Unambiguous discrimination of mixed states

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We present the conditions under which probabilistic error-free discrimination of mixed states is possible, and provide upper and lower bounds on the maximum probability of success for the case of two mixed states. We solve certain special cases exactly, and demonstrate how the problems of state filtering and state comparison can be recast as problems of mixed state unambiguous discrimination.

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I. INTRODUCTION

A characteristic feature of quantum mechanics is that if a system is prepared in one of a set of nonorthogonal pure states, then there is no measurement that can yield an errorfree determination of which state was prepared. Nonetheless, it is possible to achieve a *probabilistic* error-free discrimination, that is, one which sometimes fails, but when successful never gives an erroneous result. This sort of discrimination procedure is generally referred to as *unambiguous discrimination* (UD). The UD of two *pure* states prepared with equal prior probabilities was considered by Ivanovic and Dieks $[1]$ and the optimal procedure was given by Peres $[2]$. This was generalized to the case of unequal prior probabilities by Jaeger and Shimony $[3]$. The problem of three pure states was analyzed in Ref. $[4]$, while multiple pure states were considered in Refs. $[5,6]$.

It is a common misconception that the unambiguous discrimination of *mixed* states is impossible [7,8]. Indeed, in Ref. $[7]$ it is explicitly stated that "one cannot unambiguously discriminate mixed states.'' That such a claim cannot be correct for an arbitrary mixed-state ensemble is proven, however, by the following counterexample: any set of *orthogonal* mixed states can always be discriminated with zero probability of error.

What is less obvious is that there exist sets of *nonorthogonal* mixed states for which UD is possible. The critical feature of such sets is that their elements do not have identical supports.¹ In fact, all that is required for there to be a nonzero probability of error-free discrimination is that one of the density operators have a nonzero overlap with the intersection of the kernels of the others.

In this paper, we consider the problem of determining the *optimal* UD procedure for an arbitrary pair of mixed states. We derive strong upper and lower bounds on the probability of a conclusive result, and we provide an exact solution in the special case where both states have kernels of dimension 1.

The ability to unambiguously discriminate a pair of mixed states has many applications. Indeed, several recently studied problems can be recast as special cases of UD of mixed states. We shall focus on two tasks of this sort: *state comparison* [9] (determining whether two systems are described by the same or different pure states) and *state filtering* $[10,11]$ (discriminating one pure state from a set of pure states). We find that for the state comparison problem, our upper and lower bounds coincide, and thus automatically yield the optimal solution. For the state filtering problem, we find that our lower bound is equal to the optimal solution found in Refs. $[10,11]$. Given that our lower bound has a simple geometric interpretation, it serves to clarify the nature of the optimal state filtering procedure. In particular, it shows that the eigenbases of the optimal positive-operator valued measure (POVM) elements depend only on the subspace spanned by the states against which one is trying to filter, and not on the specific states themselves. In addition, our approach generalizes in a straightforward way to more complicated estimation tasks, such as state filtering and state comparison when the unknown states are themselves mixed.

It should be noted that our results apply not only to mixtures that arise from ignorance about which of several different pure state descriptions applies, but also to those arising as the reduced density operator of an entangled state. As such, our results can be applied to the task of achieving an UD of two entangled states of a composite system given access to only one of the subsystems. It is also worth noting that our lower bound is obtained by making implicit use of the CS decomposition, which constitutes a powerful tool in both modern linear algebra and classical signal analysis [12]. To our knowledge, this is the first application of the CS decomposition in *quantum* signal analysis.

II. GENERAL FORMULATION

We consider the task of discriminating unambiguously between two mixed states ρ_0 and ρ_1 with prior probabilities p_0 and p_1 . The measurement procedure can have up to three outcomes, associated with identifying the state as ρ_0 , identifying the state as ρ_1 , and failing to identify the state conclusively. The most general three-outcome measurement is represented in quantum mechanics by a three-element POVM, which we denote by ${E_0, E_1, E_2}$. Because the identification must never be in error, we require that

$$
Tr(\rho_0 E_1) = Tr(\rho_1 E_0) = 0.
$$
 (1)

¹The *support* of a mixed state is the space spanned by its eigenvectors with nonzero eigenvalues; the *kernel* is the space orthogonal to its support.

