Minimum error discrimination problem for pure qubit states

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The necessary and sufficient conditions for minimization of the generalized rate error for discriminating among \( N \) pure qubit states are reformulated in terms of Bloch vectors representing the states. For the direct optimization problem an algorithmic solution to these conditions is indicated. A solution to the inverse optimization problem is given. General results are widely illustrated by particular cases of equiprobable states and \( N = 2, 3, 4 \) pure qubit states given with different prior probabilities.

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I. INTRODUCTION

Essential advances in experimental techniques in recent years made possible high precision measurements which are required for distinguishing among separate nonorthogonal quantum states. These studies are stimulated by needs of quantum communication and quantum cryptography where the discrimination of quantum states is one of the key problems. In a more general context, this problem underlies many of the communication and computing schemes that have been suggested so far [1]. According to quantum-mechanical laws there is no way to discriminate perfectly among nonorthogonal states. Therefore, an actual problem is the state discrimination in an optimal way. Currently, different criteria of optimality are formulated (for a recent review, see [2]).

In this paper we will consider discrimination strategies based on the minimization of the generalized rate error (or more generally, the mean Bayes' cost [3, 4]). They are known in the literature as the minimum-error discrimination strategies.

Necessary and sufficient conditions for realizing the minimum-error (generalized) measurement were formulated independently by Holevo [5, 6] and Yuen et al [7] (see also a recent appealingly simple proof in [8]). Unfortunately, as Hunter [9] pointed out, these conditions do not provide a great insight into either the form of minimum-error measurement strategies, or into how error probability depends on the set of possible states. Moreover, the only strategy derived from these conditions corresponds to two possible states [8]. All other optimal solutions, except the one proposed by Hunter [9] for equiprobable qubit states, were first postulated and then shown to satisfy these conditions. Actually, Hunter’s solution [9] is based on solving these conditions only partly and consists in the formulation of a two-step procedure. First, he proposed to find some auxiliary operators and then to check which of these operators correspond to possible measurements. In this way, he was able to find a solution for equiprobable qubit states with a clear geometrical visualization. We have to note that our approach based on the full solution of the necessary and sufficient conditions permitted us to draw slightly different conclusions compared to those published in [9].

In the current paper, we first formulate conditions, to which the Lagrange operator should satisfy, when a measurement strategy remains to be optimal after a given set of states is enlarged by new states. Then we reformulate the known necessary and sufficient optimization conditions for pure qubit states given with arbitrary prior probabilities in terms of Bloch vectors representing the states. This permitted us to indicate an algorithmic solution of the (direct) optimization problem. Furthermore, using the new form of the necessary and sufficient optimization, conditions we succeeded to solve the inverse optimization problem, i.e., the problem of finding all sets of states and prior probabilities for which a given measurement strategy is optimal. For two-qubit states, we found a solution to the optimization problem for the case when the states are given with probabilities \( p_1 \) and \( p_2 \) such that \( p_1 + p_2 \leq 1 \). For \( p_1 + p_2 = 1 \), our solution reduces to the one first found by Helstrom [3] (see also [2]). Using this result, we derived a condition for \( N \) qubit states \( p_1, \ldots, p_N \) when they are optimally discriminated by the same orthogonal measurement which is optimal for discriminating among the states \( p_1 \) and \( p_2 \). This permitted us to formulate conditions for distinguishing projective measurements from generalized ones for optimal discrimination among three qubit states. For \( N \) equiprobable states, we have shown that the optimal (generalized) measurement may contain \( M \geq 4 \) elements of a positive operator-valued measure (POVM) only if there exists a subset of \( M \) states which may form a POVM. Otherwise, the optimal POVM contains either three or two elements. We applied our algorithm to the case of three states, two of which are given with equal probabilities. For a particular case of three mirror symmetric states, our result coincides with the one previously published by Anderson et al. [10]. For another particular case, we compared our solution to a solution obtained numerically in [11]. In contrast to [11], our approach gives exact analytic bounds for the prior probability, distinguishing projective optimal measurement from the generalized one. As another illustration of our approach, we obtained the optimal solution for four qubit states, two of which are given with the probability \( p \) and two others with the probability \( 1/2 - p \).
II. MINIMUM ERROR CONDITIONS FOR PURE QUBIT STATES

A. Minimum error conditions

Assume that we are given \( N (\geq 2) \) pure qubit states

\[
\rho_j = \rho_j^\dagger = \rho_j^2 \geq 0, \quad \text{Tr} \rho_j = 1, \quad j = 1, \ldots, N
\]

and a (discrete) probability distribution \( p_j > 0, \quad \sum_{j=1}^N p_j = 1 \). We assume also that the operator \( \rho_j \) occurs with the probability \( p_j \) and acts on the vectors of a two-dimensional Hilbert space with the usually defined inner product. A (generalized, see, e.g., [12]) measurement that discriminates between the states \( \rho_1, \ldots, \rho_N \) can be described with the help of \( N \) detection operators \( \hat{\pi}_1, \ldots, \hat{\pi}_N \) such that

\[
\hat{\pi}_j \leq 0, \quad \sum_{j=1}^N \hat{\pi}_j = I
\]

where \( I \) is the identity operator. If as a measurement result the detector \( \pi_{i_0} \) clicks we know with the probability \( \text{Tr}(\rho_{i_0} \hat{\pi}_{i_0}) \) that the chosen state is \( \rho_{i_0} \). The overall probability of correctly identifying any of the states \( \rho_j \) is then given by (see, e.g., [2])

\[
P_{\text{corr}} = \sum_{i=1}^N p_i \text{Tr}(\hat{\pi}_i \rho_i) = \text{Tr} \Gamma
\]

where we introduced

\[
\Gamma := \sum_{j=1}^N p_j \hat{\pi}_j \rho_j
\]

and \( P_{\text{err}} = 1 - P_{\text{corr}} \) is the overall probability of an erroneous guess. The minimum error discrimination strategy corresponds to such a set of detection operators \( \hat{\pi}_j \) that \( P_{\text{err}} \) takes its minimal value or equivalently \( P_{\text{corr}} \) takes its maximal value. Operator \( \Gamma \) is known in the literature as the Lagrange operator (see e.g. [3]). Since its trace defines \( P_{\text{corr}} \), we will call its matrix representation in a basis the cost matrix.

According to [3, 4], the necessary and sufficient conditions for a measurement to be optimal are

\[
\Gamma = \Gamma^\dagger, \quad G_j := \Gamma - p_j \rho_j \geq 0, \quad j = 1, \ldots, N.
\]

As it was proved by Holevo [6], instead of \( \Gamma \), one can equivalently use \( \hat{\Gamma} = (\Gamma + \Gamma^\dagger)/2 \) and at the extremum point \( \hat{\Gamma} = \Gamma \). Below, we will use also the following implication of Eq. (7)

\[
G_j \hat{\pi}_j = 0, \quad j = 1, \ldots, N.
\]

It is not difficult to see that from Eq. (8), it follows that for qubit states, if both \( \hat{\pi}_j \neq 0 \) and \( G_j \neq 0 \), then they both have a zero eigenvalue and therefore they both are proportional to projectors (cf. [3]). Indeed, since \( \hat{\pi}_j \) is Hermitian one can choose a coordinate system where it is diagonal with at least one non-zero diagonal entry. In this system from (3), it follows that at least one column of \( G_j \) and one diagonal element of \( \hat{\pi}_j \) should be equal to zero, i.e., both \( \text{det} \hat{\pi}_j = 0 \) and \( \text{det} G_j = 0 \) and both these operators are proportional to projectors. In what follows, we will extensively use this property.

We would like to note here that for an optimal strategy, some of the operators \( \hat{\pi}_j \) may become equal to zero. This happens if some of the detectors \( \hat{\pi}_j \), say for definiteness the detectors with the numbers \( j = M + 1, \ldots, N \), never click. In this case, only the states \( \rho_j \), with \( j = 1, \ldots, M \), enter the cost matrix \( \Gamma \) and their probabilities satisfy the condition \( \sum_{j=1}^M p_j < 1 \) while the first \( M \) POVM elements, \( \hat{\pi}_j, j = 1, \ldots, M \), satisfy conditions (2) and (3) with \( N = M \). We would like to stress that this property may be formulated in a more constructive way.

