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Unambiguous discrimination of mixed quantum states: Optimal solution and case study

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We present a generic study of the unambiguous discrimination between two mixed quantum states. We derive operational optimality conditions and show that the optimal measurements can be classified according to their rank. In Hilbert space dimensions less than or equal to 5, this leads to the complete optimal solution. We demonstrate our method with a physical example, namely, the unambiguous comparison of n quantum states, and find the optimal success probability.

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According to the laws of quantum mechanics, two nonorthogonal quantum states cannot be distinguished perfectly. This fact has far-reaching consequences in quantum-information processing; e.g., it allows one to generate a secret random key in quantum cryptography. In spite of the fundamental nature of the problem of state discrimination, determining the *optimal* measurement to distinguish two (mixed) quantum states is far from being trivial.

In the literature, two main paths to state discrimination have been taken [1]. First, in *minimum error discrimination*, the unavoidable error in distinguishing two states from each other is minimized. This problem has been completely solved in Ref. [2]. Second, in *unambiguous state discrimination* (USD), no error is allowed, but an inconclusive answer may occur. The optimal USD measurement minimizes the probability of an inconclusive answer [3–5]. Although USD has received much attention in recent years, and special examples have been solved, no general solution is known so far for the case of mixed states. A strategy that is analogous to USD but applicable also to linearly dependent states is discussed in Ref. [6].

The aim of this Rapid Communication is to present the optimal USD measurement for cases that cannot be reduced to the discrimination of pure states and thus to known solutions. This analysis can be applied to the unambiguous discrimination of *any* two density operators acting on a Hilbert space of up to five dimensions. This goes beyond previous results which require a high symmetry or other very special properties of the given states [7–13]. We will show the main ideas and steps toward the solution; we explain the technical details elsewhere [14].

The scenario of optimal unambiguous discrimination of two density operators is as follows: two (normalized) density operators ϱ_1 and ϱ_2, acting on a finite-dimensional Hilbert space $\mathscr{H}$ occur with *a priori* probability p_1 and p_2, respectively, where $p_1 + p_2 = 1$. We will denote the support of a density operator ϱ as the orthocomplement of its kernel, $(\operatorname{supp}\varrho)^\perp = \ker\varrho$. A measurement for USD is described by a positive operator valued measure (POVM), i.e., a family of positive semidefinite operators $\{E_1, E_2, E_?\}$ with $E_1 + E_2 + E_? = \mathbb{1}$, obeying the constraints for unambiguity, $\operatorname{tr}(E_2\varrho_1) = 0$ and $\operatorname{tr}(E_1\varrho_2) = 0$. The operator $E_?$ corresponds to the inconclusive outcome, while E_1 and E_2 correspond to the successful detection of ϱ_1 and ϱ_2, respectively. The aim is to find a POVM that maximizes the success probability $P_{\text{succ}} = p_1\operatorname{tr}(E_1\varrho_1) + p_2\operatorname{tr}(E_2\varrho_2)$. Let us introduce here the useful notation $\gamma_1 = p_1\varrho_1$ and $\gamma_2 = p_2\varrho_2$. Thus, the success probability reads $P_{\text{succ}} = \operatorname{tr}(E_1\gamma_1) + \operatorname{tr}(E_2\gamma_2)$.