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The probability *P* of successful UD is

$$
P = p_0 \text{Tr}(\rho_0 E_0) + p_1 \text{Tr}(\rho_1 E_1). \tag{2}
$$

We shall denote the kernel of ρ_b by K_b (*b*=0,1). It is clear that any intersection of K_0 and K_1 is not useful for the purposes of discriminating ρ_0 and ρ_1 since neither state has any overlap with this subspace. We shall therefore assume, in what follows, that the Hilbert space is equal to the span of the supports of ρ_0 and ρ_1 . A necessary and sufficient condition for satisfying Eq. (1) is that the POVM element E_0 (E_1) have support only in the subspace \mathcal{K}_1 (\mathcal{K}_0). It follows that for there to be a nonzero probability of success, at least one of K_0 and K_1 must be nonzero. This occurs if and only if the support of ρ_0 is not equal to the support of ρ_1 .

We seek to maximize Eq. (2) subject to Eq. (1) and the constraint that E_0 , E_1 , and E_2 be positive and sum to the identity. It suffices to vary over positive E_0 and E_1 , which satisfy

$$
I - E_0 - E_1 \ge 0. \tag{3}
$$

This optimization problem is an instance of a semidefinite programming problem for which there exist efficient numerical algorithms. (See Ref. $[6]$ for applications of semidefinite programming to UD of pure states, and Refs. $[7,8]$ for applications to the problem of optimizing the discrimination probability between mixed states for a fixed error rate, which interpolates between maximum likelihood estimation and $UD.$)

III. SOLUTIONS IN CERTAIN SPECIAL CASES

A. Mixed states with orthogonal kernels

If $K_0 \perp K_1$, the optimal POVM which satisfies Eq. (3) is clearly $E_0 = K_1$, $E_1 = K_0$, where K_b is the projector onto K_b . This yields a probability of success, $P^{\text{max}} = p_0 \text{Tr}(\rho_0 K_1)$ $+p_1Tr(\rho_1K_0)$. Note that this solution also applies when one of the kernels is zero. Note also that commuting mixed states necessarily have orthogonal kernels. It follows that this result specifies the maximum probability of UD for overlapping classical probability distributions.

B. Mixed states with one-dimensional kernels

We now turn to the special case wherein the kernels are both one-dimensional—that is, the states ρ_0 and ρ_1 have rank $n-1$, and the span of their supports is an *n*-dimensional space. Denoting by $|k_b\rangle\langle k_b|$ the projector onto \mathcal{K}_b , the POVM must be of the form ${E_0 = \alpha |k_1\rangle\langle k_1|, E_1}$ $= \beta |k_0\rangle\langle k_0|, E_\gamma = I - \alpha |k_1\rangle\langle k_1| - \beta |k_0\rangle\langle k_0|$. Our task therefore becomes to compute

$$
P^{\max} = \max_{\alpha,\beta} (\alpha p_0 \langle k_1 | \rho_0 | k_1 \rangle + \beta p_1 \langle k_0 | \rho_1 | k_0 \rangle), \qquad (4)
$$

where the maximization is subject to the constraint

$$
I - \alpha |k_1\rangle\langle k_1| - \beta |k_0\rangle\langle k_0| \ge 0. \tag{5}
$$

For convenience, we define θ to be the angle in Hilbert space between the one-dimensional kernels,

$$
\cos^2 \theta \equiv |\langle k_0 | k_1 \rangle|^2. \tag{6}
$$

Taking the minimum eigenvalue of the left hand side of Eq. (5) , we can reexpress this inequality as

$$
\frac{1}{2} [\alpha + \beta + \sqrt{(\alpha - \beta)^2 + 4 \alpha \beta \cos^2 \theta}] \le 1.
$$
 (7)