**Proposition 1.** Assume that for \( M \) states \( \rho_j, j = 1, \ldots, M \), given with the probabilities \( p_j \) such that \( \sum_{j=1}^M p_j < 1 \), the detection operators \( \hat{\pi}_j \), satisfying conditions (2) and (3) at \( N = M \), which maximizes the success probability \( P_{\text{corr}} \) for the cost matrix \( \Gamma \) at \( N = M \), are known. Then for a larger set of \( N > M \) states \( \rho_j, j = 1, \ldots, N \) given with the probabilities \( p_j \), \( \sum_{j=1}^N p_j = 1 \), such that \( \rho_j = \rho_j \) and \( \hat{\pi}_j = p_j \), \( j = 1, \ldots, M \), the optimal POVM contains all previous elements \( \hat{\pi}_j, j = 1, \ldots, M \) plus the zero elements \( \hat{\pi}_j = 0, j = M + 1, \ldots, N \) provided

\[
\Gamma - \overline{p}_j \overline{p}_j \geq 0, \quad j = M + 1, \ldots, N.
\]

The optimal success probability for the new set is \( \overline{P}_{\text{corr}} = P_{\text{corr}} \).

As the final comment of this section, we note that in what follows, we will distinguish the projective (i.e., von Neumann) measurement from the generalized one. The projective measurement may be realized only if there are no more than two detection operators in which case they should satisfy the usual condition \( \hat{\pi}_j^2 = \hat{\pi}_j \). For the generalized measurement one needs more than two detection operators.

B. Minimum error conditions in terms of Bloch vectors

We find convenient to choose Pauli matrices \( \sigma_i (i = 1, 2, 3) \) and \( \sigma_0 = I \) as a basis in the linear space of Hermitian \( 2 \times 2 \) matrices

\[
\sigma_j \sigma_k = -\sigma_k \sigma_j = i \sigma_i, \quad \sigma_j^2 = \sigma_0 = I, \\
\text{Tr} \sigma_j = 0, \quad \text{Tr}(\sigma_j \sigma_k) = 2 \delta_{j,k}, \quad j, k, l = 1, 2, 3.
\]
Thus, once \( N \) states \( \rho_j \) are given, the coefficients \( \beta_{j,k} \)
defining the states

\[
\rho_j = \sum_{k=0}^{3} \beta_{j,k} \sigma_k, \quad j = 1, \ldots, N
\]  

(11)

may be found as \( \beta_{j,k} = \frac{1}{2} \text{tr}(\rho_j \sigma_k) \in \mathbb{R} \). Normalization condition \( 1 \) imposes the following restrictions on \( \beta_{j,k} \):

\[
\beta_{j,0} = \frac{1}{2}, \quad \sum_{k=1}^{3} \beta_{j,k}^2 = \frac{1}{4}.
\]  

(12)

Therefore, any state is defined by a point on a sphere with the radius equal to 1/2 or equivalently by a 3-dimensional real vector (Bloch vector) \( \vec{\beta}_j = (\beta_{j,1}, \beta_{j,2}, \beta_{j,3}) \) of the length equal to 1/2.

As it was argued in the previous section we may look for the detection operators in the form

\[
\vec{\pi}_j = \omega_j \pi_j, \quad \pi_j = \pi_j^2 > 0, \quad \omega_j > 0.
\]  

(13)

We shall call \( \omega_j \) the frequencies. Taking into account Proposition \( 1 \) we may look for \( M \) operators \( \pi_j \) optimizing the measurement strategy for \( N \leq M \) states \( \rho_j, j = 1, \ldots, M \), given with the probabilities \( p_j, \sum_{j=1}^{M} p_j = 1 \).

The problem is solved if such a strategy is found and the remaining states (if \( M < N \)) satisfy conditions \( 1 \). Note that the optimization problem has always a solution (see \( 6, 7 \)).

Operators \( \pi_j \) will be defined in terms of unknown coefficients \( \gamma_{j,k} \),

\[
\pi_j = \sum_{k=0}^{3} \gamma_{j,k} \sigma_k
\]  

(14)

which should satisfy the relations similar to Eq. \( 12 \)

\[
\gamma_{j,0} = \frac{1}{2}, \quad \sum_{k=1}^{3} \gamma_{j,k}^2 = \frac{1}{4},
\]  

(15)

and every \( \rho_j \) is also defined by a 3-dimensional real vector \( \vec{\gamma}_j = (\gamma_{j,1}, \gamma_{j,2}, \gamma_{j,3}) \) of the length equal to 1/2. Moreover, from Eq. \( 13 \) one finds additional restrictions

\[
\sum_{j=1}^{M} \omega_j \gamma_{j,k} = 0, \quad k = 1, 2, 3, \quad M
\]  

(16)

\[
\sum_{j=1}^{M} \omega_j = 2, \quad \omega_j > 0.
\]  

(17)

According to Eq. \( 14 \) the cost matrix is also defined in terms of the vectors \( \vec{\beta}_j \) and \( \vec{\gamma}_j \),

\[
\Gamma = \sum_{k,k'=1}^{3} \Gamma_{k,k'} \sigma_k \sigma_{k'},
\]  

(18)

\[
\Gamma_{k,k'} = \sum_{j=1}^{M} \omega_j \beta_j \beta_{j,k'} \gamma_{j,k'}.
\]  

(19)

with the vectors \( \vec{\gamma}_j \) such that \( \sum_{j=1}^{M} \omega_j \vec{\gamma}_j = 0 \).

Now we can prove the following statement.

**Proposition 2.** If \( \omega_j > 0, j = 1, \ldots, M \), then conditions \( 4 \) are satisfied for \( \vec{\pi}_j = \omega_j \pi_j \), where \( \pi_j \) are given by Eq. \( 14 \) with

\[
\gamma_{j,k} = \frac{\beta_{j,k} p_j - B_k}{A - p_j}, \quad k = 1, 2, 3, \quad j = 1, \ldots, M,
\]  

(20)

where

\[
A = \text{tr} \Gamma > p_j, \quad \forall j
\]  

(21)

and \( B_k \in \mathbb{R} \) are arbitrary parameters.

**Proof.** According to Eqs. \( 18 \) and \( 10 \), one may write

\[
\Gamma = \sum_{k=0}^{3} \Gamma_{k,k} \sigma_0 + \sum_{k=1}^{3} (\Gamma_{k,0} + \Gamma_{0,k}) \sigma_k + \sum_{k \neq k'}^{3} \Gamma_{k,k'} \sigma_k \sigma_{k'}
\]  

(22)

where [see Eqs. \( 19 \), \( 12 \) and \( 15 \)]

\[
\Gamma_{k,0} = \frac{1}{2} \sum_{j=1}^{M} \omega_j p_j \beta_{j,k},
\]  

(23)

\[
\Gamma_{0,k} = \frac{1}{2} \sum_{j=1}^{M} \omega_j p_j \gamma_{j,k}.
\]  

(24)

As it was mentioned in Sec. \( 14 \) instead of \( \Gamma \) one can equivalently use \( \vec{\Gamma} = (\Gamma + \Gamma^\dagger)/2 \) which in our case is given by the first two terms at the right-hand side of Eq. \( 22 \). Therefore, below, to simplify notations, we will mean by \( \Gamma \) the same expression \( 22 \) where the last term is absent. This is justified by the property which we will show below. Namely, we will show that from Eq. \( 8 \) follows the Hermitian character of \( \Gamma \) and hence the zero contribution to \( \Gamma \) from the last term in Eq. \( 22 \). This leads to the following expression for \( G_j \):

\[
G_j = \left( \sum_{k=0}^{3} \Gamma_{k,k} - \frac{1}{2} p_j \right) \sigma_0 + \sum_{k=1}^{3} (\Gamma_{k,0} + \Gamma_{0,k} - p_j \beta_{j,k}) \sigma_k.
\]  

(25)

