

Efficient quantum tomography needs complementary and symmetric measurements

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Abstract

In this study the determinant of the average quadratic error matrix is used as the measure of state estimation efficiency. Minimizing this quantity gives us the optimal measurements in different scenarios. We present applications when von Neumann measurements or a single POVM are used, when there is no known information or a part of the parameters of the state is given. Under some restrictions the optimality is found for n -level systems. The optimal measurements have some complementary relation to each other and to the available data, moreover, symmetric informationally complete systems appear, containing a new, conditional version.

Key words and phrases: experiment design, state estimation, complementarity, measurement, quadratic error, qubit, symmetric informationally complete POVM.

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1 Introduction

State estimation or tomography is a fundamental problem in the field of quantum information theory and it can be considered as one of the foundational issues of quantum mechanics [4, 17]. The topic of quantum tomography consists of methods which reconstruct the state of the system under investigation using repeated measurements of a set of observables. The problem may be traced back to the seventies [11], the interest in a thorough mathematical analysis of the quantum state estimation procedures has been flourishing recently [2, 10, 13, 25].

In statistics the accuracy of the estimation can be quantified by the quadratic error matrix. The matrices are typically not comparable by the positive semi-definiteness, hence if different estimation schemes are compared, the determinant of mean quadratic error matrix can be used instead. This approach can be found in references [19, 20], their main result was that the complementary von Neumann measurements are optimal. A more general context appears in [3], which is much closer to our approach. The concept of complementarity was extended to quantum subsystems in [21] and the case of two qubits has a detailed analysis in [14, 24]. When all parameters of the density matrix are obtained from a single measurement, then a symmetric informationally complete POVM appears [26]. A similar result was obtained earlier by Wootters and Fields [29] for von Neumann measurements and by Scott [28] for POVMs, but optimality had a different formulation in both cases.

Some a priori information about the state can be given in various ways, for example one can minimize the relative entropy to an a priori given state, resulting in a bias toward that state [15]. The most popular subject in this field is state discrimination: when we know that the system is one of several given states and we should figure out which one [5]. Beside knowing the possible states we can have an a priori probability distribution on the true state, too. This idea was used in [6] to obtain the optimal phase estimation. The given states do not construct a discrete set, instead, they are searching among all pure states. Another continuous subset is used in [12], where we know that the state to estimate is a convex combination of two given states. In our setup we know that the state is on a given subset of the whole state space (this can be the whole state space itself) and assume an arbitrary unitarily invariant a priori probability distribution to be known.

We use the determinant of the average quadratic error matrix as a figure of merit in state estimation setup; the average is taken over the unitarily invariant states. This quantity relies on purely classical statistics, therefore it is much easier to compute than, e.g., quantum Fisher information, but still reproduces the well-known quantum phenomena and even more. So it gives us a useful tool to find the optimal measurement setup for different quantum tomography problems. We examine the assumption that the unknown state is known on some complementary subalgebras, which practically means that one should restrict the area of integration. For our calculations we use a parametrization for both the density operators and the observables (we expand them

in a fixed basis that is orthonormal with respect to the Hilbert-Schmidt inner product), but we can see that the results are independent of this parametrization. To gain analytic results, some sort of symmetry is recommended but by using numerical methods we could overcome that and solve difficult problems efficiently.

Section 2 is a very short introduction, quantum states, measurements, state estimation, complementarity and symmetric measurements are overviewed. In Section 3, we give the motivation for using the determinant of the average covariance matrix by guiding through a simple example, and then give some useful remarks about this quantity. Then the optimization problem is solved for arbitrary dimensions under some restrictions. In Section 4 the complementarity of optimal von Neumann measurements is obtained. In Section 5 a single POVM is used for the measurement, then a symmetric informationally complete POVM appears. Finally, we investigate the asymmetrical case for POVMs too (Sec. 6) and draw conclusions (Sec. 7).

2 Basic concepts

In this section, we give a brief summary of the basic concepts appearing in the present paper (for further details, see [4, 17]).

$\rho \in M_n(\mathbb{C})$ is an n -dimensional quantum state if

$$\rho \geq 0 \quad \text{and} \quad \text{Tr } \rho = 1. \quad (1)$$

We will use a basis of self-adjoint matrices to obtain a parametrization of these density matrices. In the qubit case, we use the Pauli matrices as a basis, i.e., the Bloch parametrization:

$$\rho = \frac{1}{2} \left(I + \sum_{i=1}^3 \theta_i \sigma_i \right) = \frac{1}{2} (I + \theta \cdot \sigma) = \frac{1}{2} \begin{bmatrix} 1 + \theta_3 & \theta_1 - i\theta_2 \\ \theta_1 + i\theta_2 & 1 - \theta_3 \end{bmatrix}. \quad (2)$$

In this case the whole state space of quantum states can be described using the Bloch vector: $\theta = (\theta_1, \theta_2, \theta_3)$ and the conditions in (1) are simply converted into $\theta_1^2 + \theta_2^2 + \theta_3^2 \leq 1$.

