Complete analysis for three-qubit mixed-state discrimination

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In this article, by treating minimum error state discrimination as a complementarity problem, we obtain the geometric optimality conditions. These can be used as the necessary and sufficient conditions to determine whether every optimal measurement operator can be nonzero. Using these conditions and an inductive approach, we demonstrate a geometric method and the intrinsic polytope for N-qubit mixed-state discrimination. When the intrinsic polytope becomes a point, a line segment, or a triangle, the guessing probability, the necessary and sufficient condition for the exact solution, and the optimal measurement are analytically obtained. We apply this result to the problem of discrimination to arbitrary three-qubit mixed states with given *a priori* probabilities and obtain the complete analytic solution to the guessing probability and optimal measurement.

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The goal of quantum-state discrimination is to distinguish between states of a given set as well as possible. In other words, it can be regarded as a problem to find the optimal measurement for discriminating among the given quantum states. In fact, every state in classical physics can be orthogonal to each other and therefore distinguished perfectly [1]. However, in quantum physics, a state cannot be perfectly discriminated because of the existence of nonorthogonal states [2–4]. Quantum-state discrimination [5] is classified into minimum error discrimination, originally introduced by Helstrom [2], unambiguous discrimination [6–8], and maximum confidence discrimination [9]. The purpose of minimum error strategy is to find the optimal measurement and the minimum error probability (or guessing probability) for arbitrary N-qudit mixed quantum states with arbitrary *a priori* probabilities. In the $N = 2$ case, regardless of the dimension, the Helstrom bound [2] gives an analytic solution to the problem. In the $N = 3$ case the analytic solution for pure qubit states is provided by [10,11]. In [12] the analytic solution for mixed qubit states is considered without the necessary and sufficient conditions for the solution. In other words, the full understanding for discrimination of three-qubit mixed quantum states is not provided yet.

The optimal measurement for linearly independent quantum states is the von Neumann measurement [13]. But if the given quantum states are linearly dependent, the von Neumann measurement may not be optimal. Therefore, the positive-operator-valued-measure (POVM) should be used for arbitrary quantum states. From the point where POVM can be used as a measurement and the probability to guess the quantum states correctly becomes convex, the minimum error discrimination problem may be solved by convex optimization [14]. Other efforts to solve it have been made using a dual problem [15] or complementarity problem [16]. By applying qubit-state geometry to the optimality conditions for the measurement operators and complementary states, Bae [17] obtained a geometric method to find the guessing probability and the optimal measurement for some special cases. However, they did not include the case where the optimal measurement cannot be POVM, whose every element is nonzero. In this article, we show that the case where the optimal measurement cannot be POVM, whose every element is nonzero, can be understood through the existence of parameters satisfying the geometric optimality conditions [16]. We also clarify the meaning of these geometric conditions. Through the conditions and an inductive approach, we propose a method to discriminate arbitrary N-qubit mixed quantum states with arbitrary *a priori* probabilities. In this method, we define the intrinsic polytope for discrimination problems. When the polytope becomes a point, line segment, or triangle, we find the guessing probability, the necessary and sufficient condition for the exact solution, and the optimal measurement analytically. By the number of extreme points for the intrinsic polytope and the geometric optimality conditions, we can provide a complete analysis for discrimination of the three-qubit mixed state. We also obtain its guessing probability and optimal measurement.

Let q_i and ρ_i $(i = 1,\dots,N)$ be the *a priori* probability and $d \times d$ the density matrix, where d and N denote the dimension and number of states to be discriminated. Hereafter, q_i is ordered by $q_i \geqslant q_{i+1}$. When $\{M_i\}_{i=1}^N$ is used for measurement to $\{q_i,\rho_i\}_{i=1}^N$, the probability to guess the quantum states correctly becomes $P_{\rm corr} = \sum_{i=1}^N q_i \mathrm{tr}\rho_i M_i$. The goal of the minimum error state discrimination is to obtain the maximum of $P_{\rm corr}$, called *the guessing probability* $P_{\rm guess}$, using POVM. Therefore the minimum error state discrimination can be described as

$$\begin{aligned} \max \quad & \sum_{i=1}^{N} q_i \mathrm{tr}\rho_i M_i, \\ \text{subject to} \quad & M_i \geqslant 0 \quad \forall i \in \{1,\cdots,N\}, \\ & \sum_{i=1}^{N} M_i = I_d. \end{aligned} \tag{1}$$

By semidefinite programming [14], the dual problem of Eq. (1) is obtained as follows:

$$\min \mathrm{tr}K, \quad \text{subject to } K - q_i\rho_i \geqslant 0 \quad \forall i \in \{1,\cdots,N\}, \tag{2}$$

where K is the $d \times d$ Hermitian matrix. In fact, using a nonnegative number r_i and the density matrix $\tilde{\rho}_i$, the constraints

