix}.$$

Practically, it means that the measurement of σ_3 is performed first, then comes observable σ_1 and finally σ_2.

The very concrete estimation scheme we use will be the natural extension of example 1. Denote by E_{ij} the $k \times k$ matrix units and set

$$Z_{ii} := \gamma^{\tau(i,i)}(E_{ii}) \qquad (1 \leqslant i < k),$$
$$X_{ij} := \gamma^{\tau(i,j)}(E_{ij} + E_{ji}) \qquad (i < j),$$
$$Y_{ij} := \gamma^{\tau(j,i)}(-\mathrm{i}E_{ij} + \mathrm{i}E_{ji}) \qquad (i < j),$$

where $\tau : \{(i, j) : 1 \leqslant i, j \leqslant k, (i, j) \neq (k, k)\} \to \{1, 2, \ldots, k^2 - 1\}$ is an arbitrary bijection. These self-adjoint operators commute and behave as independent random variables. The spectrum of Z_{ii} is $\{0, 1\}$ and the spectrum of X_{ij} and Y_{ij} is $\{-1, 0, 1\}$. The matrix $\mathbf{A}(k^2 - 1)$ is determined by these operator entries.

Finally, the estimation scheme $\mathbf{A}(r(k^2 - 1))$ is defined by the formulae

$$Z(r(k^2-1))_{ii} := \frac{1}{r}\sum_{m=0}^{r-1} \gamma^{m(k^2-1)}(Z_{ii}) \qquad (1 \leqslant i < k),$$

$$X(r(k^2-1))_{ij} := \frac{1}{r}\sum_{m=0}^{r-1} \gamma^{m(k^2-1)}(X_{ij}) \qquad (i < j),$$

$$Y(r(k^2-1))_{ij} := \frac{1}{r}\sum_{m=0}^{r-1} \gamma^{m(k^2-1)}(Y_{ij}) \qquad (i < j).$$

Note that to carry on the measurement of all these observables, $r(k^2 - 1)$ copies of the original quantum system are needed. The entries of $\mathbf{A}(n)$ are commuting observables, therefore there is a basis in $\mathcal{H}_n$ such that all of them are diagonal in this basis. Consequently, a single measurement can be performed theoretically instead of the measurements of the $k^2 - 1$ observables ($n = r(k^2 - 1)$).

The estimation procedure. Our aim is to estimate the $k \times k$ density matrix ρ of a quantum system. The parametrization is naturally given by the entries of the matrix. In what follows, we are given several copies of a k-level quantum system in the same state. We perform measurements on the systems one after another, that is, a system is measured only once, the next measurement is performed on the next copy of the system, so the states of the systems after the measurement are irrelevant from our viewpoint.

If we want to estimate the real part of the ijth entry of the density matrix ρ, then we measure the observable $E_{ij} + E_{ji}$. Its spectral decomposition is

$$1 \cdot \frac{1}{2}(E_{ii} + E_{ij} + E_{ji} + E_{jj}) + 0 \cdot \sum_{i \neq m \neq j} E_{mm} - 1 \cdot \frac{1}{2}(E_{ii} - E_{ij} - E_{ji} + E_{jj}),$$

and its measurement has three different outcomes: ± 1 and 0. The probabilities of the outcomes ± 1 are

$$\mathrm{Prob}(X_{ij} = \pm 1) = \tfrac{1}{2}(\rho_{ii} \pm \rho_{ij} \pm \rho_{ji} + \rho_{jj}) = \tfrac{1}{2}(\rho_{ii} + \rho_{jj}) \pm \mathrm{Re}\,\rho_{ij}. \tag{4}$$

To estimate the imaginary part, we measure $\mathrm{i}E_{ij} - \mathrm{i}E_{ji}$ with spectral decomposition

$$1 \cdot \frac{1}{2}(E_{ii} + \mathrm{i}E_{ij} - \mathrm{i}E_{ji} + E_{jj}) + 0 \cdot \sum_{i \neq m \neq j} E_{mm} - 1 \cdot \frac{1}{2}(E_{ii} - \mathrm{i}E_{ij} + \mathrm{i}E_{ji} + E_{jj}).$$

The probabilities are

$$\mathrm{Prob}(Y_{ij} = \pm 1) = \tfrac{1}{2}(\rho_{ii} \pm \mathrm{i}\rho_{ij} \mp \mathrm{i}\rho_{ji} + \rho_{jj}) = \tfrac{1}{2}(\rho_{ii} + \rho_{jj}) \pm \mathrm{Im}\,\rho_{ij}. \tag{5}$$

Finally, for the diagonal ii entry we have

$$\mathrm{Prob}(Z_{ii} = +1) = \rho_{ii}. \tag{6}$$

Altogether we have $k^2 - 1$ different measurements and each of them is repeated r times. The measurement outcomes form a set $\mathcal{X}_n$ and this is the domain of the matrix-valued estimate. To determine the estimate we need only the relative frequencies of the outcomes of the $k^2 - 1$ different measurements, all of them are performed r times. If M is one of the

measurements which has an outcome t, then we denote by $\nu(r, M, t)$ the relative frequency of t when the measurement is performed r times. According to the *law of large numbers*, $\nu(r, M, t) \to \mathrm{Prob}(M = t)$ as $r \to \infty$. (Of course, $\mathrm{Prob}(M = t)$ depends on the true state of our system.)