For the n -dimensional case we use the following parametrization:

$$\rho = \frac{1}{n} (I + \theta \cdot \sigma)$$

where $\theta \in \mathbb{R}^{n^2-1}$ is the generalized Bloch vector, $\theta \cdot \sigma = \sum_j \theta_j \sigma_j$ and $\{\sigma_j : 1 \leq j \leq n^2 - 1\}$ are generalized Pauli matrices, which form an orthonormal basis on the self-adjoint traceless matrices: $\sigma_i = \sigma_i^*$, $\text{Tr } \sigma_i = 0$ and $\text{Tr } \sigma_i \sigma_j = \delta_{i,j}$. An example for the 3-dimensional case are the multiples of Gell-Mann matrices.

A positive operator-valued measure (POVM) can in this framework be described as a set of matrices:

$$E = \{E_1, E_2, \dots, E_k\} \quad \text{with} \quad \sum_{i=1}^k E_i = I, E_i > 0.$$

Von Neumann measurements can be described as a POVM with two components and projective elements: $\{P_1, I - P_1\}$.

Having a quantum state ρ and a POVM E , the probability of obtaining an outcome related to the POVM element E_i is:

$$p_i = \text{Tr}(\rho E_i). \quad (3)$$

If we have m samples of the state ρ and we measure E on each copy independently, then let ν_i be the relative frequency of measuring the i th outcome. If m is a large number, then ν_i will be close to p_i , and if we know the POVM (because we set it), then we can make an estimation on ρ from (3) by using ν_i instead of p_i . A simple state estimation problem is described in detail in Section 3.

The heuristic concept of complementarity was born together with quantum theory. A mathematical definition is due to Accardi [1] and Kraus [9]. Let \mathcal{H} be an n -dimensional Hilbert space. Let the observables A and B have eigenvectors e_1, e_2, \dots, e_n and f_1, f_2, \dots, f_n which are orthonormal bases, they are complementary if

$$|\langle e_i, f_j \rangle|^2 = \frac{1}{n} \quad (1 \leq i, j \leq n). \quad (4)$$

If this condition holds then the two bases are also called mutually unbiased. An overview about complementarity can be found in [22] and details are in [21, 24].

Complementarity can be generalized to the case of POVMs. The POVMs $\{E_1, E_2, \dots, E_k\}$ and $\{F_1, F_2, \dots, F_m\}$ are complementary if

$$\text{Tr} E_i F_j = \frac{1}{n} \text{Tr} E_i \text{Tr} F_j \quad (1 \leq i \leq k, \quad 1 \leq j \leq m). \quad (5)$$

This is equivalent to the orthogonality of the traceless parts:

$$E_i - \frac{\text{Tr} E_i}{n} I \quad \perp \quad F_j - \frac{\text{Tr} F_j}{n} I,$$

so we will use the expression quasi-orthogonal, when we use this property of complementary operators.

The concept can be extended to subalgebras $\mathcal{A}_1, \mathcal{A}_2 \subset M_n(\mathbb{C})$. \mathcal{A}_1 and \mathcal{A}_2 are complementary if $A_1 \in \mathcal{A}_1$ and $A_2 \in \mathcal{A}_2$ are quasi-orthogonal (that is, the traceless part of matrices are orthogonal).

An orthonormal basis corresponds to the subalgebra of operators which are diagonal in this basis. Such a subalgebra is maximal Abelian, it will be called M-subalgebra.

A symmetric informationally complete POVM $\{E_i : 1 \leq i \leq k\}$ of an n -level system is described by a set of projections P_i ($1 \leq i \leq k$) such that

$$\sum_{i=1}^k P_i = \lambda I \quad \text{and} \quad \text{Tr } P_i P_j = \mu \quad (i \neq j), \quad (6)$$

where $k = n^2$, $\lambda = n$, $\mu = 1/(n+1)$ and all projections are rank-one, see [26, 27]. The existence of a symmetric informationally complete POVM (SIC POVM) is not known for every dimension n .

In this paper $k < n^2$ case will also appear, when some parameters are already known, we need to estimate fewer parameters, i.e., fewer elements in POVM are needed to make a full reconstruction. If they fulfill condition (6) with some constants and the P_i -s are complementary to the known subalgebra, then we call them conditional symmetric informationally complete POVM toward the known $n^2 - k$ parameters, because they are informationally complete only if we use the condition that we want to discriminate the states only in the unknown directions. They include the case of SIC-POVMs as a special case when no parameters are known. The existence of such a POVM can be a fundamental question in different quantum tomography problems.

3 The determinant of the average covariance matrix

Suppose that we have a qubit and some of the three parameters θ_1 , θ_2 and θ_3 are known and the unknown parameters will be estimated. For example, let us assume that θ_1 and θ_2 are known and we want to estimate θ_3 . The assumption means that the reduced state is known on the M-subalgebras generated by σ_1 and σ_2 , respectively. They are complementary subalgebras and the M-subalgebra generated by σ_3 is complementary to both. A projection of a von Neumann measurement

$$E = \frac{1}{2} (I + \lambda \cdot \sigma)$$

is used to estimate θ_3 from the result of several measurements, where $\lambda_1^2 + \lambda_2^2 + \lambda_3^2 = 1$. The expected value is

$$\text{Tr } \rho E = \frac{1}{2} \left(1 + \sum_{i=1}^3 \theta_i \text{Tr } \sigma_i E \right) = \frac{1}{2} (1 + \langle \theta, \lambda \rangle)$$

and we have

$$\theta_3 \text{Tr } \sigma_3 E = 2 \text{Tr } \rho E - \left(1 + \sum_{i=1}^2 \theta_i \text{Tr } \sigma_i E \right).$$

