Unambiguous discrimination of linearly independent pure quantum states: Optimal average probability of success

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We consider the problem of unambiguous (error-free) discrimination of N linearly independent pure quantum states with prior probabilities, where the goal is to find a measurement that maximizes the average probability of success. We derive an upper bound on the optimal average probability of success using a result on optimal local conversion between two bipartite pure states. We prove that for any $N \ge 2$ an optimal measurement in general saturates our bound. In the exceptional cases we show that the bound is tight, but not always optimal.

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One of the consequences of the superposition principle is that quantum states could be nonorthogonal, which restricts our ability to reliably determine the state of a quantum system even when the set of possible states is known. Thus a fundamental problem in quantum mechanics is to determine how well quantum states can be distinguished from one another (see [1,2] for reviews). In its simplest form, the problem is defined as follows: A quantum system is prepared in one of N known pure states $|\psi_1\rangle, |\psi_2\rangle, \dots, |\psi_N\rangle$ with associated probabilities p_1, p_2, \ldots, p_N , where $0 < p_i < 1$ for every *i* and $\sum_{i=1}^{N} p_i = 1$. We do not know which state the system is in, but wish to identify it. If the states are mutually orthogonal, the solution is straightforward. However, if the states are not mutually orthogonal, then quantum mechanics forbids us from distinguishing them perfectly. Therefore, the objective is to devise a measurement strategy that is optimal according to some reasonable quantifier of distinguishability. This scenario is typical in quantum information theory, especially in quantum communications and quantum cryptography.

In this paper we consider how well a given set of pure states can be discriminated without error. This measurement strategy, known as unambiguous discrimination, seeks *certain* knowledge of the state of the system balanced against a probability of failure. Since no error is permitted, in addition to the measurement outcomes that correctly identify the input state, an inconclusive outcome, which is not informative, must be allowed. That is, either the input state is correctly detected or the outcome is inconclusive, in which case we do not learn anything about the state. It may be noted that in other strategies such as minimum error discrimination [1,2] and maximum confidence measurements [2], we cannot in general be completely sure of the identity of the input state.

Unambiguous discrimination of pure quantum states is possible if and only if the states are linearly independent [3]. This assumption will therefore hold throughout this paper. The measurement is described by a positive operator valued measure (POVM) $\mathbf{\Pi} = {\Pi_k}$ with N + 1 outcomes, where $\Pi_k \ge 0$ and $\sum_{k=1}^{N+1} \Pi_k = I$. The POVM elements ${\Pi_k | k = 1, \dots, N}$ are associated with success and satisfy

$$\langle \psi_i | \Pi_j | \psi_j \rangle = \gamma_i \delta_{ij} \ \forall i, \ j = 1, \dots, N, \tag{1}$$

where γ_i is the probability of successfully detecting the state $|\psi_i\rangle$. Note that Eq. (1) implies that if the system is in state $|\psi_i\rangle$, the outcome $j \neq i$ for j = 1, ..., N will never occur. The operator $\Pi_{N+1} = I - \sum_{i=1}^{N} \Pi_i$ corresponds to an inconclusive outcome. Notice that the set of individual success probabilities $\{\gamma_1, ..., \gamma_N\}$ is determined only by our choice of POVM. Thus, for a given measurement Π , the average probability of success is defined as

$$P(\mathbf{\Pi}) = \sum_{i=1}^{N} p_i \gamma_i.$$
(2)

The goal is to find a measurement that maximizes the average probability of success. In particular, we are interested in the following quantity:

$$P_{\text{opt}} = \max_{\{\Pi\}} P(\Pi) = \sum_{i=1}^{N} p_i \gamma_i^{\text{opt}},$$
(3)

where the optimal solution $\gamma^{\text{opt}} = \{\gamma_i^{\text{opt}} | i = 1, ..., N\}$ is the set of individual success probabilities maximizing the average probability of success. The optimal solution is known only for N = 2 [4–7] and special cases for $N \ge 3$ [8–13]. General results include lower [14,15] and upper [16] bounds on the average probability of success, a solution for N equiprobable symmetric states [17], a formulation of the problem as a semidefinite program with results for symmetric and geometrically uniform states [18], characterization of optimal solutions [8], a graphic method for finding and classifying optimal solutions [9], and a solution for equidistant states [19].

