Optimal discrimination of mixed quantum states involving inconclusive results

1. INTRODUCTION

The non-admissibility of quantum states is one of the fundamental features of quantum mechanics. In particular, the quantum mechanical formalism allows for the existence of mixed quantum states that cannot be described by a single density matrix. This is in contrast to classical probability theory, where a mixed state is always represented by a convex combination of pure states.

Recently, several authors have proposed methods for the optimal discrimination of mixed quantum states. These methods typically involve the use of quantum operations to distinguish between different states. In this work, we focus on the problem of discriminating between mixed quantum states that cannot be distinguished using any single quantum operation.

We propose a generalization of the quantum discrimination problem to mixed quantum states. This generalization allows for the optimal discrimination of mixed states that cannot be distinguished using any single quantum operation. We formulate the problem in terms of a decision-theoretic framework, where the goal is to design a quantum operation that maximizes the probability of correctly identifying the unknown state.

Mathematically, the problem can be formulated as an optimization problem over the set of all possible quantum operations. The optimization criterion is the probability of correctly identifying the unknown state, which is a function of the quantum operation and the prior distribution over the states.

The solution to this optimization problem provides an optimal protocol for the discrimination of mixed quantum states. The protocol is characterized by a set of quantum operations, each of which is associated with a particular probability of success. The optimal protocol is obtained by an iterative optimization procedure that maximizes the probability of correctly identifying the unknown state.

In the following sections, we provide a detailed description of the optimal discrimination of mixed quantum states. We outline the mathematical formulation of the problem, present analytical results, and discuss applications to practical scenarios involving mixed quantum states.

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II. EXTREMAL EQUATIONS FOR OPTIMAL PVM

Let us begin with the formal definition of the problem. We assume that the quantum state sent to Bob is drawn from the set of $N$ mixed states $\{\rho_j\}_{j=1}^N$ with the a-priori probabilities $p_j$. Bob’s measurement on the state may yield $N + 1$ different results and is formally described by the PVM whose $N + 1$ components satisfy

$$\Pi_j \geq 0, \quad j = 0, \ldots, N, \quad \sum_{j=0}^N \Pi_j = 1,$$

(4)

where $I$ is the identity operator. The outcome $\Pi_j$ indicates failure and the probability of inconclusive results is thus given by

$$P_I = \sum_{j=0}^N p_j \text{Tr}[\rho_j \Pi_I].$$

(5)

For a certain fixed value of $P_I$ we want to maximize the relative success rate (3) which is equivalent to the maximization of the success rate (2). To account for the linear constraints (4) and (5) we introduce Lagrange multipliers $\lambda$ and $a$ where $\lambda$ is Hermitian operator and $a$ is a real number. Taking everything together we should maximize the constrained success rate functional

$$\hat{P}_S = \sum_{j=1}^N p_j \text{Tr}[\rho_j \Pi_j] - \sum_{j=0}^N \text{Tr}[\lambda \Pi_j] + a \sum_{j=1}^N p_j \text{Tr}[\rho_j \Pi_I].$$

(6)

We now derive the extremal equations that must be satisfied by the optimal PVM. We expand the PVM elements in terms of their eigenstates and eigenvalues, $\Pi_j = \sum_k r_{jk} \langle \phi_j | \phi_k \rangle$ and vary (6) with respect to $\langle \phi_j |$. After some algebraic manipulations, we arrive at the extremal equations,

$$\lambda - p_j \rho_j \Pi_j = 0, \quad j = 1, \ldots, N, \quad (7)$$

$$\lambda - a \sigma \Pi_j = 0, \quad (8)$$

where the operator $\sigma$ introduced for the sake of notational simplicity reads

$$\sigma = \sum_{j=1}^N p_j \rho_j.$$

(9)

From the constraint $\text{Tr}[\sigma \Pi_I] = P_I$ we can express $a$ in terms of $\lambda$,

$$a = P_I^{-1} \text{Tr}[\lambda \Pi_I].$$

(10)

Furthermore, if we sum all Eqs. (7) and also Eq. (8) and use the resolution of the identity (4), we obtain formula for $\lambda$,

$$\lambda = \sum_{j=1}^N p_j \rho_j \Pi_j + a \sigma \Pi_I.$$

(11)

If we combine Eqs. (10) and (11) then we can express $a$ and $\lambda$ solely in terms of $p_j$, $\rho_j$, and $\Pi_j$. This may be important, for example, if we guess the optimal PVM and want to determine the corresponding Lagrange multipliers. The extremal Eqs. (7) and (8) constitute a generalization of the extremal equations for optimal PVM for ambiguous quantum state discrimination that were derived by Holevo and Helstrom [6, 8].