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of the dual problem can be written as

$$K = q_i\rho_i + r_i\tilde{\rho}_i \quad \forall i \in \{1,\cdots,N\}. \tag{3}$$

Since the above operator K is equal for all i, the following relation holds:

$$q_i\rho_i - q_j\rho_j = r_j\tilde{\rho}_j - r_i\tilde{\rho}_i \quad \forall i, \quad j \in \{1,\cdots,N\}. \tag{4}$$

In the optimization problem, the dual problem in general has *weak duality* and may not be identical to the original one. However, if the optimization problem is convex and satisfies Slater's condition, the dual one has *strong duality* and is equivalent to the primal one. This condition is to check whether every POVM element is nonzero. Therefore our problem is equivalent to the following:

$$\min\, q_1 + r_1, \quad \text{subject to } r_i\tilde{\rho}_i - r_j\tilde{\rho}_j = q_j\rho_j - q_i\rho_i \ \ \forall i,j. \tag{5}$$

The objective function can be $q_i + r_i (i = 2,\cdots,N)$ instead of $q_1 + r_1$. By considering the Karush-Kuhn-Tucker (KKT) conditions, let us investigate the necessary conditions of $\{M_i, r_i, \tilde{\rho}_i\}_{i=1}^N$, which satisfy $P_{\text{corr}} = q_1 + r_1$. These conditions contain the constraints of the primal and dual problems as well as the complementary slackness one. The final condition can be found by connecting the measurement operators $\{M_i\}_{i=1}^N$ and $\{r_i, \tilde{\rho}_i\}_{i=1}^N$, which are complementary to the constraints of the primal and dual problems:

$$r_i \mathrm{tr}[\tilde{\rho}_i M_i] = 0 \quad \forall i \in \{1,\cdots,N\}. \tag{6}$$

The KKT conditions, summarized in the following, can be derived from the POVM constraints and the no-signaling ones [18]:

$$\begin{aligned}
&\text{(i)} \ \ M_i \geqslant 0 \quad \text{and} \quad \sum_{i=1}^N M_i = I_d \quad \forall i,\\
&\text{(ii)} \ \ r_i\tilde{\rho}_i - r_j\tilde{\rho}_j = q_j\rho_j - q_i\rho_i \quad \forall i,j,\\
&\text{(iii)} \ \ r_i \mathrm{tr}[\tilde{\rho}_i M_i] = 0 \quad \forall i.
\end{aligned} \tag{7}$$

We now obtain the guessing probability and the optimal measurement, by only these conditions. The complementarity problem is the one where a solution is found for the optimization problem by using the optimality conditions which should satisfy the parameters of the primal and dual problem. In this article $*$ is used to denote the optimality of the parameters.

Henceforth, by confining only the case of the two-level system ($d = 2$) let us obtain the geometric condition for Eq. (7). From the Bloch representation $\rho_i = \frac{1}{2}(I_2 + \vec{v}_i\cdot\vec{\sigma})$ and $\tilde{\rho}_i = \frac{1}{2}(I_2 + \vec{w}_i\cdot\vec{\sigma})$ we can derive the following relations:

$$q_i - q_j = r_j - r_i, \tag{8}$$

$$q_i\vec{v}_i - q_j\vec{v}_j = r_j\vec{w}_j - r_i\vec{w}_i \quad \forall i, \quad j \in \{1,\cdots,N\}, \tag{9}$$

where $\vec{v}_i$ and $\vec{w}_i$ are the Bloch vectors and $\vec{\sigma}$ represents the Pauli matrices. Since we assume $q_i \geqslant q_{i+1}$, we can find $r_i^* \leqslant r_{i+1}^*$ from Eq. (8). Therefore if $r_1^* \neq 0$, we have $r_i^* > 0$ $(i = 1,\ldots,N)$. Here, let us take an inductive approach to N-qubit-state discrimination, which means that by assuming that the way to discriminate $(N-1)$ states may be known, we investigate a method to discriminate among the N-qubit states. Therefore it is sufficient to consider only those cases where every optimal POVM element is nonzero. (For generality, we will later consider cases where some of the optimal POVM elements may be zero.) First, we consider cases where every optimal POVM element is nonzero and the guessing probability is greater than q_1. In this case, since r_1^* is nonzero, the condition (iii) becomes $\mathrm{tr}(\tilde{\rho}_i M_i) = 0$, which implies that the rank of $\tilde{\rho}_i$ and M_i should be one. This means that for each i, we find $||\vec{w}_i||_2 = 1$ and