What are the relevant structures of the density operators and measurement operators? The unambiguity condition $\operatorname{tr}(E_2\gamma_1) = 0$ means that the support of E_2 is a subspace of the kernel of γ_1. The second unambiguity condition reads $\operatorname{supp} E_1 \subset \ker\gamma_2$. Obeying these constraints, one has to maximize the sum of the scalar products $\operatorname{tr}(E_1\gamma_1)$ and $\operatorname{tr}(E_2\gamma_2)$, while keeping $E_?$ positive. Due to the reduction theorems in Ref. [8], the optimization problem reduces to the case of a *strictly skew* pair of (unnormalized) density operators. The operators γ_1 and γ_2 are called strictly skew, when they possess neither any parallel component, i.e., $\operatorname{supp}\gamma_1 \cap \operatorname{supp}\gamma_2 = \{0\}$, nor any orthogonal components, i.e., $\operatorname{supp}\gamma_1 \cap \ker\gamma_2 = \{0\}$ and $\operatorname{supp}\gamma_2 \cap \ker\gamma_1 = \{0\}$. A simple example for a strictly skew pair of unnormalized density operators is any pair of pure states, $\gamma_1 = p|\phi_1\rangle\langle\phi_1|$ and $\gamma_2 = (1-p)|\phi_2\rangle\langle\phi_2|$, with $0 < |\langle\phi_1|\phi_2\rangle| < 1$ and $0 < p < 1$. Both operators of such a strictly skew pair have the same rank, and the sum of both ranks cannot exceed the dimension of the underlying Hilbert space. Below we will show a constructive method to discriminate two skew density operators of rank 2. This solves optimal USD in all cases where one of the given states has rank 2, and hence in particular the case with a Hilbert space of up to five dimensions.

In the following we will only consider skew pairs of unnormalized density operators and proper USD measurements. We call a USD measurement "proper" if it satisfies $\operatorname{supp}(E_1 + E_2) \subset \operatorname{supp}(\gamma_1 + \gamma_2)$. It is sufficient to only consider proper measurements, since the subspace $\ker\gamma_1 \cap \ker\gamma_2$ cannot contribute to the success probability [15].

In Ref. [16], Eldar and collaborators showed that the optimality of a USD measurement can be proved via the existence of a certain operator that fulfills a set of conditions. However, no constructive way to find this operator was provided. Starting from these conditions we derive the following set of necessary and sufficient requirements for the optimality of a proper USD measurement:

$$E_?(\gamma_2 - \gamma_1)E_?(\mathbb{1} - E_?) = 0, \tag{1a}$$

$$\Lambda_1 E_?(\gamma_2 - \gamma_1)E_?\Lambda_2 = 0, \tag{1b}$$

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$$\Lambda_1 E_?(\gamma_2 - \gamma_1) E_? \Lambda_1 \geqslant 0, \tag{1c}$$
$$\Lambda_2 E_?(\gamma_1 - \gamma_2) E_? \Lambda_2 \geqslant 0. \tag{1d}$$

Here, Λ_1 is the projector onto $\ker \gamma_2$, and Λ_2 is the projector onto $\ker \gamma_1$. The details of the derivation are presented elsewhere [14]. Note that the methods used to arrive at Eqs. (1) cannot be generalized to the discrimination of more than two states. (For special cases, however, see Ref. [17].)

Let us point out two observations from Eqs. (1). First, neither E_1 nor E_2, but only the operator $E_?$ appears in this set of equations. This is due to the fact that from $E_?$ it is possible to uniquely reconstruct E_1 and E_2, as $E_i \gamma_i = \gamma_i - E_? \gamma_i$ holds for $i = 1, 2$. Second, neither $\gamma_1 - \gamma_2 \geqslant 0$ nor $\gamma_2 - \gamma_1 \geqslant 0$ can hold for a strictly skew pair of operators, and thus it is nontrivial to fulfill Eqs. (1c) and (1d). The set of equations (1a)–(1d) provides an efficient tool in optimal USD: one might be able to guess a measurement, e.g., from the symmetry of a given USD problem, and then verify easily whether it is optimal. Moreover, one can use these equations in a constructive way in order to find the solution for $E_?$, which then uniquely defines an optimal POVM. Below, we will show explicitly how to construct the optimal measurement from Eqs. (1) for the example of state comparison.