We now provide simple sufficient conditions on the optimality of the PVM. If the PVM satisfies the extremal Eqs. (7) and (8) and if the following inequalities hold:

$$\lambda - p_j \rho_j \geq 0, \quad j = 1, \ldots, N,$$

$$\lambda - a \sigma \geq 0,$$

then the PVM is the optimal one that maximizes the success rate $P_S$ for a given fixed probability of inconclusive results $P_I$.

To prove this statement we show that the Lagrange multipliers provide an upper bound on the success rate and that this bound is saturated by the PVM that satisfies Eqs. (7) and (8). From the definition of the success rate (2), the inequalities (12) and the normalization (4) we obtain

$$P_S \leq \sum_{j=1}^N \text{Tr}[\lambda \Pi_j] = \text{Tr}[\lambda (I - \Pi_I)].$$

(14)

Now we use the inequality (13) and finally we take into account the constraint $\text{Tr}[\sigma \Pi_I] = P_I$. We arrive at

$$P_S \leq \text{Tr}[\lambda] - a P_I.$$

(15)

This last inequality shows that $P_S$ is limited from above by the quantity that depends only on the Lagrange multipliers $\lambda$ and $a$ also on the fixed $P_I$. If the PVM $\Pi_j$ satisfies the extremal Eqs. (7) and (8) then this upper bound is reached, as can easily be checked.

We have thus established a simple criterion for checking of the PVM optimality. Of course, we would like to derive the optimal PVM $\Pi_j$ for given $p_j$, $\rho_j$, and $P_I$. The analytical solution to this problem seems to be extremely complicated. Nevertheless, recently it was pointed out that one can solve this kind of problems very efficiently numerically [3-4]. One possible simple and fruitful approach is to solve the extremal equations by means of repeated iterations [34, 35, 36, 37, 38, 39]. In principle, one could iterate directly Eqs. (7) and (8). However, the PVM elements $\Pi_j$ should be positive semidefinite Hermitian operators. All constraints can be exactly satisfied at each iteration step if the extremal equations are symmetrized. First we express $\Pi_j = p_j \lambda^{-1} \rho_j \Pi_I$ and combine it with its Hermitian conjugate. We proceed similarly also for $\Pi_I$ and we get

$$\Pi_j = p_j \lambda^{-1} \rho_j \Pi_I \rho_j \lambda^{-1}, \quad j = 1, \ldots, N,$$

$$\Pi_I = a \lambda^{-1} \sigma \Pi_I \sigma \lambda^{-1}.$$
The Lagrange multipliers $\lambda$ and $a$ must be determined self-consistently so that all the constraints will hold. If we sum Eqs. (16) and (17) and take into account that

$$\sum_{j=0}^{N} \Pi_j = 1,$$

we obtain

$$\lambda = \left[ \sum_{j=1}^{N} p_j^2 \rho_j \Pi_j + a^2 \sigma \Pi_j \sigma \right]^{1/2}. \quad (18)$$

The fraction of inconclusive results calculated for the POVM after the iteration is given by

$$F_1 = a^2 \text{Tr} \left[ \sigma \lambda^{-1} \sigma \Pi_j \sigma \lambda^{-1} \right]. \quad (19)$$

Since the Lagrange multiplier $\lambda$ is expressed in terms of $a$, Eq. (19) forms a nonlinear equation for a single real parameter $a$ (or, more precisely, $a^2$). This nonlinear equation can be very efficiently solved by Newton’s method of halving the interval. At each iteration step for the POVM elements, we thus solve the system of coupled nonlinear equations (18) and (19) for the Lagrange multipliers. These self-consistent iterations work very well and our extensive numerical calculations confirm that they typically exhibit an exponentially fast convergence [34].

We note that the maximization of the success rate $P_S$ for a fixed fraction of inconclusive results $P_I$ can also be formulated as a semidefinite program. Powerful numerical methods developed for solving this kind of problems may be applied. Here we will not investigate this issue in detail and we refer the reader to the papers [34, 40, 41] where the formulation of optimal quantum-state discrimination as a semidefinite program is described in detail. Note also that the semidefinite programming has recently found its applications in several branches of quantum information theory such as the optimization of completely positive maps [42, 43, 44], the analysis of the distillation protocols that preserve the positive partial transposition [45], or the tests of separability of quantum states [46].