The following estimate is natural:

(i) $\Phi^{\mathrm{un}}{}_{n\ ii} = \nu(r, Z_{ii}, +1)$ for $(1 \leqslant i < k)$ and

$$\Phi^{\mathrm{un}}{}_{n\ kk} = 1 - \sum_{i=1}^{k-1} \nu(r, Z_{ii}, +1),$$

(ii) $\mathrm{Re}\,\Phi^{\mathrm{un}}{}_{n\ ij} = \frac{1}{2}(\nu(r, X_{ij}, +1) - \nu(r, X_{ij}, -1))$ for $i < j$.

(iii) $\mathrm{Im}\,\Phi^{\mathrm{un}}{}_{n\ ij} = \frac{1}{2}(\nu(r, Y_{ij}, +1) - \nu(r, Y_{ij}, -1))$ for $i < j$.

In our notation, 'un' is an abbreviation of the word *unconstrained*. It may happen that Φ^{un}_n is not a positive semidefinite matrix; hence, it is not an estimate in the really strict sense. Let $\mathcal{M}_k$ denote the set of all self-adjoint $k \times k$ matrices of trace 1. It follows from the definition of the estimate that Φ^{un}_n takes its values in $\mathcal{M}_k$. Note that the set of invertible density matrices form an open subset of $\mathcal{M}_k$.

Properties of the estimate. Because of construction, the above unconstrained estimate is unbiased. That follows from the fact that the expectation value of the relative frequencies involved is the probabilities. For example, the expectation value of the diagonal elements of the estimator can be computed as

$$\mathbf{E}\Phi^{\mathrm{un}}{}_{n\ ii} = \mathbf{E}\nu(r, Z_{ii}, +1) = \mathrm{Prob}(Z_{ii} = +1) = \rho_{ii}.$$

The expectation value for the real and imaginary part of the off-diagonal elements can be computed similarly.

Given a true state ρ, Φ^{un}_n is a matrix-(or vector-)valued random variable which is the mean of r-independent copies of Φ^{un}_m, $m = k^2 - 1$. Let $G \subset \mathcal{M}_k$ be an open set such that $\rho \in G$. According to the law of large numbers,

$$\mathrm{Prob}\big(\Phi^{\mathrm{un}}_n \notin G\big) \to 0,$$

however, according to the *large deviation theorem* the convergence is exponentially fast:

$$\mathrm{Prob}\big(\Phi^{\mathrm{un}}_n \notin G\big) \leqslant C \exp(-n E_G),$$

where $E_G > 0$ is the infimum of the so-called rate function; see [5].

Theorem 1. *Assume that ρ is an invertible density matrix. The probability of that Φ^{un}_n is not a density matrix converges exponentially to 0 as $n \to \infty$.*

Proof. The expectation value of Φ^{un}_m is $\rho \in \mathcal{M}_k$. Cramér's theorem tells us that there is a function $I : \mathcal{M}_k \to \mathbb{R}^+ \cup \{+\infty\}$ such that for any open set containing ρ

$$\limsup_{n\to\infty} \frac{1}{n} \log \mathrm{Prob}\big(\Phi^{\mathrm{un}}_n \notin G\big) \leqslant -\inf\{I(D) : D \in \mathcal{M}_k \backslash G\}.$$

The RHS is strictly negative and if ρ is invertible, then we can choose G such that it consists of density matrices (that is, its elements are positive definite). This gives the proof.

The computation of the rate function I is theoretically possible, but we do not need its concrete form. □

Although the expectation value of the unconstrained estimate Φ^{un}_n is the true state, this does not mean that Φ^{un}_n is a good estimate. It may happen that the value of Φ^{un}_n is outside the state space with some probability.

Example 2. Consider the pure state

$$\rho = \frac{1}{2}\begin{bmatrix} 2 & 0 \\ 0 & 0 \end{bmatrix} = \frac{1}{2}(\sigma_0 + \sigma_3). \tag{7}$$

The following observables are measured:

$$Z_{11} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \qquad X_{12} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \qquad Y_{12} = \begin{bmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{bmatrix}.$$

The measurement of Z_{11} gives 1 (with probability 1). For the others we have

$$\mathrm{Prob}(X_{12} = \pm 1) = \mathrm{Prob}(Y_{12} = \pm 1) = \tfrac{1}{2}.$$

Let us introduce the binary valued random variable γ with

$$\gamma := \begin{cases} 1 & \text{with probability} \quad 1/2, \\ -1 & \text{with probability} \quad 1/2. \end{cases} \tag{8}$$

Then evidently $\gamma^2 = 1$ with probability 1.

The estimator can be regarded as a matrix-valued random variable in the form

$$\Phi_{3r}^{\mathrm{un}} = \begin{bmatrix} 1 & ((\beta_1 + \cdots + \beta_r) - \mathrm{i}(\gamma_1 + \cdots + \gamma_r))/2r \\ ((\beta_1 + \cdots + \beta_r) + \mathrm{i}(\gamma_1 + \cdots + \gamma_r))/2r & 0 \end{bmatrix},$$

where γ_i and β_j are identically distributed independent random variables with the same distribution as γ (8).

It is easy to see that the expectation value of the determinant of Φ_{3r}^{un} is $-1/2r$. This shows that although the expectation value of the determinant is zero in the limit (as a consequence of unbiasedness of the estimate), but the estimate has always a negative eigenvalue with positive probability. Therefore, in this example Φ_{3r}^{un} is a rather bad estimate.

Figure 1 shows a simulation with another pure state $(\sigma_0 + \sigma_1)/2$. The Hilbert–Smith distance of the estimator Φ_{3r}^{un} and the true density matrix has been computed as a function of n where each point has been generated using a new set of $n = 3r$ qubits. It is seen that the convergence is indeed very slow, not of an exponential type.