It has been an open question as to whether the optimal USD measurement is unique. This is indeed the case. The structure of the proof is as follows: As pointed out above, a USD measurement is already defined via $E_?$. It can be shown [14] that for optimal proper measurements, the rank of $E_?$ is fixed, namely, $\operatorname{rank} E_? = \operatorname{rank}(\gamma_1\gamma_2) + \dim\ker(\gamma_1 + \gamma_2)$. Assuming that there would be two optimal operators $E_?$ and $E'_?$, their convex combination $\frac{1}{2}(E_? + E'_?)$ would also describe an optimal measurement. However, for positive semidefinite operators $E_?$ and $E'_?$, the identity $\operatorname{rank}(E_? + E'_?) = \operatorname{rank} E_? = \operatorname{rank} E'_?$ can only hold if $\operatorname{supp} E_? = \operatorname{supp} E'_?$. When the support of $E_?$ is given, the operator $E_?$ is uniquely determined via Eq. (1a). Thus, the optimal proper USD measurement is unique.

The uniqueness of the optimal measurement now allows a meaningful characterization of the optimal USD measurement. We introduce a classification of the different types of optimal USD measurements according to the rank of the measurement operators E_1 and E_2. A measurement type is specified by $(\operatorname{rank} E_1, \operatorname{rank} E_2)$. This classification turns out to be vital for the construction of optimal measurement strategies from Eqs. (1). For given density operators ϱ_1 and ϱ_2 and a given *a priori* probability $p_1 = 1 - p_2$, one particular measurement type is optimal, due to the uniqueness of the optimal solution. While varying p_1, some or all of these measurement types may occur, see Fig. 1 for an illustration. With $r = \operatorname{rank} \gamma_1 = \operatorname{rank} \gamma_2$, one arrives at the constraints $\operatorname{rank} E_1 \leqslant r$, $\operatorname{rank} E_2 \leqslant r$, and

$$r \leqslant \operatorname{rank} E_1 + \operatorname{rank} E_2 \leqslant 2r. \tag{2}$$

Equation (2) follows from the geometry of unambiguous measurements and the fact that in the optimal case $\operatorname{rank} E_? = \dim\ker \gamma_1\gamma_2$ holds. The two extremal cases where either the lower or the upper bound in Eq. (2) is reached correspond to special situations.

The case of the upper bound in Eq. (2), where $\operatorname{rank} E_1 = r = \operatorname{rank} E_2$, is the well-understood *fidelity form measurement*.

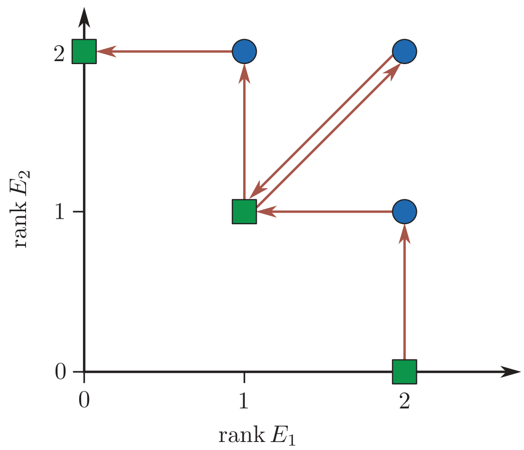

FIG. 1. (Color online) USD measurement types for $r = 2$, as allowed by the constraint in Eq. (2). Projective measurements are indicated by squares, nonprojective ones by circles. The arrows illustrate an example for a possible path between the measurement types, while the probability p_2 is varied from $p_2 = 0$ to $p_2 = 1$. The start point is necessarily type (2,0), and the end point type (0,2). The types (0,2), (2,0), and (2,2) will only occur once. Which other types are visited in between, and in which order, depends on the concrete example.