$$M_i = p_i(I_2 - \vec{w}_i\cdot\vec{\sigma}), \quad p_i > 0. \tag{10}$$

Since $\{M_i^*\}_{i=1}^N$ is POVM, $\{p_i,\vec{w}_i\}_{i=1}^N$ should satisfy

$$\sum_{i=1}^N p_i\vec{w}_i = 0, \quad \sum_{i=1}^N p_i = 1. \tag{11}$$

Therefore $\{r_i,\vec{w}_i\}_{i=1}^N$ is necessary to satisfy the following conditions (which we will call the geometric KKT conditions):

$$\begin{aligned}
&\text{(i)} \ \ r_i\vec{w}_i - r_j\vec{w}_j = q_j\vec{v}_j - q_i\vec{v}_i \quad \forall i,j,\\
&\text{(ii)} \ \ \exists\ \{p_i\}_{i=1}^N \text{ s.t. } p_i > 0\, \forall i, \quad \sum_{i=1}^N p_i\vec{w}_i = 0, \quad \sum_{i=1}^N p_i = 1,\\
&\text{(iii)} \ \ \|\vec{w}_i\|_2 = 1 \quad \forall i,\\
&\text{(iv)} \ \ r_i - r_j = q_j - q_i \quad \forall i,j.
\end{aligned} \tag{12}$$

Next, we will show that even when every optimal POVM element is nonzero and the guessing probability becomes q_1, $\{r_i,\vec{w}_i\}_{i=1}^N$ is necessary to satisfy the above condition Eq. (12). We will prove this by considering both cases $q_1 = q_2$ and $q_1 > q_2$. The case of $q_1 = q_2$ implies $\rho_1 = \rho_2$ by the KKT condition (ii), which turns out to be the case of discriminating among the same quantum states. However, we may exclude this case since we are interested in discriminating entirely different quantum states. In the case of $q_1 > q_2$, we can see that since $r_2^* > 0, \{q_1 - q_i, (q_1\vec{v}_1 - q_i\vec{v}_i)/(q_1 - q_i)\}_{i=2}^N$ satisfies the geometric KKT conditions (i), (iii), and (iv). If $r_1 = 0$, the geometric conditions (i) and (iv) do not put any restriction on $\vec{w}_1$. In addition, $\vec{w}_1$ satisfies $\|\vec{w}_1\|_2 = 1$ and the geometric KKT condition (ii). From these facts we can see that $\{r_i,\vec{w}_i\}_{i=1}^N$ should satisfy every geometric KKT condition.

Until now we showed that if every optimal POVM element is nonzero, we can find $\{r_i,\vec{w}_i\}_{i=1}^N$ by satisfying the geometric KKT conditions. Now we will prove the reverse. That is, we will prove that if $\{r_i,\vec{w}_i\}_{i=1}^N$ satisfies the geometric KKT conditions, every optimal POVM element can be nonzero. For this let us assume that $\{r_i,\vec{w}_i\}_{i=1}^N$ satisfies the geometric KKT conditions. When $\vec{R} \equiv q_i\vec{v}_i + r_i\vec{w}_i (i = 1,\ldots,N)$, the following relation holds:

$$\begin{aligned}
&\sum_{i=1}^N q_i p_i(1 - \vec{v}_i\cdot\vec{w}_i)\\
&\quad = \sum_{i=1}^N (q_1 + r_1 - r_i)p_i - \sum_{i=1}^N q_i p_i\vec{v}_i\cdot\vec{w}_i\\
&\quad = (q_1 + r_1) - \sum_{i=1}^N r_i p_i\|\vec{w}_i\|_2^2 - \sum_{i=1}^N q_i p_i\vec{v}_i\cdot\vec{w}_i\\
&\quad = (q_1 + r_1) - \sum_{i=1}^N p_i\vec{w}_i\cdot\vec{R} = q_1 + r_1.
\end{aligned} \tag{13}$$

Then by $\{M_i\}_{i=1}^N$ given in Eq. (10), we can see that P_{corr} of the primal problem is equal to $q_1 + r_1$:

$$P_{\text{corr}} = \sum_{i=1}^N q_i \text{tr}\rho_i M_i = \sum_{i=1}^N q_i p_i (1 - \vec{v}_i \cdot \vec{w}_i) = q_1 + r_1. \quad (14)$$

Therefore $\{M_i, r_i, \vec{w}_i\}_{i=1}^N$ become the optimal parameters of our primal and dual problems. Since every p_i is positive we can see that all the POVM elements are nonzero. From this, the following lemma can be obtained.

