Optimum measurement for unambiguously discriminating two mixed states: General considerations and special cases

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Abstract. Based on our previous publication [U. Herzog and J. A. Bergou, Phys. Rev. A 71, 050301(R)(2005)] we investigate the optimum measurement for the unambiguous discrimination of two mixed quantum states that occur with given prior probabilities. Unambiguous discrimination of nonorthogonal states is possible in a probabilistic way, at the expense of a nonzero probability of inconclusive results, where the measurement fails. Along with a discussion of the general problem, we give an example illustrating our method of solution. We also provide general inequalities for the minimum achievable failure probability and discuss in more detail the necessary conditions that must be fulfilled when its absolute lower bound, proportional to the fidelity of the states, can be reached.

1. Introduction
Quantum state discrimination [1] is a basic tool for quantum information and quantum communication tasks. In the standard problem, it is assumed that a quantum system is prepared, with certain prior probability, in a certain state chosen from a finite set of given states. A state discriminating measurement determines what the actual state of the system is from the set of possible states. According to the laws of quantum mechanics, perfect state discrimination yielding a correct result in each single measurement is impossible when the given states are not mutually orthogonal. For this general case various measurement strategies have been developed that are optimized with respect to different criteria. For example, the measurement for minimum-error discrimination [2] yields a definite result for the state of the system each time it is performed, but this result may be wrong and the probability of errors is as small as possible. In unambiguous discrimination, on the other hand, errors are not allowed to occur, which is possible at the expense of allowing measurement outcomes, with a certain probability of occurrence, that are inconclusive, i.e. that fail to give a definite answer.

In a measurement for optimum unambiguous discrimination the failure probability is minimized. Such a scheme was first introduced for distinguishing between two pure states [3]-[6], and only in the past few years the interest focused on investigating unambiguous state discrimination involving also mixed states [7]-[16]. While for optimum unambiguous discrimination between a pure state and an arbitrary mixed state an explicit general result has been derived for the minimum failure probability [8, 9], the problem of optimally discriminating
between two arbitrary mixed states is much more complicated and there does not exist an explicit compact solution comprising the most general case. However, a number of important results have been obtained. First, an overall lower bound has been found for the failure probability [10], being later on generalized for distinguishing between more than two mixed states [13]. Moreover, theorems have been established that reduce the problem of unambiguous discrimination to a standardized form [11]. Recently the necessary conditions have been derived that must be fulfilled when the failure probability saturates the overall lower bound [14], and explicit expressions have been provided for the optimum measurement operators in the case that the two mixed states belong to a special class [15]. In addition, the optimum measurement has been determined for a number of special cases having various degrees of generality [10], [14]-[16].

In this contribution we give a brief summary of the main results presented in our previous publication [14], along with a more detailed discussion of several issues. We also show how our method can be applied to actually solve an illustrative special example.

2. Description of the optimization problem and remarks on the solution

We start by recalling the underlying theoretical concepts for investigating a measurement capable of unambiguous discrimination of arbitrary quantum states. Any measurement for distinguishing between two mixed states, characterized by the density operators \( \rho_1 \) and \( \rho_2 \) and occurring with the prior probabilities \( \eta_1 \) and \( \eta_2 = 1 - \eta_1 \), respectively, can be formally described with the help of three positive detection operators \( \Pi_0, \Pi_1, \Pi_2 \), where

\[
\Pi_0 + \Pi_1 + \Pi_2 = I
\]

with \( I \) being the identity. These operators are defined in such a way that \( \text{Tr}(\rho_k \Pi_k) \) with \( k = 1, 2 \) is the probability that a system prepared in a state \( \rho \) is inferred to be in the state \( \rho_k \), while \( \text{Tr}(\rho \Pi_0) \) is the probability that the measurement fails to give a definite answer. The measurement is a von Neumann measurement when all detection operators are projectors, otherwise it is a generalized measurement based on a positive operator-valued measure (POVM). When the detection operators are known, schemes for realizing the measurement can be devised [17].