### III. MAXIMAL ACHIEVABLE RELATIVE SUCCESS RATE

As the fraction of inconclusive results is increased the success rate $P_S$ decreases. However, the relative success rate $P_{RS}$ grows until it achieves its maximum. If $\{\rho_j\}_{j=1}^{N}$ are linearly independent pure states, then $P_{RS,max} = 1$ because exact IDP scheme works and the unambiguous discrimination is possible. Generally, however, the maximum is lower than unity. To find this maximum, we notice that in the limit $P_I \to 1$ the POVM element $\Pi_j$ must tend to the identity operator. This means that at some point $\Pi_j$ becomes positive definite operator and all its eigenvalues are strictly positive. In that case, the extremal equation (8) can be satisfied if and only if

$$\lambda = a \sigma. \quad (20)$$

Since we are looking for some nontrivial solution to the extremal equations with $P_I < 1$, at least one of the extremal Eqs. (7) must have a nontrivial solution $\Pi_j \neq 0$. This implies that at least one of the operators $\lambda - p_j \rho_j$ must have one eigenvalue $\mu_j$ equal to zero which implies that

$$\det \left[ a \sigma - p_j \rho_j \right] = 0 \quad (21)$$

must hold at least for one of the states $\rho_j$. The optimal $\Pi_j$ is then proportional to the projector to the subspace spanned by eigenvectors corresponding to the eigenvalue $\mu = 0$.

The maximal attainable relative success rate $P_{RS}$ obtained if we insert (20) into (15), take into account that $\text{Tr}[\sigma] = \sum_j p_j = 1$ and re-normalize according to Eq. (3),

$$P_{RS} = a. \quad (22)$$

To determine the maximal $P_{RS}$ we must find the maximal $a$ that satisfies Eq. (21). Since $\sigma$ is positive definite it can be inverted, and we can equivalently express the maximal $a$ as the maximal eigenvalue of a Hermitian matrix,

$$a_j = p_j \max \left[ \text{eig} (\sigma^{-1/2} \rho_j \sigma^{-1/2}) \right]. \quad (23)$$

The maximal $P_{RS}$ is equal to the largest $a_j$,

$$P_{RS,max} = \max a_j. \quad (24)$$

For qubits, Eq. (21) leads to quadratic equation for the multiplier $a_j$ that can be solved analytically,

$$(a_j - p_j)^2 = a_j^2 \text{Tr} [\sigma^2] - 2 a_j p_j \text{Tr} [\rho_j \sigma] + p_j^2 \text{Tr} [\rho_j^2]. \quad (25)$$

It turns out that the maximal $P_{RS}$ depends only on the a-priori probabilities $p_j$, the purities of the states $\rho_j = \text{Tr} [\rho_j^2]$ and the overlaps $\mathcal{O}_{jk} = \text{Tr} [\rho_j \rho_k]$. In this context it is worth noting that it was shown recently that these parameters of the quantum states can directly be measured without the necessity to carry out a complete quantum state reconstruction [47, 48, 49].

### IV. DISCRIMINATION BETWEEN TWO MIXED QUBIT STATES

We proceed to illustrate the methods developed in the present paper on explicit example. We consider the simple yet nontrivial problem of optimal discrimination between two mixed qubit states $\rho_1$ and $\rho_2$. To simplify the discussion, we shall assume that the purities of these states as well as the a-priori probabilities are equal, $P_1 = P_2 = P$, $p_1 = p_2 = 1/2$. The mixed states can be visualized as points inside the Poincare sphere and the purity determines the distance of the point from the center of that sphere. Without loss of generality, we can assume that both states lie in the $x$-plane and are symmetrically located about the $z$-axis,

$$\rho_{1,2} = \eta \psi_{1,2}(\theta) + \frac{1 - \eta}{2} \mathbb{I}, \quad (26)$$
where the parameter $\eta$ determines the purity, $\psi_j = |\psi_j\rangle\langle\psi_j|$ denotes a density matrix of a pure state,

$$|\psi_{1,2}(\theta)\rangle = \cos \frac{\theta}{2}|0\rangle \pm i \sin \frac{\theta}{2}|1\rangle,$$  \hspace{1cm} (27)

and $\theta \in (0, \pi/2)$. From the symmetry it follows that the elements $\Pi_{1,2}$ of the optimal POVM must be proportional to the projectors $\psi_1(\phi)$ and $\psi_2(\phi)$, where the angle $\phi \in (\pi/2, \pi)$ is related to the fraction of the inconclusive results. The third component $\Pi_0$ is proportional to the projector onto state $|0\rangle$. The normalization of the POVM elements can be determined from the constraint (4) and we find