Using Eqs. \( 8 \) and \( 25 \) and assumed property \( \omega_j \neq 0 \), i.e., \( G_j \vec{\pi}_j = 0 \), we obtain a set of equations for coefficients \( \gamma_{j,k} \),

\[
\sum_{k=0}^{3} \Gamma_{k,k} - \frac{1}{2} p_j + 2 \sum_{k=1}^{3} (\Gamma_{k,0} + \Gamma_{0,k} - p_j \beta_{j,k}) \gamma_{j,k} = 0,
\]  

(26)

\[
\Gamma_{k,0} + \Gamma_{0,k} - p_j (\beta_{j,k} + \gamma_{j,k}) + 2 \gamma_{j,k} \sum_{k'=0}^{3} \Gamma_{k',k'} = 0,
\]  

(27)

\[
(\Gamma_{k,0} + \Gamma_{0,k} - p_j \beta_{j,k}) \gamma_{j,k} = (\Gamma_{k',0} + \Gamma_{0,k'} - p_j \beta_{j,k'}) \gamma_{j,k}.
\]  

(28)
If we multiply Eq. (26) by \( \gamma_{j,k} \) and subtract the result from Eq. (27), we get
\[
(\Gamma_{k,0} + \Gamma_{0,k} - p_j \beta_{j,k}) \gamma_{j,k'} = 4 \sum_{k' = 0}^{3} (\Gamma_{k',0} + \Gamma_{0,k'} - p_j \beta_{j,k'}) \gamma_{j,k'} \gamma_{j,k'},
\]
(29)
The right- and hence the left- hand side of Eq. (29) is symmetric with respect to the permutation of \( k \) and \( k' \) and therefore Eq. (28) is an implication of Eqs. (26) and (27). From the other hand, multiplying Eq. (27) by \( \gamma_{j,k} \) and summing up over \( k \) gives just Eq. (28). From Eq. (27) follows the symmetry property \( \Gamma_{k,k'} = \Gamma_{k',k} \) and, hence, the Hermitian character of the matrix \( \Gamma \). Indeed, multiplying Eq. (27) by \( \omega_{j,k,k'} \), summing up over \( j \), and using Eqs. (19) and (17) yields
\[
\Gamma_{k,k'} = - \sum_{j=1}^{M} p_j \omega_{j} \gamma_{j,k} \gamma_{j,k'} = \Gamma_{k',k}, \quad k, k' = 1, 2, 3.
\]
(30)
Thus from the set of Eqs. (28)–(28), we have to solve Eq. (27) only. For this purpose, we denote
\[
X_{j,k} := \Gamma_{k,0} + \Gamma_{0,k} - p_j (\beta_{j,k} + \gamma_{j,k}).
\]
(31)
These quantities have two remarkable properties. The first property
\[
\sum_{j=1}^{M} \omega_{j} X_{j,k} = 0, \quad k = 1, 2, 3
\]
(32)
follows from Eqs. (16), (23), and (21) and the second property
\[
\sum_{j=1}^{M} \sum_{k=1}^{3} \omega_{j} \gamma_{j,k} X_{j,k} = - \sum_{k=0}^{3} \Gamma_{k,k} = - \frac{1}{2} \text{Tr} \Gamma
\]
(33)
is a consequence of (15), (16), (18), and (19). Using Eqs. (31) and (33), we rewrite Eq. (27) as
\[
X_{j,k} = 2 \gamma_{j,k} \sum_{j'=1}^{M} \sum_{k'=1}^{3} \omega_{j'} \gamma_{j'k'} X_{j'k'},
\]
(34)
which has a solution
\[
X_{j,k} = A \gamma_{j,k},
\]
(35)
where \( A \) is for the moment an arbitrary constant. Putting thus found \( X_{j,k} \) to Eq. (33) and using Eqs. (15) and (17), we relate this constant with \( P_{corr} \), \( A = \text{Tr} \Gamma = P_{corr}. \)
To finish the proof of the statement, we solve Eq. (31) with respect to \( \gamma_{j,k} \). For this purpose, we replace in Eq. (31) \( \Gamma_{k,0} + \Gamma_{0,k} \) by the sum of Eqs. (23) and (24) which yields
\[
X_{j,k} = \frac{1}{2} \sum_{j=1}^{M} \omega_{j} p_{j} (\beta_{j,k} + \gamma_{j,k}) - p_{j} (\beta_{j,k} + \gamma_{j,k}).
\]
Then, using Eqs. (16) and (17), we find a solution to the above equation
\[
p_{j} (\beta_{j,k} + \gamma_{j,k}) = -X_{j,k} + B_{k}, \quad j = 1, \ldots, M, \quad k = 1, 2, 3.
\]
(36)
Here, parameters \( B_{k} \) remain arbitrary. From here and Eq. (35), we get Eq. (20).
Finally, we note once again that since all \( \omega_{j} \) are assumed to be different from zero, every matrix \( G_{j} \) has a zero eigenvalue (cf. (3)). Therefore, the condition \( G_{j} \geq 0 \) reduces to \( \text{Tr} G_{j} > 0 \) which upon using Eq. (26) yields \( A > p_{j} \).

Note that the proposition leaves parameter \( A \) and the frequencies \( \omega_{j} \) unspecified. Nevertheless, if we assume the frequencies to be invariant under a scaling transformation of the probabilities, i.e., after the replacement \( p_{j} \rightarrow \alpha p_{j} \), one has \( \omega_{j} \rightarrow \omega_{j} \), then from Eq. (19), it follows that \( A \) becomes a homogeneous function of the first degree with respect to the probabilities \( p_{j} \) provided the parameters \( \gamma_{j,k} \) are also invariant with respect to the same scaling. The last property agrees with Eq. (20) from which the scale invariance of the parameters \( \gamma_{j,k} \) follows if \( A \) is a homogeneous function of the first degree with respect to \( p_{j} \). Note also that under these assumptions, the detection operators \( \hat{\pi}_{j} \) become invariant with respect to the same scaling transformation.

C. Direct optimization problem
By the direct optimization problem, we mean the problem of finding the operators \( \hat{\pi}_{j} \) minimizing \( P_{corr} \) for a given set of operators \( p_{j} \). Any set of \( \hat{\pi}_{j} \) satisfying Eqs. (2), (3), and (7) with \( \Gamma \) given in Eq. (5) is a solution to this problem. Proposition 2 opens a way for an algorithmic solution to the problem.
First, we note that the operators \( \hat{\pi}_{j} = \omega_{j} \pi_{j} \) are defined by the frequencies \( \omega_{j} \) and Bloch vectors \( \gamma_{j,k} = (\gamma_{j,1}, \gamma_{j,2}, \gamma_{j,3}) \). According to Proposition 2, the vectors \( \gamma_{j} \) are defined by the parameter \( A \) and vector \( \vec{B} = (B_{1}, B_{2}, B_{3}) \). The still undefined parameters \( A, \omega_{j} \), and \( \vec{B} \) should be found form Eqs. (15), (16), and (17). Using Eq. (20), we obtain from Eq. (15) a set of equations for \( B_{k} \) and \( A \),
\[
\frac{1}{4} A^2 - \frac{1}{2} A p_{j} = \sum_{k=1}^{3} B_{k}^2 - 2 p_{j} \sum_{k=1}^{3} B_{k} \beta_{j,k}, \quad j = 1, \ldots, M.
\]
(37)
It is convenient to rewrite this system as \( M - 1 \) homogeneous equations for \( A \) and \( B_{k} \) and an equation of the second order with respect to \( A \) and \( B_{k} \). For this purpose, we subtract from the Eq. (37) at \( j = 1 \) the same equation at \( j = 2, \ldots, M \), thus obtaining
\[
4 \sum_{k=1}^{3} B_{k} (p_{1} \beta_{1,k} - p_{j} \beta_{j,k}) = A (p_{1} - p_{j}), \quad j = 2, \ldots, M.
\]
(38)
and sum up the Eqs. (37) over $j$ from 1 to $M$ which yields

$$MA^2 - 2A\alpha = 4M\sum_{k=1}^{3} B_k^2 - 8 \sum_{j=1}^{M} \sum_{k=1}^{3} B_k p_j \beta_{j,k},$$  \hspace{1cm} (39)$$