Intuition might tell us that the success probability should be a function of some distance measure between the two states (this is indeed true for minimum error discrimination, where the smallest achievable error probability is a function of the trace distance between the unnormalized density operators). Here, for the case with $\operatorname{rank} E_1 = r = \operatorname{rank} E_2$, the success probability is the square of the Bures distance, i.e., $P_{\text{fid}} = 1 - 2\operatorname{tr}|\sqrt{\gamma_1}\sqrt{\gamma_2}|$ [10,11,14,15] (while, in general, P_{fid} is an upper bound on the success probability [15]). In fact, formally, the construction of the fidelity form measurement is always possible [11], and the resulting operator $E_?$ always satisfies all conditions in Eqs. (1). However, this operator in general fails to satisfy the condition $\mathbb{1} - E_? \geqslant 0$. The measurement types for which $\operatorname{rank} E_1 + \operatorname{rank} E_2 < 2r$ occur because of this very positivity condition. In a geometric language, the optimal measurement is on the border of the allowed (positive) measurements, unless $\operatorname{rank} E_1 = r = \operatorname{rank} E_2$. One can compute two numbers p_{low} and p_{up} for given ϱ_1 and ϱ_2, such that the fidelity form measurement is optimal if and only if $p_{\text{low}} \leqslant p_1 \leqslant p_{\text{up}}$.

In the case of the lower bound of Eq. (2), where $\operatorname{rank} E_1 + \operatorname{rank} E_2 = r$, the operators E_1, E_2, and $E_?$ are projectors, i.e., the optimal measurement is a von Neumann measurement. A special situation occurs when $\operatorname{rank} E_1 = 0$ and $\operatorname{rank} E_2 = r$ or $\operatorname{rank} E_1 = r$ and $\operatorname{rank} E_2 = 0$. This is interpreted as follows: For very small p_1, it will turn out to be advantageous to ignore ϱ_1 by choosing $E_1 = 0$. This case is referred to as the *single-state detection* of ϱ_2, because the state ϱ_1 is never detected. As then $E_? = \mathbb{1} - E_2$, from Eqs. (1) only Eq. (1c) remains, and this inequality can be written as

$$\gamma_1(\gamma_2 - \gamma_1)\gamma_1 \geqslant 0. \tag{3}$$

The success probability for single-state detection of γ_2 is given by $P_{\text{succ}} = \operatorname{tr}(\Lambda_2\gamma_2)$, where Λ_2 was defined above as the projector onto $\ker \gamma_1$. Equation (3) implicitly defines a

TABLE I. Measurement types for the case $r = 2$. For details about the properties, see main text.

Rank E_1	Rank E_2	Type	Properties
0	2	(0,2)	Single-state detection, projective
1	2	(1,2)	Nonprojective measurement
2	2	(2,2)	Fidelity form measurement, nonproj.
1	1	(1,1)	Projective measurement, see example
2	1	(2,1)	Nonprojective measurement
2	0	(2,0)	Single-state detection, projective

calculable threshold for p_1, below which it is advantageous not to detect ϱ_1. This threshold is always larger than 0, i.e., single-state detection is always optimal for a finite regime. Analogous considerations hold for small p_2.

So far our considerations have been independent of r. Let us now consider specific values for r. For $r = 1$, i.e., the case of pure states, only the single-state detection measurement or the fidelity form measurement may occur. Hence the problem of unambiguous discrimination of pure states is well understood [18]. Furthermore, any USD task where the two density operators can simultaneously be brought in a diagonal form with 2×2-dimensional blocks (the "block-diagonal" case) can also be solved by treating the corresponding orthogonal subspaces independently [9,11,19]. For all other cases, only solutions for special cases are known [10–13]. For $r = 2$ there are six possible measurement types, which are summarized in Table I. The optimal measurements for types (1,2), (2,1), and (1,1) remain to be determined. For each of these types, Eqs. (1) reduce to a polynomial equation [14] and hence the analytic solution for the case $r = 2$ is completed.

Let us now study the important example of a quantum-state comparison and demonstrate explicitly how to solve Eqs. (1) for the case of measurement type (1,1), which occurs for a wide range of parameters. We consider the state comparison of n pure quantum states, where each of the states is taken from the set $\{|\psi_1\rangle, |\psi_2\rangle\}$, with corresponding *a priori* probabilities $\{\eta_1, \eta_2\}$, $\eta_1 + \eta_2 = 1$. In quantum-state comparison [10,15,19–22], one aims at answering the question of whether the given n quantum states are equal or not. Applications of this task in quantum information are, e.g., quantum fingerprinting [23] and quantum digital signatures [24]. For $n = 2$, the optimal unambiguous measurement for quantum-state comparison has been given in Refs. [10,22]. For $n \geqslant 3$, the corresponding USD task reduces to the unambiguous discrimination of two mixed states of rank 2, i.e., $r = 2$.

