Structure of minimum-error quantum state discrimination

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Abstract. Distinguishing different quantum states is a fundamental task having practical applications in information processing. Despite the effort devoted so far, however, strategies for optimal discrimination are known only for specific examples. In this paper we consider the problem of minimum-error quantum state discrimination where one attempts to minimize the average error. We show the general structure of minimum-error state discrimination as well as useful properties to derive analytic solutions. Based on the general structure, we present a geometric formulation of the problem, which can be applied to cases where quantum state geometry is clear. We also introduce equivalent classes of sets of quantum states in terms of minimum-error discrimination: sets of quantum states in an equivalent class that share the same guessing probability. In particular, for qubit states where the state geometry is found with the Bloch sphere, we illustrate that for an arbitrary set of qubit states, the minimum-error state discrimination with equal prior probabilities can be analytically solved, that is, optimal measurement and the guessing probability are explicitly obtained.
1. Introduction

In the early days, when quantum systems were applied to the communication of distant parties, in particular photonic systems which define physical limits on the sources of optical communication, there were pioneering works that investigated how quantum systems could be exploited to information processing and incorporated in the frameworks of classical information theory [1–3]. One of the most fundamental tasks for such applications is to formalize how classical messages can be retrieved from quantum states. For various purposes, different designs of measurements were then introduced and studied, for instance, measurement settings are optimized for accessible information [4], unambiguous discrimination [5–9], maximizing confidence to guess about certain states [10] or minimizing errors on average when making guesses about given states [1–3], etc. Recently, there have also been approaches that, with a pre-determined rate of inconclusive results, errors in discrimination are minimized [11, 12]. All these are fundamental and practical in quantum information theory and its applications, as well as useful tools to investigate the foundational aspects of quantum theory, see also the reviews in [13–17].

Among the different strategies in quantum state discrimination, here we are interested in minimum-error (ME) discrimination. ME discrimination optimizes measurement so that, once a quantum state is given from a set of known quantum states, one aims to make the correct guess about the state with a minimal error on average. In fact this has a number of applications in quantum information tasks; it is also of a fundamental interest since it shows the ultimate limit in the identification of a given state among a specified set of states. What is needed is, for arbitrarily given sets of quantum states, a general method of finding optimal measurement, that is, measurement that achieves minimal errors on average in the state discrimination. Despite the efforts devoted so far, however, analytic solutions are known only for restricted classes of
quantum states, e.g. cases when certain symmetries are contained. The lack of a solution in most cases is partly because ME discrimination has been largely understood as an optimization problem for which it is generally hard to have analytic solutions. Otherwise, little is known as an approach to ME discrimination. Needless to say it is important in its own right; however, the lack of a general method for state discrimination has obviously been and still is a potentially significant obstacle preventing further investigation in both quantum information theory and quantum foundation.

To be precise about known results in ME discrimination, no general method has yet been found as an analytic way of solving ME state discrimination. The known general method is a numerical approach via semidefinite programming, which efficiently returns the solution in a polynomial time [18–21]. For cases in which ME discrimination is known in an analytic form, two-state discrimination is the only case where no symmetry is assumed among given quantum states. The result was shown in 1976 and called the Helstrom bound [3]. Apart from this, if no symmetry exists among given states, no analytic solution is known, for instance, in the next simplest case of arbitrary three states, or the even simpler case of three qubit states. Otherwise, ME discrimination is known for cases when given quantum states have certain symmetries, such as the geometrically uniform structure, see [3, 4, 19, 22–27].

Note also that, although general solutions are lacking, the necessary and sufficient conditions that characterize optimal discrimination were obtained when the problem was introduced [1, 2]. That is, parameters giving optimal discrimination satisfy the conditions and conversely any parameters fulfilling the conditions can construct optimal discrimination. They have been used to run a numerical algorithm [18].

The purpose of this work is to show the general structure existing in ME discrimination, namely, the relations among optimal measurement, the guessing probability and other useful properties to analytically find optimal measurement and the guessing probability. The main idea is to view ME discrimination from various angles and different approaches, such as relations of fundamental principles, convex optimization frameworks or their generalization called the complementarity problem and different formalisms accordingly. We show that all these can be equivalently summarized into the so-called complementarity problem in the context of convex optimization, see e.g. [28]. The approach refers to a direct analysis on the optimality conditions; in fact, in this way, more parameters are included than the originally given problems; however, the advantage is that the generic structure of the given optimization problems is fully exploited. Applying the structure and the method of the complementarity problem, we provide a geometric formulation of solving ME discrimination. Thus, once the geometry is clear from the context of given quantum states, the formulation can be exploited and one can straightforwardly find the solution, such as optimal measurement and the guessing probability. As an example where the state geometry is also clear, we illustrate that ME discrimination is completely solved for an arbitrary set of qubit states given with equal prior probabilities. All these provide alternative methods of solving the ME discrimination in an analytic way, apart from the numerical optimization method.

The rest of the paper is structured as follows. In section 2, we begin with the problem of definition and an introduction to ME discrimination. We also provide an operational interpretation of the guessing probability. We obtain optimality conditions for ME discrimination from different approaches and finally put them equivalently into the framework of a complementarity problem. From the optimality conditions, we show the general structure of optimal parameters in ME discrimination, such as optimal measurement and the
guessing probability. In this way, we provide a geometric formulation of ME discrimination. In section 3, based on the general structure, we present general properties as follows. We construct equivalence classes of sets of quantum states in terms of the ME discrimination, such that for the sets in the same class, the ME discrimination is characterized in an equivalent way. We also show, conversely, how a set of states can be generated in an equivalent class. Then, for the generated states, the ME discrimination is already characterized by the equivalence class. We finally present various and equivalent forms of the guessing probability according to different approaches in which the general structure and the optimality conditions are derived and provide their operational meanings. In section 4, we apply all these to qubit states in which quantum state geometry is clearly found with the Bloch sphere. We show how the geometric formulation can be applied and illustrate that for all problems of ME discrimination, with equal prior probabilities, it can be analytically solved by using the state geometry. In section 5, we conclude the results.

2. Minimum-error discrimination and optimality conditions

In this section, let us introduce the problem of ME discrimination of quantum states and fix notations. We then analyze the optimality conditions that completely characterize optimal parameters, such as optimal measurement and the guessing probability. We review optimality conditions derived from different approaches and show that they are equivalent.

2.1. Problem definition and probability-theoretic preliminaries

Suppose that there is a device which generates different quantum states. The device has \( N \) buttons and pressing one of them, say \( x \), corresponds to an instance that a state \( \rho_x \) is generated. Denoted by \( q_x \) as the probability that the button \( x \) is pressed, \textit{a priori} probability that \( \rho_x \) is produced from the device is defined. We summarize the state generation by \( \{q_x, \rho_x\}_{x=1}^N \). Once generated, a state is then sent to a measurement device, which is prepared to make a best guess about which button has been pressed in the preparation. This corresponds to the task of distinguishing \( N \) quantum states via measurement devices.

Let \( P(x|y) \) denote the probability that when state \( \rho_y \) has been prepared, one concludes from measurement outcomes that state \( \rho_x \) is given. Or equivalently, as the conclusion follows from measurement outcomes, it is the probability that an output port \( x \) is clicked when a button \( y \) is pressed in the preparation. Then, in the ME discrimination, we are interested in minimizing the probability of making errors on average, or equivalently to have maximal probability to make correct guesses about input states, called the \textit{guessing probability}, \( P_{\text{guess}} = \max_M \sum_x q_x P(x|x) \) where the maximization runs over measurement settings \( M \).

Measurement on quantum systems is described by positive-operator-valued-measures (POVMs): a set of positive operators \( \{M_x \geq 0\}_{x=1}^N \) that fulfills, \( \sum_{x=1}^N M_x = I \). For given states \( \{q_x, \rho_x\}_{x=1}^N \), let \( \{M_x\}_{x=1}^N \) denote POVMs for quantum state discrimination. When state \( \rho_y \) is actually given, the probability that a detection event happens in measurement \( M_x \) is given by \( P(x|y) = \text{tr}[\rho_y M_x] \). The guessing probability can therefore be written as

\[
P_{\text{guess}} = \max_M \sum_{x=1}^N q_x P(x|x) = \max_{\{M_x\}_{x=1}^N} \sum_{x=1}^N q_x \text{tr}[M_x \rho_x]
\]  

(1)

with the maximization over all POVMs. From postulates of quantum theory, non-orthogonal quantum states cannot be perfectly discriminated between, i.e. \( P_{\text{guess}} < 1 \).
The ME discrimination described in the above can be rephrased in a probability-theoretical way as follows. The preparation applies random variable $X$, which corresponds to a button pressed, and the measurement shows the other random variable $Y$ for guessing about $X$ with some probabilities. The distinguishability of different probabilistic systems can be, in general, measured by the variational distance of probabilities. Then, the distance from the uniform distribution is particularly useful to describe and interpret the guessing probability. The distance of a probability distribution of random variable $P_X$ from the uniform distribution, which is $1/N$ in this case, is denoted by $d(P_X)$ or simply $d(X)$ and defined as

$$d(X) = \frac{1}{2} \sum_{x=1}^{N} \left| P_X(x) - \frac{1}{N} \right|. \quad (2)$$

Let $d(X|Y)$ denote the distance of random variable $X$ given $Y$ from the uniform.