where $\alpha = \sum_{j=1}^{M} p_j$. We thus have $M$ equations for four unknown parameters $A$ and $B_{1,2,3}$. Therefore, it is natural to expect that the system may have solutions for $M = 2, 3, 4$ and has no solutions for $M > 4$ except for some special cases. This means that except for some particular cases, the optimal measurement for $N \geq 4$ pure qubit states is realized with four operators $\hat{A}$, $\hat{B}$ where

$$\alpha = 2$$  \hspace{1cm} (40)$$

and numbers $\omega_j \geq 0$ such that $\sum_{j=1}^{N} \omega_j \gamma_{j} = 0$ and $\sum_{j=1}^{N} \omega_j = 2$ defining a POVM $\pi_j = \omega_j \pi_j$ be given. Then this POVM corresponds to an optimal measurement strategy for the states $p_j$ given with the probabilities $p_j = A p_j$  \hspace{1cm} (41)$$

by the Bloch vectors

$$\beta_{j} = \frac{(1 - q_j) \gamma_{j} + \vec{R}}{q_j}, \hspace{1cm} j = 1, \ldots, N,$$  \hspace{1cm} (42)$$

where

$$q_j = \frac{1}{2} + (2\gamma_{j} + \vec{R}) \cdot \vec{R},$$  \hspace{1cm} (43)$$

and $A = 1/F$, $F = \sum_{j=1}^{N} q_j$, $\vec{R}$ is an arbitrary real vector and by dot we denote the scalar product of the vectors from a three-dimensional Euclidean space. The optimal success probability is $P_{corr} = A$.

**Proof.** Some necessary conditions for an optimal measurement are formulated in Proposition 2. Thus, assuming the vectors $\gamma_{j}$ be given in a frame by their coordinates $\gamma_{j,k}$ and using Eq. (20), we find the coordinates $\beta_{j,k}$ of the vectors $\beta_{j}$,

$$\beta_{j,k} = \frac{(A - p_j) \gamma_{j,k} + B_k}{p_j},$$  \hspace{1cm} (44)$$

where $B_k$ are arbitrary real numbers which define a vector $\vec{B} = (B_k)$. For $\beta_{j,k}$ to be coordinates of Bloch vectors, they should satisfy Eq. (12) which may be solved with respect to $p_j$,

$$p_j = \frac{1}{2} A^2 + 2 \sum_{k=1}^{3} B_k^2 + 2 A \sum_{k=1}^{3} \gamma_{j,k} B_k}{1/2 A + 2 \sum_{k=1}^{3} \gamma_{j,k} B_k}.$$  \hspace{1cm} (45)$$

If now we put $\vec{B} = A \vec{R}$, i.e., $B_k = A R_k$, we obtain from here just Eqs. (40) and (43). At the same time, Eq. (43) reduces to Eq. (41). Equation (45) follows from the condition $\sum_{j=1}^{N} p_j = 1$.

**D. Inverse optimization problem**

By inverse optimization problem, we mean a problem of finding all possible states $\rho_j$ and the prior probabilities $p_j$ for which a given measurement strategy is optimal. For qubit states, this means that given the frequencies $\omega_j$ and parameters $\gamma_{j,k}$, we have to find $p_j$ and $\beta_{j,k}$, $j = 1, \ldots, N$, $k = 1, 2, 3$. We formulate the solution to this problem as the following proposition.

**Proposition 3.** Let the Bloch vectors $\gamma_{j}$, $j = 1, \ldots, N$ and numbers $\omega_j \geq 0$ such that $\sum_{j=1}^{N} \omega_j \gamma_{j} = 0$ and $\sum_{j=1}^{N} \omega_j = 2$ defining a POVM $\pi_j = \omega_j \pi_j$ be given. Then this POVM corresponds to an optimal measurement strategy for the states $p_j$ given with the probabilities $p_j = A p_j$ (40) by the Bloch vectors

$$\beta_{j} = \frac{(1 - q_j) \gamma_{j} + \vec{R}}{q_j}, \hspace{1cm} j = 1, \ldots, N,$$  \hspace{1cm} (41)$$

where

$$q_j = \frac{1}{2} + (2\gamma_{j} + \vec{R}) \cdot \vec{R},$$  \hspace{1cm} (42)$$

and $A = 1/F$, $F = \sum_{j=1}^{N} q_j$, $\vec{R}$ is an arbitrary real vector and by dot we denote the scalar product of the vectors from a three-dimensional Euclidean space. The optimal success probability is $P_{corr} = A$.

**Proof.** Some necessary conditions for an optimal measurement are formulated in Proposition 2. Thus, assuming the vectors $\gamma_{j}$ be given in a frame by their coordinates $\gamma_{j,k}$ and using Eq. (20), we find the coordinates $\beta_{j,k}$ of the vectors $\beta_{j}$,

$$\beta_{j,k} = \frac{(A - p_j) \gamma_{j,k} + B_k}{p_j},$$  \hspace{1cm} (44)$$

where $B_k$ are arbitrary real numbers which define a vector $\vec{B} = (B_k)$. For $\beta_{j,k}$ to be coordinates of Bloch vectors, they should satisfy Eq. (12) which may be solved with respect to $p_j$,

$$p_j = \frac{1}{2} A^2 + 2 \sum_{k=1}^{3} B_k^2 + 2 A \sum_{k=1}^{3} \gamma_{j,k} B_k}{1/2 A + 2 \sum_{k=1}^{3} \gamma_{j,k} B_k}.$$  \hspace{1cm} (45)$$

If now we put $\vec{B} = A \vec{R}$, i.e., $B_k = A R_k$, we obtain from here just Eqs. (40) and (43). At the same time, Eq. (43) reduces to Eq. (41). Equation (45) follows from the condition $\sum_{j=1}^{N} p_j = 1$.

**III. PARTICULAR CASES**

**A. N=2**

Although the case of two qubit states is studied in details [2,3], we find instructive to show how the known
solution follows from our approach. Moreover, in view of Proposition 4, we need to consider the case where \( p_1 + p_2 = \alpha < 1 \) which was not studied so far.

We find convenient to choose a frame in the three-dimensional Euclidian space such that the given states \( \rho_1 \) and \( \rho_2 \) are defined by the Bloch vectors \( \vec{\beta}_1 \) and \( \vec{\beta}_2 \) with coordinates \( \vec{\beta}_1 = (\beta_{11}, \beta_{12}, 0) \) and \( \vec{\beta}_2 = (\beta_{21}, -\beta_{12}, 0) \).

From Eq. (10) at \( k = 3 \), we learn that \( B_3 = 0 \). After solving the compatibility condition of two remaining Eqs. (10) (with \( k = 1 \) and \( k = 2 \)) together with Eq. (48), we find \( B_1 \) and \( B_2 \) as linear functions of \( A \),

\[
B_1 = \frac{\beta_{11}}{4D^2} [A(p_1 - p_2)^2 + 8\beta_{12}^2 p_1p_2(p_1 + p_2)], \quad (46)
\]

\[
B_2 = \frac{\beta_{12}}{4D^2} [A(p_1 + p_2) - 8\beta_{11}^2 p_1p_2], \quad (47)
\]

where

\[
D = [\beta_{11}^2(p_1 - p_2)^2 + \beta_{12}^2(p_1 + p_2)^2]^{1/2}. \quad (48)
\]

Placing thus found \( B_1 \) and \( B_2 \) to Eq. (45) at \( j = 1 \), we solve this equation with respect to \( A \),

\[
A = \frac{1}{2}(p_1 + p_2) + D. \quad (49)
\]

Here from two roots of Eq. (47), we kept the biggest one. With the values \( A \) and \( B_{1,2} \) given in Eq. (10) and Eqs. (10) and (47), one can transform the left-hand side of Eq. (10) at \( k = 1 \) to a form \( (\omega_2 - \omega_1) \) times a nonzero factor so that one finds from the system (10) and (17) that \( \omega_1 = \omega_2 = 1 \).