State comparison of n states is equivalent to the discrimination of (cf. Ref. [22])

$$\gamma_e = (\eta_1 |\psi_1\rangle\langle\psi_1|)^{\otimes n} + (\eta_2 |\psi_2\rangle\langle\psi_2|)^{\otimes n}, \tag{4}$$

$$\gamma_d = (\eta_1 |\psi_1\rangle\langle\psi_1| + \eta_2 |\psi_2\rangle\langle\psi_2|)^{\otimes n} - \gamma_e. \tag{5}$$

Due to Theorem 2 in Ref. [8], it remains to consider the reduced operators γ_e^r and γ_d^r, which are given by the projection of γ_e and γ_d onto (supp γ_e + ker γ_d), respectively. It is straightforward to see that for $n \geqslant 3$ this discrimination task cannot be reduced further and that no block-diagonal structure is present unless $\eta_1 = \eta_2 = \frac{1}{2}$.

We next construct a basis of supp γ_e and of ker γ_d. A convenient basis of supp γ_e is given by

$$|\phi_\pm\rangle \propto |\psi_1\rangle^{\otimes n} \pm |\psi_2\rangle^{\otimes n}. \tag{6}$$

We define $c = \langle\psi_1|\psi_2\rangle$ with $0 < c < 1$. Using $|\psi_1^\perp\rangle \propto |\psi_2\rangle - c|\psi_1\rangle$ and $|\psi_2^\perp\rangle \propto |\psi_1\rangle - c|\psi_2\rangle$, a basis of ker γ_d can be constructed as

$$|\omega_\pm\rangle \propto |\psi_1^\perp\rangle^{\otimes n} \pm |\psi_2^\perp\rangle^{\otimes n}. \tag{7}$$

Now a Gram-Schmidt orthogonalization of $\{|\phi_+\rangle, |\phi_-\rangle, |\omega_+\rangle, |\omega_-\rangle\}$ yields the orthonormal basis $\{|\phi_+\rangle, |\phi_-\rangle, |\sigma_+\rangle, |\sigma_-\rangle\}$ of supp γ_e + ker γ_d. Then $\{|\sigma_+\rangle, |\sigma_-\rangle\}$ is an orthonormal basis of ker $\gamma_e^r \cap$ supp $(\gamma_e^r + \gamma_d^r)$, while $\{|\omega_+\rangle, |\omega_-\rangle\}$ is an orthonormal basis of ker $\gamma_d^r \cap$ supp $(\gamma_e^r + \gamma_d^r)$. In fact, they form Jordan bases (see, e.g., Refs. [15,25]) of these subspaces, i.e., $\langle\sigma_\mp|\omega_\pm\rangle = 0$. The remaining overlaps $\langle\sigma_\pm|\omega_\pm\rangle$ are equal for odd n (*degenerate Jordan angles*). We now study for general but odd $n \geqslant 3$ the solution of the conditions in Eqs. (1) while restricting our considerations to the measurement type (1,1).

The measurements of type (1,1) are von Neumann measurements, where E_e and E_d both have rank 1, i.e., $E_e = |\chi_e\rangle\langle\chi_e|$ and $E_d = |\chi_d\rangle\langle\chi_d|$. In particular, the vectors $|\chi_e\rangle$ and $|\chi_d\rangle$ must be orthogonal and normalized. We use the parametrization $|\chi_e\rangle \propto |\omega_+\rangle + x^*|\omega_-\rangle$ and $|\chi_d\rangle \propto x|\sigma_+\rangle - |\sigma_-\rangle$, where x is a complex variable.[1]

We now evaluate the necessary and sufficient conditions for optimality in Eqs. (1). Equation (1) is satisfied for any x. Let us abbreviate $\langle\omega_a|\gamma_e|\omega_b\rangle = G_e^{ab}$ and $\langle\sigma_a|\gamma_d|\sigma_b\rangle = G_d^{ab}$, where $a, b \in \{+, -\}$. Equation (1b) now becomes a scalar equation which is only quadratic in x; in matrix notation, Eq. (1b) reads

$$(1, x)(G_e - G_d)(-x, 1)^T = 0. \tag{8}$$

Similarly, the positivity conditions (1c) and (1d) simplify to scalar inequalities.