**Lemma 2.1 ([29]).** The guessing probability about $X$ given $Y$ can be expressed by

$$P_{\text{guess}} := P_{\text{guess}}(X|Y) = \frac{1}{N} + d(X|Y). \quad (3)$$

**Proof.** Note that the guessing probability is $P_{\text{guess}} = \sum_{y=1}^{N} P_Y(y) P_{X|Y}(y|y)$. It is then straightforward to write the distance, as follows:

$$d(X|Y) = \sum_{y=1}^{N} P_Y(y) d(X|Y = y) = \frac{1}{2} \sum_{y=1}^{N} P_Y(y) \sum_{x=1}^{N} \left| P_{X|Y}(x|y) - \frac{1}{N} \right|.$$

As the probability of making correct guesses is not smaller than the random guess, we can assume that $P_{X|Y}(y|y) \geq 1/N$ for all $y = 1, \ldots, N$ and $P_{X|Y}(x|y) \leq 1/N$ for $x \neq y$ and this does not lose any generality. Thus it follows that, when $Y = y$,

$$\sum_{x=1}^{N} \left| P_{X|Y}(x|y) - \frac{1}{N} \right| = P_{X|Y}(y|y) - \frac{1}{N} - \sum_{x \neq y} \left( P_{X|Y}(x|y) - \frac{1}{N} \right) = 2P_{X|Y}(y|y) - \frac{2}{N}.$$

From these two relations, it holds that

$$d(X|Y) = P_{\text{guess}} - \sum_{y=1}^{N} P_Y(y) \frac{1}{N} = P_{\text{guess}} - \frac{1}{N}$$

and thus equation (3) is shown. \qed

This shows that the guessing probability about random variable $X$ given $Y$ corresponds to the distance of the probability $P_{X|Y}$ from the uniform distribution. As only input and output random variables are taken into account, the expression in equation (3) generally works for any physical system, either quantum or classical, employed from preparation to measurement.
Then, the distance \(d(X|Y)\) depends on the physical systems employed between preparation and measurement. Once quantum systems are applied, the distance \(d(X|Y)\) must be expressed in terms of properties or relations of given quantum states. The expression for quantum systems is shown in lemma 3.2.

2.2. Optimality conditions

As is shown in equation (1), optimal discrimination is obtained with POVM elements that maximize the probability of making correct guesses. There have been different approaches to characterize optimal measurement. Here, we review known results and show that they are equivalent to one another.

2.2.1. Optimality conditions from analytic derivation. The necessary and sufficient conditions that POVMs must satisfy to fulfill optimal discrimination have been obtained from the very beginning when the problem was introduced in [1, 2]. For given states \(\{q_x, \rho_x\}_{x=1}^N\) to discriminate among, POVM elements \(\{M_x\}_{x=1}^N\) achieve the guessing probability if and only if they satisfy

\[
M_x(q_x \rho_x - q_y \rho_y) M_y = 0 \quad \forall x, y = 1, \ldots, N, \tag{4}
\]

\[
\sum_{x=1}^N q_x \rho_x M_x - q_y \rho_y \geq 0 \quad \forall y = 1, \ldots, N. \tag{5}
\]

That is, for a state discrimination problem, if one finds a set of POVMs that satisfy two of the conditions above, then optimal discrimination is immediately obtained. Note also that for a given problem of state discrimination, optimal measurement is generally not unique.

2.2.2. Optimality condition from convex optimization. The optimality conditions can also be derived from a different context, the formalism of convex optimization [21]. The optimization problem in equation (1) with the convex and affine constraints on POVMs can be written as

\[
\max \sum_{x=1}^N q_x \text{tr}[M_x \rho_x] \quad \text{s.t.} \quad \sum_{x=1}^N M_x = I \quad \text{and} \quad M_x \geq 0 \quad \forall x = 1, \ldots, N. \tag{6}
\]

For convenience, we call equation (6) the primal problem. Note that the primal problem in the above is feasible.

To derive its dual problem, let us first construct the Lagrangian \(L\) as follows:

\[
L([M_x]_{x=1}^N, [\sigma_x]_{x=1}^N, K) = \sum_{x=1}^N q_x \text{tr}[M_x \rho_x] + \sum_{x=1}^N \text{tr}[\sigma_x M_x] + \text{tr} \left[ K \left( I - \sum_{x=1}^N M_x \right) \right]
\]

\[
= \sum_{x=1}^N \text{tr}[M_x (q_x \rho_x + \sigma_x - K)] + \text{tr} K,
\]

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where \( \{ \sigma_x \}_{x=1}^N \) are positive-semidefinite Hermitian operators and \( K \) is a Hermitian operator. Note that \( \{ \sigma_x \}_{x=1}^N \) and \( K \) are called dual parameters. To derive the dual problem, we first have to maximize the Lagrangian over primal parameter \( \{ M_x \}_{x=1}^N \). If it holds that \( q_x \rho_x + \sigma_x - K > 0 \) for some \( x \), then the primal problem becomes not feasible since the maximization may go to \( +\infty \). Thus, we have \( q_x \rho_x + \sigma_x - K \leq 0 \) for all \( x \), where the equality holds if and only if the Lagrangian is maximized. Combined together with the other constraint that \( \sigma_x \geq 0 \) for all \( x \), the constraint can be finally rewritten as, \( K \geq q_x \rho_x \) for all \( x \). This also shows that the operator \( K \) must be positive. Note that since the Lagrangian is maximized, we now have

\[
\max \{ M_x \}_{x=1}^N \sum_{x=1}^N q_x \operatorname{tr}[M_x \rho_x] \leq \max \{ M_x \}_{x=1}^N \mathcal{L}(\{ M_x \}_{x=1}^N, \{ \sigma_x \}_{x=1}^N, K) |_{q_x \rho_x + \sigma_x - K \leq 0} = \operatorname{tr} K,
\]

which is called the weak duality.

The dual problem to equation (6) is therefore obtained as follows:

\[
\begin{align*}
\min & \quad \operatorname{tr}[K] \\
\text{s.t.} & \quad K \geq q_x \rho_x \quad \forall \ x = 1, \ldots, N.
\end{align*}
\]

Putting optimal discrimination problems into this convex optimization framework, the solution, i.e. the guessing probability, is returned efficiently in a polynomial time. In general, solutions from primal and dual problems in the convex optimization are not necessarily the same. It generally holds that either of the solutions is larger than or equal to the other, from the property called weak duality, as is shown in the above. In this problem of state discrimination, it turns out that solutions from both problems coincide each other, which follows from the so-called constraint quantification. This property is called the strong duality. Thus, we have

\[
P_{\text{guess}} = \max \{ M_x \}_{x=1}^N \sum_{x=1}^N q_x \operatorname{tr}[M_x \rho_x] = \min \{ K \}_{K \geq q_x \rho_x} \operatorname{tr}[K].
\]

That is, the guessing probability is obtained by solving either the primal or the dual problem.

Apart from solving either the primal or the dual problem, a third approach in the convex optimization, which we are mainly going to consider here, is the so-called complementarity problem that directly analyzes the constraints characterizing the optimal parameters in both primal and dual problems and finds all of the optimal parameters [30]. As both the primal and dual parameters from both convex constraints are taken into account, the approach itself is not considered to be more efficient in numerics than primal or dual problems. Its advantage, however, lies in the fact that the general structure existing in an optimization problem is fully exploited.

Those constraints which characterize optimal solutions are called optimality conditions and can be written as the so-called Karush–Kuhn–Tucker (KKT) conditions. In general, KKT conditions are only necessary since solutions of primal and dual problems can be unequal. As we have mentioned, from the constraint qualification the strong duality holds and consequently the KKT conditions in this case are also sufficient. The list of KKT conditions for the discrimination problem is, then, constraints in equations (6) and (7) and two more conditions in the following.

Lemma 2.2 (Optimality conditions). For a set of states \( \{ q_x, \rho_x \}_{x=1}^N \), the optimal ME discrimination is characterized by a symmetry operator denoted by \( K^* \) and complementary
states \( \{ r^*_x, \sigma^*_x \}_{x=1}^N \), where \( r^*_x \geq 0 \), which satisfy the followings, for \( x = 1, \ldots, N \):

\[
\text{(symmetry operator)} \quad K^* = q_x \rho_x + r^*_x \sigma^*_x, \\
\text{(orthogonality)} \quad r^*_x \text{tr}[M^*_x \sigma^*_x] = 0,
\]

where POVM elements \( \{ M^*_x \}_{x=1}^N \) in the above are an optimal measurement giving the guessing probability.

Conversely, for given states \( \{ q_x, \rho_x \}_{x=1}^N \), any set of parameters, \( K, \{ r_x, \sigma_x \}_{x=1}^N \) and \( \{ M_x \}_{x=1}^N \) fulfilling KKT conditions, equations (6)–(9), characterize the optimal state discrimination. If parameters satisfy KKT conditions, they are optimal and we write them by \( K^* \), \( \{ r^*_x, \sigma^*_x \}_{x=1}^N \) and \( \{ M^*_x \}_{x=1}^N \), throughout.

Note that, with optimal parameters, the guessing probability is given by \( P_{\text{guess}} = \text{tr}[K^*] \) from the dual problem in equation (7).

Let us explain how one can obtain two conditions in equations (8) and (9). In the context of convex optimization, the condition of symmetry operator in equation (8) follows from the Lagrangian stability: \( \nabla M_x \mathcal{L} = 0 \) for all \( x \). The orthogonality condition in equation (9) is obtained from the complementary slackness [21]. In state discrimination, therefore, those parameters satisfying KKT conditions, equations (6)–(9), are characterized as optimal measurements and complementary states to give guessing probabilities.

We in particular call \( K^* \) as the symmetry operator in the ME discrimination of states \( \{ q_x, \rho_x \}_{x=1}^N \) due to the following reasons. First, the operator is uniquely determined for the ME discrimination of given states, whereas optimal measurement is not unique e.g. [36]. Later, the proof is provided in lemma 2.4. This means that for given quantum states, the symmetry operator, rather than optimal measurement, characterizes ME discrimination. Next, due to the uniqueness, the operator preserves the properties concerning the guessing probability in ME discrimination. Note that the guessing probability is of practical importance when exploiting sets of quantum states in a communication task. Then, as we will explicitly show later in examples, the guessing probability does not generally depend on detailed relations (e.g. angles or distances between states) of given states \( \{ q_x, \rho_x \}_{x=1}^N \) but a single parameter, the operator \( K^* \) constructed by given states.

Let us also be precise about the result that the guessing probability does not depend on detailed relations of given quantum states. We point out that the observation from the two-state discrimination [3], where the trace-distance defining the relation between the two states is the parameter dictating the guessing probability, cannot generalize to more than two states. In addition we show, by examples, that it clearly fails to generalize the observation for ME discrimination of more than two states. As is going to be shown in section 4, one of three states can be modified independently, while the guessing probability remains the same. We emphasize that the operator \( K^* \) directly dictates and corresponds to the guessing probability, rather than any other parameters in ME discrimination. We also note that this property is along the conclusion in [31] that distinguishability is a global property that cannot be reduced to the distinguishability of each pair of states.