Lemma 1—Geometric KKT conditions. The fact that every optimal POVM element can be nonzero is equivalent to the fact that $\{r_i, \vec{w}_i\}_{i=1}^N$ satisfying the geometric KKT conditions exists.

Let us denote $P\{\vec{x}_i\}_{i=1}^N$ as the polytope formed by $\{\vec{x}_i\}_{i=1}^N$. When the number of extreme points of $P\{q_i, \rho_i\}_{i=1}^N (\equiv P\{q_i \vec{v}_i\}_{i=1}^N)$ is the same as the number of quantum states to be discriminated, the geometric meaning of Eq. (12) can be easily expressed. Then the geometric condition (i) indicates that $P\{q_i, \rho_i\}_{i=1}^N$ is congruent to $P\{r_i \vec{w}_i\}_{i=1}^N$. The geometric condition (ii) implies that the origin of the Bloch sphere lies in the relative interior of $P\{r_i \vec{w}_i\}_{i=1}^N$. The geometric condition (iii) ensures that the distances from the origin to the extreme points of $P\{r_i \vec{w}_i\}_{i=1}^N$ become $\{r_i\}_{i=1}^N$. The final condition (iv) shows that the difference between the distances should be the same as that between the *a priori* probabilities. Since $\{r_i, \vec{w}_i\}_{i=1}^N$ satisfying the geometric KKT conditions (i)–(iii) certainly exists, the crucial element for obtaining the guessing probability is condition (iv).

Let us explain how to discover the guessing probability when $\{r_i, \vec{w}_i\}_{i=1}^N$ cannot satisfy the geometric KKT conditions. In this case at least one of the optimal POVM elements is zero. Therefore, if we denote $P_{\text{guess}}^{(N)}(\{q_i, \rho_i\}_{i=1}^N)$ the guessing probability function for N-qubit states, we may write it as

$$P_{\text{guess}} = \max_S \left(\textstyle\sum_{j\in S} q_j\right) P_{\text{guess}}^{(|S|)}\left(\left\{q_i / \textstyle\sum_{j\in S} q_j, \rho_i\right\}_{i\in S}\right), \quad (15)$$

where S is the proper subset of $\{1, \cdots, N\}$. For now, using S and lemma 1, we will obtain the guessing probability and the optimal measurement when $P\{q_i, \rho_i\}_{i=1}^N$ becomes a special case. First, let us consider when $P\{q_i, \rho_i\}_{i=1}^N$ becomes a point. For this purpose, suppose that $\{r_i, \vec{w}_i\}_{i=1}^N$ satisfies the geometric KKT conditions. Then the conditions (i) and (iii) imply the equality of $\vec{w}_i (i = 1, \ldots, N)$. Applying this result to condition (ii), we find that $\sum_{i=1}^N p_i = 0$ and $\sum_{i=1}^N p_i = 1$, which contradicts each other. Therefore we can see that when $P\{q_i, \rho_i\}_{i=1}^N$ forms a point, every optimal POVM element cannot be nonzero. Since for any proper subset S of $\{1, \ldots, N\}$, $P\{q_i / \sum_{j\in S} q_j, \rho_i\}_{i\in S}$ becomes a point, the nonzero element of the optimal POVM is only one. Therefore, we find corollary 1.

Corollary 1. If the number of the extreme points to $P\{q_i, \rho_i\}_{i=1}^N$ is one, every optimal POVM element except M_1 is zero, and the guessing probability is q_1.

The second case is when $P\{q_i, \rho_i\}_{i=1}^N$ forms a line segment. Let us denote the two indices corresponding to the extreme points as α and $\beta (> \alpha)$. Then the geometric KKT condition (i) indicates that $P\{r_i \vec{w}_i\}_{i=\alpha,\beta}$ should be a line segment with the same length to $P\{q_i, \rho_i\}_{i=\alpha,\beta}$. Condition (ii) requires that $P\{r_i \vec{w}_i\}_{i=\alpha,\beta}$ contain the origin O. This implies that the length of the line segment becomes

$$r_\alpha \|\vec{w}_\alpha\|_2 + r_\beta \|\vec{w}_\beta\|_2 = \|q_\alpha \vec{v}_\alpha - q_\beta \vec{v}_\beta\|_2 = r_\alpha + r_\beta. \quad (16)$$