Let us denote by ν the random outcome of the measurement of E , the expected value is $p = \text{Tr } \rho E$ and it is Bernoulli distributed. The natural unbiased estimate of θ_3 is

$$\hat{\theta}_3 = \frac{1}{\text{Tr } \sigma_3 E} \left(2\nu - 1 - \sum_{i=1}^2 \theta_i \text{Tr } \sigma_i E \right). \quad (7)$$

The variance is

$$\text{Var}(\hat{\theta}_3) = \frac{4p(1-p)}{\lambda_3^2} = \frac{1 - \langle \lambda, \theta \rangle^2}{\lambda_3^2}. \quad (8)$$

We want to argue that the optimal estimate corresponds to the projection $\lambda_1 = \lambda_2 = 0$, $\lambda_3 = \pm 1$, i.e. measuring in the unknown direction. This estimator has the variance $1 - \theta_3^2$. However, the inequality

$$\frac{1 - \langle \lambda, \theta \rangle^2}{\lambda_3^2} \geq 1 - \theta_3^2 \quad (9)$$

is not true in general, for example $\lambda = \theta$ is possible for pure states and then the left-hand side is zero. So if we want to minimize $\text{Var}(\hat{\theta}_3)$, it is not true that $\frac{I+\sigma_3}{2}$ is the best observable.

Since θ_1, θ_2 are given, the only unitarily invariant vector to $(\theta_1, \theta_2, \theta_3)$ is $(\theta_1, \theta_2, -\theta_3)$, if we take the average of the left hand side of (9) on these states we obtain

$$\langle \text{Var}(\hat{\theta}_3) \rangle = \frac{1}{2} \cdot \frac{1 - (\lambda_1 \theta_1 + \lambda_2 \theta_2 + \lambda_3 \theta_3)^2}{\lambda_3^2} + \frac{1}{2} \cdot \frac{1 - (\lambda_1 \theta_1 + \lambda_2 \theta_2 - \lambda_3 \theta_3)^2}{\lambda_3^2}.$$

We can solve the minimization problem

$$\langle \text{Var}(\hat{\theta}_3) \rangle \rightarrow \min, \quad \lambda_1^2 + \lambda_2^2 + \lambda_3^2 = 1$$

using the Schwarz inequality, and get that in the optimal case $\lambda_1 = \lambda_2 = 0$, $\lambda_3 = \pm 1$. Thus, the measurement of $\frac{I+\sigma_3}{2}$ is optimal indeed, yet only in the average sense.

Note that in (7) ν has Bernoulli distribution, with $p(1-p)$ variance. If m measurements are performed, we will have $\nu = (\nu_1 + \nu_2 + \dots + \nu_m)/m$, where ν_i is the outcome of the i -th measurement. Then the variance will be $\frac{mp(1-p)}{m^2} = \frac{1}{m}p(1-p)$, so we can conclude that if we have multiple measurements the variance changes only by a constant factor, hence the minimization problem remains unaffected.

In the following sections, we will always use the same kind of naturally derived estimators; one can prove that those are unbiased and efficient. We should also always bear in mind that if we have only a few measurements, we can easily get a Bloch-vector as a result of the estimation, which does not satisfy the positivity condition in (1). But in practical cases, we have many measurements, hence the law of large numbers ensures us that the estimator will give a state near the original one, and the probability of getting a physically impossible state (a density matrix with at least one

negative eigenvalue) will converge to zero exponentially, due to the large deviation theory. That is why we do not have to deal with any physical restrictions, even if we calculate the variance only for one measurement in each case.

If we have multiple parameters, we can still get a multidimensional estimator from the measurement outcomes, but in that case, a covariance matrix will take the role of the variance. The average covariance matrix can be calculated by taking the piecewise average of the elements, but since the matrices are not comparable in general, we need an $M_n(\mathbb{C}) \rightarrow \mathbb{R}$ function which gives us a number as the objective function to minimize. After examining some candidates we concluded that the best choice is to take the determinant of the matrix and that this needs to be done after the averaging process, so we have the following optimization problem:

$$\det \langle Cov(\hat{\theta}) \rangle \rightarrow \min,$$

where $\hat{\theta}$ is the estimator of the unknown parameters. This way we obtain an easily calculable quantity, and by solving the minimization problem, the optimal measurements.

If we want to take the average of this covariance matrix on the whole state space, we have to give a unitarily invariant measure on the state space. On the other hand, if we integrate on the unitarily invariant states of an initial state with respect to the normalized Haar measure and the minimum is independent of the initial state, we get optimal measurements independently from the (unitarily invariant) probability measure. Thus, we can obtain a stronger result than we would by using a particular measure.

Finally, let us note that using a POVM instead of von Neumann measurements is not a crucial difference. If there are n unknown parameters, we need to have n independent positive operators in the POVM. We only have the restriction $\sum E_i = I$, so $n + 1$ operators are sufficient and we can construct the estimator from the outcomes related to the first n components. The only difference is that in this case, the n outcomes would not be independent, off-diagonal elements appear in the covariance matrix, too.