Once the coordinates \( B_{1,2,3} \) of the vector \( \vec{B} \) and the optimal success probability \( P_{\text{corr}} = A \) are found, we may calculate detection operators

\[
\pi_1 = \left( \begin{array}{c} \frac{1}{2} \\ \pi \end{array} \right), \quad \pi_2 = I - \pi_1, \quad (50)
\]

\[
\pi = \frac{1}{2D} [\beta_{11}(p_1 - p_2) - i\beta_{12}(p_1 + p_2)] \quad (51)
\]

and the cost matrix

\[
\Gamma = \frac{1}{4} \begin{pmatrix} 2A & \gamma^* \\ \gamma & 2A \end{pmatrix}, \quad (52)
\]

\[
\gamma = \frac{1}{D} \{i\beta_{12}(p_1 - p_2)(2D + p_1 + p_2)
+ \beta_{11}[(p_1 - p_2)^2 + 2D(p_1 + p_2)]\}. \quad (53)
\]

Here we observe the invariance of the detection operators (50) with respect to scaling of the probabilities \( p_j \to \alpha p_j \) mentioned above.

If we notice that the parameters \( \beta_{11} \) and \( \beta_{12} \) may be expressed in terms of the Bloch vectors \( \vec{\beta}_1 \) and \( \vec{\beta}_2 \),

\[
\beta_{11} = \frac{(\vec{\beta}_2 + \vec{\beta}_1) \cdot \vec{\beta}_2}{\|\vec{\beta}_2 + \vec{\beta}_1\|}, \quad \beta_{12} = \frac{(\vec{\beta}_2 - \vec{\beta}_1) \cdot \vec{\beta}_2}{\|\vec{\beta}_2 - \vec{\beta}_1\|}, \quad (54)
\]

where by \( \|\vec{\beta}\| \) the length of the vector \( \vec{\beta} \) is denoted, we may present parameter \( D \) and with it the optimal success probability \( A \) (49) in an explicitly covariant form

\[
D = \left[ \frac{p_1^2 + p_2^2}{4} - 2p_1p_2 \frac{\beta_1 \cdot \beta_2}{\|\beta_2 + \beta_1\|} \right]^{1/2}. \quad (55)
\]

Another covariant form for \( A \) corresponds to using the absolute value of the overlap between the state vectors \( \langle \psi_1 | \psi_2 \rangle = s_{1,2}, \rho_1 = |\psi_1\rangle \langle \psi_1|, \rho_2 = |\psi_2\rangle \langle \psi_2| \),

\[
|s_{1,2}|^2 = \text{Tr}(\rho_1 \rho_2) = \frac{1}{2} + 2\beta_1 \cdot \beta_2 \quad (56)
\]

which yields

\[
A = \frac{p_1 + p_2}{2} + \frac{1}{2} [(p_1 + p_2)^2 - 4p_1p_2 |s_{1,2}|^2]^{1/2}. \quad (57)
\]

For \( p_1 + p_2 = 1 \), the last equation gives the value known as the Helstrom bound (3) (see also (2)).

Once the problem for two states given with the probabilities \( p_1 \) and \( p_2 \), \( p_1 + p_2 \leq 1 \), is solved, we can apply Proposition 4 for formulating conditions for \( N > 2 \) qubit states which are optimally discriminated by the same orthogonal measurement which optimally distinguishes the given states \( \rho_1 \) and \( \rho_2 \). For that, assuming that the states \( \rho_j \) are given with the probabilities \( p_j \), we have to calculate both the trace and the determinant of the matrix \( G_j = \Gamma - p_j \hat{\rho}_j \). After some algebra, one finds

\[
\text{Tr} G_j = A - p_j, \quad (58)
\]

\[
\det G_j = \frac{D}{2} (A - p_j) - \frac{A(p_1 - p_2)^2}{8D}
+ \frac{p_j(p_1 - p_2)}{2D} \left[ (p_1 \beta_1 - p_2 \beta_2) \cdot \beta_j \right]
+ p_j \left[ p_1(\beta_1 - \beta_j) + p_2(\beta_2 - \beta_j) \right] \cdot \beta_j. \quad (59)
\]

If both \( \text{Tr} G_j > 0 \) and \( \det G_j \geq 0, \ j = 3, \ldots, N \), then the optimal measurement is the projective measurement which optimally distinguishes \( \rho_1 \) from \( \rho_2 \) given with the probabilities \( p_1 \) and \( p_2 \), \( p_1 + p_2 < 1 \).

For \( N \) equiprobable states, given with the probability \( p = 1/N \), we have \( p_j = p \) and \( A = p + D \) so that Eq. (59) reduces to

\[
\det G_j = p^2 (\beta_1 + \beta_2) \cdot (\beta_j - \beta_1). \quad (60)
\]

**B. \( N = 3 \)**

For three given states \( \rho_1, \rho_2, \) and \( \rho_3 \), it may happen that the optimal measurement is the projective measurement. In such a case, because of the aforementioned scale invariance of the detection operators for \( N = 2 \), there are three possibilities for the optimal discrimination among the states \( \rho_1, \rho_2, \) and \( \rho_3 \). The optimal measurement may
be the projective measurement which optimally discriminates among any two from three given states. Therefore, to distinguish these possibilities below, we will need to put additional labels to quantities \( A \) and \( G_j \). In cases where there is no confusion, we will use the previous notations also. Thus, \( A \) defined by Eqs. (49) and (55) will be denoted as \( A_{1,2} \) so that

\[
A_{1,2} := \frac{1}{2} (p_1 + p_2) + \left[ \frac{p_1^2 + p_2^2}{4} - 2p_1 p_2 \beta_1 \cdot \beta_2 \right]^{1/2}
\]  

and \( \det G_j \) given in Eq. (59) at \( j = 3 \) will be denoted \( \det G_{1,2,3} \); i.e., \( \det G_{1,2,3} := \det G_3 \). For the set of labels \( \{1, 2, 3\} \), we will use also cyclic permutations \( \{1, 2, 3\} \rightarrow \{2, 3, 1\} \rightarrow \{3, 1, 2\} \). Using these notations, we may apply the proposition 4 to formulate conditions distinguishing projective optimal measurements from generalized ones for discriminating among three qubit states.

**Proposition 4.** Let the different states \( \rho_1, \rho_2, \rho_3 \) be given with the probabilities \( p_1, p_2, p_3 \) and \( \beta_1, \beta_2, \beta_3 \) as their Bloch vectors. The optimal measurement discriminating among these states is the projective measurement if the inequalities \( A_{i,j} > p_k \) and \( G_{i,j,k} \geq 0 \) hold for one cyclic permutation of the labels \( \{i, j, k\} = \{1, 2, 3\} \) at least. Otherwise, i.e., if no cyclic permutation exists such that both above inequalities hold, the optimal measurement is generalized. In the first case, the optimal success probability is \( P_{\text{corr}} = A_{i,j} \). In the second case, \( P_{\text{corr}} = A \) where \( A \) should be found from the system of equations (37), (16), and (17).

Proof. First we note that since the states are assumed to be different from each other, the optimal POVM contains more than one element. The statement becomes evident if one notices that the optimal solution exists always and the optimal POVM contains three elements if it cannot contain two elements.}

Note nevertheless that for the general case of three qubit states, solution to the system of equations (37), (16), and (17) is rather involved. Therefore, below we will consider some particular cases.

1. **Equiprobable states**

Let us consider \( p_1 = p_2 = p_3 = p = 1/N \) (\( N = 3 \)). In this case, \( A = p \left( 1 + \sqrt{\frac{1}{4} - 2\beta_1 \cdot \beta_2} \right) > p \) and whether the optimal measurement is projective or generalized is defined by the sign of \( \det G_{1,2,3} \). Thus, using Eq. (60) at \( j = 3 \), we may formulate a modification of Proposition 4 for this particular case.