The equality in the second line comes from the condition (iii). Also, by applying condition (iv) to Eq. (16) we have

$$\begin{aligned} r_\alpha &= \frac{1}{2}[\|q_\alpha \vec{v}_\alpha - q_\beta \vec{v}_\beta\|_2 - (q_\alpha - q_\beta)], \\ r_\beta &= \frac{1}{2}[\|q_\alpha \vec{v}_\alpha - q_\beta \vec{v}_\beta\|_2 + (q_\alpha - q_\beta)], \\ \vec{w}_\alpha &= \frac{q_\alpha \vec{v}_\alpha - q_\beta \vec{v}_\beta}{\|q_\alpha \vec{v}_\alpha - q_\beta \vec{v}_\beta\|_2}, \quad \vec{w}_\beta = \frac{q_\beta \vec{v}_\beta - q_\alpha \vec{v}_\alpha}{\|q_\alpha \vec{v}_\alpha - q_\beta \vec{v}_\beta\|_2}. \end{aligned} \quad (17)$$

Since r_α, r_β should be non-negative, we find $\|q_\alpha \vec{v}_\alpha - q_\beta \vec{v}_\beta\|_2 \geqslant q_\alpha - q_\beta$. It supplies the necessary and sufficient condition for $\{r_i, \vec{w}_i\}_{i=\alpha,\beta}$ to satisfy the geometric KKT conditions. If $\{q_i, \rho_i\}_{i=\alpha,\beta}$ satisfies the condition, the guessing probability becomes

$$\begin{aligned} P_{\text{guess}} &= \frac{1}{2}[(q_\alpha + r_\alpha) + (q_\beta + r_\beta)] \\ &= \frac{1}{2}(q_\alpha + q_\beta + \|q_\alpha \vec{v}_\alpha - q_\beta \vec{v}_\beta\|_2) \\ &= \frac{q_\alpha + q_\beta}{2}\left[1 + \left\|\frac{q_\alpha \vec{v}_\alpha}{q_\alpha + q_\beta} - \frac{q_\beta \vec{v}_\beta}{q_\alpha + q_\beta}\right\|_2\right]. \end{aligned} \quad (18)$$

From this result, our problem can be thought as one of discriminating $\{q_i/(q_\alpha + q_\beta), \rho_i\}_{i=\alpha,\beta}$, with the probability $(q_\alpha + q_\beta)$. However, if the condition does not hold, we have to find the index set S which provides the guessing probability given by Eq. (15). However, by this assumption, since for any S $P\{q_i / \sum_{j\in S} q_j, \rho_i\}_{i\in S}$ forms a point or a line segment, the problem becomes how to discriminate two quantum states. From the Helstrom bound, we can obtain corollary 2.

Corollary 2. If the number of the extreme points to $P\{q_i, \rho_i\}_{i=1}^N$ is two, the guessing probability becomes

$$P_{\text{guess}} = \max_{i\neq j} \tfrac{1}{2}(q_i + q_j + \|q_i \rho_i - q_j \rho_j\|_1). \quad (19)$$

When a and $b(>a)$ are the indices giving the optimal value, if $\|q_a \vec{v}_a - q_b \vec{v}_b\|_2 < q_a - q_b$, every optimal POVM element except M_1 is zero. However, if $\|q_a \vec{v}_a - q_b \vec{v}_b\|_2 \geqslant q_a - q_b$, the optimal POVM elements are given as

$$\begin{aligned} M_a &= \frac{1}{2}\left[I_2 + \left(\frac{q_a \vec{v}_a - q_b \vec{v}_b}{\|q_a \vec{v}_a - q_b \vec{v}_b\|_2}\right) \cdot \vec{\sigma}\right], \\ M_b &= \frac{1}{2}\left[I_2 + \left(\frac{q_b \vec{v}_b - q_a \vec{v}_a}{\|q_a \vec{v}_a - q_b \vec{v}_b\|_2}\right) \cdot \vec{\sigma}\right], \\ M_i &= 0 \quad \forall i \neq a,b. \end{aligned} \quad (20)$$

Now let us consider the case when $N = 3$, and the intrinsic polytope forms a triangle. We define two sides of the triangle as

$$l_1 \equiv \| q_2 \vec{v}_2 - q_1 \vec{v}_1 \|_2, \quad l_2 \equiv \| q_3 \vec{v}_3 - q_1 \vec{v}_1 \|_2, \quad (21)$$

and the difference between the *a priori* probabilities as

$$e_1 \equiv q_1 - q_2, \quad e_2 \equiv q_1 - q_3. \quad (22)$$

Now suppose that $\{r_i,\vec{w}_i\}_{i=1}^N$ satisfies the geometric KKT conditions. In this case the number of extreme points is equal to that of the quantum states to be discriminated. Then $P\{r_i\vec{w}_i\}_{i=1}^3$ is congruent to $P\{q_i,\rho_i\}_{i=1}^3$, and the origin O exists inside the relative interior. When T_i represents the vertex $r_i\vec{w}_i$ of the triangle $P\{r_i\vec{w}_i\}_{i=1}^3$ and $r_i(i=1,2,3)$ is the distance from O to the vertex T_i, we have the following relations:

$$r_2 - r_1 = e_1, \quad r_3 - r_1 = e_2. \tag{23}$$

The necessary and sufficient condition that $\{r_i,\vec{w}_i\}_{i=1}^3$, satisfying that the geometric KKT conditions can exist, can be obtained by the property of hyperbola, as follows:

$$\begin{aligned}
&\text{(i)}\ \ l_1 > e_1, \quad l_2 > e_2,\\
&\text{(ii)}\ \ \frac{l_1\cos\theta_1 + e_1}{l_1+e_1} < \frac{l_1-e_1}{l_2-e_2}, \quad \frac{l_2\cos\theta_1 + e_2}{l_2+e_2} < \frac{l_2-e_2}{l_1-e_1},\\
&\text{(iii)}\ \ \frac{l_1^2-e_1^2}{2(l_1\cos\chi+e_1)} < \frac{l_1\sin\theta_2}{\sin(\chi+\theta_2)},
\end{aligned} \tag{24}$$

where θ_i denotes the inside angle of vertex T_i, and the angle χ which is $\angle OT_1T_2$, is given as

$$\chi = \chi_2 - \chi_1, \quad \chi_1 = \cos^{-1}\left(\frac{l_1(l_2^2-e_2^2) - l_2(l_1^2-e_1^2)\cos\theta_1}{\sqrt{l_1^2(l_2^2-e_2^2)^2 + l_2^2(l_1^2-e_1^2)^2 - 2l_1l_2(l_1^2-e_1^2)(l_2^2-e_2^2)\cos\theta_1}}\right),$$

$$\chi_2 = \cos^{-1}\left(\frac{e_2(l_1^2-e_1^2) - e_1(l_2^2-e_2^2)}{\sqrt{l_1^2(l_2^2-e_2^2)^2 + l_2^2(l_1^2-e_1^2)^2 - 2l_1l_2(l_1^2-e_1^2)(l_2^2-e_2^2)\cos\theta_1}}\right). \tag{25}$$

Therefore, if $\{q_i,\rho_i\}_{i=1}^3$ satisfies the conditions, r_1^* becomes $\frac{l_1^2-e_1^2}{2(l_1\cos\chi+e_1)}$ and the guessing probability P_{guess} is given by

$$P_{\text{guess}} = q_1 + \frac{l_1^2-e_1^2}{2(l_1\cos\chi+e_1)}. \tag{26}$$

The optimal POVM can be found by substituting $\{p_i,\vec{w}_i\}_{i=1}^3$ into Eq. (10). Through a lengthy calculation, we find $\{p_i,\vec{w}_i\}_{i=1}^3$, such as

$$\begin{aligned}
p_1 &= \frac{l_1l_2\sin\theta_1 - r_1l_1\sin\chi - r_1l_2\sin(\theta_1-\chi)}{l_1l_2\sin\theta_1 + e_2l_1\sin\chi + e_1l_2\sin(\theta_1-\chi)},\\
p_2 &= \frac{r_2l_2\sin(\theta_1-\chi)}{l_1l_2\sin\theta_1 + e_2l_1\sin\chi + e_1l_2\sin(\theta_1-\chi)},\\
p_3 &= \frac{r_3l_1\sin\chi}{l_1l_2\sin\theta_1 + e_2l_1\sin\chi + e_1l_2\sin(\theta_1-\chi)},
\end{aligned} \tag{27}$$

and

$$\begin{aligned}
\vec{w}_1 &= \frac{\sin(\theta_1-\chi)}{l_1\sin\theta_1}(q_2\vec{v}_2 - q_1\vec{v}_1) + \frac{\sin\chi}{l_2\sin\theta_1}(q_3\vec{v}_3 - q_1\vec{v}_1),\\
\vec{w}_2 &= \frac{r_1\vec{w}_1 - (q_2\vec{v}_2 - q_1\vec{v}_1)}{r_1+e_1}, \quad \vec{w}_3 = \frac{r_1\vec{w}_1 - (q_3\vec{v}_3 - q_1\vec{v}_1)}{r_1+e_2}.
\end{aligned} \tag{28}$$

However, the case where this condition is not satisfied turns out to be a problem of discriminating two quantum states. Therefore the guessing probability to the case can be given by corollary 2. Now we can have lemma 2.

