Unambiguous discrimination of mixed states: A description based on system-ancilla coupling

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We propose a general description on the unambiguous discrimination of mixed states according to the system-environment coupling, and present a procedure to reduce this to a standard semidefinite programming problem. In the two states case, we introduce the canonical vectors and partly simplify the problem to the case of discrimination between pairs of canonical vectors. By considering the positivity of the two by two matrices, we obtain a series of new upper bounds of the total success probability which depends on both the prior probabilities and specific state structures.

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I. INTRODUCTION

Quantum state discrimination (QSD) is one of the fundamentally important problems in quantum information science. Especially in quantum communication and quantum cryptography, many novel schemes are based on the fact that nonorthogonal states cannot be discriminated determinately. Henceforth study on the discrimination of quantum states has a close relation to the security of quantum cryptographic protocols. On the other hand, since there is no measurement that can perform a perfect identification, several strategies have been proposed in QSD based on different criteria. One of these is the minimum-error discrimination [1], which permits incorrect outcomes during the measurement procedure. The other one is unambiguous discrimination (UD) of quantum states. This sort of discrimination procedure never gives an erroneous result, but sometimes it fails. Here we consider the latter case which has received much attention recently.

In the pure states case, UD has been widely considered [2, 3]. While in mixed states case, it seems to be a hard problem. In many earlier works, some useful bounds of the total success probability $P$, together with several useful reduction theorem, have been presented [4, 5, 6, 7, 8, 9, 10, 11]. However, totally solving this problem seems not so easy at all. What’s more, even for the simple case, e.g., UD between two mixed states, which has been wildly studied recently, there still exists many questions which are not clear to us.

The standard description of UD among mixed states are usually formulated as this: given a set of mixed states $\{\rho_1, \rho_2, \ldots, \rho_N\}$ with the corresponding prior probabilities $\{\eta_1, \eta_2, \ldots, \eta_N\}$, the aim of discriminating these states unambiguously is to find a $N + 1$-element positive operator value measurement (POVM) $\{E_0, E_1, E_2, \ldots, E_N\}$ with $\sum_{i=0}^{N} E_i = I$ and $\text{Tr}(E_k \rho_l) = \rho_k \delta_{kl} (k \neq l)$, such that the measurement operator $E_k$ gets a result with the probability $p_k$ only when the input state is $\rho_k$. Here $E_0$ denotes the inconclusive measurement where the identification fails. The average failure probability is described by $Q = \sum_{k=1}^{N} Q_k$ with $Q_k = \eta_k \text{Tr}(E_0 \rho_k)$ being the failure probability of identifying $\rho_k$. Equivalently, one can also concentrate on the total success probability $P = 1 - Q = \sum_{k=1}^{N} \eta_k \text{Tr}(E_k \rho_k)$.

From the general viewpoint, UD can be regarded as some kind of physically accessible transformation on a finite number of input states $\xi : \{\rho_1, \rho_2, \ldots, \rho_N\} \rightarrow \{\sigma_1, \sigma_2, \ldots, \sigma_N\}$ [12]. The major character of this transformation is that it is probabilistic, accurate, and the output states $\sigma_k$ must be orthogonal to each other so that they can be identified perfectly. There are several equivalent approaches to describe a completely positive (CP) map [13]. For example, it can be represented in a Kraus operator sum form. Also it can be implemented by employing a unitary transformation on the system plus ancilla, i.e. $\xi(p) = \text{Tr}_{E'}[U \rho \otimes \rho_E U^\dagger I \otimes P_{E'}]$, where $\rho_E$ is the initial state of the ancilla system, $I$ denotes the identity operator in output Hilbert space $\mathcal{H}_2$, $P_{E'}$ is a projector in $\mathcal{H}_{E'}$, and $\mathcal{H}_1 \otimes \mathcal{H}_E = \mathcal{H}_2 \otimes \mathcal{H}_{E'}$.