4 The optimal von Neumann measurement

The n -level quantum system is described by the algebra $M_n(\mathbb{C})$. Consider the following decomposition

$$M_n(\mathbb{C}) = \mathbb{C}I \oplus \mathcal{A} \oplus \mathcal{B},$$

where \mathcal{A} and \mathcal{B} are linear subspaces and orthogonality is defined with respect to the Hilbert-Schmidt inner product $\langle A, B \rangle = \text{Tr } A^* B$.

A state has the density matrix

$$\rho = I/n + \rho_{\mathcal{A}} + \rho_{\mathcal{B}}. \tag{10}$$

We assume that the component $\rho_{\mathcal{B}}$ should be estimated. Let the dimension of \mathcal{B} be k . The positive contractions E^1, \dots, E^k are used for independent measurements (on several identical copies of the n -level system): A measurement corresponds to the POVM $\{E^i, I - E^i\}$. These operators have the expansion

$$E^i = e_i I + E_{\mathcal{A}}^i + E_{\mathcal{B}}^i \quad (1 \leq i \leq k). \quad (11)$$

The expectations are

$$p_i := \text{Tr } \rho E^i = e_i + \text{Tr } \rho_{\mathcal{A}} E_{\mathcal{A}}^i + \text{Tr } \rho_{\mathcal{B}} E_{\mathcal{B}}^i \quad (1 \leq i \leq k).$$

We fix an orthonormal basis F_1, \dots, F_k in \mathcal{B} . The unknown component has the expansion

$$\rho_{\mathcal{B}} = \theta_1 F_1 + \dots + \theta_k F_k,$$

where $\theta = (\theta_1, \dots, \theta_k)$ are the parameters to be estimated. Similarly,

$$E_{\mathcal{B}}^i = e_{i1} F_1 + e_{i2} F_2 + \dots + e_{ik} F_k$$

is an orthogonal expansion.

The estimates $\hat{\theta}_i$ are solutions of the equations

$$\varepsilon_i = e_i + \text{Tr } \rho_{\mathcal{A}} E_{\mathcal{A}}^i + \sum_{j=1}^k e_{ij} \hat{\theta}_j,$$

where ε_i is the random result of the i th measurement, $1 \leq i \leq k$. In another form

$$\begin{bmatrix} \varepsilon_1 \\ \vdots \\ \varepsilon_k \end{bmatrix} = \begin{bmatrix} e_1 \\ \vdots \\ e_k \end{bmatrix} + \begin{bmatrix} \text{Tr } \rho_{\mathcal{A}} E_{\mathcal{A}}^1 \\ \vdots \\ \text{Tr } \rho_{\mathcal{A}} E_{\mathcal{A}}^k \end{bmatrix} + \begin{bmatrix} e_{11} & \cdots & e_{1k} \\ \vdots & \ddots & \vdots \\ e_{k1} & \cdots & e_{kk} \end{bmatrix} \hat{\theta}^t$$

or in a different notation

$$\begin{bmatrix} \varepsilon_1 \\ \vdots \\ \varepsilon_k \end{bmatrix} = \begin{bmatrix} e_1 + \text{Tr } \rho_{\mathcal{A}} E_{\mathcal{A}}^1 \\ \vdots \\ e_k + \text{Tr } \rho_{\mathcal{A}} E_{\mathcal{A}}^k \end{bmatrix} + T \hat{\theta}^t,$$

where T is the $k \times k$ matrix from the previous formula. Therefore,

$$\hat{\theta}^t = T^{-1} \left(\begin{bmatrix} \varepsilon_1 \\ \vdots \\ \varepsilon_k \end{bmatrix} - \begin{bmatrix} e_1 + \text{Tr } \rho_{\mathcal{A}} E_{\mathcal{A}}^1 \\ \vdots \\ e_k + \text{Tr } \rho_{\mathcal{A}} E_{\mathcal{A}}^k \end{bmatrix} \right).$$

We have

$$\hat{\theta}^t - \theta^t = T^{-1} \left(\begin{bmatrix} \varepsilon_1 \\ \vdots \\ \varepsilon_k \end{bmatrix} - \begin{bmatrix} p_1 \\ \vdots \\ p_k \end{bmatrix} \right).$$

The quadratic error matrix is the expected value of

$$T^{-1} \begin{bmatrix} \varepsilon_1 - p_1 \\ \vdots \\ \varepsilon_k - p_k \end{bmatrix} [\varepsilon_1 - p_1, \dots, \varepsilon_k - p_k] (T^{-1})^t = T^{-1} \left[(\varepsilon_i - p_i)(\varepsilon_j - p_j) \right]_{i,j=1}^k (T^{-1})^t.$$

Due to the independence of the measurements the expected value of

$$\left[(\varepsilon_i - p_i)(\varepsilon_j - p_j) \right]_{i,j=1}^k$$

will be diagonal.