**Proposition 5.** For three different equiprobable states \( \rho_j \) given by their Bloch vectors \( \beta_j \), \( j = 1, 2, 3 \), the optimal POVM includes three elements if the following inequalities,

\[
(\beta_1 + \beta_2) \cdot (\beta_4 - \beta_3) < 0, \\
(\beta_3 + \beta_1) \cdot (\beta_2 - \beta_3) < 0, \\
(\beta_2 + \beta_3) \cdot (\beta_1 - \beta_2) < 0
\]

hold. Otherwise, i.e., if at least one of these inequalities is violated the optimal measurement is projective.

If for instance \( (\beta_1 + \beta_2) \cdot (\beta_2 - \beta_3) \geq 0 \) then the optimal measurement is the one which optimally distinguishes the state \( \rho_1 \) from \( \rho_2 \). In the coordinate system where

\[
\beta_1 = (\beta_{1,1}, \beta_{1,2}, \beta_{1,3}), \\
\beta_2 = (\beta_{2,1}, -\beta_{1,2}, \beta_{1,3}), \\
\beta_3 = (\beta_{3,1}, \beta_{3,2}, \beta_{1,3}),
\]

\( \beta_{1,1} \geq 0, \beta_{1,2} > 0, \beta_{1,3} \geq 0 \)

the optimal success probability reads

\[
P_{\text{corr}} = A_{1,2} = \frac{1}{3} (1 + 2\beta_{1,2}). \tag{69}
\]

For the generalized measurement, the system of Eqs. (37), (16), and (17) in the frame (65)–(67) acquires a simple form and one easily obtains that the vector \( B \) points to the positive direction of the \( z \) axis, \( B = (0, 0, \sqrt{2} \beta_{1,3}) \), and the optimal success probability depends on the common projection of the vectors onto the same axis

\[
P_{\text{corr}} = A = p \left( 1 + \sqrt{1 - 4\beta_{1,3}^2} \right), \quad p = \frac{1}{3}. \tag{70}
\]

For the frequencies \( \omega_j \), one gets

\[
\omega_{1,2} = \frac{+\beta_{1,1} \beta_{1,3} - \beta_{1,2} \beta_{1,3}}{\beta_{1,2}(\beta_{1,1} - \beta_{1,3})}, \quad \omega_3 = \frac{2\beta_{1,1}}{\beta_{1,1} - \beta_{1,3}}. \tag{71}
\]

From the proposition 5 it follows that inequalities (62)–(64) imply positivity of the frequencies (71).

From Eq. (20), we find the vectors \( \gamma_j, \ j = 1, 2, 3 \), defining the detection operators \( \pi_j, \gamma_j = (1 - 4\beta_j^2)^{-1/2}(\beta_{1,1}, \beta_{1,2}, 0) \). We thus see that these vectors lay in the \( z = 0 \) plane and differ from the projection of the vectors \( \beta_j \) onto the same plane by the factor \( (1 - 4\beta_j^2)^{-1/2} \). In particular, if the vectors \( \beta_1, \beta_2, \) and \( \beta_3 \) are coplanar, i.e., if \( \beta_{1,3} = 0 \), the measurement is generalized provided these vectors themselves may form a POVM.

It is also useful to represent the success probability (70) in a covariant form

\[
P_{\text{corr}} = p \left( 1 + \sqrt{1 - 4\beta \cdot \beta} \right), \quad p = \frac{1}{3}. \tag{72}
\]
where by oblique cross, we denote the vector product and by brackets the mixed product of three-dimensional vectors.

Once the operators \( \pi_j \) and frequencies \( \omega_j \) are determined we may calculate the cost matrix \( \Gamma \). Thus from Eq. (5), it follows that this matrix is diagonal \( \Gamma = \text{diag}(A/2 + \beta_{j,3}, A/2 - \beta_{j,3}) \).

Now, assuming that the states \( \rho_1, \rho_2, \) and \( \rho_3 \) are discriminated by a generalized measurement and using Proposition 1, we can formulate conditions when the optimal measurement for discriminating among \( N \) states plays a fundamental role since for \( N = 4 \), the statement is proven. Let \( \bar{\beta} \) be given by their Bloch vectors \( \bar{\beta}_j = (\beta_{j,1}, \beta_{j,2}, \beta_{j,3}), j = 1, \ldots, N, \) is the same which is optimal for the first three states. This is the case if both the trace and determinant of the matrices \( G_j = \Gamma - p \rho_j, j = 4, \ldots, N, \) are non-negative. Since the trace is always positive, \( \text{Tr} G_j = p \sqrt{1 - 4 \beta_{j,3}^2} > 0 \), it remains to analyze the sign of the determinant \( \det G_j = \beta_{j,1} (\beta_{j,3} - \beta_{j,1}) \).

The optimization problem for three equiprobable states is given in Eq. (73).

The statement (ii) is a particular case of a solution previously indicated by Yeon et al. [7].

Thus it remains to prove the statement (iii). For that, we will use the induction method and first prove the statement for \( N = 4 \). If for \( N = 4 \) there exists a vector \( \bar{B} \neq 0 \) satisfying Eq. (73), then the system (55) has a nontrivial solution and we easily find that in the coordinate system (65)-(67), the vector \( \bar{B} \) points to the positive direction of the \( z \) axis. Using Eqs. (20), (17), and (16) at \( k = 3 \), we find its exact value, \( \bar{B} = (0, 0, p \beta_{j,3}), p = 1/4 \).

To find the frequencies \( \omega_j, j = 1, \ldots, 4, \) we have to solve two from three equations given in Eq. (10) (at \( k = 1, 2 \)) together with Eq. (17). From these equations one can always express say \( \omega_1, \omega_2, \) and \( \omega_3 \) in terms of \( \omega_4 \) but only solutions with all \( \omega_k \geq 0, k = 1, \ldots, 4, \) are suitable for our purpose. It is important to stress that \( \omega_{1,2,3} \) are linear (and hence monotonous) functions of \( \omega_4 \).

If we put \( \omega_4 = 0 \), we find unique values for \( \omega_1, \omega_2, \) and \( \omega_3 \) since corresponding linear inhomogeneous system has a unique solution. If additionally all these frequencies are nonnegative, \( \omega_j \geq 0, j = 1, 2, 3, \) then the optimal measurement contains three POVM elements \( \pi_1, \pi_2, \) and \( \pi_3 \) and the statement is proven. Let at \( \omega_4 = 0 \) at least one of \( \omega_j, j = 1, 2, 3 \) is negative, say, for definiteness \( \omega_1 < 0, \) and \( \omega_2 \geq 0, \omega_3 \geq 0 \). If the optimal measurement with four POVM elements exists, then taking into account a monotonous dependence of \( \omega_{1,2,3} \) on \( \omega_4 \), we conclude that there exists a value \( \omega_4 = \omega_{40} > 0 \) such that \( \omega_1 = 0, \omega_2 \geq 0, \omega_3 \geq 0 \) and the optimal measurement contains no more than three POVM elements \( \pi_4, \pi_3, \) and \( \pi_2 \) which also tells us that the statement is proven. If the optimal measurement with four POVM elements does not exist, then it contains either three or two POVM elements since by assumptions that the given states are different from each other it cannot contain one element. Thus for \( N = 4 \), the statement is proven.