In fact, two distinct sets of quantum states can have the same symmetry operator. Then, since the symmetry operator gives the complete characterization of the ME discrimination such as the guessing probability and complementarity states, the ME discrimination for the two sets

\[\text{For a specific example one can refer to the case of linearly dependent quantum states, e.g. [36].}\]
is analyzed in terms of the same symmetry operator. This motivates one to construct equivalence classes of sets of quantum states via the symmetry operator in the ME discrimination and shows a general structure in ME discrimination, see section 3.

In the below, we show that optimality conditions in equations (8) and (9) are equivalent to those in equations (4) and (5).

**Remark 2.1.** KKT conditions in equations (8) and (9) are equivalent to the optimality conditions shown in equations (4) and (5).

**Proof.** To prove the equivalence, it suffices to show that KKT conditions imply optimality conditions in equations (4) and (5). In the following, we derive equations (4) and (5) from KKT conditions.

First, since the symmetry operator in equation (8) gives the guessing probability, we have

$$P_{\text{guess}} = \text{tr}[K^*] = \text{tr} \left[ \sum_{x=1}^{N} q_x \rho_x M_x^* \right].$$

(10)

It follows that

$$K^* = \sum_{x=1}^{N} q_x \rho_x M_x^*$$

with optimal POVMs fulfilling equation (10). From equation (8), noting that $r_x^* \sigma_x^* \geq 0$, we have $K^* - q_x \rho_x \geq 0$ for all $x = 1, \ldots, N$. This already proves the condition in equation (5).

Next, from the symmetry operator in equation (8), the equality in equation (10) also implies the following:

$$\text{tr}[K^*] = \text{tr} \left[ \sum_{x=1}^{N} q_x \rho_x M_x^* \right] = \text{tr} \left[ \sum_{x=1}^{N} (K^* - r_x^* \sigma_x^*) M_x^* \right] = \text{tr}[K^*] - \sum_{x=1}^{N} \text{tr}[r_x^* \sigma_x^* M_x^*]$$

$$\Rightarrow \sum_{x=1}^{N} \text{tr}[r_x^* \sigma_x^* M_x^*] = 0.$$

Since $\text{tr}[r_x^* \sigma_x^* M_x^*] \geq 0$ for each $x$, we conclude that $\text{tr}[M_x^* r_x^* \sigma_x^*] = 0$ for all $x$. Moreover, since $\sigma_x^* \geq 0$, $M_x^* \geq 0$ and $r_x^* \geq 0$, we have $r_x^* \sigma_x^* M_x^* = 0$ for all $x$. We apply this identity to the following, together with the relation $q_x \rho_x = K^* - r_x^* \sigma_x^*$ in equation (8):

$$M_x^*(q_x \rho_x - q_y \rho_y) M_y^* = M_x^*((K^* - r_x^* \sigma_x^*) - (K^* - r_y^* \sigma_y^*)) M_y^* = M_x^* (r_y^* \sigma_y^* M_y^* - (M_y^* r_y^* \sigma_y^*)) M_y^* = 0.$$

Thus, it is shown that the KKT conditions imply the optimality condition in equation (4).

2.2.3. Optimality conditions from fundamental principles. In [32], it is shown that the no-signaling principle can generally determine the ME quantum state discrimination. This is shown by proving that if measurement devices are non-signaling, the guessing probability in the state discrimination cannot be larger than that characterized within quantum theory. Here, we briefly sketch the main framework of the derivation and show that the optimality conditions in equations (8) and (9) can be alternatively derived from the fundamental principles.

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Two operational tasks in quantum theory are exploited. One is the ensemble steering, which states that there always exists a bipartite quantum state, such that by sharing the state, one party can prepare any ensemble decomposition of the other party’s state. This was first asserted by Schrödinger [33] and later formalized as the Gisin–Hughston–Jozsa–Wootters (GHJW) theorem [34, 35]. The other is the no-signaling principle that information cannot be transmitted faster than the speed of light. Then, the result in [32] is that optimal quantum state discrimination is a consequence when two correlations are compatible: (i) from quantum correlations, called ensemble steering, that ensemble decompositions of quantum states can be steered by a party at a distance, and (ii) the no-signaling condition on probability distributions, that probability distributions of input and output random variables at a location cannot be exploited to instantaneous communication. From two fundamental principles, optimality conditions in equations (8) and (9) can be reproduced as follows.

Suppose that two parties share entangled states and one party prepares quantum states (to be discriminated among) to the other far in the distance using ensemble steering. For states \( \{q_x, \rho_x\}_{x=1}^N \) for the ME discrimination, the other parties are with the following identical ensemble in different decompositions:

\[
\rho = p_x \rho_x + (1 - p_x) \sigma_x \quad \text{for } x = 1, \ldots, N \tag{11}
\]

for some states \( \{\sigma_x\}_{x=1}^N \) with \( q_x = p_x / \sum_{y=1}^N p_y \). Notice that an identical ensemble \( \rho \) has different decompositions according to indices \( x = 1, \ldots, N \). Existence of states \( \{\sigma_x\}_{x=1}^N \) that compose the identical ensemble in the above together with a given set \( \{\rho_x\}_{x=1}^N \) follows from the GHJW theorem in [34, 35]. Note that \( \{q_x\}_{x=1}^N \) are prior probabilities and thus \( \sum_{x=1}^N q_x = 1 \); that \( \{p_x\}_{x=1}^N \) are probabilities to steer quantum states \( \{\rho_x\}_{x=1}^N \) in the ensembles and thus we do not necessarily have \( \sum_{x=1}^N p_x = 1 \).

If a measurement device is set only to discriminate among states \( \{\rho_x\}_{x=1}^N \), the capability of optimal discrimination of \( \{q_x, \rho_x\}_{x=1}^N \) cannot work with an arbitrarily high probability. This is because, if the ME discrimination works arbitrarily well, it would violate the no-signaling principle. For instance, suppose that the ensemble decomposition is concluded by the ME discrimination of states \( \{\rho_x\}_{x=1}^N \): that is, concluding that \( \rho_x \) is found in the discrimination, one guesses that the ensemble corresponds to \( p_x \rho_x + (1 - p_x) \sigma_x \). While no information is announced about the preparation of ensemble decompositions among \( x = 1, \ldots, N \), the no-signaling condition is fulfilled and therefore the ME discrimination of \( \{\rho_x\}_{x=1}^N \) must not allow one to gain knowledge about the preparation. Given no information about the preparation, it must be a random guess about ensemble decompositions. Thus, state discrimination can be constrained such that the strategy above gives at its best the random guess.

In [32] it is shown that the ME discrimination must satisfy the following condition to fulfill two constraints in the above:

\[
\sum_{x=1}^N p_x P(x|x, \{\rho_x\}_{x=1}^N) \leq 1, \tag{12}
\]

where \( P(x|x, \{\rho_x\}_{x=1}^N) \) is the probability of giving outcome \( x \) when one of the states \( \{\rho_x\}_{x=1}^N \) is given i.e. the probability of correctly discriminating among states \( \{\rho_x\}_{x=1}^N \). The equality holds if and only if, for an ensemble prepared in equation (11) with some \( x \), a measurement device responds only to quantum states \( \rho_x \) but not to states \( \sigma_x \), that is, \( P(x|x, \{\sigma_x\}_{x=1}^N) = 0 \). Note that, with the measurement postulate, this is equivalent to \( \text{tr}[M_x \sigma_x] = 0 \) for some POVM \( M_x \), which is indeed the optimality condition in equation (9).
the ME discrimination among quantum states \( \{ \rho_x \}_{x=1}^N \) that are given with prior probabilities \( \{ q_x = p_x / \sum_{y=1}^N p_y \}_{x=1}^N \). All these are summarized as follows.

**Lemma 2.3.** When quantum states \( \{ q_x, \rho_x \}_{x=1}^N \) are prepared by ensemble steering, as shown in equation (11), the guessing probability is upper bounded by the no-signaling condition

\[
P_{\text{guess}} \leq \frac{1}{\sum_{x=1}^N p_x} \quad \text{with equality if and only if } P(x|x, \{ \sigma_x \}_{x=1}^N) = 0 \quad \text{for } x = 1, \ldots, N, \tag{13}
\]

where \( \{ p_x \}_{x=1}^N \) are from equation (11). With the measurement postulate, the equality holds when POVM \( M_x \) does not respond to \( \sigma_x \) but only to \( \rho_x \) for each \( x \), that is

\[
\text{tr}[M_x \sigma_x] = 0, \tag{14}
\]

which reproduces the condition in equation (9). Then, the upper bound is equal to the guessing probability from quantum theory, e.g. equation (7).

**Proof.** The upper bound can be derived from equation (12). We also recall \( q_x = p_x / \sum_{y=1}^N p_y \). Since \( \sum_{x=1}^N q_x = 1 \), the upper bound in equation (13) is obtained. \( \square \)

Consequently, two constraints in equations (11) and (14) are optimality conditions for probabilities in the ME discrimination. Optimality conditions in equations (11) and (14) are equivalent to those in lemma 2.2: equation (11) is equivalent to the symmetry operator in equation (8). We also remark that this approach of constraining with the no-signaling principle is valid for generalized probability theories, as long as the steering effect is allowed to do, i.e. that different decompositions of an identical ensemble in equation (11) can be prepared at a distance.

### 2.3. Geometric formulation

From the different approaches to ME discrimination, we have shown different forms of the optimality conditions, which are also shown to be equivalent to the KKT conditions. Compared to previously known forms of the conditions in equations (4) and (5), the usefulness of expressing the optimality conditions in KKT conditions in lemma 2.2 is that conditions about states (in the state space) and optimal measurement are separated.

We here interpret the symmetry operator in terms of the quantum state geometry and put forward a geometric approach to optimal state discrimination. This shows that optimal discrimination of quantum states, which is supposed to be explained on the level of probability distributions from measurement outcomes, can be explained only with quantum states and their geometry.

We first recall the optimality conditions in lemma 2.2: for a problem of ME discrimination, there exists a symmetry operator \( K^* \) which characterizes optimal discrimination and directly gives the guessing probability. Once the operator is obtained, the rest is straightforward. First, complementary states \( \{ r_x^*, \sigma_x^* \}_{x=1}^N \) can be found as \( K^* - q_x \rho_x \) from equation (8). Since \( K^* \) is uniquely determined by given states, this also means the uniqueness of complementary states in the ME discrimination.