The random variables ε_i have Bernoulli distribution and their variance is

$$(1 - \text{Tr } \rho E^i) \text{Tr } \rho E^i.$$

We want to take the average:

$$\int (1 - \text{Tr } \rho E^i) \text{Tr } \rho E^i d\mu(\rho),$$

where we integrate on the unitarily invariant states, and μ is the corresponding normalized Haar measure. For the sake of simplicity, assume that the operators E^i have the same spectrum. Then the integral is constant: it does not depend on the actual E_i , so the average of the quadratic error matrix is

$$cT^{-1}(T^{-1})^t.$$

The determinant is minimal if the determinant of the matrix T is maximal. Geometrically, the determinant is the volume of the parallelepiped determined by the row vectors. To maximize the determinant, the row vectors should be long. This implies that $E_{\mathcal{A}}^i = 0$ in (11), since otherwise we could project E^i on to $\mathbb{C}I \oplus \mathcal{B}$, and still have the same elements in T . So we have

$$E^i = e + e_{i1}F_1 + \dots + e_{ik}F_k \quad (1 \leq i \leq k),$$

and then the determinant of the matrix

$$\begin{bmatrix} 1/n & 0 & \dots & 0 \\ e & e_{11} & \dots & e_{1k} \\ \vdots & \vdots & \ddots & \vdots \\ e & e_{k1} & \dots & e_{kk} \end{bmatrix}$$

is $\det T$. The angle of the first row and any other row is fixed. To have a large determinant the rows of T should be orthogonal. In this case, the operators E^1, \dots, E^k are quasi-orthogonal.

Theorem 1 *If the positive contractions E^1, \dots, E^k have the same spectrum, then the determinant of the average of the quadratic error matrix is minimal if the operators E^1, \dots, E^k are complementary to each other and to \mathcal{A} .*

Example 1 If two qubits are given and the reduced states of both qubits are known, then the ideal state estimation is connected to the observables

$$\sigma_{11}, \sigma_{22}, \sigma_{33}, \sigma_{12}, \sigma_{23}, \sigma_{31}, \sigma_{13}, \sigma_{21}, \sigma_{32},$$

where $\sigma_{ij} = \sigma_i \otimes \sigma_j$. □

5 The optimal POVM

Once again we are in the n -dimensional case, but in this section we will use POVMs for state estimation. Assume that $\mathcal{A} = \{0\}$, which means that all parameters are unknown. Then

$$E_i = e_i I + E_{\mathcal{B}}^i = e_i(I + f_i \cdot \sigma) \quad (1 \leq i \leq n^2),$$

where $e_i \in \mathbb{R}$, $f_i \in \mathbb{R}^{n^2-1}$, $f_i \cdot \sigma = \sum_j f_{ij} \sigma_j$ and $\{\sigma_j : 1 \leq j \leq n^2 - 1\}$ are generalized Pauli matrices, $\text{Tr } \sigma_i = 0$, $\text{Tr } \sigma_i^2 = 1$, $\text{Tr } \sigma_i \sigma_j = 0$. The positivity condition of E_i is not known, but we have a necessary condition:

Lemma 1 *If the $n \times n$ matrix $I + g \cdot \sigma$ is positive, then $\sum_k g_k^2 \leq n^2 - n$. If $\sum_k g_k^2 = n^2 - n$, then $I + g \cdot \sigma = nP$ with a projection P of rank 1.*

Proof. $A = g \cdot \sigma$ is self-adjoint, $\text{Tr } A = 0$. Let $\lambda_1, \lambda_2, \dots, \lambda_n$ be the eigenvalues of A . Then

$$\sum_{k=1}^{n^2-1} g_k^2 = \text{Tr } A^2 = \sum_{t=1}^n \lambda_t^2.$$

Since $\sum_{t=1}^n \lambda_t = 0$ from $\text{Tr } A = 0$ and $\lambda_t \geq -1$ from $I + A \geq 0$, we have the upper bound. Namely, $\sum_{t=1}^n \lambda_t^2$ is maximal, if $\lambda_1, \lambda_2, \dots, \lambda_n$ is a permutation of the numbers $-1, -1, \dots, -1, n-1$. In this case $I + A$ has eigenvalues $0, 0, \dots, 0, n$, so it is a multiple of a projection. □

The computations are similar to the von Neumann case. The probabilities of different outcomes are

$$\begin{bmatrix} p_1 \\ \vdots \\ p_d \end{bmatrix} = \begin{bmatrix} e_1 \\ \vdots \\ e_d \end{bmatrix} + T \begin{bmatrix} \theta_1 \\ \vdots \\ \theta_d \end{bmatrix}$$

where $d = n^2 - 1$ and $T = (e_1, e_2, \dots, e_d)^T (f_1, f_2, \dots, f_d)$ dyadic matrix.

If $\nu_1, \nu_2, \dots, \nu_d$ are the relative frequencies of the outcomes (of different measurements on identical copies), then the estimator is

$$\begin{bmatrix} \hat{\theta}_1 \\ \vdots \\ \hat{\theta}_d \end{bmatrix} = T^{-1} \begin{bmatrix} \nu_1 - e_1 \\ \vdots \\ \nu_d - e_d \end{bmatrix}. \quad (12)$$

The mean quadratic error matrix is

$$V(\theta) = T^{-1} W (T^{-1})^*$$

with W denoting the covariance matrix of the random variables $\nu_1, \nu_2, \dots, \nu_d$. These are multinomially distributed, so

$$W = \begin{bmatrix} p_1(1-p_1) & -p_1p_2 & \dots & -p_1p_d \\ -p_1p_2 & p_2(1-p_2) & \dots & -p_2p_d \\ \vdots & \vdots & \dots & \vdots \\ -p_1p_d & -p_2p_d & \dots & p_d(1-p_d) \end{bmatrix}.$$