In this paper, we consider to discriminate mixed states unambiguously from the system-ancilla coupling viewpoint. By constructing the whole unitary transformation on the combinations of the inputs and the auxiliary system, we obtain the necessary and sufficient conditions on the existence of a UD strategy. We point out that in the more general case to find the optimal UD strategy can be reduced to a standard semidefinite programming problem. Especially, in the case of UD between two mixed states, we obtain a series of new upper bounds of the success probability which are closely related to the structure of the input quantum states together with the ratio of prior probabilities. In some sense our result confirms the conjecture made by Bergou et al [11].
II. GENERAL DESCRIPTION OF UNAMBIGUOUS DISCRIMINATION

Let us start with the general UD of \( N \) mixed states. For any mixed state \( \rho_k \), it can always be regarded as the mixture of pure states, i.e. \( \rho_k = \sum_m |\psi_m^{(k)}\rangle \langle \psi_m^{(k)}| \), where \( |\psi_m^{(k)}\rangle \) are nonnormalized state vectors. Here for simplicity, we assume that \( |\psi_m^{(k)}\rangle \) are linearly independent. 

Firstly, we suppose the intersection of the supports of two density matrices \( \rho_k \) and \( \rho_l \) is empty (except for a trivial zero vector). This also indicates that all vectors \( \{ |\psi_m^{(k)}\rangle, \ldots, |\psi_m^{(l)}\rangle \} \) are linearly independent. By introducing suitable auxiliary system, we consider the following unitary realization of the CP map \( \xi \)

\[
U|\tilde{\psi}_m^{(k)}\rangle_1|0\rangle_E = |\tilde{\phi}_m^{(k)}\rangle_2a|P_0\rangle_p + |\tilde{\beta}_m^{(k)}\rangle_2a|P_0\rangle_p. \tag{1}
\]

Here \( \mathcal{H}_{E'} = \mathcal{H}_a \otimes \mathcal{H}_p \), \( |0\rangle \) is the fixed initial state of the environment, \(|P_0\rangle\) is the state of the probe system satisfying \( \langle P_0|\tilde{\phi}_m^{(k)}\rangle = 0 \), and we also use the tilde "\( \tilde{\cdot} \)" to denote a nonnormalized state vector. The output state \( \sigma_k \) can be obtained by tracing over the subsystem \( a \) after we get a measurement outcome corresponding to the probe \(|P_0\rangle\), i.e. \( \sigma_k = \sum_m \text{Tr}_a[|\tilde{\phi}_m^{(k)}\rangle \langle \tilde{\phi}_m^{(k)}|] \).

On the other hand, if the intersection of the supports of two density matrix \( \rho_k \) and \( \rho_l \) is not empty, there exists at least one state vector \( |\psi\rangle \in \text{supp}(\rho_k) \cap \text{supp}(\rho_l) \). From the definition of the CP map, we have

\[
U|\psi\rangle|0\rangle_E = |\tilde{\phi}(k)\rangle|P_0\rangle + |\tilde{\beta}(l)\rangle|P_0\rangle = |\tilde{\phi}(l)\rangle|P_0\rangle + |\tilde{\beta}(l)\rangle. \tag{2}
\]

Since \( |\tilde{\phi}(k)\rangle \neq |\tilde{\phi}(l)\rangle \) (the output states are different from each other), Eq. (2) is satisfied only when \( |\tilde{\phi}(k)\rangle = |\tilde{\phi}(l)\rangle = 0 \), hence any state contained in \( \text{supp}(\rho_k) \cap \text{supp}(\rho_l) \) has no contribution to the desired transformation. Thus it’s enough to consider the case \( \text{supp}(\rho_k) \cap \text{supp}(\rho_l) = \{0\} \), which reproduces the known results \([7]\).

The inner-product preservation of unitary transformation leads us to the following equation

\[
\tilde{X} - \tilde{Y} = \tilde{B} \geq 0 \tag{3}
\]

with

\[
\tilde{w} = \begin{pmatrix}
\tilde{w}_{kk} & \cdots & \tilde{w}_{kl} \\
\vdots & \ddots & \vdots \\
\tilde{w}_{lk} & \cdots & \tilde{w}_{ll}
\end{pmatrix} \quad \{w \in \{X, Y, B\}\}. \tag{4}
\]