Lemma 2—Three-quantum-state discrimination. When arbitrary three quantum states $\{q_i,\rho_i\}_{i=1}^3$ are given with given *a priori* probabilities, the guessing probability can be classified into the following three cases: (i) When the number of the extreme points to $P\{q_i,\rho_i\}_{i=1}^3$ is one, the guessing probability becomes q_1 by the corollary 1. (ii) When the number of the extreme points is two or three and the condition of Eq. (24) cannot be satisfied, the guessing probability can be found by the corollary 2. (iii) When the number of the extreme points is three and the condition of Eq. (24) is satisfied, the guessing probability can be given by Eq. (26).

Here as an example let us consider the quantum discrimination of three symmetric quantum states. The symmetric property implies that for ρ_1, ρ_2, and ρ_3, $\text{tr}\rho_1\rho_2 = \text{tr}\rho_2\rho_3 = \text{tr}\rho_3\rho_1$. Their purity is assumed to be the same as $\text{tr}\rho_1^2 = \text{tr}\rho_2^2 = \text{tr}\rho_3^2 \leqslant 1$. This symmetric condition can be expressed by

$$\vec{v}_i\cdot\vec{v}_j = \begin{cases} r & (i=j),\\ \gamma & (i\neq j),\end{cases} \tag{29}$$

where $\vec{v}_i$ is the Bloch vector of ρ_i. If their *a priori* probabilities are the same as $\frac{1}{3}$ ($q_1=q_2=q_3=\frac{1}{3}$), the guessing probability P_{guess} becomes $\frac{1}{3}+r_1^*$. Since $P\{q_i\vec{v}_i\}_{i=1}^3 = P\{\vec{v}_i/3\}_{i=1}^3$ is the equilateral triangle whose side is given by $\sqrt{2(t-s)}/3$ ($t\equiv 1-\gamma$ and $s\equiv 1-r$), $\{r_i,\vec{w}_i\}_{i=1}^3$, satisfying that the geometric KKT conditions naturally exist. The circumradius of the triangle $P\{r_i\vec{w}_i\}_{i=1}^3$ becomes $\frac{1}{3}\sqrt{\frac{2(t-s)}{3}}$. Therefore we find

$$r_1 = r_2 = r_3 = \frac{1}{3}\sqrt{\frac{2(t-s)}{3}}. \tag{30}$$

The guessing probability P_{guess} turns out to be

$$P_{\text{guess}} = \frac{1}{3}\left(1+\sqrt{\frac{2(t-s)}{3}}\right), \tag{31}$$

which agrees with the result in [19].

In conclusion, by considering the minimum-error quantum-state discrimination as the complementarity problem, we obtained four geometric optimality conditions in the case of qubit geometry. We clearly showed that there is a relation between these conditions and the optimal measurement. By these conditions and the intrinsic polytope for the discrimination problem, we can provide a method to discriminate N-qubit mixed quantum states. We are also able to obtain the guessing probability and the optimal measurements. We applied these results to discriminating three-qubit mixed quantum states to show that discrimination for the three-qubit mixed quantum states can be classified by the geometric KKT conditions and the number of extreme points for the intrinsic polytope. The analytic expression of the guessing probability and the optimal measurement for three-qubit mixed quantum states was obtained. Furthermore, we have shown that for the special case of three symmetric quantum states, our result is consistent.

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APPENDIX

Suppose that two points T and T', whose distance is l, are given in a two-dimensional plane. The points where the difference in distances between two points T and T' becomes e form a hyperbola. When the distance from these points to $T(T')$ becomes $r(r')$, the hyperbola can be divided into two curves $r' - r = e$ and $r - r' = e$. Let us denote the curve $r' - r = e$ as $C_e\{T,T'\}$. The distance r can be obtained from the hyperbolic equation as follows:

$$r = \frac{l^2 - e^2}{2(l\cos\theta + e)}, \tag{A1}$$

where θ is the angle between the segment to r and the line segment $\overline{TT'}$. Now let us consider a triangle formed by three different points T_1, T_2, and T_3 in a two-dimensional plane. We denote the interior of the triangle, $C_{e_1}\{T_1,T_2\}$, and $C_{e_2}\{T_1,T_3\}$ as $\triangle$, C_1, and C_2. Also, let us represent the intersection of $\triangle$, C_1, and C_2 as $\Omega(\Omega = \triangle \cap C_1 \cap C_2)$. Now we will find the necessary and sufficient condition where Ω is nonempty. Since the condition for $\triangle \cap C_i$ to be nonempty is $l_i > e_i$, we obtain the condition (i) of Eq. (24) in the main text. Here l_1 and l_2 are the length of $\overline{T_1T_2}$ and $\overline{T_1T_3}$, respectively.