Assume the statement be correct for \( N \) Bloch vectors (the main assumption) and prove it for \( N + 1 \) vectors. For the general case in the coordinate system (65)-(67) from Eqs. (68), (20), (17), and (16), we find the same value for the vector \( \bar{B} \) as it was for \( N = 4 \) with the sole difference that now \( p = 1/(N + 1) \). To find \( N + 1 \) frequencies \( \omega_j \), we have to solve the same Eqs. (10) at \( k = N + 1 \) from which we can always express three of them, say, \( \omega_1, \omega_2, \) and \( \omega_3 \) as linear (and hence monotonous once again) functions of \( \omega_j, j = 4, \ldots, N + 1 \). Let us put \( \omega_j = 0, j = 4, \ldots, N + 1 \). If we find \( \omega_j \geq 0, j = 1, 2, 3, \) the statement is proven. Therefore, assume that at least one of these frequencies is negative, say, for definiteness \( \omega_1 < 0, \omega_2 > 0, \omega_3 > 0 \). The situation here is a bit more complicated than it was for \( N = 4 \) since the dependence of every \( \omega_j, j = 1, 2, 3, \) on the other frequencies may be increasing with respect to some frequencies and decreasing for some others. If there exists a measurement with \( N + 1 \) POVM elements, different scenarios may take place but in all cases, there should exist a set of nonnegative frequencies. In particular, it may happen that there exists such values of \( \omega_j = \omega_{j0} \geq 0, \)
\[ j = 4, \ldots, N+1 \text{ that } \omega_1 = 0 \text{ and } \omega_2 \geq 0, \omega_3 \geq 0. \] Another possibility may be for instance such that at \( \omega_1 = 0 \), at least one of two other frequencies becomes negative, say, \( \omega_2 < 0 \), but with a variation of the frequencies \( \omega_j, j = 4, \ldots, N+1 \) the frequency \( \omega_3 \) should become positive and hence should cross the point \( \omega_2 = 0 \). In other words, the set of the values which \( \omega_{1,2,3} \) take under the variation of \( \omega_2 \in [0,2], j = 4, \ldots, N+1 \) necessarily contains a point where at least one of \( \omega_1, \omega_2, \) and \( \omega_3 \) vanishes. This means that the optimal measurement should contain no more than \( N \) POVM elements. For \( \omega_1 = 0 \) and \( \omega_j \geq 0, j = 2, \ldots, N+1 \), these are \( \pi_2, \ldots, \pi_{N+1} \). Therefore, the matrix \( \Sigma = p \sum_{j=2}^{N+1} \omega_j \pi_j \rho_j \) satisfies conditions (6) and (7) with \( p_j = p = 1/(N+1) \). Since \( p \) is simply a scaling factor both for \( \Gamma \) and in Eq. (7), these conditions remain valid after the replacement \( N \to N+1 \). This means that the same measurement is optimal for \( N \) states \( \rho_2, \ldots, \rho_{N+1} \) and according to the main assumption, there exists an optimal measurement which contains either two or three POVM elements.

From this proposition we can extract the following corollary:

**Corollary 1.** For \( N \geq 4 \) equiprobable states \( \rho_j \) given by their Bloch vectors \( \vec{\beta}_j \), the optimal measurement may contain \( M \geq 4 \) POVM elements only if there exists a subset of \( M \) states which form a POVM.

**Proof.** Indeed, if for \( N \) states only \( \vec{B} = 0 \) satisfies Eqs. (7), and the states \( \rho_j \) cannot form a POVM, then one has to examine all \( N \) subsets of \( N - 1 \) states and check whether there exists a subset which may form a POVM. If the answer is positive, for instance the vectors \( \rho_j, j = 1, \ldots, N-1 \), form a POVM, i.e., there exist numbers \( \omega_j \geq 0 \) such that \( \sum_{j=1}^{N-1} \omega_j \rho_j = I \) or equivalently such that \( \sum_{j=1}^{N-1} \omega_j = 2 \) and \( \sum_{j=1}^{N-1} \omega_j \beta_j = 0 \), then as a POVM for \( N \) states, we may choose just these frequencies together with the states \( \pi_j = \rho_j, j = 1, \ldots, N \) and put \( \omega_N = 0 \). For this POVM, the cost matrix (5) reads \( \Gamma = p \sum_{j=1}^{N} \omega_j \rho_j^2 = p \sum_{j=1}^{N-1} \omega_j \rho_j = pI \). Therefore, for any state \( \rho \) given by the Bloch vector \( \vec{\beta} = (\beta_1, \beta_2, \beta_3) \) for the trace and determinant of the matrix \( G = \Gamma - p \rho \), one gets \( \text{Tr} G = p, \text{det} G = p^2 (1 - \beta_1^2 - \beta_2^2 - \beta_3^2) = 0 \). This result means that the chosen POVM is optimal for discriminating among all \( N \) states \( \rho_j \).

If the answer is negative, i.e., if such a subset of \( N - 1 \) states does not exist, one has to examine all subsets of \( N - 2 \) states, etc. From here, it is clear that if there exists a subset of \( M \leq N \) states which may form a POVM, then the optimal POVM for discriminating among \( N \) states consists of the POVM thus found supplemented by other states (for \( M < N \)) with zero frequencies. If for a subset of the states there exists a vector \( \vec{B} \neq 0 \) as a solution to the Eqs. (7), then according to the point (iii) of the proposition 6 the optimal measurement cannot contain more than three POVM elements.

2. Two from three states are equally likely

Consider the case when \( p_1 = p_2 = p \) and \( p_3 = 1 - 2p, 0 < p \leq 1/2 \). Proposition 6 permits us to indicate the cases when three states given with the above probabilities are discriminated by the same projective measurement as two states given with equal probabilities. It is convenient to choose a frame such that

\[
\vec{\beta}_1 = (\beta_{1,1}, 0, \beta_{1,3}), \quad \vec{\beta}_2 = (-\beta_{1,1}, 0, \beta_{1,3}), \quad \beta_{1,1} > 0, \quad \beta_{1,3} = \sqrt{1/4 - \beta_{1,1}^2} > 0.
\]

From Eq. (61), we find \( A_{1,2} = p(1 + 2\beta_{1,1}) \geq 1 - 2p \) or equivalently \( p \geq (3 + 2\beta_{1,1})^{-1} \). Another condition follows from nonnegativity of \( \text{det} G_{1,2,3} \) given in Eq. (60) at \( j = 3 \)

\[
\text{det} G_{1,2,3} = p \beta_{1,1} (3p + 2p \beta_{1,1} - 1) + 2p (2p - 1) (1/4 - \beta_{1,3}^2) \geq 0.
\]

Since both \( \beta_{1,1} \) and \( \beta_{1,3} \) are assumed to be positive and hence \( 1 + 3\beta_{1,1} + 2\beta_{1,3}^2 - 4\beta_{1,3} \beta_{1,3} > 0 \) from here, it follows that

\[
P \geq \frac{2}{5 + \cos(2\theta) + \sin(2\theta)} > \frac{1}{3 + \sin(2\theta)}.
\]

and one recognizes the condition found in [11] for distinguishing the optimal projective measurement from the generalized one for discriminating among three mirror symmetric states.

Another simplification occurs at \( \beta_{1,3} = 0 \),

\[
\text{det} G_{1,2,3} = \frac{p}{2} (1 + 2\beta_{1,1})(2p + 2p \beta_{1,1} - 1),
\]

which leads to

\[
P \geq \frac{1}{2 + 2\beta_{1,1}} = \frac{1}{2 + \sin(2\theta)} > \frac{1}{3 + \sin(2\theta)}.
\]

Note that this case was previously studied numerically in [11] and we find instructive to compare our analytic solution with the numerical one. For this purpose, we additionally put \( \beta_{3,2} = 0, \beta_{3,1} = \frac{1}{2} \), and \( \beta_{1,1} = -\beta_{2,1} = \frac{b}{2}, \beta_{1,3} = \beta_{2,3} = \frac{1}{2} \sqrt{1 - b^2}, b > 0 \). Solving simultaneously Eqs. (83) and the compatibility condition for the system (10), we find the vector

\[
\vec{B} = \left( \frac{A(3p - 1)}{2p \sqrt{1 - b^2}}, 0, 0 \right),
\]

which being put to Eq. (83) with \( \alpha = 1 \) gives a second-order equation with respect to \( A \). This equation has the roots \( A = 0 \) and

\[
A = \frac{2p^2(1 - 2p)(b^2 - 1)}{1 - 6p + p^2(8 + b^2)}.
\]
With these values of $B_j$ and $A$ we solve the system of equations (10), (17)

$$\omega_{1,2} = \pm \frac{1 + p[4(p - 1) + b^2(5p - 2)]}{b[1 + p(-6 + (8 + b^2)p)]^2} \times [-1 + p(4 - 4p + b[\mp 2 + (\pm 6 + b)p])] , \quad (76)$$

$$\omega_3 = 2 - \omega_1 - \omega_2 . \quad (77)$$

From here, it follows that the equation $\omega_3 = 0$ has only one real root inside the interval $0 < p < 1/2$, which is $p = p_r = (2 + b)^{-1} = (2 + 2\beta_{1,1})^{-1}$ and if $p > p_r$, $\omega_3 < 0$. The equation $\omega_2 = 0$ has no real roots inside this interval and the equation $\omega_1 = 0$ has one root also

$$p = p_l = (b - 2 + \sqrt{2b(1 + b)})/(b^2 + 6b - 4) .$$

Thus, for $p_l < p < p_r$, these states are discriminated by a generalized measurement. Otherwise, they are discriminated by a projective measurement. In contrast to the paper [11], we give exact analytic bounds for the probability $p$ distinguishing optimal generalized measurements from projective ones.