Here \( \tilde{w}_{kl} \) are all block matrices with \( \tilde{X}_{kl} = |\tilde{\psi}_m^{(k)}\rangle \langle \psi_n^{(l)}|, \ \tilde{Y}_{kl} = |\tilde{\phi}_m^{(k)}\rangle \langle \phi_n^{(l)}|, \ \text{and} \ \tilde{B}_{kl} = |\tilde{\beta}_m^{(k)}\rangle \langle \beta_n^{(l)}| \) respectively. Also we can find that all the three matrices \( \tilde{X}, \tilde{Y}, \tilde{B} \) are Hermitian, and positive semidefinite. Since \( \sigma_k \) are orthogonal to each other, we have \( \langle \tilde{\phi}_m^{(k)}| \tilde{\phi}_n^{(l)} \rangle = 0 (k \neq l) \). This indicates \( \tilde{Y} \) is quasi-diagonal and can be written as \( \tilde{Y} = \text{diag}\{\tilde{Y}_{kk}, \ldots, \tilde{Y}_{ll}\} \).

Contrarily, if there exists a positive semidefinite \( \tilde{Y} \) matrix satisfying Eq. (4), we can always choose suitable state vectors \( |\phi_m^{(k)}\rangle \) and \( |\beta_m^{(k)}\rangle \) such that \( \tilde{X} = \tilde{B} + \tilde{Y} \). With the standard Gram-Schmidt orthogonalization procedure, the desired the unitary transformation can be easily obtained.

We conclude the above discussion by the following theorem.

**Theorem 1.** \( N \) mixed states \( \{\rho_1, \rho_2, \ldots, \rho_N\} \) can be unambiguously discriminated if and only if there exists a positive semidefinite quasi-diagonal matrix \( \tilde{Y} \) such that \( \tilde{X} - \tilde{Y} \geq 0 \). Moreover, if the input states are chosen with prior probabilities \( \{\eta_1, \eta_2, \ldots, \eta_N\} \) and \( \sum_k \eta_k = 1 \), the total success probability will be \( P = \sum_k \eta_k \text{Tr}(\tilde{Y}_{kk}) \).

This theorem characterize the general properties of UD among \( N \) mixed states in the system-ancilla framework. One can also easily check that it is consistent with earlier works \([4, 5, 6, 7, 8, 9, 10, 11]\). In a more realistic situation, people often concentrate on the total success probability of some physical transformation. This indicates that we should make the probability \( P \) as high as possible. Mathematically, this is equivalent to maximizing

\[
P = \sum_k \eta_k \text{Tr}(\tilde{Y}_{kk}) \tag{5}
\]

under the constraints

\[
\tilde{X} - \tilde{Y} \geq 0, \text{and} \tilde{Y} \geq 0. \tag{6}
\]

Usually given the input mixed states, we can get to know the matrix \( \tilde{X} \) exactly. Therefore the only thing we should do is to find the optimal positive semidefinite matrix \( \tilde{Y} \) which maximizes the success probability \( P \). By redefining a series of new matrices \( F_0 = \text{diag}\{\tilde{X}, 0\}, F_k^{pq} = \text{diag}\{E_k^{pq}, -E_k^{pq}\}, \text{and} G_k^{pq} = \text{diag}\{iE_k^{pq}, -iE_k^{pq}\} \), where \( i \) is the basic imaginary unit, and \( E_k^{pq} \) are matrices corresponding the block matrices \( \tilde{Y}_{kk} \) with \( \{F_k^{pq}\}_{mn} = \delta_{mp}\delta_{nq} \), the problem under consideration can be reformulated as

\[
\max_{\tilde{Y}} \sum_k \eta_k \text{Tr}(\tilde{Y}_{kk}) \tag{7}
\]

subject to

\[
F_0 - \sum_{k,p,q} \left\{ \text{Re}[\tilde{Y}_{kk}] F_k^{pq} + \text{Im}[\tilde{Y}_{kk}] G_k^{pq} \right\} \geq 0,
\]

where \( \text{Re}[\tilde{Y}_{kk}] \) and \( \text{Im}[\tilde{Y}_{kk}] \) represent the real and imaginary parts of the matrices elements \( \{\tilde{Y}_{kk}\}_{pq} \) respectively. This is a standard semi-definite programing (SDP) problem \([11]\), and can be solved by numeric method efficiently (one can also find another method to reduce this to a SDP problem in \([12]\), which is equivalent to our result). Therefore in principle, the optimal success probability of UD of mixed states can be found numerically. Actually once we have found the optimal matrix \( \tilde{Y} \), with the standard procedure, we can construct the corresponding unitary implementation of the discrimination operation.
III. UNAMBIGUOUS DISCRIMINATION OF TWO MIXED STATES