$$\Pi_{1,2}(\phi) = \frac{1}{2 \sin^2(\phi/2)} \psi_{1,2}(\phi),$$  \hspace{1cm} (28)

$$\Pi_0(\phi) = \left(1 - \frac{1}{\tan^2(\phi/2)}\right) |0\rangle\langle 0|.$$

The relative success rate for this POVM reads

$$P_{RS} = \frac{1 + \eta \cos(\phi - \theta)}{2(1 + \eta \cos \theta \cos \phi)}$$  \hspace{1cm} (29)

and the fraction of inconclusive results is given by

$$P_{I} = \frac{1}{2} \left(1 + \eta \cos \theta \right) \left(1 - \frac{1}{\tan^2(\phi/2)}\right).$$  \hspace{1cm} (30)

The formulas (29) and (30) describe explicitly the dependence of the relative success rate $P_{RS}$ on the fraction of the inconclusive results $P_I$. From Eqs. (10) and (11) one can determine the Lagrange multipliers $\lambda$ and $\alpha$ for the POVM (28) and check that the extremal Eqs. (7), (8), (12) and (13) are satisfied which proves that the POVM (28) is indeed optimal.

The maximum $P_{RS,\text{max}}$ (24) is achieved if the angle $\phi$ is chosen as follows,

$$\cos \phi_{\text{max}} = -\eta \cos \theta.$$  \hspace{1cm} (31)

On inserting the optimal $\phi_{\text{max}}$ back into Eq. (29) we get

$$P_{RS,\text{max}} = \frac{1}{2} \left[1 + \frac{\eta \sin \theta}{\sqrt{1 - \eta^2 \cos^2 \theta}} \right].$$  \hspace{1cm} (32)

Making use of Eqs. (24) and (25) we can express the $P_{RS,\text{max}}$ in terms of the overlap $O_\phi$ and the purity $P$,

$$P_{RS,\text{max}} = \frac{1}{2} \left[1 + \sqrt{\frac{P - O_\phi}{2 - P - O_\phi}} \right].$$  \hspace{1cm} (33)

If we calculate $O$ and $O_\phi$ for the density matrices (26) and insert them into (33) then we recover the formula (22).

The optimal POVM (28) can be also obtained numerically. We demonstrate feasibility of iterative solution of the symmetrized extremal equations (16), (17), (18), and (19) for mixed quantum states (26) with the angle of separation $\theta = \pi/4$. The trade-off of the relative success rate and the probability of inconclusive results is shown in Fig. 1 for various purities of the states being discriminated. For the given probability $P_I$ of inconclusive results and the given purity of the states the extremal equations were solved self-consistently by means of repeated iterations. The success rate $P_{RS}$ is evaluated from the obtained optimal POVM and re-normalized according to Eq. (3). The numerically obtained dependence of $P_{RS}$ on $P_I$ is in excellent agreement with the analytical dependence following from formulas (29) and (30). Typically, a sixteen digit precision is reached after several tens of iterations. The trade-off curves shown in Fig. 1 reveal the monotonous growth of $P_{RS}$ until the maximal plateau (32) is reached.

**V. CONCLUSIONS**

In conclusion, we have considered a generalized discrimination scheme for mixed quantum states. The present scenario interpolates between the Helstrom and IDP schemes. We allow for a certain fixed fraction of inconclusive results and maximize the success rate. We have derived the extremal equations for the optimal POVM that describes the discrimination device. The extremal equations can be efficiently solved numerically by means of the devised simple iterative algorithm or, alternatively, by using the powerful techniques of semidefinite programming.

We have shown that the relative success rate $P_{RS}$ monotonically grows as the fraction of inconclusive results $P_I$ is increased and at certain point it reaches its upper bound $P_{RS,\text{max}}$. For purely linearly independent states this bound is $P_{RS,\text{max}} = 1$ which corresponds to the IDP unambiguous discrimination scheme. For mixed states this bound is in general lower than unity and we have derived a simple formula for it.
The present scheme may be important for quantum cryptographic schemes where the receiver and/or eavesdropper want to discriminate nonorthogonal states. Although these schemes are usually based on pure states, in realistic cases the unavoidable noise and decoherence will reduce the purity of these states and one would have to deal with mixed states. Various modifications of our method can be suggested for such application. For instance, if the involved states are in some sense asymmetric, one may impose the condition that the probabilities of inconclusive results or successful discrimination of the states $p_j$ should all be identical, and minimize the error rate with this additional constraint.

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