If the inner angle of the vertex T_i is θ_i, we can classify the triangle into four types, according to θ_1: (i) $-\frac{e_1}{l_1}, -\frac{e_2}{l_2} < \cos\theta_1$; (ii) $-\frac{e_1}{l_1} < \cos\theta_1 \leqslant -\frac{e_2}{l_2}$; (iii) $-\frac{e_2}{l_2} < \cos\theta_1 \leqslant -\frac{e_1}{l_1}$; (iv) $\cos\theta_1 \leqslant -\frac{e_1}{l_1}, -\frac{e_2}{l_2}$. And the condition where $C_1 \cap C_2$ becomes nonempty in each case is as follows: (i) $\frac{l_2\cos\theta_1+e_2}{l_2+e_2} < \frac{l_2-e_2}{l_1-e_1} < \frac{l_1+e_1}{l_1\cos\theta_1+e_1}$, (ii) $\frac{l_2-e_2}{l_1-e_1} < \frac{l_1+e_1}{l_1\cos\theta_1+e_1}$, (iii) $\frac{l_2\cos\theta_1+e_2}{l_2+e_2} < \frac{l_2-e_2}{l_1-e_1}$, and (iv) no condition needed. These conditions can be put into the two restrictive ones:

$$\frac{l_1\cos\theta_1 + e_1}{l_1 + e_1} < \frac{l_1 - e_1}{l_2 - e_2}, \quad \frac{l_2\cos\theta_1 + e_2}{l_2 + e_2} < \frac{l_2 - e_2}{l_1 - e_1}, \tag{A2}$$

which is the condition (ii) of Eq. (24) in the main text. Indeed, if C_1 and C_2 meet together, they intersect only at a single point because the equation derived by Eq. (A1),

$$\frac{l_1^2 - e_1^2}{2(l_1\cos\chi + e_1)} = \frac{l_2^2 - e_2^2}{2[l_2\cos(\theta_1 - \chi) + e_2]}, \tag{A3}$$

can be satisfied by unique $\chi \in (0,\theta_1)$. When we denote the intersection point as O, χ is $\angle OT_1T_2$, which is given as follows:

$$\begin{aligned}\chi &= \chi_2 - \chi_1, \quad \chi_1 = \cos^{-1}\left(\frac{l_1\left(l_2^2 - e_2^2\right) - l_2\left(l_1^2 - e_1^2\right)\cos\theta_1}{\sqrt{l_1^2\left(l_2^2 - e_2^2\right)^2 + l_2^2\left(l_1^2 - e_1^2\right)^2 - 2l_1l_2\left(l_1^2 - e_1^2\right)\left(l_2^2 - e_2^2\right)\cos\theta_1}}\right),\\ \chi_2 &= \cos^{-1}\left(\frac{e_2\left(l_1^2 - e_1^2\right) - e_1\left(l_2^2 - e_2^2\right)}{\sqrt{l_1^2\left(l_2^2 - e_2^2\right)^2 + l_2^2\left(l_1^2 - e_1^2\right)^2 - 2l_1l_2\left(l_1^2 - e_1^2\right)\left(l_2^2 - e_2^2\right)\cos\theta_1}}\right).\end{aligned} \tag{A4}$$

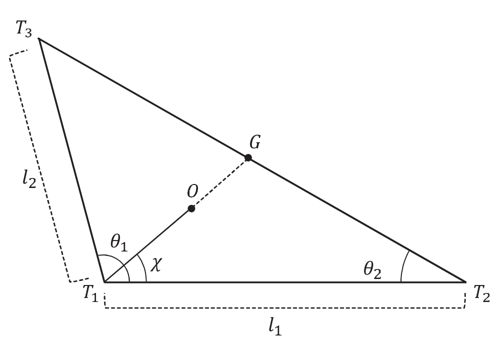

FIG. 1. For the point O to be located inside the triangle, $\overline{T_1O}$ must be shorter than $\overline{T_1G}$.

Here let us find the condition for $O \in \triangle$. This can be found from the fact that when G is the intersection point between the half line from the vertex T_1 to the point O and the line segment $\overline{T_2T_3}$, the length of $\overline{T_1G}$ becomes $\frac{l_1\sin\theta_2}{\sin(\chi+\theta_2)}$. From Fig. 1 we can see that the point O can be located inside the triangle if the length of $\overline{T_1O}$ becomes less than that of $\overline{T_1G}$:

$$\frac{l_1^2 - e_1^2}{2(l_1\cos\chi + e_1)} < \frac{l_1\sin\theta_2}{\sin(\chi + \theta_2)}. \tag{A5}$$

Therefore we showed that three conditions given by Eq. (24) in the main text are the necessary and sufficient conditions for nonempty Ω.

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