In the above discussion, we have given a general description on UD among $N$ mixed input states. To be specific, in the following, we will focus on a particular case, i.e. UD between two mixed states. This is a basic and very important case in the study of UD, and much attention has been paid to this problem recently. In [3], Rudolph et al. present the lower bound on the failure probability $Q$, and later, it has been pointed out that there exist mixed states for which the lower bound cannot be reached for any prior probabilities. Based on these facts, Raynal et al. [9,10] investigated a large class of two mixed states discrimination, they also found the necessary and sufficient conditions for two mixed state to saturate these bounds. In all these works, $Q$ is considered in three different regions, depending on the ratio between two prior probabilities. Recently, Bergou et al. [11] have considered the discrimination of two subspaces and they find that for this special case there are many parameter regions which can give different minimal failure probabilities. The regions depend on both the prior probabilities and the specific structure of the two subspaces. The lower bound $2\sqrt{m^2n^2}F$ of the failure probability $Q$ can be reached only when the prior probabilities lie in some specific regions. Later they conjecture that this phenomenon occurs for any two mixed states. In the following, we will show that this result is indeed universal.

When restricted to two-state case, Eq. (3) can be simplified as

$$
\begin{bmatrix}
\tilde{X}_{11} & \tilde{X}_{12} \\
\tilde{X}_{21} & \tilde{X}_{22}
\end{bmatrix} - 
\begin{bmatrix}
\tilde{Y}_{11} & 0 \\
0 & \tilde{Y}_{22}
\end{bmatrix} \geq 0,
$$

(8)

where $\tilde{X}_{kl}$ arise from the decompositions of $\rho_1$ and $\rho_2$. Usually there exist many other ensembles which can generate the same operators, i.e. $\rho_1 = (|\psi_1^{(1)}\rangle, |\psi_2^{(1)}\rangle, \ldots)(|\psi_1^{(1)}\rangle, |\psi_2^{(1)}\rangle, \ldots)^T = (|\tilde{\psi}_1\rangle, |\tilde{\psi}_2\rangle, \ldots)U^T(U(|\tilde{\psi}_1\rangle, |\tilde{\psi}_2\rangle, \ldots)^T = (|\tilde{\rho}_1\rangle, |\tilde{\rho}_2\rangle, \ldots)(|\tilde{\rho}_1\rangle, |\tilde{\rho}_2\rangle, \ldots)^T$, where $U$ (or $V$ for $\rho_2$) is a unitary matrix and $T$ represents the transpose of the matrix. This is known as the unitary freedom for density matrices [16]. Hence we can also write down the correspondence of Eq. (3) according to this new decomposition

$$
\tilde{X}' \times - \tilde{Y}' \geq 0.
$$

(9)

Since $\tilde{X}' = \text{diag}(U, V) \tilde{X} \text{diag}(U^T, V^T)$, we can immediately obtain that this will not affect the total success probability $P$ we consider here (This is also general for $N$ input mixed states).

Keeping in mind that $U$ and $V$ can be arbitrary, we can choose the two matrices appropriately such that $U \tilde{X}_{12}V^T = \text{diag}(\{f_1, f_2, \ldots, f_t\}, 0)$, where we assume $\tilde{X}_{11}$ and $\tilde{X}_{22}$ are $u \times u$ and $v \times v$ matrices respectively with $u \leq v$, $f_m$ are the singular values of $X_{12}$, and $\tilde{0}$ is a $(u - t) \times (v - t)$ zero matrix. This implies there exist some kinds of decompositions of $\rho_1$ and $\rho_2$, namely, $\rho_1 = \sum_m |\tilde{r}_m\rangle \langle \tilde{r}_m|$ and $\rho_2 = \sum_n |\tilde{s}_n\rangle \langle \tilde{s}_n|$, which satisfies the following equations

$$
\langle \tilde{r}_m | \tilde{s}_n \rangle = \left\{ \begin{array}{ll}
f_m \delta_{mn} & (m, n) \leq t, \\
0 & \text{otherwise}.
\end{array} \right.
$$

(10)

The singular values $f_m$ have very interesting properties and we characterize this by the following theorem [17].