Solving for P^{max} under this constraint, we find that if $\cos\theta$ $\langle \sqrt{A_{\text{min}}/A_{\text{max}}} \rangle$ then $\alpha^{\text{opt}} = (1 - \sqrt{A_1 / A_0} \cos \theta)/\sin^2 \theta$, $\beta^{\text{opt}} = (1 - \sqrt{A_1 / A_0})$ $-\sqrt{A_0/A_1} \cos \theta / \sin^2 \theta$; otherwise $\alpha^{opt}=1$, $\beta_{opt}=0$ (*A*₁ $\langle A_0 \rangle$ or $\alpha^{\text{opt}}=0$, $\beta^{\text{opt}}=1$ ($A_0 \langle A_1 \rangle$). This yields

$$
P^{\max} = \begin{cases} \frac{A_0 + A_1 - 2\cos\theta\sqrt{A_0 A_1}}{\sin^2\theta} & \text{if } \cos\theta < \sqrt{\frac{A_{\min}}{A_{\max}}} \\ A_{\max} & \text{otherwise.} \end{cases}
$$
(8)

Here, $A_0 = p_0(k_1|\rho_0|k_1)$, $A_1 = p_1(k_0|\rho_1|k_0)$, and A_{\min} $\min\{A_0, A_1\}, A_{\text{max}} = \max\{A_0, A_1\}.$ This solution, considered as a function of $|k_0\rangle$ and $|k_1\rangle$, will be denoted as $P_{1D}^{\max}(|k_0\rangle,|k_1\rangle).$

The problem of unambiguously discriminating two nonorthogonal pure states $|\psi_0\rangle$, $|\psi_1\rangle$ is a special case of the one-dimensional kernel problem. Although $\cos \theta$ is defined to be the overlap of the one-dimensional kernels, clearly $|\langle \psi_0|\psi_1\rangle| = \cos \theta$, and Eq. (8) becomes

$$
P^{\max} = \begin{cases} 1 - 2\sqrt{p_0 p_1} |\langle \psi_0 | \psi_1 \rangle| & \text{if } |\langle \psi_0 | \psi_1 \rangle| < \sqrt{\frac{p_{\min}}{p_{\max}}} \\ p_{\max} (1 - |\langle \psi_0 | \psi_1 \rangle|^2) & \text{otherwise,} \end{cases}
$$
(9)

in agreement with Ref. [3]. In the case of equal prior probabilities, we have $P^{\text{max}}=1-\frac{|\langle \psi_0 | \psi_1 \rangle|}{\langle \psi_1 | \psi_1 \rangle}$, as expected from Ref. $[2]$.

IV. LOWER BOUND

We consider a strategy that achieves UD of an arbitrary pair of mixed states and which is strongly dependent on the geometrical relationship between the two subspaces \mathcal{K}_0 and \mathcal{K}_1 :

Theorem. Consider two arbitrary mixed states ρ_0 and ρ_1 . Denote the dimensionality of their kernels \mathcal{K}_0 and \mathcal{K}_1 by r_0 and r_1 , and assume that $r_0 \ge r_1$. There exist orthonormal bases $\{ |k_b^j\rangle \}_{j=1}^{r_b}$ for $\mathcal{K}_b(b=0,1)$ such that for $1 \leq j \leq r_0$, 1 $\leq i \leq r_1$

$$
\langle k_0^j | k_1^i \rangle = \delta_{ij} \cos(\theta_j), \qquad (10)
$$

where the θ_i are the canonical angles between \mathcal{K}_0 and \mathcal{K}_1 [13]. In this case,

$$
P^{\max} \leq \sum_{j=1}^{r_1} P_{1D}^{\max}(|k_0'\rangle, |k_1'\rangle) + \sum_{j=r_1+1}^{r_0} \langle k_0^j | \rho_1 | k_0^j \rangle \quad (11)
$$

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expresses a lower bound on the maximum probability of discriminating unambiguously between ρ_0 and ρ_1 .