Before we state our results it is necessary to briefly review all possible classes of optimal solution [8], precise definitions of which are given in Ref. [20]. For a given set of N linearly independent pure states let \mathcal{R} be the set of all candidate optimal solutions. This set, said to be the critical feasible region, is an (N - 1)-dimensional region (hypersurface) in the N-dimensional real vector space \mathbb{R}^N and is completely determined by the input states and the constraints imposed by the problem. Once we specify the prior probabilities, the optimal solution, which is an element of \mathcal{R} , becomes unique in the sense that there is no other solution that is also optimal for the same set of prior probabilities. Different sets of prior probabilities in general lead to different optimal solutions within the set \mathcal{R} .

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The optimal solution is either an interior or a boundary point of \mathcal{R} . If it is an interior point then it means that the optimal measurement is able to discriminate all states, i.e., for every *i*, $0 < \gamma_i^{\text{opt}} \leq 1$. On the other hand, if it is a boundary point, then at least one of the optimal individual success probabilities is zero. We say that an interior point is nonsingular if the solution is nondegenerate, i.e., it can be the optimal solution only for a unique set of prior probabilities. An interior point can also be singular if the solution is degenerate, i.e., it can be the optimal solution for different sets of prior probabilities. It should be noted that interior singular points are exceptions and may not even exist for a given set of states. Thus there are only three possible classes of optimal solution: interior nonsingular, interior singular, and boundary.

Using the conditions in [8], it is easy to show that for a given set of states, every interior nonsingular point is the optimal solution for some set of prior probabilities. Noting that the critical feasible region is of dimension N - 1, the dimension of the interior part is also N - 1, whereas the dimensions of the boundary regions are strictly less than N - 1. Therefore, for almost all assignments of prior probabilities, the optimal solution will be an interior nonsingular point. In other words, for any given instance of an unambiguous state discrimination problem, the optimal solution in general will be an interior nonsingular point of the critical feasible region.

In this work we derive an upper bound on the optimal average probability of success using a result [21,22] on optimal local conversion between two bipartite pure states. We prove that the bound is saturated when the optimal solution is an interior nonsingular point of the critical feasible region: the set of all candidate optimal solutions. From the previous argument we therefore conclude that for any given set of $N \ge 2$ linearly independent pure states with prior probabilities, the upper bound in general equals the optimal average probability of success.

When the optimal solution is either an interior singular point or a boundary point, we show that the upper bound is tight. However, we also show that it is not achieved in general by an optimal boundary solution. The question whether an optimal solution that is an interior singular point always saturates our bound remains open.

We begin by obtaining an upper bound on the optimal average probability of success.

Theorem 1. Suppose a quantum system is prepared in one of the linearly independent pure states $|\psi_1\rangle, \ldots, |\psi_N\rangle$ with prior probabilities p_1, \ldots, p_N , respectively, where $0 < p_i < 1$ for every *i* and $\sum_{i=1}^{N} p_i = 1$. For an optimal unambiguous state discrimination measurement, the average success probability P_{opt} is bounded by

$$P_{\text{opt}} \leqslant \min_{\{\theta_j\}} \left\| \sum_{j=1}^N \sqrt{p_j} e^{i\theta_j} |\psi_j\rangle \right\|^2.$$
 (4)

Essentially we are required to minimize the norm of the vector $\sum_{j=1}^{N} \sqrt{p_j} e^{i\theta_j} |\psi_j\rangle$ with respect to the real parameters $\{\theta_j | j = 1, ..., N\}$ we are free to vary. Because of this we can always set one of the θ_i , say, θ_1 , equal to zero and minimize the norm with respect to the remaining N - 1 parameters. However, it is often useful to express inequality (4) in a form where the

PHYSICAL REVIEW A 90, 030301(R) (2014)

parameters defining the inner products of the states become explicit. Let $\langle \psi_i | \psi_j \rangle = |\langle \psi_i | \psi_j \rangle | e^{\phi_{ij}}$, i < j. We then have

$$P_{\text{opt}} \leqslant 1 + \min_{\{\theta_i\}} \sum_{1 \leqslant i < j \leqslant N} 2\sqrt{p_i p_j} |\langle \psi_i | \psi_j \rangle| \cos(\theta_j - \theta_i + \phi_{ij}).$$
(5)

We shall use (5) in the examples later in the paper and Ref. [20].