The properties of the unconstrained estimate Φ_n^{un} depend very much on the true state. If the eigenvalues of the true state are strictly positive (and not very small), then the estimate is rather good and the convergence is visible from the simulations; see figures 2 and 3. The simulations are essentially simpler in the 2×2 case, when the boundary of the state space consists of pure states and the positivity of the estimate can be seen from the length of the Bloch vector. In the 3×3 case the boundary is more complicated, it consists of the non-invertible densities.

3. Constrained estimate

There are cases when Φ_n^{un} is not a positive semidefinite matrix, sometimes we call Φ_n^{un} *unconstrained estimate*. The expectation value of Φ_n^{un} is the true state of the system, so it is an *unbiased estimate*.

We can use the method of least squares to get a density matrix:

$$\Phi_n := \mathrm{argmin}_\omega \mathrm{Tr}\big(\Phi_n^{\mathrm{un}} - \omega\big)^2 = \mathrm{argmin}_\omega \sum_{i,j} \big(\Phi_n^{\mathrm{un}}\big)_{ij} - \omega_{ij}\big)^2, \tag{9}$$

where ω runs over the density matrices. The density matrices form a closed convex set $\mathcal{D}_k$, therefore the minimizer is unique. Note that for a qubit the closest positive semidefinite matrix

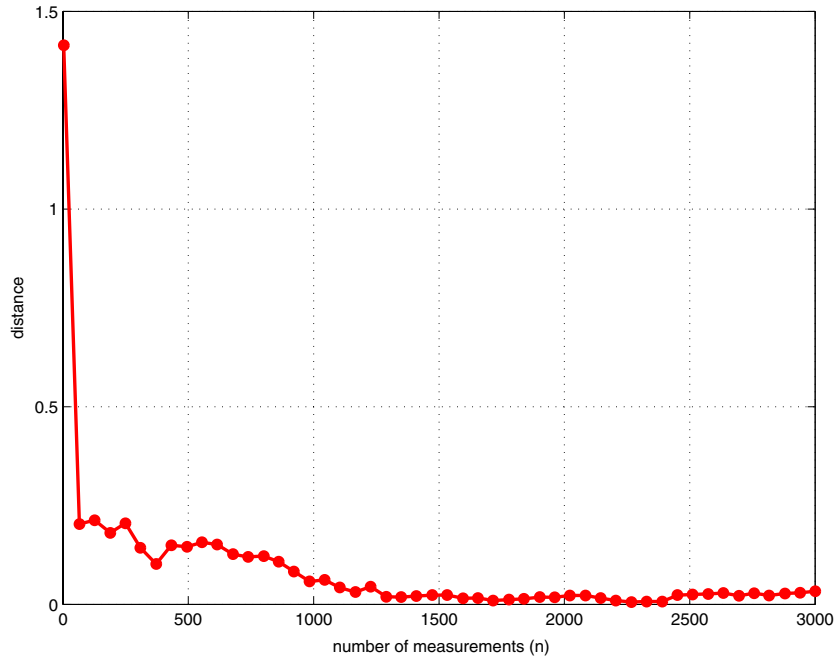

Figure 1. The Hilbert–Schmidt distance between the true pure state $(\sigma_0+\sigma_1)/2$ and Φ_n^{un} converges very slowly to 0 as $n \to \infty$.

is easy to find. When the values of the estimate are 2×2 matrices, they can be identified by vectors in $\mathbb{R}^3$. When the estimate is unconstrained, it my happen that the values can go out of the Bloch ball (see figure 4 for an example).

If the values of the estimates are simply the Bloch vectors, then

$$\Phi_n = \begin{cases} \Phi_n^{\mathrm{un}} & \text{if} \quad \left\|\Phi_n^{\mathrm{un}}\right\| \leqslant 1, \\ \frac{\Phi_n^{\mathrm{un}}}{\left\|\Phi_n^{\mathrm{un}}\right\|} & \text{otherwise.} \end{cases} \tag{10}$$

Theorem 2. *The constrained estimate Φ_n is asymptotically unbiased.*

Proof. We can use the fact that Φ_n^{un} is unbiased and to show that Φ_n is an asymptotically unbiased estimate we study their difference. Let $p(x)$ be the probability of the measurement result $x \in \mathcal{X}_n$. Denote by X the set of outcomes such that $\Phi_n^{\mathrm{un}}(x) \neq \Phi_n(x)$. Then evidently

$$\sum_x \Phi_n^{\mathrm{un}}(x)p(x) - \sum_x \Phi_n(x)p(x) = \sum_{x\in X} \left(\Phi_n^{\mathrm{un}}(x) - \Phi_n(x)\right)p(x). \tag{11}$$

If $\mathcal{D}_k \subset \mathcal{M}_k$ is the set of density matrices, then X is the set of outcomes x such that $\Phi_n^{\mathrm{un}}(x) \notin \mathcal{D}_k$. Let us fix a norm on the space $\mathcal{M}_k$. (Note that all norms are equivalent.)