Proof. The proof is constructive. Let X_b be any $n \times r_b$ dimensional matrix whose orthonormal columns span \mathcal{K}_b . Define an $r_b \times r_b$ unitary matrix U_b , and an $r_0 \times r_1$ matrix *S* via a singular-value decomposition $[13]$,

$$
X_0^\dagger X_1 = U_0 S U_1^\dagger. \tag{12}
$$

The matrix *S* is of the form $S = \begin{bmatrix} C \\ O \end{bmatrix}$, where *C* is a diagonal matrix of the form $C = \text{diag}(\cos \theta_1, \dots, \cos \theta_{r_1}), \theta_i$ $\in [0,\pi/2]$, while *O* is an $(r_0-r_1)\times r_1$ matrix of 0's. Defining $\theta_j = \pi/2$ for $j > r_1$, and denoting by $|k_b^i\rangle$ the *i*th column of $X_b U_b$, we have constructed *canonical* bases for K_0 and K_1 , that is, bases satisfying $\langle k_0^j | k_1^i \rangle = \delta_{ij} \cos \theta_i$, as required in the theorem.

The measurement achieving the lower bound is associated with the POVM that has $E_0 = \sum_{i=1}^{r_1} \alpha_i |k_1^i\rangle \langle k_1^i|$ and E_1 $=\sum_{i=1}^{r_0} \beta_i |k_0^i\rangle\langle k_0^i|$. Constraint (3) takes the form

$$
I - \sum \alpha_i |k_1^i\rangle\langle k_1^i| - \sum \beta_i |k_0^i\rangle\langle k_0^i| \ge 0. \tag{13}
$$

Since the two-dimensional subspace spanned by $|k_0^j\rangle$ and $|k_1^j\rangle$ for $1 \le j \le r_1$ is orthogonal to all other such subspaces and is orthogonal to $|k_0^j\rangle$ for $r_1 < j \le r_0$, constraint (13) reduces to constraints of the form (5) for $1 \le j \le r_1$, and constraints of the form $I - \beta_j |k_0^j\rangle \langle k_0^j| \ge 0$ for $r_1 < j \le r_0$. In this manner, we have reduced the problem to r_1 separate optimizations of the form already considered in Sec. III B. Solving each of these yields the first term on the right-hand side of Eq. (11) in the theorem. The remaining $r_0 - r_1$ optimizations are achieved by taking $\beta_j = 1$, which yields the second term on the right-hand side of Eq. (11) .

In order to understand the geometry of the eigenbases for the POVM elements in this lower bound, it is helpful to realize that the canonical angles θ_i form the unique geometrical invariants describing the relationship between two subspaces. They can be defined iteratively: θ_1 is the smallest angle between any pair of vectors drawn from \mathcal{K}_0 and \mathcal{K}_1 , and $|k_0^1\rangle, |k_1^1\rangle$ are the corresponding pair of vectors. θ_2 is the smallest such angle after these two vectors are removed, and so on. In this way, one obtains a simple geometrical picture of the measurement achieving the lower bound. We note that we have not found any example of UD wherein this lower bound is not optimal. Nonetheless, given that the eigenbases for E_0 , E_1 depend only on the subspaces spanned by ρ_0 , ρ_1 , and not on the states themselves, there is no reason to expect it to be optimal in the general case.

V. UPPER BOUND

Theorem. An upper bound on the maximum probability of unambiguously discriminating two mixed states, ρ_0 and ρ_1 , is

$$
P^{\max} \leqslant \begin{cases} 1 - 2\sqrt{p_0 p_1} F(\rho_0, \rho_1) & \text{if } F(\rho_0, \rho_1) < \sqrt{\frac{p_{\min}}{p_{\max}}}, \\ p_{\max} [1 - F(\rho_0, \rho_1)^2] & \text{otherwise}, \end{cases} \tag{14}
$$

where $F(\rho_0, \rho_1) = \text{Tr}[\sqrt{\rho_0} \sqrt{\rho_1}]$ is the fidelity.