**Lemma 2.4.** The symmetry operator and complementary states in a problem of ME discrimination are unique.
Proof. We first show that the symmetry operator $K^*$ is unique for given states $\{q_x, \rho_x\}_{x=1}^N$. Suppose that for given states $\{q_x, \rho_x\}_{x=1}^N$, there exist two symmetry operators $K^*$ and $\tilde{K}^*$ such that both give the same guessing probability i.e. $P_{\text{guess}} = \text{tr}[K^*] = \text{tr}[\tilde{K}^*]$ while

$$K^* = q_x \rho_x + r_x^* \sigma_x^* \quad \forall x,$$

$$\tilde{K}^* = q_x \rho_x + r_x^* \tilde{\sigma}_x^* \quad \forall x$$

with corresponding complementary states $\{r_x^*, \sigma_x^*\}_{x=1}^N$ and $\{r_x^*, \tilde{\sigma}_x^*\}_{x=1}^N$, respectively. Note that the parameters $\{r_x^*\}_{x=1}^N$ remain the same in both cases of complementary states: this follows from equation (8) that the guessing probability is also given as $P_{\text{guess}} = q_x + r_x^*$ for each $x$. In addition, let us assume that $\{M_x^*\}_{x=1}^N$ and $\{\tilde{M}_x^*\}_{x=1}^N$ are optimal measurements, respectively, such that, $P_{\text{guess}} = \text{tr}[K^*] = \text{tr}[\sum_x q_x \rho_x M_x^*]$ and also $P_{\text{guess}} = \text{tr}[\tilde{K}^*] = \text{tr}[\sum_x q_x \rho_x \tilde{M}_x^*]$, or equivalently from the optimality condition in equation (9), $r_x^* \text{tr}[\sigma_x^* M_x^*] = 0$ and $r_x^* \text{tr}[\tilde{\sigma}_x^* M_x^*] = 0$.

Now, with two equations in equation (15), let us compute $\sum_x K^* M_x^*$ and $\sum_x \tilde{K}^* M_x^*$ as follows, since $\sum_x M_x^* = \sum_x \tilde{M}_x^* = I$,

$$K^* = \sum_x K^* M_x^* = \sum_x q_x \rho_x \tilde{M}_x^* + \sum_x r_x^* \sigma_x^* \tilde{M}_x^* = \tilde{K}^* + \sum_x r_x^* \sigma_x^* \tilde{M}_x^*, \quad (16)$$

$$\tilde{K}^* = \sum_x \tilde{K}^* M_x^* = \sum_x q_x \rho_x M_x^* + \sum_x r_x^* \tilde{\sigma}_x^* M_x^* = K^* + \sum_x r_x^* \tilde{\sigma}_x^* M_x^*, \quad (17)$$

where we have used the fact that $K^* = \sum_x q_x \rho_x M_x^*$ and $\tilde{K}^* = \sum_x q_x \rho_x \tilde{M}_x^*$. From equations (16) and (17), we have

$$K^* + \tilde{K}^* = \tilde{K}^* + K^* + \sum_x r_x^* \sigma_x^* \tilde{M}_x^* + \sum_x r_x^* \tilde{\sigma}_x^* M_x^*$$

$$\Rightarrow \sum_x r_x^* \sigma_x^* \tilde{M}_x^* + \sum_x r_x^* \tilde{\sigma}_x^* M_x^* = 0$$

$$\Rightarrow \sum_x r_x^* \sigma_x^* \tilde{M}_x^* = 0 \text{ and } \sum_x r_x^* \tilde{\sigma}_x^* M_x^* = 0. \quad (18)$$

To conclude equation (18), we have recalled that all operators of measurement and complementary states are positive semidefinite. Plugging equation (18) to equations (16) and (17), we have that $K^* = \tilde{K}^*$. This proves that for a set of quantum states, the symmetry operator is unique.

Then, from equation (8) and the uniqueness of the symmetry operator, it is shown that complementary states are also uniquely determined, $\forall x, r_x^* \sigma_x^* = K - q_x \rho_x$. \hfill $\Box$

For obtained complementary states, it is not difficult to find POVM elements satisfying the orthogonality condition in equation (9). An optimal POVM for state $\rho_x$ can be found in the kernel of the state $\sigma_x^*$, $\mathcal{K}[\sigma_x^*] = \text{span}\{|\psi\rangle : \sigma_x^* |\psi\rangle = 0\}$, i.e. $M_x^* \in \mathcal{K}[\sigma_x^*]$. In doing this, POVM elements should be chosen such that $\text{span}\{M_x^*\}_{x=1}^N = \text{span}\{\rho_x\}_{x=1}^N$ so that the completeness condition $\sum_{x=1}^N M_x = I$ is fulfilled. Note also that it holds, $\text{span}\{\rho_x\}_{x=1}^N = \text{span}\{\sigma_x^*\}_{x=1}^N$. If given states $\{\rho_x\}_{x=1}^N$ are linearly independent, optimal POVM elements must be of rank-one [37].
Since complementary states are unique, one can alternatively solve the ME discrimination in terms of complementary states, without referring directly to optimal measurement. This is also because optimal POVMs are generally not unique: for complementary states \( \{ \sigma_x^* \}_{x=1}^N \), optimal POVMs \( \{ M_x^* \}_{x=1}^N \) specified by the optimality condition tr\[ \sigma_y^* M_x^* \] are not unique [36]. From lemma 2.2, optimal discrimination is solved once those parameters satisfy the KKT conditions. If the underlying geometry of given states is clear, complementary states can be found from given states to discriminate among, in the following way.

Let \( \mathcal{P}(\{ q_x, \rho_x \}_{x=1}^N) \) denote the polytope of given states constructed in the state space, where each vertex of the polytope is specified by \( q_x, \rho_x \). The condition of symmetry operator in equation (8) can be written as

\[
q_x \rho_x - q_y \rho_y = r_y^* \sigma_y^* - r_x^* \sigma_x^* \quad \forall \ x, y = 1, \ldots, N.
\]

This means that the unknown polytope of complementary states \( \mathcal{P}(\{ r_x^*, \sigma_x^* \}_{x=1}^N) \) is congruent to the polytope of given states. Note that, here, we say that two polytopes are congruent if all of the vertices of one polytope are identical to those of the other. This already determines the polytope \( \mathcal{P}(\{ r_x^*, \sigma_x^* \}_{x=1}^N) \) of the states we search for. Then, the optimal discrimination follows by locating \( \mathcal{P}(\{ r_x, \sigma_x \}_{x=1}^N) \) in the state space such that, together with given polytope \( \mathcal{P}(\{ q_x, \rho_x \}_{x=1}^N) \), the symmetry operator can be constructed. This is equivalent to the condition that corresponding lines are anti-parallel, see equation (19). An approach to construct the symmetry operator can be done by rewriting the symmetry operator in equation (8) as

\[
K^* = \frac{1}{N} \sum_{x=1}^N q_x \rho_x + \frac{1}{N} \sum_{x=1}^N r_x^* \sigma_x^*.
\]

Note an interpretation of \( K^* \), that a symmetry operator corresponds to the sum of two centers of two respective polytopes \( \mathcal{P}(\{ q_x, \rho_x \}_{x=1}^N) \) and \( \mathcal{P}(\{ r_x^*, \sigma_x^* \}_{x=1}^N) \). Then, given the two congruent polytopes in the state space, a symmetry operator can be obtained by rotating the not-yet-fixed one \( \mathcal{P}(\{ r_x, \sigma_x \}_{x=1}^N) \) with respect to the fixed one \( \mathcal{P}(\{ q_x, \rho_x \}_{x=1}^N) \), such that operators from two constructions in equations (8) and (20) are identical.

To apply the geometric formulation in the above, one should be able to describe the geometry of quantum states in the state space. The difficulty is clearly the lack of a general picture to quantum state space apart from two-dimensional cases, qubit state space.

3. General structures

In this section, we show general structures of ME discrimination: equivalence classes of sets of quantum states, construction of the ME discrimination and general expressions of the guessing probability. We mainly exploit results shown in the previous section, that for ME discrimination there always exists a symmetry operator which completely characterizes the optimal discrimination. We first define equivalence classes of sets of quantum states in terms of a symmetry operator. As an approach converse to optimal discrimination for given states, we present a systematic way of constructing a set of quantum states for which the optimal discrimination is immediately known from a given symmetry operator. We then show a general and analytic expression of the guessing probability.

From now on, unless specified otherwise, for simplicity let \( K \) and \( \{ r_x, \sigma_x \} \) without * denote a symmetry operator and complementary states, respectively.
3.1. Equivalence classes

From lemma 2.2, a symmetry operator gives a complete characterization of optimal parameters in ME discrimination. Once a symmetry operator is found, it is straightforward to find the complementary states and optimal measurements. Note that the guessing probability is given by the trace norm of a symmetry operator, see equation (7). Therefore, if two different sets of quantum states share an identical symmetry operator, the ME discrimination is characterized in an equivalent way in terms of the identical symmetry operator.

**Definition 3.1 (Equivalence classes).** Two sets of quantum states, say \( \{q_x, \rho_x\}_{x=1}^{N} \) and \( \{q'_x, \rho'_x\}_{x=1}^{L} \), are equivalent in the ME state discrimination if their symmetry operators are identical up to unitary transformations i.e. an identical spectrum. We write two equivalent sets as

\[
\{q_x, \rho_x\}_{x=1}^{N} \sim \{q'_x, \rho'_x\}_{x=1}^{L},
\]

and the equivalence class characterized by a symmetry operator \( K \) is denoted by \( A_K \). Then sets of quantum states in the same equivalence class have the same guessing probability.

3.2. Construction of a set of quantum states from a symmetry operator

In this subsection, conversely to solving a problem of ME discrimination (or equivalent to finding the symmetry operator), we here introduce a systematic way of generating a set of quantum states for a given symmetry operator. This means that, for the generated quantum states, optimal discrimination is already characterized by the symmetry operator. That is, elements of an equivalent class identified by a symmetry operator are generated in this way.