With the help of a computer algebra system, we obtain for $n = 3$ the optimal success probability

$$P_{\text{succ}}^{(1,1)} = \frac{1}{4}\frac{(1-c^2)^2}{1-c^6}\{(c^4 + 4c^2 + 1)\,\alpha + (1-c^2)(2 + \sqrt{W}\,)\}, \tag{9}$$

with $W = [(1-c^6)\alpha^2 + 4(1 - \alpha - \alpha c^4)](1-\alpha) + \alpha^2 c^2$ and $\alpha = 4\,\eta_1\eta_2$. Note that this expression is only valid if in addition the inequalities (1c) and (1d) hold. The success probability is illustrated as a contour plot in Fig. 2. Above the dashed line, the optimal measurement is of type (1,1) and the success probability is given by Eq. (9). We find from numerical analysis that the optimal measurement is a fidelity form measurement in the remaining cases. Note that for a wide range of the parameters, the optimal measurement is a von Neumann measurement and hence may be implemented physically without the need of an auxiliary system.

In summary, we have presented a strategy to find the optimal measurement for unambiguous discrimination of two mixed quantum states acting on a five-dimensional Hilbert space. Our

[1] This parametrization does not include the case $|\chi_e\rangle = |\omega_+\rangle, |\chi_d\rangle = |\sigma_-\rangle$. However, this case is optimal only if $\eta_1 = \eta_2 = \frac{1}{2}$.

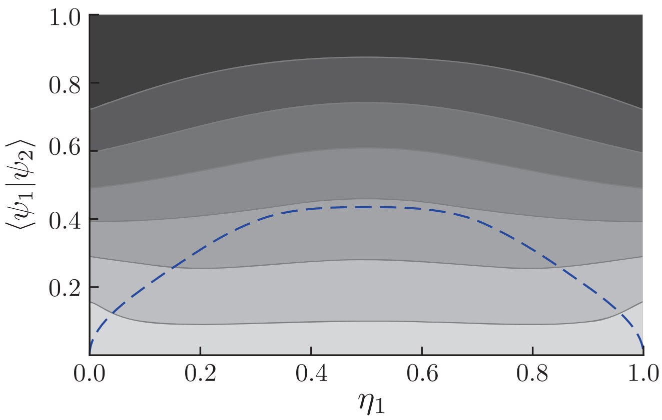

FIG. 2. (Color online) Maximal success probability for comparison of three pure quantum states, taken from the set $\{|\psi_1\rangle, |\psi_2\rangle\}$, as a function of the *a priori* probability η_1 and the overlap $\langle\psi_1|\psi_2\rangle$. Darker areas correspond to lower success probability. The dashed line indicates the bound from the conditions (1c) and (1d).

method can in principle also be applied to the discrimination of two quantum states in general dimensions. Our results are also useful in other contexts, e.g., quantum-state filtering: in Ref. [7] it has been shown how to optimally distinguish between one pure state from a given set and the remaining ones. With our method one could filter a subset of states from the whole set. In connection with quantum algorithms, one could thus distinguish between two sets of Boolean functions, rather than between one function and a set of functions. The results presented in this paper could also be used to prove optimality for the universal programmable state discriminator suggested in Ref. [26]. As the optimal measurement is unique, the optimal device discussed in Ref. [26] cannot be simplified. Furthermore, in Ref. [11] the importance of unambiguous discrimination in the context of quantum key distribution was shown with particular emphasis on the case of states of rank 2. As an outlook, our strategy seems a promising path for the generalization to unambiguous state discrimination of more than two states.

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