Let $\varepsilon > 0$ be arbitrary. We split X into two subsets:

$$X_1 = \left\{x \in X : \text{distance}\left(\Phi_n^{\mathrm{un}}(x), \mathcal{D}_k\right) \leqslant \varepsilon\right\} \qquad \text{and} \qquad X_2 = X\backslash X_1.$$

Note that distance $\left(\Phi_n^{\mathrm{un}}(x), \mathcal{D}_k\right) = \left\|\Phi_n^{\mathrm{un}}(x) - \Phi_n(x)\right\|$. Then

$$\sum_{x\in X} \left\|\Phi_n^{\mathrm{un}}(x) - \Phi_n(x)\right\| p(x) \leqslant \sum_{x\in X_1} \left\|\Phi_n^{\mathrm{un}}(x) - \Phi_n(x)\right\| p(x) + \sum_{x\in X_2} \left\|\Phi_n^{\mathrm{un}}(x) - \Phi_n(x)\right\| p(x).$$

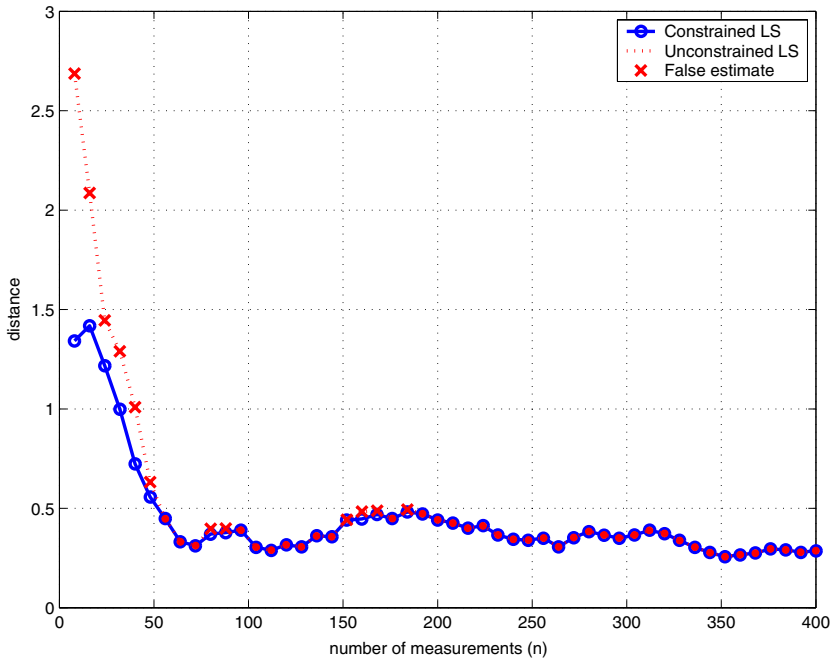

Figure 2. The Hilbert–Schmidt distance between the true 3×3 state with eigenvalues 0.1186, 0.2871, 0.5943 and the estimate. When the number of the measurement is more than 200, the unconstrained estimate gives really a positive semidefinite matrix.

The first term is majorized by ε and the second one by $C\,\mathrm{Prob}(X_1)$. Since the first is arbitrary small and the latter goes to 0, we can conclude that (11) goes to 0. □

Computing the constrained estimate. The computation of the minimizer of (9) is easier if Φ_n^{un} is diagonal. Since Φ_n^{un} is self-adjoint, changing the basis we may assume that $\Phi_n^{\mathrm{un}} = \mathrm{Diag}(x_1, x_2, \ldots, x_n)$ and $x_1, x_2, \ldots, x_k < 0$ and $x_{k+1}, x_{k+2}, \ldots, x_n \geqslant 0$. The minimizer is obviously diagonal, hence we need to solve

$$\mathrm{argmin}_{y_i} \sum_i (x_i - y_i)^2$$

under the constraint $y_i \geqslant 0$ and $\sum_i y_i = 1$. According to the inequality between the quadratic and arithmetic means, we have

$$\sum_{i=1}^n (x_i - y_i)^2 \geqslant \sum_{i=1}^k x_i^2 + \sum_{i=k+1}^n (x_i - y_i)^2 \geqslant \sum_{i=1}^k x_i^2 + \frac{1}{n-k}\left(\sum_{i=k+1}^n (x_i - y_i)\right)^2$$
$$= \sum_{i=1}^k x_i^2 + \frac{1}{n-k}\left(\sum_{i=1}^k y_i - x_i\right)^2.$$

If

$$y_i = x_i + c \quad \left(i = k+1, k+2, \ldots, n, \quad c = \frac{1}{n-k}\sum_{i=1}^k x_i, \quad c < 0\right)$$

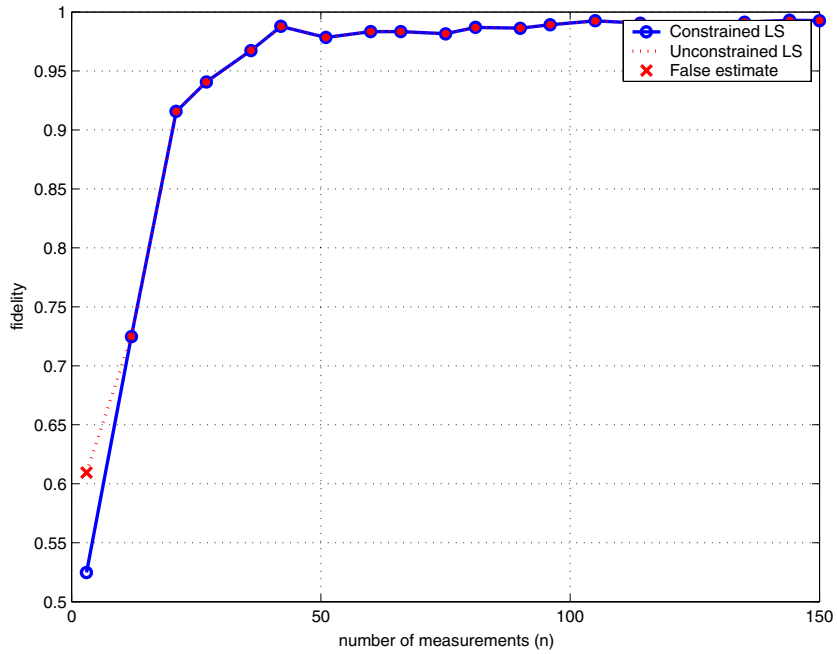

Figure 3. The fidelity between the true 2×2 mixed state with eigenvalues 0.1235, 0.8765 and the estimate. When the number of the measurement is more than 10, the unconstrained and the constrained estimates are the same.