The main idea is to exploit the structure of ME discrimination shown in the section 2.2. Suppose that a symmetry operator is given by \( K \in \mathcal{B}(H) \) which is simply a (bounded) positive operator over a Hilbert space \( H \). As the guessing probability is to be given as \( \text{tr}[K] \) at the end (see equation (7)), we note that the operator is not larger than the identity operator in the space. To construct a set of quantum states \( \{q_x, \rho_x\}_{x=1}^{N} \) having operator \( K \) as their symmetry operator, the first thing to do is to normalize the operator to interpret it as a quantum state and then make its purification. Let \( \tilde{K} \) denote the operator after normalization, \( \tilde{K} = K / \text{tr}[K] \). We write its purification as \( |\psi_K\rangle_{AB} \in \mathcal{H} \otimes \mathcal{H} \) such that \( \tilde{K} = \text{tr}_A |\psi_K\rangle_{AB} \langle \psi_K| \); the purification is unique up to local unitary transformations on the \( A \) system.

Then, the next is to construct \( N \) two-outcome and complement measurements on the \( A \) system, \( M^x = \{ M^x_0, M^x_1 \} \) with \( M^x_0 + M^x_1 = I \) for \( x = 1, \ldots, N \). Since each measurement is complete, the resulting state in the \( B \) system on average (i.e. ensemble average) is described by the operator \( \tilde{K} \). Decompositions of operator \( \tilde{K} \) are determined by the choice of measurement \( M^x \) on the \( A \) system: let \( \rho_x (\sigma_x) \) denote the state that resulted from the detection event appearing in Alice’s measurement \( M^x_0 \) \( (M^x_1) \); we assume that the detection event happens with probability \( p_x (1 - p_x) \). In this way, there are \( N \) different decompositions of operator \( \tilde{K} \),

\[
\tilde{K} = p_x \rho_x + (1 - p_x) \sigma_x \quad \text{for } x = 1, \ldots, N, \tag{21}
\]

where \( \{\rho_x\}_{x=1}^{N} \) are those states that we are interested in discriminating. Given that a measurement device is prepared to discriminate among these states \( \{\rho_x\}_{x=1}^{N} \), the a priori probability that \( \rho_x \) is generated is given by \( p_x / \sum_{x=1}^{N} p_x \), which we write by \( q_x \).

The ensemble decomposition in equation (21) corresponds to the case shown in equation (11), or also equivalently in equation (8), that an identical ensemble is decomposed into...
When a symmetry operator $K$ is given, a set of POVM elements exists $\{M^x_I\}_{x=1}^N$ on the $A$ system of the purification $|\psi_K\rangle_{AB}$, such that those states $\{\rho_x\}_{x=1}^N$ are prepared in the $B$ system with probabilities $\{p_x\}_{x=1}^N$, respectively, where $p_x = q_x \text{tr}[K]$ for each $x = 1, \ldots, N$. Then, the other POVM elements $\{M^x_F\}_{x=1}^N$, which fulfill that $M^x_O + M^x_I = I$ for each $x$, uniquely find complementary states $\{\sigma_x\}_{x=1}^N$ in the $B$ system.

Before proceeding, we present an example that shows how the method of constructing a set of quantum states can be applied, when a symmetry operator is given. It is simple but also useful to see how all that has been explained works out. Further examples are also presented in section 4.

Example (Equivalence class of a normalized identity operator). Suppose that a symmetry operator is given as the identity operator in a $d$-dimensional Hilbert space, $K = I/d$. Take one spectral decomposition of the identity, we write it using an orthonormal basis $\{|k\rangle\}_{k=1}^d$: $I = \sum_{k=1}^d |k\rangle \langle k|$. Since the symmetry operator is normalized, the guessing probability for quantum states to be constructed is to be $P_{\text{guess}} = 1$. The purification is the maximally entangled state, $|\psi_K\rangle = \sum_{k=1}^d |k\rangle |k\rangle \sqrt{d}$. Applying measurement $\{M^0_O = |x\rangle \langle x|, M^x_I = I - M^0_O\}_{x=1}^d$ on the $A$ system, the following ensemble is prepared in the $B$ system:

$$K = \frac{1}{d} |x\rangle \langle x| + \frac{d-1}{d} \sigma_x,$$

where $\sigma_x = \frac{1}{d-1} \sum_{y \neq x} |y\rangle \langle y| \quad \forall \ x = 1, \ldots, d$.

This defines a problem of state discrimination for orthogonal states $\{1/d, |x\rangle \langle x|\}_{x=1}^N$. Complementary states are shown in the above; it is also straightforward to find optimal measurements. Thus, it is shown that $\{1/d, |x\rangle \langle x|\}_{x=1}^N \in \mathcal{A}_{1/d}$.

3.3. Analytic expression of the guessing probability

In this subsection, we present various expressions of the guessing probability in ME state discrimination. They are equivalent but of different forms depending on how they are derived. The first one based on the optimality conditions corresponds to a quantum analogy of the probabilistic-theoretic measure shown in equation (3). The next one is in accordance with other physical theories, ensemble steering on quantum states and the no-signaling principle on measurement outcomes.

3.3.1. Quantum analogy to the probability-theoretic expression. Let us first present a general form of the guessing probability (for quantum states) in the framework of probability-theoretic measures. We first recall from lemma 2.1 that the guessing probability about random variable $X$ given $Y$ is generally expressed as the distance of probability $P_{X|Y}$ deviated from the uniform distribution. This holds true in general, no matter what physical systems are applied to mediate
while the preparation and the measurement. Then, it remains to determine the form of \( d(X|Y) \) once quantum systems are applied.

We recall the KKT conditions of the ME discrimination for \( \{q_x, \rho_x\}_{x=1}^N \), as follows:

\[
K = q_x \rho_x + r_x \sigma_x \quad \text{for } x = 1, \ldots, N \text{ with complementary states } \{r_x, \sigma_x\}_{x=1}^N.
\]

Using the simple identity that

\[
P_{\text{guess}} = \frac{1}{N} \text{tr} \left[ \sum_x q_x \rho_x + r_x \sigma_x \right] = \frac{1}{N} \text{tr} K + R,
\]

where \( R = \frac{1}{N} \sum_x r_x \), we have

\[
P_{\text{guess}} = \frac{1}{N} \text{tr} K = \frac{1}{N} + R,
\]

This compares to equation (3): the distance \( d(X|Y) \) corresponds to the dual parameter \( R \), which now corresponds to the norm of the ensemble average of complementary states.

The parameter \( R \) in the expression in equation (22) in fact has a geometrical meaning in the state space. Recall from section 2.3 that each complementary state is determined as a vertex of the polytope that is congruent to the polytope constructed by given states, \( \mathcal{P}(\{q_x, \rho_x\}_{x=1}^N) \). Then, each state \( r_x \sigma_x \) plays the role of the (trace) distance between each vertex \( q_x \rho_x \) of the polytope and the symmetry operator, i.e.

\[
r_x = \text{tr} [r_x \sigma_x] = \text{tr} [K - q_x \rho_x] = \| K - q_x \rho_x \|_1,
\]

where we note that \( K \geq q_x \rho_x \) for all \( x = 1, \ldots, N \), from the dual problem in equation (7).

**Proposition 3.2.** The guessing probability for quantum states \( \{q_x, \rho_x\}_{x=1}^N \) constructed from a symmetry operator \( K \) is

\[
P_{\text{guess}} = \frac{1}{N} + R(K||\{q_x, \rho_x\}_{x=1}^N) \text{ with } R(K||\{q_x, \rho_x\}_{x=1}^N) = \frac{1}{N} \sum_{x=1}^N \| K - q_x \rho_x \|_1,
\]

where \( R(K||\{q_x, \rho_x\}_{x=1}^N) \) shows the averaged trace distance of given states \( \{q_x, \rho_x\}_{x=1}^N \) deviated from their symmetry operator \( K \), see also equation (3) in lemma 2.1 for comparison.

### 3.3.2. General expression for probabilistic and physical models.

The next form of guessing probability (for discrimination among states \( \{q_x, \rho_x\}_{x=1}^N \) ) is obtained by the compatibility between ensemble steering on quantum states and the no-signaling condition on probability distributions of measurement outcomes. Then, as is shown in lemma 2.3, the guessing probability is given by

\[
P_{\text{guess}} = \frac{1}{p_1 + \cdots + p_N} \quad \text{with } p_x = q_x P_{\text{guess}} \quad \text{for } x = 1, \ldots, N,
\]

since the bound in equation (13) is tight. From the ensemble steering shown in equation (11), the guessing probability can be interpreted as follows. Each parameter \( p_x \) of \( \{p_x\}_{x=1}^N \) in the above shows the probability that a party can prepare a quantum state \( \rho_x \) to the other party at a distance via the ensemble steering. Therefore, the guessing probability corresponds to the maximal average probability to prepare a set of chosen quantum states to a distant party via the ensemble steering.

**Theorem 3.1 (Steerability and state discrimination).** While ensemble steering is allowed within quantum theory, the steerability of a quantum state in the ensemble is generally proportional to the guessing probability for those states prepared in the ensemble.

\[\text{New Journal of Physics 15 (2013) 073037 (http://www.njp.org/)}\]
3.3.3. Simplification for equal prior probabilities. Finally, for the ME discrimination for \( \{q_x, \rho_x\}_{x=1}^N \), a huge simplification can be made when prior probabilities are equal i.e. \( q_x = 1/N \) for all \( x \). The simplification is shown in the expression of \( R \) in equation (23), that it holds \( r_x = r_y \) for all \( x, y = 1, \ldots, N \) if \( q_x = 1/N \). Note also that since the symmetry operator in equation (8) shows that \( r_{\text{guess}} = \text{tr}[K] = q_x + r_x = q_y + r_y \) \( \forall x, y \); now since \( q_x = q_y = 1/N \), it holds that \( r_x = r_y \) for all \( x, y \). From lemma 3.2, this means that the distances of given states from the symmetry operator are all equal. Thus, for convenience, let us write

\[
r_x := r_x \quad \forall x = 1, \ldots, N \quad \text{and then } r = R(K \parallel \{1/N, \rho_x\}_{x=1}^N).
\]  

(25)

The problem of ME discrimination becomes even simpler. There is only a single parameter \( r \) to find, to solve optimal quantum state discrimination for the uniform prior.

Applying the geometric formulation shown in section 2.3, the geometrical meaning of the parameter \( r \) in equation (25) can be found in a simple way. From the KKT condition in equation (8), we have the following relation, see also equation (19):

\[
\frac{1}{N} \rho_x - \frac{1}{N} \rho_y = r \sigma_y - r \sigma_x \quad \text{and then } r = \frac{\| \frac{1}{N} \rho_x - \frac{1}{N} \rho_y \|_1}{\| \sigma_x - \sigma_y \|_1}.
\]

(26)

Then, the parameter \( r \) corresponds to the ratio between two polytopes in the state space, the given one \( \mathcal{P}(\{\frac{1}{N}, \rho_x\}_{x=1}^N) \) constructed from given states and the other one \( \mathcal{P}(\{\sigma_x\}_{x=1}^N) \) only of complementary states.