The proof of the theorem relies on two facts. First, any set of linearly independent quantum states can be unambiguously discriminated [3]. This simply means that one can always find a measurement, which may not be optimal, that unambiguously discriminates all states. Second, a pure bipartite entangled state with *d* nonzero Schmidt coefficients can be converted, with some nonzero probability, to a maximally entangled state in $d \otimes d$ by local operations and classical communication (LOCC). The optimal probability of such a local conversion can be obtained using the result in [21,22] and is stated in the following lemma (proof in [20]).

Lemma 1. Let $|\Psi\rangle_{AB} = \sum_{i=1}^{d} \sqrt{\alpha_i} |i\rangle_A |i\rangle_B$ be a bipartite pure entangled state, where $\{\sqrt{\alpha_i}\}$ are the Schmidt coefficients such that $\alpha_1 \ge \cdots \ge \alpha_d > 0$ and $\sum_{i=1}^{d} \alpha_d = 1$. Then the optimal probability with which $|\Psi\rangle_{AB}$ can be locally converted to a maximally entangled state in $d \otimes d$ is given by $d\alpha_d$.

Proof of Theorem 1. For convenience we first sketch the main idea behind the proof. We shall begin with a scenario of local conversion between two bipartite states (say, source and target), where the target state is maximally entangled. The source state is so constructed that (a) any measurement, say, Π , on Alice's side that unambiguously discriminates the states $\{|\psi_i\rangle| j = 1, ..., N\}$ constitutes a local protocol for the aforementioned state transformation and (b) the probability of local conversion, say, $P(\Pi)$, thus obtained is exactly equal to the average probability of success in an unambiguous discrimination scenario, where the measurement Π distinguishes the states $\{p_i, |\psi_i\rangle| = 1, \dots, N\}$. However, for any Π , $P(\mathbf{\Pi})$ is bounded by the optimal local conversion probability obtained from Lemma 1. An upper bound on the optimal average probability of success follows by choosing Alice's measurement to be optimal for unambiguous discrimination, that is, $\Pi = \Pi^{\text{opt}}$. Further refinement leads us to inequality (4). We now give the formal proof in three key steps.

(i) Consider a bipartite scenario with two spatially separated observers, Alice and Bob, with Alice holding quantum systems A_1 and A_2 of dimensions $N' \ge N$ and N, respectively, and Bob holding a quantum system B of dimension N. Alice and Bob share the pure state

$$|\psi^{\theta}\rangle_{AB} = \sum_{j=1}^{N} \sqrt{p_j} e^{i\theta_j} |\psi_j\rangle_{A_1} \otimes |\Phi_j\rangle_{A_2B}, \qquad (6)$$

where θ represents the collection of parameters $\{\theta_i | i = 1, ..., N\}$ allowed to vary and $\{|\Phi_j\rangle| j = 1, ..., N\}$ is a set of *N* mutually orthonormal maximally entangled states in $N \otimes N$ defined as

$$\begin{split} |\Phi_{j}\rangle &= \frac{1}{\sqrt{N}} \sum_{k=1}^{N} \exp\left(\frac{2\pi i (k-1)(j-1)}{N}\right) |k\rangle |k\rangle,\\ j &= 1, \dots, N. \end{split}$$
(7)

UNAMBIGUOUS DISCRIMINATION OF LINEARLY ...

Suppose Alice and Bob wish to convert $|\psi^{\theta}\rangle_{AB}$ to a maximally entangled state, say, $|\Phi\rangle_{AB}$ in $N \otimes N$, by LOCC. This can be achieved by a local protocol, which is not necessarily optimal, where Alice performs a generalized measurement (POVM) $\mathbf{\Pi} = \{\Pi_k | k = 1, \dots, N+1\}$ on system A_1 that unambiguously discriminates the states $\{|\psi_i\rangle| j = 1, \dots, N\}$. The POVM elements $\{\Pi_k | k = 1, ..., N\}$ satisfy Eq. (1), where the outcomes j = 1, ..., N correspond to success and the outcome i = N + 1 corresponds to failure. If the outcome is j, the measurement successfully detects the state $|\psi_i\rangle$ for j = 1, ..., N. From the expression of $|\psi^{\theta}\rangle_{AB}$ given by Eq. (6) it is evident that this occurs with probability $p_i \gamma_i$ and for each of these cases the corresponding maximally entangled state $|\Phi_i\rangle$ is created between Alice and Bob. For j = N + 1, the outcome is inconclusive and therefore will not be our concern.