are positive, then the minimizer is $(y_1, y_2, \ldots, y_n)$, where $y_1 = y_2 = \cdots = y_k = 0$ and the other y_i's are defined above. If the n-tuple $(y_1, y_2, \ldots, y_n)$ contains negative entries, then we repeat the procedure, the negative entries are replaced with 0 and the actual value of c is added to the other entries. After finitely many steps we arrive at the minimizer. Figure 5 shows the details for $n = 3$.

In the general case, we can change the basis such that Φ_n^{un} becomes diagonal, since the Hilbert–Schmidt distance is invariant under this transformation. So let $U\Phi_n^{\mathrm{un}}U^* = \mathrm{Diag}(x_1, x_2, \ldots, x_n)$ for a unitary U. Then we compute the minimizer $\mathrm{Diag}(y_1, y_2, \ldots, y_n)$ using the above procedure and

$$\Phi_n = U^* \mathrm{Diag}(y_1, y_2, \ldots, y_n)U.$$

Note that there are other computationally feasible methods for computing the constrained estimate, the details and simulation results can be found in [10].

4. Estimations for a qubit

The mean quadratic error matrix may be used to measure the efficiency of an estimate. If the unknown state is parametrized by $(\theta_1, \theta_2, \ldots, \theta_m)$, then the *mean quadratic error* is an $m \times m$ matrix defined as

$$V_n(\theta)_{i,j} := \sum_{x \in \mathcal{X}_n} (\Phi_n(x)_i - \theta_i)(\Phi_n(x)_j - \theta_j)p(x) \qquad (1 \leqslant i, j \leqslant m),$$

where $\mathcal{X}_n$ is the set of measurement outcomes.

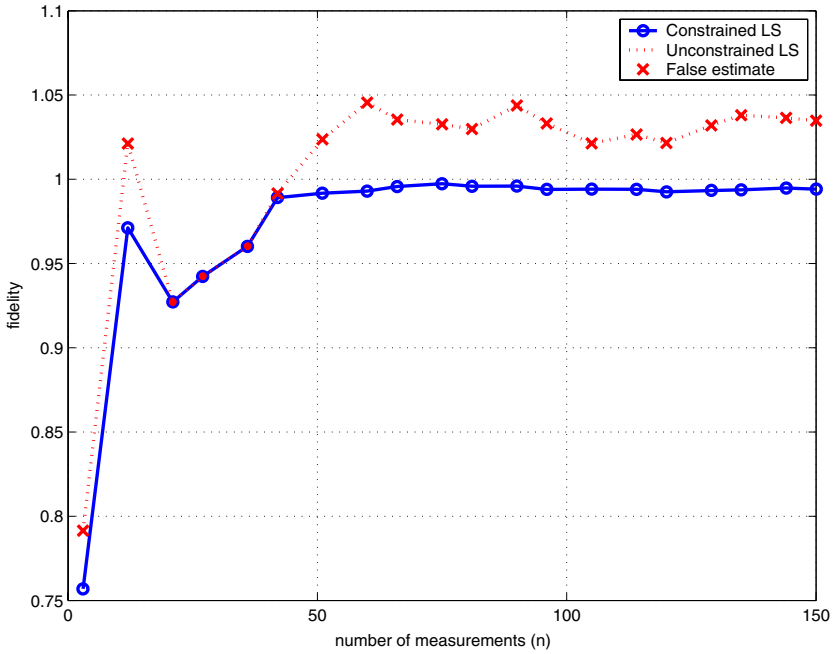

Figure 4. The fidelity between the true 2×2 pure state and the estimates. The unconstrained estimate is often outside of the Bloch ball and in this case the (real part of the complex) fidelity can be greater than 1. The constrained estimate converges to the true state.

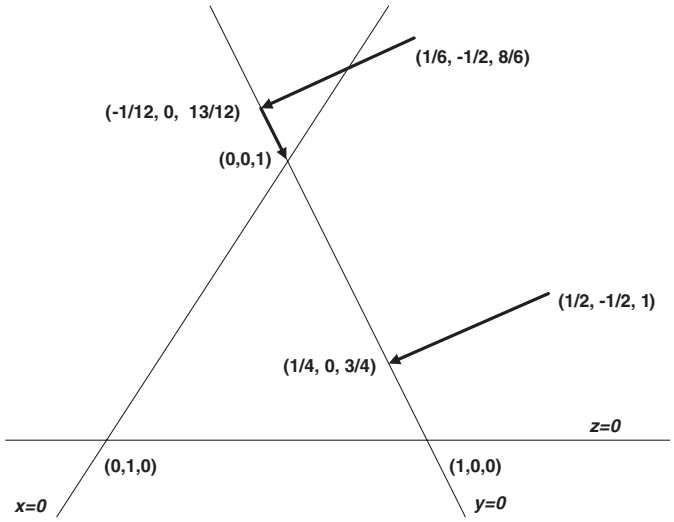

Figure 5. The constrained estimate for 3×3 matrices. The plain $x + y + z = 1$ of $\mathbb{R}^3$ is shown. The triangle $\{(x, y, z) : x, y, z \geqslant 0\}$ corresponds to the diagonal density matrices. Starting from the unconstrained estimate $\mathrm{Diag}(1/2, -1/2, 1)$, the constrained $\mathrm{Diag}(1/4, 0, 3/4)$ is reached in one step. Starting from $\mathrm{Diag}(1/6, -1/2, 8/6)$, two steps are needed.