**Theorem 2.** Given two mixed states density matrices $\rho_1$ and $\rho_2$, there exist two sets of canonical vectors $\{|\tilde{r}_1\rangle, |\tilde{r}_2\rangle, \ldots\}$ and $\{|\tilde{s}_1\rangle, |\tilde{s}_2\rangle, \ldots\}$, which generate $\rho_1$ and $\rho_2$ respectively, such that Eq. (17) is satisfied. And the fidelity of the two density matrices can be formulated as

$$
F = \sqrt{\rho_1^{1/2} \rho_2^{1/2}} = \sum_m f_m.
$$

Proof: The only thing we should do now is to prove the second part of this theorem. Consider the spectral decompositions of $\rho_1$ and $\rho_2$

$$
\rho_1 = \sum_i \alpha_i |\alpha_i\rangle \langle \alpha_i|, \quad \rho_2 = \sum_h \beta_h |\beta_h\rangle \langle \beta_h|.
$$

(11)

According to the definition of fidelity $F$, we obtain

$$
(\rho_1^{1/2} \rho_2^{1/2})_{ij} = \sum_h \sqrt{\alpha_i} \sqrt{\beta_h} \langle \alpha_i | \beta_h \rangle = \sqrt{\alpha_j} \sqrt{\beta_h} \langle \beta_h | \alpha_j \rangle.
$$

(12)

Now we definite a new matrix

$$
A_{ih} = \sqrt{\alpha_i} \sqrt{\beta_h} \langle \alpha_i | \beta_h \rangle.
$$

(13)

The fidelity $F$ can be rewritten as this

$$
F = \text{Tr} \sqrt{\rho_1^{1/2} \rho_2^{1/2}} = \text{Tr} \sqrt{AA^\dagger}.
$$

(14)

Since $A$ is a complex matrix, using a singular value decomposition, we have $A = U \text{diag}(\{f_1, f_2, \ldots, f_t\}, 0) V_i$ with $f_m \geq 0$ for all $1 \leq m \leq t$. Thus the fidelity becomes

$$
F = \text{Tr} \sqrt{AA^\dagger} = \sum_m f_m.
$$

(15)

On the other hand, because of the unitary freedom in the ensemble representation of density matrices, we can find two unitary operations $U_2$ and $V_2$ such that $U_2 \tilde{X}_{12} V_2 = A$. Therefore $A$ and $X_{12}$ have the same singular values, which completes the proof.

Theorem 2 indicates for any two mixed states, it is always possible to find two sets of canonical vectors $\{|\tilde{r}_1\rangle, |\tilde{r}_2\rangle, \ldots\}$ and $\{|\tilde{s}_1\rangle, |\tilde{s}_2\rangle, \ldots\}$ so that $|\tilde{r}_m\rangle$ only have a nonzero overlap with $|\tilde{s}_m\rangle$. When $(n, m) \geq t$, one can easily check that $|\tilde{r}_m\rangle$ and $|\tilde{s}_n\rangle$ lie in the subspace orthogonal to the supports of $\rho_1$ and $\rho_1$ respectively. From the reduction theorem in [15], we conclude that UD between $\rho_1$ and $\rho_2$ is equivalent to that between the two newly
defined density matrices $\rho_1' = \sum_{m=1}^t |\tilde{r}_m\rangle\langle\tilde{r}_m|/N_1$ and $\rho_2' = \sum_{m=1}^t |\tilde{s}_m\rangle\langle\tilde{s}_m|/N_2$ with $N_1 = \text{Tr}(\sum_{m=1}^t |\tilde{r}_m\rangle\langle\tilde{r}_m|)$ and $N_2 = \text{Tr}(\sum_{m=1}^t |\tilde{s}_m\rangle\langle\tilde{s}_m|)$ being the corresponding normalization factors. According to the system-ancilla model (Theorem 1), Eq. (5) can always be reduced to a $2t \times 2t$ matrix
\[
\left( \begin{array}{cc}
X_{11} - \tilde{Y}_{11} & \text{diag}\{f_1, \ldots, f_t\} \\
\text{diag}\{f_1, \ldots, f_t\} & X_{22} - \tilde{Y}_{22}
\end{array} \right) \geq 0,
\]
(16)
where we have used the same notations for simplicity.