The above local protocol, with some nonzero probability, converts the state $|\psi^{\theta}\rangle_{AB}$ to a maximally entangled state in $N \otimes N$. Note that for every successful outcome, the maximally entangled state created between Alice and Bob can be converted to the designated state $|\Phi\rangle_{AB}$ by local unitaries. Thus the probability of creating a maximally entangled state between Alice and Bob with this local protocol is $P(\Pi) = \sum_{j=1}^{N} p_j \gamma_j$, which is the same as the average probability of success in unambiguous discrimination of the states $\{p_j, |\psi_j\rangle|_j = 1, \dots, N\}$ with the measurement Π .

Now suppose that the POVM $\Pi = \Pi_{opt}$, that is, the measurement is optimal for unambiguous discrimination of the states $\{p_j, |\psi_j\rangle| j = 1, ..., N\}$. Then $P_{opt} = \sum_{j=1}^{N} p_j \gamma_j^{opt}$, which by our previous argument is also the probability, not necessarily optimal, of locally converting the state $|\psi^{\theta}\rangle_{AB}$ to $|\Phi\rangle_{AB}$. However, P_{opt} cannot exceed the optimal local conversion probability $p(\psi^{\theta}_{AB} \rightarrow \Phi_{AB})$ that can be obtained by applying Lemma 1. Therefore,

$$P_{\text{opt}} \leqslant p(\psi_{AB}^{\theta} \to \Phi_{AB}).$$
 (8)

(ii) To obtain an expression for $p(\psi_{AB}^{\theta} \to \Phi_{AB})$ we first write $|\psi^{\theta}\rangle_{AB}$ in its Schimdt-decomposed form

$$|\psi^{\theta}\rangle = \frac{1}{\sqrt{N}} \sum_{k=1}^{N} ||\eta_k\rangle| |\eta'_k k\rangle_{A_1 A_2} |k\rangle_B, \qquad (9)$$

where $|\eta_k\rangle$ (unnormalized) is given by

$$|\eta_k\rangle = \sum_{r=1}^N \sqrt{p_r} e^{i\theta_r} \exp\left(\frac{2\pi i}{N}(r-1)(k-1)\right) |\psi_r\rangle \quad (10)$$

and $|\eta'_k\rangle = \frac{1}{\||\eta_k\rangle\|} |\eta_k\rangle$ is the normalized state. Observe that (9) is indeed the Schmidt decomposition of $|\psi^{\theta}\rangle_{AB}$ owing to $\langle \eta'_k k | \eta'_m m \rangle = \langle \eta'_k | \eta'_m \rangle \langle k | m \rangle = \langle \eta'_k | \eta'_m \rangle \delta_{km}$. The Schmidt coefficients are given by $\frac{\||\eta_k\rangle\|}{\sqrt{N}}$, k = 1, ..., N, where for every $k, \||\eta_k\rangle\| > 0$. Thus all Schmidt coefficients are nonzero. Then from Lemma 1 it follows that

$$p(\psi_{AB}^{\theta} \to \Phi_{AB}) = \min_{k} \{ \||\eta_{k}\rangle\|^{2} |k = 1, \dots, N \}.$$
 (11)

It can be easily seen that $p(\psi_{AB}^{\theta} \to \Phi_{AB})$ depends on $\{\theta_i | i = 1, ..., N\}$, inner products of the states $\{|\psi_r\rangle|r = 1, ..., N\}$,

PHYSICAL REVIEW A 90, 030301(R) (2014)

and the probabilities $\{p_i | i = 1, ..., N\}$. Of all these only the real parameters θ_i can be varied, everything else remaining fixed for a given set $\{p_i, |\psi_i\rangle| i = 1, ..., N\}$.

Noting that P_{opt} does not depend on $\{\theta_i\}$, inequality (8) therefore holds for *any* set $\{\theta_i\}$ and in particular any set that minimizes $p(\psi_{AB}^{\theta} \rightarrow \Phi_{AB})$. Therefore,

$$P_{\text{opt}} \leqslant \min_{\{\theta_i\}} p(\psi_{AB}^{\theta} \to \Phi_{AB})$$
 (12)

gives us the best possible bound on P_{opt} using this approach.