In the case of a qubit with $m = k^2 - 1 = 3$, the Bloch parametrization can be used:

$$\rho = \frac{1}{2}\begin{bmatrix} 1+\theta_3 & \theta_1 - \mathrm{i}\theta_2 \\ \theta_1 + \mathrm{i}\theta_2 & 1+\theta_3 \end{bmatrix}.$$

Then $\theta = (\theta_1, \theta_2, \theta_3)^t$ belongs to the unit ball of $\mathbb{R}^3$. ($(\theta_1, \theta_2, \theta_3)^t$ means a column vector, so ^{t} may be regarded as the transpose.)

The estimation scheme. Throughout this section the 2-level case ($k = 2$) is considered, and the observables are derived from the 'standard' ones being the Pauli matrices:

$$\sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \qquad \sigma_2 = \begin{bmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{bmatrix}, \qquad \sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

All of them has the spectrum $\{+1, -1\}$, that is, the possible outcomes of their measurement are ± 1. All three observables have the spectral decomposition

$$\sigma_i = (+1)E_{i,+} + (-1)E_{i,-}, \qquad (i = 1, 2, 3),$$

where $E_{i,\pm}$ are eigenprojections.

The probability of having outcome ± 1 for σ_i is

$$\operatorname{Tr} \rho E_{i,+} = \tfrac{1}{2}(1 \pm \theta_i), \qquad (i = 1, 2, 3).$$

Applying a slightly different version of the estimator introduced in section 2, it has the form

$$\Phi_{3r}^{\mathrm{un}} = \begin{bmatrix} 2\nu(r, \sigma_1, +1) - 1 \\ 2\nu(r, \sigma_2, +1) - 1 \\ 2\nu(r, \sigma_3, +1) - 1 \end{bmatrix}.$$

Note that the above estimator maps the set of measurement outcomes to the set of Bloch vectors while that presented in section 2 maps onto the set of density matrices. The observables are also not the same for the two estimators: the above one uses the Pauli matrix σ_3 instead of Z_{ii}.

Example 3. Assume that the observables

$$A(i) = \mathbf{u}(i) \cdot \sigma \qquad (1 \leqslant i \leqslant 3), \qquad \sigma = (\sigma_1, \sigma_2, \sigma_3)$$

are measured in the true state

$$\rho_\theta = \frac{1}{2}(I + \theta \cdot \sigma) = \frac{1}{2}\begin{bmatrix} 1+\theta_3 & \theta_1 - \mathrm{i}\theta_2 \\ \theta_1 + \mathrm{i}\theta_2 & 1-\theta_3 \end{bmatrix}, \tag{12}$$

where $\mathbf{u}(1)$, $\mathbf{u}(2)$ and $\mathbf{u}(3)$ are unit vectors in $\mathbb{R}^3$. The spectral decomposition of $A(i)$ is

$$1 \cdot \tfrac{1}{2}(I + \mathbf{u}(i) \cdot \sigma) + (-1) \cdot \tfrac{1}{2}(I - \mathbf{u}(i) \cdot \sigma)$$

and

$$p_i := \operatorname{Prob}(A(i) = 1) = \frac{1 + \mathbf{u}(i) \cdot \theta}{2}.$$

If the measurements are performed r times, then $\operatorname{Prob}(A(i) = +1)$ is estimated by the relative frequency $\nu(r, A(i), +1)$ of the outcome +1. The equations

$$\nu(r, A(i), +1) = \frac{1 + \mathbf{u}(i) \cdot \hat{\theta}}{2} \qquad (1 \leqslant i \leqslant 3)$$

should be solved to find an estimate. The solution is

$$\hat{\theta} = 2T^{-1}(\nu(r, A(1), +1), \nu(r, A(2), +1), \nu(r, A(3), +1))^t - T^{-1}\mathbf{1} \tag{13}$$

where ^{t} denotes the transpose (of a row vector), $\mathbf{1} = (1, 1, 1)^t$ and the matrix T is

$$T = \begin{bmatrix} \mathbf{u}(1)_1 & \mathbf{u}(1)_2 & \mathbf{u}(1)_3 \\ \mathbf{u}(2)_1 & \mathbf{u}(2)_2 & \mathbf{u}(2)_3 \\ \mathbf{u}(3)_1 & \mathbf{u}(3)_2 & \mathbf{u}(3)_3 \end{bmatrix}.$$