Equation (10) supplies enough information which can be used to demonstrate our main results. Actually, since $X - Y$ is positive semidefinite, from the standard linear algebra theory, we have that every principal minor of $X - Y$ can be used to demonstrate our main results. Actually, since $X_{11}$ and $X_{22}$ are not diagonal matrices, generally, for different canonical vectors of the input states, the question can be in part reduced to UD between pairs of state vectors $|\tilde{r}_m\rangle$ and $|\tilde{s}_m\rangle$. Such question has been solved in many earlier works, and the results are listed as follows
\[
P_m = \eta_1 y_m + \eta_2 z_m
\leq \sum_m P_m^{\text{max}}
\begin{cases}
\eta_2(s_m - f_m^2/r_m) & 0 \leq \sqrt{\frac{m}{n_2}} \leq \frac{f_m}{r_m} \\
\eta_1 r_m + \eta_2 s_m - 2\sqrt{\eta_1\eta_2 f_m} & \frac{f_m}{r_m} \leq \sqrt{\frac{m}{n_2}} \leq \frac{s_m}{f_m} \\
\eta_1(r_m - f_m^2/s_m) & \sqrt{\frac{m}{n_2}} \geq \frac{s_m}{f_m}.
\end{cases}
\]
(18)

The above expression shows that for every $m$, the maximal value that $P_m$ can achieve has a close relation with the specific configuration of $\sqrt{\frac{m}{n_2}}$, $r_m$, $s_m$, and $f_m$. Generally, for different $m$, $P_m$ will have very different expressions. Therefore, the total success probability $P = \sum_m P_m$ cannot always be represented as a function of the fidelity $F = \sum_m f_m$.

Specifically, in the following we will focus on some special cases. Firstly, if for all $m = 1, \ldots, t$, we have $\frac{f_m}{r_m} \leq \sqrt{\frac{m}{n_2}} \leq \frac{s_m}{f_m}$, then according to the above equation, the upper bound of the total success probability can be rewritten as
\[
P = \sum_m P_m \leq \sum_m P_m^{\text{max}} = \sum_m \eta_1 r_m + \eta_2 s_m - 2\sqrt{\eta_1\eta_2 f_m} = 1 - 2\sqrt{\eta_1\eta_2}F.
\]
(19)
The corresponding lower bound of the failure probability becomes $Q = 1 - P \geq 2\sqrt{\eta_1\eta_2}F$. This bound has been proved to be the minimal value of $Q$ for any type of input configurations. However, our result shows that even in this special case, the lower bound of $Q$ can only be possibly saturated. This occurs, for example, when the canonical vectors are orthogonal to each other. In general, since $X_{11}$ and $X_{22}$ are not diagonal matrices, this lower bound cannot always be reached.

In the second example, we assume that $\sqrt{\frac{m}{n_2}} \geq \frac{f_m}{r_m}$ for all $1 \leq m \leq t$. A simple algebra will lead us to the following bound of the total success probability $P \leq \eta_1(1 - \sum_m f_m^2/s_m)$. If we introduce a new operator $C_2 = \sum_m |s_m\rangle\langle s_m|$ composed of the normalized canonical vectors of $\rho_2$, we can reformulate $P$ as $P \leq \eta_1(1 - \text{Tr}(\rho_1 C_2))$, or equivalently $Q \geq \eta_2 + \eta_1 \text{Tr}(\rho_1 C_2)$. When $|s_m\rangle$ are orthogonal to each other, $C_2$ is nothing but the projection onto the support of $\rho_2$.

Thirdly, if we have $\sqrt{\frac{m}{n_2}} \leq \frac{f_m}{r_m}(\forall m)$, the total success probability satisfies $P \leq \eta_2(1 - \sum_m f_m^2/r_m) = \eta_2(1 - \text{Tr}(\rho_2 C_1))$ with $C_1 = \sum_m |r_m\rangle\langle r_m|$. Correspondingly, the failure probability becomes $Q \geq \eta_1 + \eta_2 \text{Tr}(\rho_2 C_1)$.