In unambiguous discrimination errors do not occur which is equivalent to [1]

\[
\rho_1 \Pi_2 = \rho_2 \Pi_1 = 0.
\]

The total probability that the measurement fails can then be written as

\[
Q = \eta_1 \text{Tr}(\rho_1 \Pi_0) + \eta_2 \text{Tr}(\rho_2 \Pi_0) = 1 - \eta_1 \text{Tr}(\rho_1 \Pi_1) - \eta_2 \text{Tr}(\rho_2 \Pi_2),
\]

where in the second line Eqs. (1) and (2) have been used. In order to determine the measurement, we have to find explicit expressions for the detection operators. For this purpose we introduce the spectral representations of the given density operators,

\[
\rho_1 = \sum_{l=1}^{d_1} |r_l\rangle \langle r_l|, \quad \rho_2 = \sum_{m=1}^{d_2} |s_m\rangle \langle s_m|,
\]

where \( r_l, s_m \neq 0 \), and \( \langle r_l | r_m \rangle = \delta_{l,m} = \langle s_l | s_m \rangle \). Moreover, we introduce the projection operators

\[
P_1 = \sum_{l=1}^{d_1} |r_l\rangle \langle r_l|, \quad P_2 = \sum_{m=1}^{d_2} |s_m\rangle \langle s_m|.
\]
Now we decompose each eigenstate of \( \rho_1 \) into a component lying within the support of \( \rho_2 \), i.e., within the Hilbert space spanned by the eigenstates of \( \rho_2 \) belonging to nonzero eigenvalues, and a second component being perpendicular to it, \( |r_i\rangle = P_2|r_i\rangle + |r_i\rangle^\perp \). By applying the Gram-Schmidt orthogonalisation procedure [18] we can construct a complete orthonormal basis \( \{|v_i\}\rangle \) in the subspace spanned by the non-normalized state vectors \( |r_i\rangle^\perp \), \( i = 1 \ldots , d_1 \), and we denote the projector onto this subspace by \( P_{1\perp} \). In an analogous way, after decomposing the eigenstates of \( \rho_2 \), we determine the projector \( P_{2\perp} \). When \( d_{1\perp} \) and \( d_{2\perp} \) are the dimensionalities of the corresponding bases, these projectors take the form

\[
P_{1\perp} = I - P_2 = \sum_{i=1}^{d_{1\perp}} |v_i\rangle\langle v_i|, \quad P_{2\perp} = I - P_1 = \sum_{j=1}^{d_{2\perp}} |w_j\rangle\langle w_j|, \quad (6)
\]

where \( \langle v_i|v_j\rangle = \langle w_i|w_j\rangle = \delta_{i,j} \). Since by construction \( \rho_2|v_i\rangle = 0 \) for \( 0 \leq i \leq d_{1\perp} \) and \( \rho_1|w_j\rangle = 0 \) for \( 0 \leq j \leq d_{2\perp} \), the most general Ansatz for the detection operators \( \Pi_1 \) and \( \Pi_2 \) can be written as

\[
\Pi_1 = \sum_{i,j=1}^{d_{1\perp}} \alpha_{ij}|v_i\rangle\langle v_j|, \quad \Pi_2 = \sum_{i,j=1}^{d_{2\perp}} \beta_{ij}|w_i\rangle\langle w_j|. \quad (7)
\]

Clearly, unambiguous discrimination is possible with a non-zero probability of success when the supports of the two density operators are not identical, since in this case at least one of the operators \( \Pi_1 \) and \( \Pi_2 \) does not vanish. On the other hand, the measurement result is always inconclusive when the supports coincide, \( P_1 = P_2 = I \), because in this case \( \Pi_1 = \Pi_2 = 0 \) and therefore \( P_0 = 1 \). We also note that there exists a modified Ansatz for \( \Pi_2 \) [14], referring to the eigenstates of \( \rho_1 \) and already taking into account that the failure probability is to be made as small as possible. This Ansatz implicitly contains one of the reduction theorems derived in [11]. For the purposes of this contribution, however, it is sufficient to rely on the representation in Eq. (7).