In particular, if each of the three measurements is performed once and the result is $\varepsilon = (\varepsilon_1, \varepsilon_2, \varepsilon_3)^t$, then the unconstrained estimate (in Bloch vector form) is

$$\Phi_3^{\mathrm{un}}(\varepsilon) = 2T^{-1}\varepsilon - T^{-1}\mathbf{1}.$$

Similarly to (13), we have

$$\theta = 2T^{-1}p - T^{-1}\mathbf{1}. \tag{14}$$

The mean quadratic error matrix is the expectation of

$$\begin{aligned}\big(\big(\Phi_3^{\mathrm{un}}(\varepsilon) - \theta\big)\big(\Phi_3^{\mathrm{un}}(\varepsilon) - \theta\big)^t\big) &= 4(T^{-1}\varepsilon - T^{-1}p)(T^{-1}\varepsilon - T^{-1}p)^t \\ &= 4T^{-1}((\varepsilon - p)(\varepsilon - p)^t)(T^{-1})^*\end{aligned}$$

and the computation yields

$$V_3^{\mathrm{gen}}(\theta) = 4T^{-1}\begin{bmatrix} 1 - (\mathbf{u}(1)\cdot\theta)^2 & 0 & 0 \\ 0 & 1 - (\mathbf{u}(2)\cdot\theta)^2 & 0 \\ 0 & 0 & 1 - (\mathbf{u}(3)\cdot\theta)^2 \end{bmatrix}(T^{-1})^*. \tag{15}$$

When each measurement is performed r times, then

$$V_n^{\mathrm{gen}}(\theta) = \frac{3}{n}V_3^{\mathrm{gen}}(\theta),$$

where $n = 3r$. If the observables σ_1, σ_2 and σ_3 are measured, then

$$V_n^{\mathrm{comp}}(\theta) = \frac{3}{n}\begin{bmatrix} 1 - \theta_1^2 & 0 & 0 \\ 0 & 1 - \theta_2^2 & 0 \\ 0 & 0 & 1 - \theta_3^2 \end{bmatrix}. \tag{16}$$

Theorem 3. *In the context of the previous example, the determinant of the average mean quadratic error matrix is the smallest, if the vectors* $\mathbf{u}(1)$, $\mathbf{u}(2)$ *and* $\mathbf{u}(3)$ *are orthogonal, that is, the observables* $A(1)$, $A(2)$ *and* $A(3)$ *are complementary.*

Proof. On the parameter space, the Bloch ball, we consider the normalized Lebesgue measure. (Any rotationally invariant measure may be considered and gives similar result.) Since

$$\begin{aligned}\int V_n^{\mathrm{gen}}(\theta)\,\mathrm{d}\theta &= T^{-1}\left(I - \int \mathrm{Diag}((\mathbf{u}(1)\cdot\theta)^2, (\mathbf{u}(2)\cdot\theta)^2, (\mathbf{u}(2)\cdot\theta)^2)\,\mathrm{d}\theta\right)(T^{-1})^* \\ &= C(T^*T)^{-1}\end{aligned}$$

with some positive constant C, the determinant is minimal if $\mathrm{Det}(T^*T) = (\mathrm{Det}\,T)^2$ is maximal. $\mathrm{Det}\,T$ is the volume of the parallelepipedone determined by the three vectors $\mathbf{u}(1)$, $\mathbf{u}(2)$ and $\mathbf{u}(3)$, and it is maximal when they are orthogonal. □

The content of the theorem is similar to the result of [14]; however, in the approach of Wootters and Fields the mean quadratic error was not minimized but the information gain was maximized. The complementary (or unbiased) measurements are optimal from both viewpoints. The optimality of the complementarity has been the motivation to study this concept and to extend it to subsystems [11, 12].

Example 4. Let $\sigma_i = P_i - Q_i$ be the spectral decomposition and let

$$F_i = \frac{P_i}{3} \qquad \text{and} \qquad F_{i+3} = \frac{Q_i}{3} \qquad (1 \leqslant i \leqslant 3)$$

be a POVM, denoted by A^{stand}. The corresponding measurement is sometimes called *standard qubit tomography* [13] and it has six outcomes with probabilities

$$p_i = \frac{1+\theta_i}{6}, \qquad p_{i+3} = \frac{1-\theta_i}{6} \qquad (1 \leqslant i \leqslant 3).$$

It is important to note that (opposed to the previous example) there is only one kind of measurement in this case, i.e. $n = r$.

The appropriate unconstrained and density matrix valued state estimate

$$\Phi_1^{\text{stand}}(i) = \tfrac{1}{2}(I + 3\sigma_i) = -I + 3P_i, \qquad \Phi_1^{\text{stand}}(i+3) = \tfrac{1}{2}(I - 3\sigma_i) = -I + 3Q_i$$

is unbiased. The symbols i stands for the different outcomes of the measurement corresponding to F_i and F_{i+3} $(1 \leqslant i \leqslant 3)$.

The estimator can also be given in Bloch vector form for n measurements as

$$\Phi_n^{\text{stand}} = 3\sum_{j=1}^{6} \nu(n, A^{\text{stand}}, j) e_j,$$

where

$$\begin{aligned} e_1 &= (1,0,0)^t, & e_4 &= -e_1, \\ e_2 &= (0,1,0)^t, & e_5 &= -e_2, \\ e_3 &= (0,0,1)^t, & e_6 &= -e_3 \end{aligned}$$

and $\nu(n, A^{\text{stand}}, j)$ denotes the relative frequency of the jth outcome of the POVM A^{stand}.