(iii) To evaluate the right-hand side of (12) we proceed as follows. First, we observe that

$$\min_{\{\theta_i\}} p(\psi_{AB}^{\theta} \to \Phi_{AB}) = \min_k \{\min_{\{\theta_i\}} \||\eta_k\rangle\|^2 |k = 1, \dots, N\}.$$
(13)

Next, we prove the following equality:

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$$\min_{\{\theta_i\}} \||\eta_k\rangle\|^2 = \min_{\{\theta_i\}} \||\eta_j\rangle\|^2$$
(14)

for every pair (k, j). To prove Eq. (14) we first express $||\eta_k\rangle||^2$ as

$$\||\eta_k\rangle\|^2 = \left\|\sum_{r=1}^N \sqrt{p_r} e^{i\theta'_r(k)} |\psi_r\rangle\right\|^2,$$
 (15)

where $\theta'_r(k) = \theta_r + \frac{2\pi}{N}(r-1)(k-1)$ for r = 1, ..., N. Now suppose that the set $\{\theta_r | r = 1, ..., N\}$ minimizes $|||\eta_k\rangle||^2$. Noting that (15) has exactly the same form of $|||\eta_1\rangle||^2$, the set $\{\theta'_r(k)|r = 1, ..., N\}$ therefore minimizes $|||\eta_1\rangle||^2$. A similar argument holds for every $i, i \neq k$. We have therefore proved (14) and consequently

$$\min_{\{\theta_i\}} p(\psi_{AB}^{\theta} \to \Phi_{AB}) = \min_{\{\theta_i\}} \||\eta_k\rangle\|^2 \ \forall k = 1, \dots, N.$$
(16)

Inequalities (12) and (16) for k = 1 together prove the theorem.

We now show that the upper bound in (4) is saturated when the optimal solution is a nonsingular interior point of the critical feasible region \mathcal{R} . Therefore, in a generic case the optimal average probability of success is equal to the upper bound given by Theorem 1.

Theorem 2. Let a quantum system be prepared in one of the linearly independent pure states $|\psi_1\rangle, \ldots, |\psi_N\rangle$ with prior probabilities p_1, \ldots, p_N , respectively, where $0 < p_i < 1$ for every *i* and $\sum_{i=1}^{N} p_i = 1$. For an optimal unambiguous state discrimination measurement, suppose that the solution is an interior nonsingular point of the critical feasible region. Then

$$P_{\text{opt}} = \min_{\{\theta_i\}} \left\| \sum_{j=1}^N \sqrt{p_j} e^{i\theta_j} |\psi_j\rangle \right\|^2.$$
(17)

Proof. In [8] it was shown that if γ^{opt} is an interior nonsingular point of the critical feasible region, then P_{opt} can be expressed as

$$P_{\text{opt}} = \left\| \sum_{j} \sqrt{p_{j}} e^{i\theta'_{j}} |\psi_{j}\rangle \right\|^{2}, \qquad (18)$$

but no explicit expressions of the phases $e^{i\theta'_j}$ were given. However, it was noted that P_{opt} must be the value of a stationary point if the phases are allowed to change freely. Note that without the explicit knowledge of the phases or knowing how to obtain them (a stationary point may be a minimum or maximum), Eq. (18) is not very useful.

However, the upper bound in Theorem 1 [inequality (4)], which holds irrespective of the class of optimal solution, fills this gap. Consequently,

$$P_{\text{opt}} = \min_{\{\theta_i\}} \left\| \sum_j \sqrt{p_j} e^{i\theta_j} |\psi_j\rangle \right\|^2.$$
(19)

This proves the theorem and also shows that the stationary point must be a minimum.

It is not clear whether our bound saturates for the other two classes of optimal solution, as the expression (18) was obtained [8] assuming that the optimal solution is an interior nonsingular point of the critical feasible region. However, by considering examples from each of the other two classes, we first show that the upper bound given by Theorem 1 is tight for both. The third example shows that for a boundary solution, the optimal value could be strictly less than the value obtained from our bound. Therefore, an optimal boundary solution will not in general saturate our bound.