It is our aim to determine the particular measurement that is optimally suited for unambiguous discrimination of the given states. For this purpose we have to insert the general Ansatz for \( \Pi_1 \) and \( \Pi_2 \) into the second line of Eq. (3) and determine the parameters \( \alpha_{ij} \) and \( \beta_{ij} \) that minimize the failure probability \( Q \) under the constraint that the operator \( I - \Pi_1 - \Pi_2 \) is positive. So far complete analytical solutions, for arbitrary prior probabilities of the two mixed states, have only been found for special cases [10, 14, 16]. All of them are characterized by the fact that the two density operators to be discriminated have a certain mutual geometrical structure, where after suitable numbering of the eigenvectors we can write for any \( l \) and \( m \)

\[
\langle v_i|r_l\rangle = \langle v_i|r_l\rangle \delta_{i,l}, \quad \langle w_j|s_m\rangle = \langle w_j|s_m\rangle \delta_{j,m}, \quad (8)
\]

for \( i = 1, \ldots , d_{1\perp} \) and \( j = 1, \ldots , d_{2\perp} \). From this assumption it follows that \( \text{Tr}(\rho_1\Pi_1) = \sum_{l=1}^{d_{1\perp}} \alpha_{il}|v_i|v_l\rangle^2 \) and, similarly, \( \text{Tr}(\rho_2\Pi_2) \) also depends on the diagonal elements \( \beta_{ii} \) only. As a consequence, the states \( \{|v_i\}\rangle \) and \( \{|w_j\}\rangle \) are eigenstates of the optimum detection operators \( \Pi_1 \) and \( \Pi_2 \), respectively, and the solution of the optimization problem therefore is facilitated.

To elucidate our approach, let us treat a simple analytically solvable example in which we want to optimally discriminate two density operators with \( d_1 = 2 \) and \( d_2 = 3 \). We assume that their supports have a common subspace and jointly span a four-dimensional Hilbert space. In particular, in terms of the basis vectors \( |u_i\rangle \) \( i = 1, \ldots , 4 \) with \( \langle u_i|u_j\rangle = \delta_{i,j} \), we choose

\[
\rho_1 = \frac{|u_2\rangle\langle u_2| + (|u_3\rangle - |u_4\rangle)(\langle u_3| - \langle u_4|)}{4}, \quad \rho_2 = \sum_{i=1}^{3} \frac{|u_i\rangle\langle u_i|}{3}. \quad (9)
\]
Although for solving the problem one could apply one of the reduction theorems derived in [11], here we proceed in a direct way. We find immediately that in Eq. (6) $d_{1\perp} = 1$ with $|v_1\rangle = |u_4\rangle$, while $d_{2\perp} = 2$ with $|w_1\rangle = |u_1\rangle$ and $|w_2\rangle = (|u_3\rangle + |u_4\rangle)/\sqrt{2}$. Making use of Eqs. (7) and (6) the failure probability can be written as $Q = 1 - \eta_1 \alpha_{11}/4 - \eta_2 (2 \beta_{11} + \beta_{22})/6$. In order to minimize $Q$ under the constraint that $\Pi_0$ is positive, we put $\beta_{12} = 0$. The four eigenvalues of $\Pi_0$ are then found to be equal to 1, 1 − $\beta_{11}$, and 2 − $\beta_{22} - \alpha_{11} \pm \sqrt{\alpha_{11}^2 + \beta_{22}^2}$. They all are positive provided that $\beta_{11} \leq 1$ and $\beta_{22} \leq (2 - 2\alpha_{11})(2 - \alpha_{11})$. For making $Q$ as small as possible we choose the equality signs. After substituting these expressions, we minimize the resulting function $Q(\alpha_{11})$, taking into account that 0 ≤ $\alpha_{11}$ ≤ 1. We find that $Q$ takes its minimum when $\alpha_{11} = 0$ if $3\eta_1 \leq \eta_2$, $\alpha_{11} = 2(1 - \sqrt{\eta_2/3\eta_1})$ if $\eta_2 \leq 3\eta_1 \leq 4\eta_2$, and $\alpha_{11} = 1$ if $3\eta_1 \geq 4\eta_2$. This yields the minimum failure probability

$$Q_{\text{min}} = \begin{cases} 1 - \frac{2\eta_2}{3} & \text{if } 3\eta_1 \leq \eta_2 \\ \frac{\eta_1}{6} + \frac{1}{3}(1 + \sqrt{3\eta_1 \eta_2}) & \text{if } \eta_2 \leq 3\eta_1 \leq 4\eta_2 \\ 1 - \frac{\eta_1}{4} - \frac{2\eta_2}{3} & \text{if } 3\eta_1 \geq 4\eta_2, \end{cases}$$

(10)

where $\eta_2 = 1 - \eta_1$. In the inner parameter region the optimum measurement is a generalized measurement, while in the two outer regions it is a von Neumann measurement, where the detection operators are projectors.