**Proposition 3.3.** The guessing probability for quantum states given with the uniform prior is determined by only a single parameter as

\[
P_{\text{guess}} = \frac{1}{N} + r,
\]

(27)

where \( r \) is the ratio between two polytopes, one from given states and the other from complementary states.

4. Examples: solutions in qubit state discrimination

In this section, we apply general results shown so far to an arbitrary set of qubit states. Since qubits are the unit of quantum information processing, the results presented here are not only of theoretical interest as they characterize the quantum capabilities of state-discrimination-based tasks, but they are also useful for practical applications. Note that, for ME discrimination for qubit states, general solutions are known for two qubit states. For more than two states, optimal discrimination is known for qubit states containing some symmetry, such as a geometrically uniform structure. Recently, there have been analytical approaches to qubit state discrimination, one exploiting the dual problem in equation (7) [38] and the other from the complementarity problem that analyzes the KKT conditions in equations (8) and (9) [30]. In the latter, an analytic method is provided to solve ME discrimination for any set of qubit states with the uniform prior. In the following subsections, we present the optimal discrimination of qubit states when qubit states may not contain any symmetry among them. That is, we present the symmetry operator, complementary states and the optimal measurement.

Let us collect general results to be used for qubit state discrimination. As for qubit states, a useful and clear geometric picture is present with the Bloch sphere, in which the state geometry is also clear with a Hilbert–Schmidt distance. The other useful fact is that for qubit states,
the Hilbert–Schmidt distance is proportional to the trace distance. From this, the geometry formulation in the section 2.3 can also be applied.

**Lemma 4.1.** For qubit states, the Hilbert–Schmidt and the trace distances, denoted by $d_{\text{HS}}$ and $d_T$ respectively, are related by a constant as follows:

$$d_{\text{HS}}(\rho, \sigma) = \sqrt{2} d_T(\rho, \sigma)$$

for any qubit states $\rho$ and $\sigma$.

The lemma is useful when the trace distance between qubit states is computed via the geometry in the Bloch sphere: once the actual distance measured in the Bloch sphere is computed in the Hilbert–Schmidt norm via the geometry, from lemma in the above the distance can be converted to the trace norm.

The next useful fact is the orthogonality relation. In the two-dimensional Hilbert space, if two non-negative and Hermitian operators $O_1$ and $O_2$ fulfill the orthogonality condition $\text{tr}[O_1 O_2] = 0$, see equation (9), the only possibility is that the two operators are of rank-one and, once normalized, they are a resolution of the identity operator. That is, if $O_1 \propto |\phi\rangle \langle \phi|$ satisfies the orthogonality, then the other is uniquely determined $O_2 \propto |\phi^\perp\rangle \langle \phi^\perp|$, since in two-dimensional space, the resolution of the identity is given as $I = |\phi\rangle \langle \phi| + |\phi^\perp\rangle \langle \phi^\perp|$ for any vector $|\phi\rangle$. This means that as long as the optimal strategy in state discrimination is not the application of the null measurement for some state (i.e. $M_x = 0$ for some $x$), optimal POVM elements and complementary states, that would fulfill the optimality condition in equation (9), each must be of rank-one and uniquely determined from the aforementioned relation in the above. All these are summarized in the following, exploiting the optimality condition in equation (9).

**Lemma 4.2.** The following are the conditions for optimal measurement and complementary states in optimal discrimination of qubit states:

1. If complementary states are not pure states, then the optimal strategy to have a minimal error is to apply the null-measurement, i.e. no-measurement for some states gives an optimal strategy [30, 39].

2. For cases where the optimal strategy is not the null measurement, optimal POVM elements are of rank-one [30, 38] and are uniquely determined by complementary states that are also of rank-one [30].

**Proof.**

1. Let us decompose a complementary state $\sigma_x$ in the following way: $\sigma_x = s_x |\varphi_x\rangle \langle \varphi_x| + (1 - s_x) |\varphi^\perp_x\rangle \langle \varphi^\perp_x|$ with some $|\varphi_x\rangle$ and $|\varphi^\perp_x\rangle$ in the two-dimensional space. One can always find two orthogonal vectors to decompose a qubit state in this way. Suppose that $s_x > 0$ so that $\sigma_x$ is not of rank-one. Then, suppose that there exists a POVM element $M_x$ such that $\text{tr}[M_x \sigma_x] = 0$. This means that $\langle \varphi_x| M_x |\varphi_x\rangle = \langle \varphi^\perp_x| M_x |\varphi^\perp_x\rangle = 0$. Since $I = |\varphi_x\rangle \langle \varphi_x| + |\varphi^\perp_x\rangle \langle \varphi^\perp_x|$, it follows that $\text{tr}[M_x] = \text{tr}[M_x I] = 0$. Since $M_x$ is non-negative, we have $M_x = 0$, i.e. no-measurement.

2. Now it is clear that, when two positive operators e.g. $\sigma_x$ and $M_x$ fulfill the orthogonality relation, both of them must be of rank-one. Once a complementary state is given, the only choice for its corresponding POVM element that satisfies the orthogonality is where the POVM is in the kernel of the complementary state $K[\sigma_x]$. Since $\dim \mathcal{H} = 2$ and $\sigma_x$ are of
rank-one, it follows that \( \dim \mathcal{K}[\sigma_i] = 1 \). Thus, the POVM element is also of rank-one and uniquely determined in the one-dimensional kernel space of a complementary state. \( \square \)

Lemma shown in the above applies directly to the geometric formulation presented in section 2.3 for qubit states. Recall that most complementary states for which the optimal measurement is not the null POVM element are of rank-one, that is, pure states. This means that complementary states lie at the surface of the Bloch sphere; the polytope of them \( \mathcal{P}(\sigma_i) \) is therefore the maximal within the Bloch sphere. The shape of the polytope \( \mathcal{P}(\sigma_i) \) is also known to be congruent to the polytope \( \mathcal{P}(\rho_i) \) of given states, see the formulation in section 2.3.

Furthermore, let us recall the following. For the uniform prior probabilities \( q_i = 1/N \), as is shown in equation (27), there is only a single parameter to find in order to solve the optimal discrimination. The parameter is expressed by \( r \) in equation (27), corresponding to the ratio between two polytopes \( \mathcal{P}(\sigma_i) \) and \( \mathcal{P}(\rho_i) \), see the expression in equation (26). Note also that \( r = r_i \) for all \( i = 1, \ldots, N \) when finding the complementary states \( \{\sigma_i, \rho_i\} \) as it is shown in equation (25).

**Lemma 4.3.** The guessing probability for qubit states given with the uniform prior probabilities is in the following form:

\[
P_{\text{guess}} = \frac{1}{N} + r
\]

with the parameter \( r \), the ratio between two polytopes in the state space, \( \mathcal{P}(\rho_i) \) constructed from given states and its similar polytope that is also maximal in the Bloch sphere.

**Proof.** Two polytopes \( \mathcal{P}(\sigma_i) \) and \( \mathcal{P}(\rho_i) \) are congruent and therefore two polytopes \( \mathcal{P}(\sigma_i) \) and \( \mathcal{P}(\rho_i) \) are similar with the ratio \( r \). For qubit state discrimination, from lemma 4.2 it holds that most complementary states are of rank-one lying at the surface of the Bloch sphere and hence \( \mathcal{P}(\sigma_i) \) is the maximal in the Bloch sphere. Therefore, the ratio \( r \) is given from \( \mathcal{P}(\rho_i) \) and its similar and maximal one \( \mathcal{P}(\sigma_i) \). This completes the proof. \( \square \)

In what follows, we apply all these results to qubit state discrimination. We also write qubit states using Bloch vectors as \( \rho_i = \rho(\vec{v}_i) = \frac{1}{2}(I + \vec{v}_i \cdot \vec{\sigma}) \), where \( \vec{\sigma} = (X, Y, Z) \) are Pauli matrices.

### 4.1. Two states

When two quantum states are given, the state space spanned by them is effectively two-dimensional. Consequently, discrimination of them is equivalently restricted to two qubit states. This does not lose any generality. Then, for two-state discrimination \( \{q_i, \rho_i\} \), optimal discrimination was shown in [3],

\[
P_{\text{guess}} = \frac{1}{2}(1 + \|q_1 \rho_1 - q_2 \rho_2\|_1).
\]

We now reproduce the result using the geometric formalism presented in section 2.3.

The optimal discrimination is obtained if complementary states are found, since complementary states provide the symmetry operator that gives the guessing probability and also defines optimal measurements, see lemma 2.2. Thus, we now show how to find complementary states from given states. We first rewrite equation (19) for the two states

\[
q_1 \rho_1 - q_2 \rho_2 = r_2 \sigma_2 - r_1 \sigma_1,
\]
Figure 1. Discrimination of two states \( \{q_x, \rho_x\}_{x=1}^2 \). In both figures (A) and (B), given states \( q_1 \rho_1 \) and \( q_2 \rho_2 \) are depicted by two lines \( OX_1 \) and \( OX_2 \), respectively. The line \( OK \) corresponds to the symmetry operator, which is the same in both figures and therefore the guessing probability for two cases is the same, i.e. two cases (A) and (B) are in the same equivalence class. From the geometric formation in section 2.3, complementary states can be found as a polytope congruent to the given polytope \( X_1 X_2 \) of given states. From lemma 4.2, complementary states are on the surface. Therefore, \( R_1 R_2 \) is the polytope congruent to \( X_1 X_2 \); then \( OC_1 \) and \( OC_2 \) are complementary states \( \sigma_1 \) and \( \sigma_2 \) respectively, from which optimal POVM elements for states \( \rho_1 \) and \( \rho_2 \) are \( OC_1 \) and \( OC_2 \) respectively. The KKT condition in equation (8) holds as \( OK = OX_1 + OR_1 = OX_2 + OR_2 \) and the other in equation (9) \( OC_1 \perp OC_2 \).

where \( \{r_x, \sigma_x\}_{x=1}^2 \) are complementary states to find. Recall lemma 4.2, complementary states are of rank-one and thus lie at the surface of the Bloch sphere. Then, equation (30) in the above means (i) two polytopes (lines in this case) by given states and by complementary states, respectively, are congruent and also parallel. Thus, given the line defined by \( q_1 \rho_1 - q_2 \rho_2 \) in the Bloch sphere, two complementary states can be found by finding a diameter (since they are pure states) such that the diameter is parallel to the given line, see figure 1. Two parameters \( r_1 \) and \( r_2 \) can be found to satisfy the relation in equation (30). Then, the symmetry operator is found as \( q_x \rho_x + r_x \sigma_x \) for \( x = 1, 2 \), and optimal measurements are also defined in the diameter of complementary states as \( M_1 \propto \sigma_2 \) and \( M_2 \propto \sigma_1 \).