Example I: boundary point. We begin by considering an example for N = 3 [13], where the given states $|\psi_1\rangle = (1 \ 0 \ 0)^T$, $|\psi_2\rangle = \sqrt{\frac{1}{3}}(1 \ 1 \ 1)^T$, and $|\psi_3\rangle = \frac{1}{\sqrt{3}}(1 \ 1 \ -1)^T$ are equally likely. Noting that the inner products are all real, inequality (5) becomes (set $\theta_1 = 0$)

$$P_{\text{opt}} \leq 1 + \min_{\{\theta_2, \theta_3\}} \frac{2}{3\sqrt{3}} \bigg[\cos \theta_2 + \cos \theta_3 + \frac{1}{\sqrt{3}} \cos(\theta_3 - \theta_2) \bigg].$$

By simple numerical minimization using *Mathematica* we find that $P_{opt} \leq 0.4444$. In [13] it was shown that $\gamma^{opt} = \{0, \frac{2}{3}, \frac{2}{3}\}$, from which we obtain $P_{opt} = \frac{4}{9} = 0.4444$. Thus the upper bound is achieved. As one of the individual success probabilities is zero, the optimum point is therefore on the boundary.

It is easy to construct an example for any $N \ge 4$ starting from the one we just discussed. Here we give an example for N = 4, from which it will be evident how to generalize for higher N. Consider the set of states $\{|\psi_i\rangle|i = 1, ..., 4\}$, where the first three states are from the above example and the new state $|\psi_4\rangle$ has the property that $|\psi_4\rangle \perp |\psi_i\rangle$ for i = 1,2,3. We choose the prior probabilities as $p_i = \frac{1-p}{3}$ for i = 1,2,3 and $p_4 = p$, where 0 . In this case, using inequality (5) we find that

$$P_{\text{opt}} \leq p + 0.4444(1-p).$$

To show that the above bound is tight, we find the optimal set of the individual success probabilities. Noting that $|\psi_4\rangle$ is orthogonal to every other state, it is easy to obtain that $\gamma^{\text{opt}} = \{0, \frac{2}{3}, \frac{2}{3}, 1\}$ and $P_{\text{opt}} = p + \frac{4}{9}(1 - p)$, thereby achieving the upper bound.

Example II: interior singular point. We begin by considering such an example for N = 3 [8]. Consider the vectors $|\psi_1\rangle = (1 \ 0 \ 0)^T$, $|\psi_2\rangle = \sqrt{\frac{1}{5}}(1 \ 2 \ 0)^T$, and $|\psi_3\rangle = \frac{2}{\sqrt{17}}(1 \ 1 \ \frac{3}{2})^T$, with prior probabilities $p_1 = 0.30$, $p_2 = 0.35$, and $p_3 = 0.35$, respectively. We see that the inner products are real. Using inequality (5), a simple numerical minimization using MATHEMATICA shows that $P_{\text{opt}} \leq 0.4430$, which agrees with the optimal value [8]. Following the method used in the previous example, we can therefore generalize this example for any $N \ge 4$.

Example III: In this example we show that the upper bound does not saturate in general for an. This example is from [8], where the states $|\psi_1\rangle = (1 \quad 0 \quad 0)^T$, $|\psi_2\rangle = \sqrt{\frac{1}{5}}(1 \quad 2 \quad 0)^T$, and $|\psi_3\rangle = \frac{2}{\sqrt{17}}(1 \quad 1 \quad \frac{3}{2})^T$ occur with prior probabilities $p_1 = 0.10$, $p_2 = 0.80$, and $p_3 = 0.10$, respectively. Once again using inequality (5), a simple numerical minimization using *Mathematica* shows that $P_{\text{opt}} \leq 0.4758$, which is pretty close to the optimal value $P_{\text{opt}} = 0.4632$ [8].

To conclude, we studied the problem of unambiguous discrimination of N linearly independent pure quantum states, where the measurement strategy is such that either the input state is correctly identified (zero error) or we learn nothing about it. The objective is to find a measurement that maximizes the average probability of success. This problem has been extensively studied over the years, but the exact solution is known only for N = 2 and special cases for $N \ge 3$. In this paper we obtained an upper bound on the optimal average probability of success using a result [21,22] on optimal local conversion between two bipartite pure states. We showed that for $N \ge 2$ an optimal measurement in general saturates our bound, thereby providing an exact expression of the optimal average probability of success in the generic case. In the exceptional cases we have shown that the bound is tight, but not always attained for an optimal boundary solution. The question whether an optimal solution that is an interior singular point always saturates our bound remains open.

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UNAMBIGUOUS DISCRIMINATION OF LINEARLY ...

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