3. General inequalities for the failure probability

Although for discriminating two completely arbitrary mixed states a closed expression for the minimum achievable failure probability is lacking, lower bounds can be derived for its value, in dependence on the prior probabilities of the states. For this purpose we first observe that by using the relation between the arithmetic and the geometric mean as well as the Cauchy-Schwarz-inequality [18] we obtain from the first line of Eq. (3) that [13]

$$Q \geq 2\sqrt{\eta_1 \eta_2 \text{Tr}(\rho_1 \Pi_0)\text{Tr}(\rho_2 \Pi_0)} \geq 2\sqrt{\eta_1 \eta_2 \max U |\text{Tr}(U \sqrt{\rho_1} \Pi_0 \sqrt{\rho_2})|},$$

(11)

where $U$ describes an arbitrary unitary transformation. Using $\Pi_0 = I - \Pi_1 - \Pi_2$, as well as the condition for error-free discrimination, Eq. (2), we arrive at the inequality

$$Q \geq 2\sqrt{\eta_1 \eta_2 \max U |\text{Tr}(U \sqrt{\rho_1} \sqrt{\rho_2})|} = 2\sqrt{\eta_1 \eta_2} F(\rho_1, \rho_2),$$

(12)

where $F = \text{Tr}[(\sqrt{\rho_2} \rho_1 \sqrt{\rho_2})^{1/2}]$ is the fidelity [18].

We can specify the lower bound for the failure probability still further when we investigate the conditions that must be fulfilled when the bound $2\sqrt{\eta_1 \eta_2} F$ is saturated, i. e. when the equality signs hold in Eqs. (11) and (12). Obviously this is true if and only if

$$\eta_1 \text{Tr}(\rho_1 \Pi_0) = \eta_2 \text{Tr}(\rho_2 \Pi_0) = \sqrt{\eta_1 \eta_2} F.$$

(13)

At this point it is important to note that the possible values of $\text{Tr}(\rho_1 \Pi_0)$ and $\text{Tr}(\rho_2 \Pi_0)$ are restricted which is a consequence of the structure of the detection operators $\Pi_1$ and $\Pi_2$. Since the detection operators determine probabilities and, therefore, their eigenvalues are between 0 and 1, we get from Eqs. (7) and (6) the relation

$$0 \leq \text{Tr}(\rho_1 \Pi_1) \leq \text{Tr}(P_{1\perp} \rho_1) = 1 - \text{Tr}(P_2 \rho_1).$$

(14)

Taking into account that $\text{Tr}(\rho_1 \Pi_1) = 1 - \text{Tr}(\rho_1 \Pi_0)$ because of Eqs. (1) and (2), and making use of the symmetry with respect to interchanging the indices 1 and 2, we arrive at the basic inequalities [14]

$$\text{Tr}(\rho_1 \Pi_0) \geq \text{Tr}(P_2 \rho_1), \quad \text{Tr}(\rho_2 \Pi_0) \geq \text{Tr}(P_1 \rho_2).$$

(15)
Obviously due to the requirement that the discrimination be error-free, expressed by Eq. (2), the two state-selective failure probabilities $\text{Tr}(\rho_1 \Pi_0)$ and $\text{Tr}(\rho_2 \Pi_0)$ each exceed a certain minimum which is larger than zero unless the supports of the density operators to be discriminated are orthogonal. Combining Eqs. (13) and (15) we find that the lower bound can only be saturated when $\text{Tr}(P_2 \rho_1) / F \leq \sqrt{\eta_2 / \eta_1} \leq F / \text{Tr}(P_1 \rho_2)$ [14]. From these considerations it is easy to obtain the general inequalities for the failure probability [15]