From the geometric method, the guessing probability can be explicitly written as follows. Note that, from equation (30), (i) \( \text{tr}[q_1 \rho_1 - q_2 \rho_2] = q_1 - q_2 \) and (ii) \( r_1 + r_2 = \| r_1 \sigma_1 - r_2 \sigma_2 \|_1 = \| q_1 \rho_1 - q_2 \rho_2 \|_1 \).
Thus, for $x = 1, 2$

$$r_x = \frac{1}{2}(\|q_1 \rho_1 - q_2 \rho_2\| + (-1)^x(q_1 - q_2)).$$

(31)

Thus, from the general expression shown in equation (22) for $N = 2$, the guessing probability is

$$P_{\text{guess}} = \text{tr}[K] = \frac{1}{2} + \frac{1}{2}(r_1 + r_2) = \frac{1}{2}(1 + \|q_1 \rho_1 - q_2 \rho_2\|)$$

with

$$K = \frac{1}{2}(q_1 \rho_1 + q_2 \rho_2) + \frac{1}{2}(r_1 \sigma_1 + r_2 \sigma_2).$$

(32)

Thus, it is shown that the Helstrom bound is reproduced.

In particular, when $q_1 = q_2 = 1/2$, from proposition 3.3 it follows that $r = r_1 = r_2 = \| \rho_1 - \rho_2 \| / 2$. Then, from the expresso in equation (32), the symmetry operator has an even simpler form

$$K = \frac{1}{2}(1/2 \rho_1 + 1/2 \rho_2) + 1/2 (r I),$$

since two complementary states correspond to the diameter and their average is simply proportional to the identity.

In this case, let us also show how the formulation in lemma 4.3 can be applied. First, note again that the polytope constructed by given states is the line $q_1 \rho_1 - q_2 \rho_2$ in the Bloch sphere. Since it is a line, the largest polytope similar to the line is clearly a diameter that has the length 2 in trace norm. The parameter $r$ in equation (27) that we look for is the ratio between two lines,

$$\| \frac{1}{2} \rho_1 - \frac{1}{2} \rho_2 \| : 2 = r : 1 \quad \text{and thus } r = \frac{1}{2} \| \frac{1}{2} \rho_1 - \frac{1}{2} \rho_2 \|.$$

With the above, the guessing probability is $P_{\text{guess}} = 1/2 + r$, which reproduces the Helstrom bound in equation (29) when $q_1 = q_2 = 1/2$.

4.2. Three states

We now move to cases of three qubit states. For three states, no general solution for ME discrimination has been known to date, apart from specific cases where they are symmetric. Here, for three states given with equal prior probabilities, we apply lemma 4.3 and show how to find optimal discrimination.

4.2.1. Three-state example I: isosceles triangles. We first suppose that three pure states lying at a half-plane are given with equal prior probabilities 1/3, i.e. $\{1/3, \rho_x = |\psi_x\rangle\langle\psi_x|\}_{x=1}^3$. In particular, we suppose that the polytope constructed by the three states forms an isosceles triangle on a half plane of the Bloch sphere. For convenience, we parameterize the three states as follows, for some $\theta_0$:

$$|\psi_1\rangle = \cos \frac{1}{2} (\theta_0 + \theta)|0\rangle + \sin \frac{1}{2} (\theta_0 + \theta)|1\rangle,$$

$$|\psi_2\rangle = \cos \frac{1}{2} \theta_0|0\rangle + \sin \frac{1}{2} \theta_0|1\rangle,$$

$$|\psi_3\rangle = \cos \frac{1}{2} (\theta_0 - \theta)|0\rangle + \sin \frac{1}{2} (\theta_0 - \theta)|1\rangle,$$

(33)

where let us suppose $\theta \in [0, \pi]$, see figure 2.

We now apply lemma 4.2 to discriminate among these three states, referring to the geometry shown in figure 2. The maximal polytope which is similar to the given one $X_1 X_2 X_3$ is $S_1 S_2 S_3$. There are many ways of putting the maximal polytope in the plane, however,
Figure 2. Discrimination of three qubit states \( \{ q_x = 1/3, \rho_x = |\psi_x\rangle\langle\psi_x| \}_{x=1}^3 \) in a half-plane is shown. It is straightforward to generalize this to three qubit states having the same purity. In the half-plane, each state \( \rho_x/3 \) corresponds to line \( OX_x \) for \( x = 1, 2, 3 \). The three states are defined such that two states \( \rho_1 \) and \( \rho_3 \) are equally distant from state \( \rho_2 \); the distance is specified by angle \( \theta \). Then, the polytope of the given states corresponds to the triangle \( X_1X_2X_3 \), an isosceles triangle. Since they are given with equal probabilities, lemma 4.3 is applied as follows. The largest triangle similar to \( X_1X_2X_3 \) is given by \( S_1S_2S_3 \). The ratio between the two triangles is, \( r = \sin(\theta)/3 \). Thus, the guessing probability is \( P_{\text{guess}} = (1 + \sin\theta)/3 \). Note that \( OS_x \) for \( x = 1, 2, 3 \) correspond to complementary states. Since the complementary state \( OS_2 \) is not pure, optimal POVM for the state \( \rho_2 \) is the null measurement, \( M_2 = 0 \).

In figure 2, the guessing probability for the three states is plotted as angle \( \theta \) varies. One can easily find that for \( \theta \geq \pi/2 \), the ratio is \( r = 1/3 \) and thus the guessing probability is, \( 2/3 \).

Let us then find the optimal measurement. Note that \( OS_1, OS_2 \) and \( OS_3 \) correspond to complementary states, \( \sigma_1, \sigma_2 \) and \( \sigma_3 \), respectively. It is shown that \( \sigma_2 \) is not a pure state, i.e. not of rank-one. This means that, to fulfill the optimality condition in equation (9), the optimal POVM element is the null measurement, i.e. \( M_2 = 0 \), no-measurement on the state. The other complementary states can be written explicitly as follows:

\[
\sigma_1 = |\varphi_1\rangle\langle\varphi_1|, \quad |\varphi_1\rangle = \cos\left(\frac{\theta_0}{2} - \frac{\pi}{4}\right) |0\rangle + \sin\left(\frac{\theta_0}{2} - \frac{\pi}{4}\right) |1\rangle,
\]

\[
\sigma_3 = |\varphi_3\rangle\langle\varphi_3|, \quad |\varphi_3\rangle = \cos\left(\frac{\theta_0}{2} + \frac{\pi}{4}\right) |0\rangle + \sin\left(\frac{\theta_0}{2} + \frac{\pi}{4}\right) |1\rangle
\]
and the optimal POVM elements are

\[ M_1 = |\varphi_3\rangle\langle \varphi_3|, \quad M_2 = 0, \quad M_3 = |\varphi_1\rangle\langle \varphi_1|, \quad \text{so that } \sum_{x=1}^{3} M_x = I. \]

One can see that with these POVMs, the guessing probability is obtained

\[ P_{\text{guess}} = \frac{1}{3} \text{tr}[\rho_1 M_1] + \frac{1}{3} \text{tr}[\rho_2 M_2] + \frac{1}{3} \text{tr}[\rho_3 M_3] = \frac{1}{3} + \frac{1}{3} \sin \theta \]

as it is shown in equation (34). Optimal POVM elements show that for discrimination among the three states given with probability 1/3, the optimal strategy corresponds to the measurement setting where the device only responds to the two most distant states out of the three.

4.2.2. Three-state example II: geometrically uniform states. The example shown in the previous can be extended to the so-called geometrically uniform states [23, 27], which correspond to the case that \( \theta = 2\pi/3 \). It is straightforward to exploit the method shown in the above from lemma 4.2, then the guessing probability is 2/3. In fact, as is shown, the guessing probability is found, \( P_{\text{guess}} = 2/3 \) for any three pure (qubit) states given with equal probabilities if the polytope of them in the Bloch sphere contains the origin.

4.2.3. Three-state example III: arbitrary triangles on a half-plane. We now consider a set of three pure states given with equal probabilities 1/3 and suppose that the polytope constructed by the three states forms an arbitrary triangle in a half-plane of the Bloch sphere: \( \{1/3, \rho_x = |\psi_x\rangle\langle \psi_x|\}_{x=1}^{3} \). As a contrast to the example isosceles triangles shown in the above, we also suppose that the polytope of given states contains the origin of the Bloch sphere, see figure 3.

To apply the geometric formulation in lemma 4.3, we also refer to figure 3. Note that the three states \( \rho_x/3 \) for \( x = 1, 2, 3 \) correspond to \( OX_x, x = 1, 2, 3 \), respectively; thus the polytope of given states is the triangle \( X_1X_2X_3 \). Then, the next thing to do is to find a maximal polytope similar to \( X_1X_2X_3 \) within the Bloch sphere. The triangle \( S_1S_2S_3 \) in figure 3 could be a possibility. The ratio \( r \) corresponds to, for instance, \( X_1X_2/S_1S_2 \), which is also equal to \( OX_1/OS_1 \): therefore \( r = 1/3 \), then the guessing probability is

\[ P_{\text{guess}} = \frac{1}{3} + r = \frac{2}{3}. \]

Note that this is the guessing probability for many cases of three pure states. This can be generalized to cases where three states have the same purity, as follows.

Remark 4.1. Suppose that three qubit states having an equal purity denoted by \( f \) are given with equal prior probabilities 1/3. Here, the purity corresponds to the norm of a Bloch vector. Then, if the polytope of the three states in the Bloch sphere contains the origin, the guessing probability is

\[ P_{\text{guess}} = \frac{1}{3} + \frac{1}{3} f. \]

This is independent of the other details of given quantum states, e.g. the angles between them.