To obtain the average mean quadratic error matrix, we integrate W on the rotation invariant states H with respect to the normalized Haar measure μ . We have to calculate two types of integrals:

$$\begin{aligned} \int_H -p_i p_j d\mu(\theta) &= - \int_H (e_i + e_i \langle f_i, \theta \rangle) (e_j + e_j \langle f_j, \theta \rangle) d\mu(\theta) \\ &= - \int_H e_i e_j d\mu(\theta) - e_i e_j \int_H \langle f_i, \theta \rangle d\mu(\theta) - \int_H e_i e_j \langle f_j, \theta \rangle d\mu(\theta) - e_i e_j \int_H \langle f_i, \theta \rangle \langle f_j, \theta \rangle d\mu(\theta) \\ &= -e_i e_j + 0 + 0 - e_i e_j \alpha \langle f_i, f_j \rangle. \end{aligned}$$

The integrals in the middle are zeros because of the symmetry: $\int_H \langle v, \theta \rangle d\mu(\theta) = 0$. The last integral comes from:

$$\int_H \langle f_i, \theta \rangle \langle f_j, \theta \rangle d\mu(\theta) = \int_H \left(\sum_{\ell=1}^d f_{i,\ell} \theta_\ell \right) \left(\sum_{m=1}^d f_{j,m} \theta_m \right) d\mu(\theta) = \sum_{\ell=1}^d \left(\int_H \theta_\ell^2 d\mu(\theta) \right) f_{i,\ell} f_{j,\ell}$$

The quantity $\int_H \theta_\ell^2 d\mu(\theta)$ does not depend on ℓ : it is a constant α depending on the domain of the integration; this way we obtained the stated formula.

Similarly,

$$\int_H p_i(1-p_i) d\mu(\theta) = e_i(1-e_i) - e_i^2 \alpha \langle f_i, f_i \rangle,$$

so we can calculate the average quadratic error matrix:

$$F^{-1} \begin{bmatrix} e_1^{-1} - 1 - \alpha \langle f_1, f_1 \rangle & -1 - \alpha \langle f_1, f_2 \rangle & \dots & -1 - \alpha \langle f_1, f_d \rangle \\ -1 - \alpha \langle f_1, f_2 \rangle & e_2^{-1} - 1 - \alpha \langle f_2, f_2 \rangle & \dots & -1 - \alpha \langle f_2, f_d \rangle \\ \vdots & \vdots & \dots & \vdots \\ -1 - \alpha \langle f_1, f_d \rangle & -1 - \alpha \langle f_2, f_d \rangle & \dots & e_d^{-1} - 1 - \alpha \langle f_d, f_d \rangle \end{bmatrix} (F^{-1})^*,$$

where $F = (f_1, f_2, \dots, f_d)$.

The minimizer should be symmetric, hence $e_i = 1/n^2$, $\langle f_i, f_i \rangle = x$ and $\langle f_i, f_j \rangle = y$, if $i \neq j$, $i, j \leq n^2 - 1$. Then the determinant has the form A/B , where

$$A = (n^2 - \alpha(x - y))^{n^2-2} (1 - \alpha(x + (n^2 - 2)y))$$

and

$$B = (x - y)^{n^2-2} \cdot (x + (n^2 - 2)y)$$

Therefore, we minimize

$$\frac{A}{B} = \left(\frac{n^2}{x - y} - \alpha \right)^{n^2-2} \left(\frac{1}{x + (n^2 - 2)y} - \alpha \right). \quad (13)$$

We can also calculate the length of $f_{n^2} = - \sum_{i=1}^{n^2-1} f_i$:

$$\langle f_{n^2}, f_{n^2} \rangle = (n^2 - 1) \cdot (x + (n^2 - 2)y) \leq n^2 - n \quad (14)$$

where the latter inequality is the condition for positivity, see Lemma 1. On the other hand, we have the condition

$$x \leq n^2 - n. \quad (15)$$

If both inequalities were sharp, then (13) would not be minimal, because we could increase both x and y with a sufficiently small ε and then the value of (13) would be smaller. If the equality holds in (14), then the second term of (13) will be constant. So we want to have the difference of x and y as large as possible, hence x should be maximal (and then y is minimal). If the equality holds in (15), then from (14) we have $y \leq -(n^2 - n)/(n^2 - 1)$, and on this domain (13) has a negative derivative. So the minima are taken at

$$x = n^2 - n, \quad \text{and} \quad y = -\frac{n^2 - n}{n^2 - 1}.$$

Lemma 1 gives

$$E_i = \frac{1}{n^2} (I + f_i \cdot \sigma) = \frac{1}{n} P_i$$

with some projections P_i and

$$\text{Tr } P_i P_j = \frac{1}{n^2} \langle I + f_i \sigma, I + f_j \sigma \rangle = \frac{1}{n} + \frac{1}{n^2} y = \frac{1}{n+1}.$$

We arrived at a system (6). The following statement is obtained.

Theorem 2 *If a symmetric informationally complete system exists, then the optimal POVM is described by its projections P_i as $E_i = P_i/n$ ($1 \leq i \leq n^2$).*

For a qubit the existence of the symmetric informationally complete POVM is obvious, there are other known examples in lower dimensions, but in n dimensions the existence is not known.

6 A non-symmetrical qubit case for POVM

In contrast to the previous section where we constructed an optimal POVM without any information on the state, in the upcoming part we will show some special, non-trivial cases, where some information is known. This is a much harder task, therefore the achieved results are not so strong, nevertheless, it is even more interesting than the fully unknown case.