Proof. Let $|\psi_b\rangle$ be a purification of ρ_b [14]. Clearly, UD of $|\psi_0\rangle$, $|\psi_1\rangle$ with priors p_0 , p_1 can be achieved with a maximal probability of success that is greater than or equal to the maximum probability of success in the UD of ρ_0 , ρ_1 with the same priors. This follows from the fact that any discrimination procedure for the latter task serves also as a discrimination procedure for the former task. Thus,

$$
P^{\max}(p_0 \rho_0, p_1 \rho_1) \leq \min_{|\psi_0\rangle, |\psi_1\rangle} P^{\max}(p_0|\psi_0\rangle \langle \psi_0|, p_1|\psi_1\rangle \langle \psi_1|),
$$

where the minimization is over all purifications of ρ_b . We know, however, that $P^{\max}(p_0|\psi_0\rangle\langle\psi_0|,p_1|\psi_1\rangle\langle\psi_1|)$ is given by Eq. (9) . Minimizing either of the expressions on the righthand side of Eq. (9) requires maximizing $|\langle \psi_0|\psi_1\rangle|$. Uhlmann's theorem $[14]$ states that the maximum overlap between purifications of two density operators is equal to the fidelity between the density operators. Applying this observation yields the desired upper bound.

In the case of equal prior probabilities, the upper bound has the simple form $P^{\text{max}} \leq 1 - F(\rho_0, \rho_1)$. Numerical studies of rank-2 mixed states in a four-dimensional Hilbert space indicate that even for randomly chosen ρ_0 and ρ_1 , our upper and lower bounds are generally very close.

VI. SOME APPLICATIONS

A. State comparison

In Ref. [9], Barnett, Chefles, and Jex introduced the following problem: given two systems, each of which is in one of two (generally nonorthogonal) states $\{|\psi_1\rangle,|\psi_2\rangle\}$, with what probability can one determine whether the two systems are in the same state or in different states? Here, we consider the case where this determination must be made without error, if at all. Assuming equal likelihood for either possibility, we can clearly interpret the problem as one of achieving UD of the two mixed states

$$
\rho_0 = \frac{1}{2} |\psi_1 \psi_1\rangle \langle \psi_1 \psi_1| + \frac{1}{2} |\psi_2 \psi_2\rangle \langle \psi_2 \psi_2|
$$

$$
\rho_1 = \frac{1}{2} |\psi_1 \psi_2\rangle \langle \psi_1 \psi_2| + \frac{1}{2} |\psi_2 \psi_1\rangle \langle \psi_2 \psi_1|,
$$
 (15)

as was recognized by the authors of Ref. $[9]$.

These are rank-2 mixed states in a four-dimensional space; as such, their kernels are also two-dimensional. We let $|\bar{\psi}_i\rangle$ be the state orthogonal to $|\psi_i\rangle$, and choose phases such that $\langle \bar{\psi}_1 | \bar{\psi}_2 \rangle$ is real. It is clear that K_0 is spanned by $\{[\bar{\psi}_1 \bar{\psi}_2], [\bar{\psi}_2 \bar{\psi}_1]\},$ while K_1 is spanned by $\{[\bar{\psi}_1 \bar{\psi}_1], [\bar{\psi}_2 \bar{\psi}_2]\}.$ Using the techniques of Sec. IV, we find that the canonical basis vectors in K_0 are $|k_0^1\rangle = |\bar{\psi}_1 \bar{\psi}_2\rangle + |\bar{\psi}_2 \bar{\psi}_1\rangle$, $|k_0^2\rangle$ $= |\overline{\psi}_1 \overline{\psi}_2 \rangle - |\overline{\psi}_2 \overline{\psi}_1 \rangle$, while those of \mathcal{K}_1 are $|k_1^1 \rangle = |\overline{\psi}_1 \overline{\psi}_1 \rangle$ $+\vert \bar{\psi}_2 \bar{\psi}_2 \rangle$, $\vert k_1^2 \rangle = \vert \bar{\psi}_1 \bar{\psi}_1 \rangle - \vert \bar{\psi}_2 \bar{\psi}_2 \rangle$ (all suitably normalized).

Since $\langle k_0^2 | k_1^2 \rangle = 0$, these two states can be included in their respective POVM elements with weight 1, i.e., $\alpha_2 = 1 = \beta_2$. The remaining pair of states have overlap cos $\theta_1 = \langle k_0^1 | k_1^1 \rangle$, and we can use the solution for one-dimensional kernels. Performing this calculation, we find that our lower bound is 1 $-F(\rho_0, \rho_1)$. Since this is equal to our upper bound, we automatically know that this is optimal, and we have the optimal POVM by construction.