For mixed states $\rho_1$ and $\rho_2$, we always have $(r_m, s_m) < 1$. This indicates that the failure probability $Q$ can never reach the bound $2\sqrt{\eta_1\eta_2}F$ for the latter two cases. Generally, different canonical vectors of the input states will separate the parameter space into different regions, and the lower bound of $Q$ is determined by both the prior probabilities and the structure of states. Moreover, in each region, the lower bound of $Q$ can not always be reached. Mathematically, to judge whether the lower bound can be saturated is equivalent to determinating whether there exists a positive semidefinite matrix $\tilde{Y} \geq 0$ such that Eq. (5) is satisfied. This problem is often called semidefinite feasibility problem (SDFP). Unfortunately, the complexity of SDFP is still not known, and currently we can only say that it cannot be a NP-complete problem unless NP=NP-complete. Therefore to judge whether the bound of $Q$ can be reached or not seems to be a hard problem. But in some special case (for example, the canonical vectors are orthogonal to each other, or $X - Y$ is a diagonally dominant matrix), some known results in linear algebra theory will be helpful to solve this problem.

IV. EXAMPLES

In many related works, the upper bound of the success probability $P$ is only considered in three different intervals, which depends on the ratio of $\eta_1$ and $\eta_2$ together with the fidelity $F$ and supports of the input states. Here by introducing the decomposition in Theorem 2, we find a series of parameter regions related to the specific input states. In addition, from the system-ancilla coupling viewpoint, one can also derive the corresponding results in $\tilde{B}$ and $\tilde{C}$. For example, if we definite $B = X' - \tilde{Y}'$ in Eq. (9), then since $B$ is positive semidefinite, we have
\[
\sqrt{\text{Tr}(\tilde{B}_{11})/\text{Tr}(\tilde{B}_{22})} \geq \text{Tr}(\tilde{B}_{12})\]

for any kind of decompositions of \(p_1\) and \(p_2\) (for the definitions of \(\tilde{B}_{ij}\), see Eq. \([8]\)). Therefore we obtain \(\sqrt{\text{Tr}(\tilde{B}_{11})/\text{Tr}(\tilde{B}_{22})} \geq F\), where equality holds only when \(\tilde{B}_{11} = \alpha \tilde{B}_{22}\) with \(\alpha \in \mathbb{R}\). This also indicates that the output states corresponding to the failure measurement results cannot be used for further discrimination operations, which is consistent with the discussions in \([6]\). To reveal the relation and difference between the bounds listed above and those in the previous works, in the following we will investigate a specific example.

Consider two rank-2 mixed states \(p_1 = \frac{1}{2}(|r_1\rangle\langle r_1| + |r_2\rangle\langle r_2|)\) and \(p_2 = \frac{1}{2}(|s_1\rangle\langle s_1| + |s_2\rangle\langle s_2|)\) with \(\langle r_1|s_2\rangle = 0\), \(\langle r_1|s_1\rangle = \cos\theta_1\), and \(\langle r_2|s_2\rangle = \cos\theta_2\). To simplify our consideration, we also assume \(\langle r_1|r_2\rangle = \langle s_1|s_2\rangle = 0\). Actually, discrimination of such kind of mixed states has been extensively studied in \([11]\). Here we also use it to manifest the difference of the upper bounds presented in several related works. Suppose \(0 < \cos\theta_1 \leq \cos\theta_2 < 1\). Then based on our former discussions, optimal success probability \(P\) can be obtained exactly in five parameter regions, \([0, \cos\theta_1]\), \([\cos\theta_1, \cos\theta_2]\), \([\cos\theta_2, 1/\cos\theta_2]\), \([1/\cos\theta_2, 1/\cos\theta_1]\), \([1/\cos\theta_1, \infty]\). Alternatively, one can also obtain the corresponding upper bound of \(P\) according to \([9]\) and \([8]\). Table 1 shows the details of \(P\) in each of these regions.