\[ Q \geq \begin{cases} 
\frac{\eta_1 F^2}{\text{Tr}(P_1 \rho_2)} + \eta_1 \text{Tr}(P_1 \rho_2) & \text{if } \sqrt{\frac{\eta_2}{\eta_1}} \geq \frac{F}{\text{Tr}(P_1 \rho_2)} \\
2 \sqrt{\eta_1 \eta_2} F & \text{if } \frac{\text{Tr}(P_2 \rho_1)}{F} \leq \sqrt{\frac{\eta_2}{\eta_1}} \leq \frac{F}{\text{Tr}(P_1 \rho_2)} \\
\frac{\eta_2 F^2}{\text{Tr}(P_2 \rho_1)} + \eta_2 \text{Tr}(P_2 \rho_1) & \text{if } \sqrt{\frac{\eta_2}{\eta_1}} \leq \frac{\text{Tr}(P_2 \rho_1)}{F}, \end{cases} \tag{16} \]

where the conditions on the right-hand side still can be modified taking into account that $\eta_2 = 1 - \eta_1$.

Clearly, the necessary condition for the saturation of the bound $Q = 2 \sqrt{\eta_1 \eta_2} F$ can be only fulfilled, for certain values of the prior probabilities, if

\[ \text{Tr}(P_2 \rho_1) / \text{Tr}(P_1 \rho_2) \leq F^2. \tag{17} \]

When at least one of the states to be discriminated is pure, there exists always a parameter interval for the prior probabilities where the failure probability reaches the fidelity bound $Q = 2 \sqrt{\eta_1 \eta_2} F$, as can be seen from the exact solution [8, 9]. For two arbitrary mixed states, however, this statement does not hold true [14]. In fact, the condition expressed by Eq. (17) can be violated even when the supports of the two density operators do not have a common subspace.

\textbf{Figure 1.} The parameter space of the two special density operators from Eq. (18). In the shaded area the inequality (17) is satisfied, $F^2 \geq \frac{1}{4}$, and the white corners represent the part of the parameter space where it is violated, $F^2 < \frac{1}{4}$. The boundaries of the shaded area are given by $s = 0$ for $0 \leq r \leq 1/2$, by $(r - 1/2)^2 + (s - 1/2)^2 = 1/4$ for $1/2 \leq r \leq 1$, $0 \leq s \leq 1/2$ and for $0 \leq r \leq 1/2$, $1/2 \leq s \leq 1$, and by $s = 1$ for $1/2 \leq r \leq 1$.

As an illustration, we specify Eq. (4) and consider the density operators

\[ \rho_1 = r |r_1 \rangle \langle r_1| + (1-r) |r_2 \rangle \langle r_2|, \quad \rho_2 = s |s_1 \rangle \langle s_1| + (1-s) |s_2 \rangle \langle s_2|, \tag{18} \]
where $\langle r_i | s_j \rangle = \frac{1}{\sqrt{2}} \delta_{i,j}$. It is easy to check that in this case Eqs. (8) hold. A short calculation shows that $F = \frac{1}{\sqrt{2}} [\sqrt{r s} + \sqrt{(1-r)(1-s)}]$ and $\text{Tr}(P_1 \rho_2) = \text{Tr}(P_2 \rho_1) = 1/2$. As becomes obvious from Fig. 1, there exists a parameter space for $(r,s)$ where the necessary condition (17) is violated and the fidelity bound cannot be reached for any value of the prior probabilities. We still mention that for $r = s$ the exact solution for the minimum failure probability in our example is given by Eq. (16) when on the left-hand side the equality sign holds, as has been shown in [14]. In this case again in the intermediate parameter region, where the fidelity bound is reached, the optimum measurement is a generalized measurement, while in the outer two regions it is a von Neumann measurement.

4. Conclusions

In this contribution we briefly rederived some of our recent results [14] on the problem of optimum unambiguous discrimination of two mixed states, and we discussed two illustrative special cases. It is worth noting that even for the lowest-dimensional non-specialized case, where two completely arbitrary density operators of rank two have to be distinguished, so far there does not exist a general analytical solution.

Acknowledgments

J. B. acknowledges useful discussions with E. Feldman and M. Hillery.

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