B. State filtering

A problem that has been considered recently by Sun, Bergou, and Hillery [10] is that of unambiguously discriminating whether a state is $|\psi_1\rangle$ or whether it is in the set $\{\ket{\psi_2},\ket{\psi_3}\}\$ when the prior probabilities of the three states are η_1, η_2 , and η_3 , respectively. This task has been called *state filtering*. It is straightforward to see that it is an instance of UD of mixed states. Specifically, it is the problem of unambiguously discriminating

$$
\rho_0\!=\!|\psi_1\rangle\langle\psi_1|,\quad\rho_1\!=\!\frac{\eta_2}{\eta_2\!+\eta_3}|\psi_2\rangle\langle\psi_2|+\frac{\eta_3}{\eta_2\!+\eta_3}|\psi_3\rangle\langle\psi_3|,
$$

with prior probabilities $p_0 = \eta_1, p_1 = \eta_2 + \eta_3$. It is easy to find our lower bound for this problem. Since \mathcal{K}_1 is one dimensional, we associate it with a unique vector $|k_1\rangle$. The kernel K_0 is two-dimensional, and so there is flexibility in the basis that diagonalizes E_1 . Our lower bound dictates that we use the basis $|k_0^1\rangle$, $|k_0^2\rangle$, where $|k_0^1\rangle$ is the vector in \mathcal{K}_0 that is maximally parallel to $|k_1\rangle$, and $|k_0\rangle$ is the vector in \mathcal{K}_0 that is orthogonal to both $|k_1\rangle$ and $|k_0\rangle$. Our lower bound is $P_L = P_{1D}^{\text{max}}(|k_0^1\rangle, |k_1\rangle) + \langle k_0^2 | \rho_1 | k_0^2 \rangle$. Defining the canonical angle θ by $\cos \theta = \langle k_1 | k_0 \rangle$ and appealing to the geometry of the problem, we find $A_0 = p_0(1-\cos^2\theta)$ of the problem, we find $A_0 = p_0(1 - \text{cc}$
and $A_1 = p_1 F(\rho_0, \rho_1)^2 \tan^2 \theta$. Finally, defining *F* $\equiv F(\rho_0, \rho_1)/\sqrt{p_0 / p_1}$, the lower bound takes the following form:

$$
P^{\max} \geqslant \begin{cases} 1 - p_0 \cos^2 \theta - \frac{p_1}{\cos^2 \theta} F(\rho_0, \rho_1)^2, & \tilde{F} \leqslant \cos^2 \theta \\ 1 - 2\sqrt{p_0 p_1} F(\rho_0, \rho_1), & \cos^2 \theta \leqslant \tilde{F} \leqslant 1 \\ p_1 [1 - F(\rho_0, \rho_1)^2], & \tilde{F} \geqslant 1. \end{cases}
$$

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This coincides precisely with the optimal solution derived in Ref. $[10]$. Thus, our lower bound is found to be optimal in this case.

By recasting state filtering as an instance of UD of a pure state and a mixed state, it has become apparent that the particular ensemble of states from which the mixed state is formed (in this case, $|\psi_2\rangle$ and $|\psi_3\rangle$ with priors η_2 and η_3) is not significant. As such, our analysis applies also to the case wherein the second set of states contains an arbitrary number of elements, in agreement with the solution found in Ref. [11]. Moreover, the mixed state need not even arise as a result of ignorance of the pure state, but rather may arise as a result of the system being entangled with another degree of freedom. This is confirmed by the fact that the probability of success depends only on ρ_1 . The problem of UD between multiple sets of pure states $[15]$ is a straightforward generalization of state filtering that can be recast as a problem of UD of mixed states in a similar way.

VII. CONCLUSION

We have shown that UD of a pair of mixed states is possible when these have distinct supports. We have provided the maximum probability of success for the case of mixed states with orthogonal or one-dimensional kernels. In the general case, we have determined an upper bound based on the probability of UD for purifications of the states, and a lower bound based on the geometrical invariants between their kernels. In addition to the tasks discussed here, there are likely to be many others for which UD of mixed states may be useful, such as quantum random access codes, quantum oblivious transfer, and entanglement distillation, to name a few.

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