The quadratic error matrix for n-independent measurements is

$$V_n^{\text{stand}}(\theta) = \frac{1}{n}\begin{bmatrix} 3-\theta_1^2 & -\theta_1\theta_2 & -\theta_1\theta_3 \\ -\theta_1\theta_2 & 3-\theta_2^2 & -\theta_2\theta_3 \\ -\theta_1\theta_3 & -\theta_2\theta_3 & 3-\theta_3^2 \end{bmatrix}. \tag{17}$$

Proposition 1. *In the context of the previous example, the complementary measurement is more efficient than the standard one, i.e. its mean quadratic error matrix is smaller.*

Proof. To compare the efficiency of the standard measurement and the complementary measurement, we study the mean quadratic error matrices (16) and (17). The difference $V_n^{\text{stand}}(\theta) - V_n^{\text{comp}}(\theta)$ has the form

$$\begin{aligned} &\frac{1}{n}\begin{bmatrix} 3-\theta_1^2 & -\theta_1\theta_2 & -\theta_1\theta_3 \\ -\theta_1\theta_2 & 3-\theta_2^2 & -\theta_2\theta_3 \\ -\theta_1\theta_3 & -\theta_2\theta_3 & 3-\theta_3^2 \end{bmatrix} - \frac{3}{n}\begin{bmatrix} 1-\theta_1^2 & 0 & 0 \\ 0 & 1-\theta_2^2 & 0 \\ 0 & 0 & 1-\theta_3^2 \end{bmatrix} \\ &\qquad = \frac{1}{n}\begin{bmatrix} 2\theta_1^2 & -\theta_1\theta_2 & -\theta_1\theta_3 \\ -\theta_1\theta_2 & 2\theta_2^2 & -\theta_2\theta_3 \\ -\theta_1\theta_3 & -\theta_2\theta_3 & 2\theta_3^2 \end{bmatrix} = \frac{1}{n}\begin{bmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{bmatrix} \circ \left(\begin{bmatrix} \theta_1 \\ \theta_2 \\ \theta_3 \end{bmatrix} \cdot [\theta_1\theta_2\theta_3] \right), \end{aligned}$$

where $\circ$ stands for the Hadamard (or Schur) product. Since the Hadamard product of two positive semidefinite matrices is positive semidefinite, we have $V_n^{\text{stand}}(\theta) \geqslant V_n^{\text{comp}}(\theta)$. The complementary measurement is more effective, than the standard one. □

Example 5. Consider the following Bloch vectors

$$a_1 = \frac{1}{\sqrt{3}}(1,1,1), \qquad a_2 = \frac{1}{\sqrt{3}}(1,-1,-1),$$
$$a_3 = \frac{1}{\sqrt{3}}(-1,1,-1), \qquad a_4 = \frac{1}{\sqrt{3}}(-1,-1,1),$$

and form the positive operators

$$F_i = \tfrac{1}{4}(\sigma_0 + a_i \cdot \sigma) \qquad (1 \leqslant i \leqslant 4). \tag{18}$$

They determine a measurement, $\sum_{i=1}^{4} F_i = I$. The probability of the outcome i is

$$p_i = \operatorname{Tr} F_i \rho_\theta = \tfrac{1}{4}(1 + a_i \cdot \theta).$$

The above POVM is called *minimal qubit tomography* by Rehácek, Englert and Kaszlikowski [13] and in the following it is denoted by $A^{\min}$. In this case $n = r$, again.

The matrix-valued estimator

$$\Phi_1^{\min}(i) = -\sigma_0 + 6F_i \qquad (1 \leqslant i \leqslant 4).$$

is unbiased. If the measurement is performed n times, then the average (written in Bloch vector-valued form) is

$$\Phi_n^{\min} = 3\sum_{i=1}^{4} \nu(n, A^{\min}, i)a_i \tag{19}$$

where $\nu(n, A^{\min}, i)$ is the relative frequency of the ith outcome from the n measurements of $A^{\min}$. The mean quadratic error matrix is

$$V_n^{\min}(\theta) = \frac{1}{n}\begin{bmatrix} 3-\theta_1^2 & \sqrt{3}\theta_3 - \theta_1\theta_2 & \sqrt{3}\theta_2 - \theta_1\theta_3 \\ \sqrt{3}\theta_3 - \theta_1\theta_2 & 3-\theta_2^2 & \sqrt{3}\theta_1 - \theta_2\theta_3 \\ \sqrt{3}\theta_2 - \theta_1\theta_3 & \sqrt{3}\theta_1 - \theta_2\theta_3 & 3-\theta_3^2 \end{bmatrix}. \tag{20}$$

Unfortunately, the above matrix is not comparable with the mean quadratic error matrix (16), i.e. their difference is indefinite. However, $\operatorname{Tr} V_n^{\text{comp}} \leqslant \operatorname{Tr} V_n^{\min}$.

5. Conclusion

The estimation of the density matrix of a k-level quantum system is studied in this paper. The essential ingredients of an estimation scheme are identified. Those are the parametrization of the density operator ρ, the observables to be measured, and the estimator mapping the measured values to an estimate of the density operator. The considered parametrization is given by the real and imaginary part of the entries, and they are estimated by independent measurements. A special set of commuting observables is defined in order to obtain measured values that are classical random variables.

The unconstrained estimate gives a matrix which may not be positive definite and the constrained estimate is the closest density matrix with respect to the Hilbert–Schmidt distance. The constrained estimate is given by a simple procedure starting with the diagonalization of the unconstrained one.

It is established that the properties of the estimation procedure depend very much on the invertibility of the true state. In case of an invertible true state, the unconstrained estimate becomes proper relatively fast. It has been found that for pure states the unconstrained estimates, that are self-adjoint by construction, may not be positive semidefinite and this requires to apply a regularization called constrained estimation procedure.

The estimation procedures carried out by different estimators are compared on the basis of the biasedness of the estimates and their mean quadratic error matrices. In particular, several estimation schemes are compared for the unknown state of a qubit when a single qubit is measured at a time, and its density matrix is parametrized using the Bloch vector. It is shown that the average mean quadratic error matrix is the smallest if the applied observables are complementary. The results are illustrated by computer simulations.

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