C. $N=4$

Let two states $\rho_1$ and $\rho_2$ be given with the probability $p$ and two other states $\rho_3$ and $\rho_4$ with the probability $1/2 - p$, $0 < p < 1/2$. Let us choose the coordinate system such that the $z = 0$ plane is the plane of the Bloch vectors $\vec{\beta}_1$, $\vec{\beta}_2$ and they are symmetrically disposed with respect to $x$ axis, i.e.,

$$\vec{\beta}_1 = (\beta_{1,1}, \beta_{1,2}, 0) , \quad \vec{\beta}_2 = (\beta_{1,1}, -\beta_{1,2}, 0) ,$$

and assume that $\beta_{1,1} \geq 0$ and $\beta_{1,2} > 0$. Here, we will consider the case where the vectors $\vec{\beta}_3$ and $\vec{\beta}_4$ are placed into the $x = 0$ plane and symmetrically disposed with respect to $z$ axis, i.e.,

$$\vec{\beta}_3 = (0, \beta_{3,2}, \beta_{3,3}) , \quad \vec{\beta}_4 = (0, \beta_{3,2}, -\beta_{3,3})$$

with $\beta_{3,2} \geq 0$ and $\beta_{3,3} > 0$.

From the system (37), we find both the vector $\vec{B} = (B_1, 0, 0)$ and the optimal success probability $P_{corr} = A, \ B_1 = \frac{2p\beta_{1,1}(1 - 6p + 8p^2)}{1 - 8p + 16p^2(1 - \beta_{1,1}^2)\beta_{1,1}} , \ A = \frac{8p\beta_{1,1}^3}{4p - 1}B_1 , \quad (78)$

if for discrimination of these states, one needs four detection operators.

From here, we see that $P_{corr}$ does not depend on the states $\rho_3$ and $\rho_4$. In particular, these states may be orthogonal to each other ($\beta_{3,2} = 0$) in which case they correspond to opposite parts of the Bloch sphere. With these values of $B_1, B_2, B_3,$ and $A$, from the system of equations (10) and (17), we find the frequencies

$$\omega_{1,2} = \pm \frac{1 + 4p[p - 1 + 4(3p - 1)\beta_{1,2}^2]}{\beta_{1,2}[1 + 4p(-2 + p[3 + 4\beta_{1,2}^2])]^2} \times [-1 + 4p(4 - 4p\beta_{1,2}^2)] , \quad (79)$$

$$\omega_3 = \omega_4 = 1 - \frac{1}{2}(\omega_1 + \omega_2) . \quad (80)$$

Note that for $\beta_{3,2} = 0$, when the states $\rho_3$ and $\rho_4$ are orthogonal to each other, $\omega_1 = \omega_2$. From here it follows that for a fixed value of $\beta_{1,1}$ (and hence $\beta_{1,2}$), $\omega_4$ is not positive, $\omega_4 \leq 0$, if

$$p \geq 1 - \frac{2\beta_{1,2}}{8\beta_{1,1}^2} := p_r$$

and $\omega_1 > 0$ if

$$p > \frac{\beta_{1,2} - \beta_{3,2} + \sqrt{\beta_{1,2}(\beta_{1,2} + 2\beta_{3,2} + 4\beta_{1,2}\beta_{3,2}^2)}}{8\beta_{1,2}^2 - 2\beta_{3,2}^2 + 4\beta_{1,2}^2\beta_{3,2}^2} := p_l$$

where $\omega_2 > 0$ inside the interval $p_l < p < p_r$. Note that for $\beta_{1,2}, \beta_{3,2} \in [0, 1/2]$, the difference $p_r - p_l$ is not negative, $p_r - p_l \geq 0$. Thus, for the $p$ values from the interval $p \in (p_l, p_r)$, the states are discriminated with four detection operators $\sigma_j = \omega_j \sigma_j, j = 1, \ldots, 4$. For $p > p_r$, they are discriminated by a projective measurement which optimally distinguishes $\rho_1$ from $\rho_2$. For the success probability, one finds from Eq. (78) at $p = p_r$, the value $P_{corr} = 1/2$. Note that Eqs. (56) and (57) at $p_l = p_r = p_r$ yield the same value for the success probability. With $p$ growing from $p_l$ up to $1/2$, the success probability linearly increases until the value $1/2 + \beta_{1,2}$.

At $p = p_1$, $\omega_1$ vanishes, $\omega_1 = 0$, and for $p \leq p_1$, the states are optimally discriminated by the same measurement which optimally discriminates among the states $\rho_2, \rho_3,$ and $\rho_4$. From Eqs. (79) and (80) at $p = p_1$, we obtain corresponding frequencies

$$\omega_3 = \omega_4 = \frac{\beta_{1,2} + \beta_{3,2}}{\beta_{1,2} + 2\beta_{3,2} + 4\beta_{1,2}\beta_{3,2}^2} , \quad \omega_2 = 2 - 2\omega_3 . \quad (81)$$

Note that for $0 < \beta_{1,2}, \beta_{3,2} < 1/2$ all the frequencies (81) are positive. On the other hand, for $\beta_{3,2} = 0$, when the state $\rho_3$ is orthogonal to $\rho_4, p_1 = 1/4, \omega_3 = \omega_4 = 1,$ and $\omega_1 = \omega_2 = 0$. The success probability in this case is $P_{corr} = A = 1/2$. Note also that the same value follows from Eqs. (49) and (53) at $p_1 = p_2 = p_3 = p_4$. When $p \to 0$, the success probability tends linearly to zero.

IV. CONCLUSION

The known necessary and sufficient conditions for discriminating between nonorthogonal qubit states with the minimum error are formulated in terms of Bloch vectors representing the states. This permitted us to indicate an algorithmic solution to the direct optimization problem and give a complete solution to the inverse optimization problem. By the direct optimization problem, we mean the problem of finding the optimal measurement strategy when the states to be discriminated are given together with their prior probabilities. Accordingly, the
inverse optimization problem is the problem of specifying all possible states and their prior probabilities which may be optimally discriminated by the given generalized measurement.

An intermediate (or mixed) optimization problem may also be important for practical usage. We formulate it as follows. Assume that the minimum-error discrimination strategy for $N$ given states is known. Is it possible to enlarge this set of states in such a way that they are optimally discriminated by the same measurement strategy? If yes, what are the conditions to which the additional states should satisfy? A simple analysis of the necessary and sufficient conditions for minimizing the generalized rate error tells us that the answer to this question is positive. We formulated conditions in terms of Bloch vectors when a set of $N$ qubit states is discriminated by the same orthogonal measurement which is optimal for discriminating among two states given with arbitrary prior probabilities. We applied this result to formulate conditions when three qubit states are optimally discriminated either by the generalized measurement or by the projective one. In particular for $N$ equiprobable states, we have shown that the optimal generalized measurement may contain $M \geq 4$ POVM elements only if the states themselves may form a POVM. Otherwise, it contains either three or two POVM elements. For three equiprobable states, we found conditions which distinguish projective optimal measurements from generalized ones.

To illustrate our approach, we considered an example of three states, two of which are equally likely. For a particular case of three mirror symmetric states, we reproduced a result previously published in [10]. To illustrate the advantage of the analytic solution compared to a numerical one, we considered another particular case previously reported in [11]. For this case in contrast to [11], we were able to present the strict analytic bounds for the prior probability for distinguishing the optimal generalized measurement from the projective one. As the final illustration of our approach, we solved the optimization problem for four qubit states, two of which are given with the probability $p$ and two others with the probability $1/2 - p$.

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