| \(\sqrt{\eta_1/\eta_2}\) | \(P\) | \(P_{Ra}(P_{Ru})\) |
|---|---|---|
| \([0, \cos\theta_1]\) | \(\frac{1}{2}\eta_2(\sin^2\theta_1 + \sin^2\theta_2)\) | \(\frac{1}{2}\eta_2(\sin^2\theta_1 + \sin^2\theta_2) + \frac{1}{2}\eta_1\left(\frac{\cos\theta_1 - \cos\theta_2}{\cos\theta_1 + \cos\theta_2}\right)^2\) (or \(\eta_1(1 - F^2)\)) |
| \([\cos\theta_1, Ra_1(F)]\) | \(\frac{1}{2} - \sqrt{\eta_1\eta_2}\cos\theta_1 + \frac{1}{2}\eta_1\sin^2\theta_2\) | \(1 - 2\sqrt{\eta_1\eta_2}F\) (or \(1 - 2\sqrt{\eta_1\eta_2}F\)) |
| \([Ra_1(F), \eta_{\infty}]\) | \(\frac{1}{2} - \sqrt{\eta_1\eta_2}\cos\theta_1 + \frac{1}{2}\eta_1\sin^2\theta_2\) | \(\frac{1}{2}\eta_1\left(\sin^2\theta_1 + \sin^2\theta_2\right) + \frac{1}{2}\eta_1\left(\frac{\cos\theta_1 - \cos\theta_2}{\cos\theta_1 + \cos\theta_2}\right)^2\) (or \(\eta_1(1 - F^2)\)) |

TABLE I: Bounds of the maximal success probabilities presented in several related works. Here \(P\) denotes the bound according to Eq. \([13]\). \(P_{Ra}\) and \(P_{Ru}\) are the results obtained from \([8]\) and \([9]\) respectively. \(F = (\cos\theta_1 + \cos\theta_2)/2\) is the fidelity of the two input mixed states. \(Ra_1 = \text{Tr}(P_{Ra_2})/F = (\cos^2\theta_1 + \cos^2\theta_2)/(\cos\theta_1 + \cos\theta_2)\) and \(Ra_2 = F/\text{Tr}(P_{Ra_1}) = (\cos\theta_1 + \cos\theta_2)/(\cos^2\theta_1 + \cos^2\theta_2)\) are parameters according to \([8]\) with \(P_1\) and \(P_2\) being the supports of \(\rho_1\) and \(\rho_2\) separately.

The above table shows that when \(\cos\theta_1 = \cos\theta_2\), the three bounds \(P, P_{Ra}\), and \(P_{Ru}\) are equal to each other. However, for the general case \(\cos\theta_1 \neq \cos\theta_2\), one can easily obtain \(P \leq P_{Ra}\) and \(P \leq P_{Ru}\), and equalities hold only when \(\cos\theta_2 \leq \sqrt{\eta_1/\eta_2} \leq 1/\cos\theta_2\). For example, if \(\cos\theta_1 \leq \sqrt{\eta_1/\eta_2} \leq Ra_1\), we have \(P_{Ra} - P = \frac{1}{2}\sqrt{\eta_2}[2x\cos\theta_1 - \cos^2\theta_1 - 2x^2\cos\theta_1\cos\theta_2/(\cos^2\theta_1 + \cos^2\theta_2)] = f(x)\), where we have assumed \(x = \sqrt{\eta_1/\eta_2}\). Since \(f(\cos\theta_1) = \eta_2\cos^2\theta_1(\cos\theta_1 - \cos\theta_2)^2/[2(\cos^2\theta_1 + \cos^2\theta_2)] \geq 0\) and \(f(Ra_1) = \eta_2\cos^2\theta_1(\cos\theta_1 - \cos\theta_2)^2/[2(\cos\theta_1 + \cos\theta_2)^2] \geq 0\), one immediately sees that \(P \leq P_{Ra}\) for any \(\sqrt{\eta_1/\eta_2}\) in \([\cos\theta_1, Ra_1]\). These observations indicate that the bound presented in this work is independent of those of former works, and sometimes it can provide tighter bound of the total success probability \(P\), as we have expected.

V. CONCLUSION

To summarize, we have proposed a general description on the UD of mixed states from the system-ancilla model, and presented a procedure to reduce this to a standard SDP problem, which makes the problem to be solvable numerically. On the UD between two mixed states, we have introduced the canonical vectors and partly reduced the original problem to the UD between pairs of canonical vectors. We present a series of new upper bounds on the total success probability which depends on both the ratio of the prior probabilities and the input state structures. This indicates that the results in \([11]\) are universal for any type of input states. It also should be mentioned that throughout the paper we mainly concentrate on the diagonal elements of the corresponding matrices. In practice, the non-diagonal elements also play important roles which deserves further investigation.

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