Let us assume, first of all, that we have a qubit: θ_1, θ_2 are not known, but θ_3 is given, so the density operator is only partially unknown. In this case the POVM will have three components $\{E_1, E_2, E_3\}$, the sufficient number of components to make the state estimation. Of course we can use a greater number of components but in that case the construction of the estimator is not trivial.

We use the parametrization

$$E_1 = a_0(I + a \cdot \sigma), \quad E_2 = b_0(I + b \cdot \sigma), \quad E_3 = c_0(I + c \cdot \sigma),$$

where $a_0, b_0, c_0 \in \mathbb{R}$, and a, b, c are vectors in \mathbb{R}^3 . From $E_1 + E_2 + E_3 = I$, we have $a_0 + b_0 + c_0 = 1$ and $a_0 a + b_0 b + c_0 c = 0$. The positivity conditions are:

$$0 \leq a_0, b_0, c_0 \quad \|a\|, \|b\|, \|c\| \leq 1.$$

Similarly to the previous section we should minimize a determinant of the form A/B , where

$$A = \det V, \quad B = \det^2 \begin{bmatrix} a_1 & a_2 \\ b_1 & b_2 \end{bmatrix} = \det \begin{bmatrix} \langle a^*, a^* \rangle & \langle a^*, b^* \rangle \\ \langle a^*, b^* \rangle & \langle b^*, b^* \rangle \end{bmatrix} =: \det C,$$

$$V = \begin{bmatrix} pa_0^{-1} - p^2 & -pq \\ -pq & qb_0^{-1} - q^2 \end{bmatrix} - \beta(1 - \theta_3^2) \begin{bmatrix} \langle a^*, a^* \rangle & \langle a^*, b^* \rangle \\ \langle a^*, b^* \rangle & \langle b^*, b^* \rangle \end{bmatrix} =: D - c \cdot C$$

$$p = 1 + a_3 \theta_3, \quad q = 1 + b_3 \theta_3, \quad a^* = (a_1, a_2), \quad b^* = (b_1, b_2),$$

where β is a constant depending on the particular unitarily invariant surface of the integration, $0 \leq \beta \leq 1$, so c is a given constant on interval $[0, 1 - \theta_3^2]$.

For the minimizer we can assume some symmetry conditions: $a_0 = b_0 = c_0 = \frac{1}{3}$, and we will minimize A and maximize B independently to obtain the optimum:

$$A = (d_{11} - c c_{11})(d_{22} - c c_{22}) - (d_{12} - c c_{12})^2 \rightarrow \min, \quad (16)$$

$$B = c_{11}c_{22} - (c_{12})^2 \rightarrow \max. \quad (17)$$

Let us suppose first that a_3 and b_3 are given (then the elements of D are constants) and we want to optimize the other variables.

We know that

$$\langle a + b, a + b \rangle = c_{11} + c_{22} + 2c_{12} + (a_3 + b_3)^2 \leq 1. \quad (18)$$

If $c_{12} \geq 0$, then from (18) we have $c_{11} + c_{22} \leq 1$, hence $B \leq 1/4$.

If $c_{12} < 0$, then B is maximal if c_{12} is maximal, from (18) we have an upper bound:

$$c_{12} \leq \frac{1 - (a_3 + b_3)^2 - c_{11} - c_{22}}{2}. \quad (19)$$

Substituting this upper bound in (17) we have to maximize it in c_{11} and c_{22} . Using derivation we can obtain that it is maximal if c_{11} and c_{22} are maximal:

$$c_{11} = a_1^2 + a_2^2 \leq 1 - a_3^2 \quad \text{and} \quad c_{22} = b_1^2 + b_2^2 \leq 1 - b_3^2. \quad (20)$$

Substituting this upper bound in (17) we get

$$B = \frac{3}{4} - a_3^2 - a_3 b_3 - b_3^2. \quad (21)$$

which is optimal if $a_3 = b_3 = 0$. Then $B = 3/4$, so it is a global optimum.

Lemma 2 *The following inequality is always true:*

$$d_{12} - c_{12} \leq 0$$

Proof. We have

$$d_{12} - c_{12} = -(1 + \theta_3 a_3)(1 + \theta_3 b_3) - c(a_1 b_1 + a_2 b_2).$$

Since $c \leq 1 - \theta_3^2$ and

$$a_1 b_1 + a_2 b_2 = \langle a^*, b^* \rangle \geq -\|a^*\| \|b^*\| \geq -\sqrt{1 - a_3^2} \sqrt{1 - b_3^2},$$

so it is enough to show that

$$(1 + \theta_3 a_3)(1 + \theta_3 b_3) \geq (1 - \theta_3^2) \sqrt{1 - a_3^2} \sqrt{1 - b_3^2}.$$

The right-hand side does not depend on the signs, the left-hand side is minimal if $\theta_3 a_3 \leq 0$, $\theta_3 b_3 \leq 0$, so it suffices to prove for positive a_3, b_3, θ_3 that

$$(1 - \theta_3 a_3)(1 - \theta_3 b_3) \geq (1 - \theta_3^2) \sqrt{1 - a_3^2} \sqrt{1 - b_3^2}.$$

This is true since from the Cauchy-Schwarz inequality follows that

$$a_3 \theta_3 + \sqrt{1 - a_3^2} \sqrt{1 - \theta_3^2} \leq 1 \quad \implies \quad 1 - a_3 \theta_3 \geq \sqrt{1 - a_3^2} \sqrt{1 - \theta_3^2},$$

and a similar statement is true for b_3 . □

Using this lemma, we get that A is minimal if c_{12} is maximal, and from there the solution is almost the same as in the previous case, we only have more complicated calculations. We substitute the upper bound (19) in to (16) and we can obtain that it is minimal if c_{11} and c_{22} are maximal. Using the bounds (20) we get for A a function of a_3 and b_3 ; using differentiation we can obtain that $a_3 = b_3 = 0$ gives the optimal solution here, too.

So in both cases we have equality in (20), so $\langle a^*, a^* \rangle = \langle b^*, b^* \rangle = 1$ and equality in (19), so $\langle a^*, b^* \rangle = -1/2$. Since $\|a\| = \|b\| = 1$,

$$\frac{3}{2}E_1 = \frac{1}{2}(I + a \cdot \sigma), \quad \frac{3}{2}E_2 = \frac{1}{2}(I + b \cdot \sigma)$$

are projections. We have $\|c\| = \|a + b\| = 1$ and this implies that $3E_3/2$ is a projection as well.

Theorem 3 *The optimal POVM for the unknown θ_1 and θ_2 can be described by projections P_i ($i = 1, 2, 3$):*

$$E_i = \frac{2}{3}P_i, \quad \sum_{i=1}^3 P_i = \frac{3}{2}I, \quad \text{Tr } \sigma_3 P_i = 0, \quad \text{Tr } P_i P_j = \frac{1}{4} \quad \text{for } i \neq j.$$

The optimal POVM is quasi-orthogonal to the subalgebra generated by σ_3 and symmetric in the other directions. This result is in some sense the combination of Theorem 1 and Theorem 2, with complementarity and symmetricalness both occurring in the same problem. The conditions of (6) are valid, but with different constants than in the SIC-POVM case.

It is an interesting question whether the existence of a conditional SIC-POVM in Theorem 3 is just a coincidence and it follows from the geometrical structure of $M_2(\mathbb{C})$, or there are such objects in higher dimensions. The following example solves this problem:

Example 2 Let the elements of a POVM in $M_3(\mathbb{C})$ be

$$E_1 = \frac{1}{7} \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}, \quad E_2 = \frac{1}{7} \begin{bmatrix} 1 & \varepsilon^6 & \varepsilon^2 \\ \varepsilon & 1 & \varepsilon^3 \\ \varepsilon^5 & \varepsilon^4 & 1 \end{bmatrix}, \quad E_3 = \frac{1}{7} \begin{bmatrix} 1 & \varepsilon^2 & \varepsilon^3 \\ \varepsilon^5 & 1 & \varepsilon \\ \varepsilon^4 & \varepsilon^6 & 1 \end{bmatrix},$$

$$E_4 = \frac{1}{7} \begin{bmatrix} 1 & \varepsilon^4 & \varepsilon^6 \\ \varepsilon^3 & 1 & \varepsilon^2 \\ \varepsilon & \varepsilon^5 & 1 \end{bmatrix}, \quad E_5 = \overline{E_2}, \quad E_6 = \overline{E_3}, \quad E_7 = \overline{E_4},$$

where $\varepsilon = \exp(2\pi i/7)$. This POVM fulfills the conditions in (6) with constants $k = 7$, $\lambda = 7/3$ and $\mu = 2/9$. Moreover it is quasi-orthogonal to diagonal matrices, so it is a conditional SIC-POVM with respect to the diagonal matrices. \square

It is still an open question, however, that exactly in which cases a conditional SIC-POVM exists. Furthermore, does it minimize the determinant of the average covariance matrix? The answer to the first question is definitely a difficult problem, because it contains the question of the existence of SIC-POVMs. Our conjecture to the second question is that conditional SIC-POVMs are optimal if they exist, and so they can play an important role in quantum information theory, but an exhaustive investigation exceeds the scope of this paper.

7 Discussion and conclusions

A density matrix $\rho \in M_n(\mathbb{C})$ has $n^2 - 1$ real parameters. If there are no known parameters, several two-valued POVMs $\{F_1, I - F_1\}$, $\{F_2, I - F_2\}$, \dots , $\{F_{n^2-1}, I - F_{n^2-1}\}$ or a single POVM $\{E_1, E_2, \dots, E_{n^2}\}$ are considered. The estimator can be constructed as a linear function of the outcomes, and since they are multinomially and binomially distributed, their variance can be calculated easily. By averaging them on the invariant states and taking the determinant of the average covariant matrix, we will get comparable results. The optimum is at the quasi-orthogonal measurements (Theorem 1) and at a symmetric informationally complete system (Theorem 2), respectively. If partial information is known, the concept is the same as previously, but as there are some known parameters, the domain of integration is restricted. From Theorem 1, it turns out that in the von Neumann case the optimal measurements are not only complementary to each other, but to the known subalgebras as well. For POVMs a qubit case is described in detail: conditionally symmetric informationally complete systems turn out to be optimal. The latter is a new concept, an example for the qutrit case is obtained too, further investigations are suggested.

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