The triangle \( S_1S_2S_3 \) in figure 3 does not show complementary states yet, since the optimality condition in equation (19), or equivalently equation (8), is not fulfilled. Therefore, one has to put or rotate \( S_1S_2S_3 \) to \( C_1C_2C_3 \) in figure 3, so that equation (19) holds true: \( X_xX_y \parallel C_yC_x \) for all \( x, y = 1, 2, 3 \), where \( \parallel \) means that two lines are parallel. Then, all of the optimality conditions are satisfied.
Figure 3. A general method of applying lemma 4.3 to arbitrarily given three qubit states is shown. Note that prior probabilities are equal, 1/3, given states correspond to $OX_x$ for $x = 1, 2, 3$ and the polytope of given states is $X_1X_2X_3$. To make the explanation simple, we suppose that a maximal triangle similar to $X_1X_2X_3$, which is $S_1S_2S_3$, is covered by the Bloch sphere. In case one of them does not lie at the surface, one can proceed as in figure 2. Then, the ratio between the two triangles can give the guessing probability. Then, complementary states can be found by rotating $S_1S_2S_3$ such that the optimality condition in equation (26) is fulfilled. Then, the polytope of complementary states $C_1C_2C_3$ is defined, where one can see that $X_xX_y$ is parallel with $C_yC_x$ for $x$ and $y$. An optimal measurement can also be found as $OP_x$, $x = 1, 2, 3$, since $OP_x$ is opposite to $OC_x$ from the optimality condition in equation (9).

Complementary states are then those states that correspond to $OC_x$ for $x = 1, 2, 3$. It also follows that optimal POVM elements are $OP_x$ for $x = 1, 2, 3$ as each of them is orthogonal to its corresponding complementary state, see the optimality condition in equation (9). Thus, optimal POVM elements are $\{M_x \propto OP_x\}_{x=1}^3$. Since the convex hull $P_1P_2P_3$ contains the origin, it is also straightforward to have the completeness, $\sum_{x=1}^3 M_x = I$. Here, it is noteworthy that optimal POVMs can be in vectors which are not parallel to corresponding states: in figure 3, we found that $OX_x \parallel OP_x$ for some $x$.

4.2.4. Three-state example IV: arbitrary triangles. Finally, let us show how the geometric formulation in lemma 4.3 can be generally applied to a set of arbitrary three qubit states when they are given with equal probabilities, $\{1/3, \rho_x\}_{x=1}^3$. We explain this, referring to figure 4. Arbitrary three states are depicted by $OX_x$ for $x = 1, 2, 3$ respectively.

Once they are given, they define a plane of the triangle $X_1X_2X_3$ in the Bloch sphere and there exists a half-plane parallel to the plane. To find the guessing probability for the states, one has to first find a maximal triangle that is similar to the triangle $X_1X_2X_3$ in the Bloch sphere. Then, the maximal one must lie on the half-plane parallel to $X_1X_2X_3$, to fulfill the optimality condition in equation (19), or equivalently equation (8). Then, the maximal one is
Figure 4. Arbitrary three qubit states are given with equal prior probabilities \(1/3\). They are denoted by \(OX_x\) for \(x = 1, 2, 3\). The polytope of given states \(X_1X_2X_3\) defines a plane; then the complementary states and optimal POVM elements lie on the half-plane which is parallel to the defined plane. See section 4.2.4 for more details.

rotated such that the condition in equation (19) is fulfilled and finally ends up with \(C_1C_2C_3\). Then, complementary states are immediately found as \(OC_x\) for \(x = 1, 2, 3\), from which optimal measurement also follows as those POVM elements orthogonal to complementary states.

4.3. Four states

We now consider discrimination among four qubit states. We begin with a simple case: pairs of orthogonal states. Then, cases where four states define a quadrilateral are considered. Finally, we also show how the geometric formulation can be applied when four states form a tetrahedron in the Bloch sphere.

4.3.1. Four-state example I: rectangles. Let us first consider pairs of orthogonal states, say \(\frac{1}{4}, \rho_x = |\psi_x\rangle\langle \psi_x|\) for \(x = 1, 2, 3, 4\). The four states define a plane in the Bloch sphere and then form a rectangle on the plane. To be explicit, they can be written as follows, for some \(\theta_0\) and \(\theta\):

\[
|\psi_1\rangle = \cos \frac{\theta_0}{2} |0\rangle + \sin \frac{\theta_0}{2} |1\rangle,
\]

\[
|\psi_2\rangle = \cos \left(\frac{\theta_0}{2} - \theta\right) |0\rangle + \sin \left(\frac{\theta_0}{2} - \theta\right) |1\rangle,
\]

\[
|\psi_3\rangle = \cos \left(\frac{\theta_0}{2} - \frac{\pi}{2}\right) |0\rangle + \sin \left(\frac{\theta_0}{2} - \frac{\pi}{2}\right) |1\rangle,
\]

\[
|\psi_4\rangle = \cos \left(\frac{\theta_0}{2} - \theta - \frac{\pi}{2}\right) |0\rangle + \sin \left(\frac{\theta_0}{2} - \theta - \frac{\pi}{2}\right) |1\rangle.
\]

which are shown in figure 5. The half-plane in which the four states lie is then defined in the Bloch sphere.

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Figure 5. Discrimination of pairs of two orthogonal states, \( \{1/4, \rho_x = |\psi_x\rangle\langle\psi_x|\}_{x=1}^4 \) (see also equation (36)), is shown. Each state \( \rho_x/4 \) corresponds to \( OX_x \) for \( x = 1, 2, 3, 4 \). Complementary states can be found easily by enlarging and inverting the given polytope \( X_1X_2X_3X_4 \) so that the optimality condition in equation (26) is fulfilled. Then, the complementary states form the rectangle \( C_1C_2C_3C_4 \), from which optimal measurement can also be found as, \( \{M_x \propto OM_x\}_{x=1}^4 \), see equation (37). The ratio between two rectangles is \( 1/4 \), thus the guessing probability \( 1/2 \).

Referring to figure 5, we apply the geometric formulation in lemma 4.3 and show the optimal parameters, optimal measurement and complementary states. The polytope of given states is the rectangle \( X_1X_2X_3X_4 \). It is straightforward to see that the largest one similar to \( X_1X_2X_3X_4 \) is the rectangle having its diagonal in length 2 (in terms of trace-norm). Then, we rotate it so that the relation in equation (19), or the optimality condition in equation (8), is satisfied; then we have the rectangle \( C_1C_2C_3C_4 \). The complementary states are found as \( OC_x \) for \( x = 1, 2, 3, 4 \), from which optimal POVM elements are also obtained \( \{M_x \propto OM_x\}_{x=1}^4 \). Therefore, we have optimal parameters as follows:

\[
M_1 = \sigma_3 = |\psi_1\rangle\langle\psi_1|, \quad M_2 = \sigma_4 = |\psi_2\rangle\langle\psi_2|, \\
M_3 = \sigma_1 = |\psi_3\rangle\langle\psi_3|, \quad M_4 = \sigma_2 = |\psi_4\rangle\langle\psi_4|.
\]

From these, the guessing probability can be obtained. Or, applying lemma 4.2, one can see the ratio, for instance,

\[
r = \frac{X_1X_2}{C_1C_2} = \frac{OX_1}{OC_1} = \frac{1}{4} \quad \text{and thus} \quad P_{\text{guess}} = \frac{1}{4} + r = \frac{1}{2}.
\]

We remark that, as it is shown in the above, the guessing probability is equal in the range of angle \( 0 \leq \theta \leq \pi/2 \).

The analysis shown in the above implies that the guessing probability does not depend on detailed relations among given quantum states but on a property assigned by the set of them. This shows the freedom of choosing four states such that the guessing capability about states
Figure 6. Arbitrary four states lying on a half-plane of the Bloch sphere are
given, denoted by \( \{ q_x = 1/4, \rho_x \}_{x=1}^4 \). Each state \( \rho_x/4 \) corresponds to \( OX_x \) where \( x = 1, 2, 3, 4 \). Applying lemma 4.3, the aim is to find a rectangle which
is maximal in the Bloch sphere and similar to the given one \( X_1X_2X_3X_4 \).
Then, the maximal rectangle is rotated such that the optimality condition in
equation (26) is satisfied, which then results in \( C_1C_2C_3C_4 \). Thus, complementary
states are found in \( OC_x \) for \( x = 1, 2, 3, 4 \). Note that vertices of \( C_1C_2C_3C_4 \)
may not lie on the surface of the Bloch sphere. For such vertices, optimal
POVM elements are the null measurement. Optimal measurement follows
straightforwardly as \( \{ M_x \propto OM_x \}_{x=1}^4 \).

does not change. More precisely, this can be seen in terms of the symmetry operator, which in
this case is
\[
K = \frac{1}{4} \rho_x + r \sigma_x = \frac{1}{2} I
\]
(39)
consistently to equation (38). That is, all sets of four states of pairs of orthogonal states share
the same the symmetry operator in equation (39), meaning that all of them are in the same
equivalence class, see definition 3.1.

Remark 4.2. Four states of any two pairs of orthogonal qubit states are in the same equivalence
class, \( A_{1/2} \).

4.3.2. Four-state example II: quadrilateral. Next, let us consider arbitrary four qubit states
defined on a half-plane, which are given with the equal probabilities \( 1/4 \). For generality, we
do not assume any internal symmetry among given states \( \{ 1/4, \rho_x \}_{x=1}^4 \) except the assumption
that they are on a half-plane in the Bloch sphere. It is then straightforward to generalize this to
arbitrary four states defined on any plane in the sphere.

We now refer to figure 6 to show how the geometric formulation in lemma 4.3 can be
applied to those four states. The polytope of four states is shown as the quadrilateral \( X_1X_2X_3X_4 \)
where each vertex corresponds to \( \rho_x/4 \) for \( x = 1, 2, 3, 4 \). Then, one has to expand the given
quadrilateral so that they are maximal in the Bloch sphere. In this way, the ratio between two
quadrilaterals can be found.
Figure 7. It is shown that the four given states $OX_x$ ($x = 1, 2, 3, 4$) form a tetrahedron $X_1X_2X_3X_4$ in the Bloch sphere. They are given with prior probabilities $1/4$; it is not assumed that they are equally spaced from one another in the sphere. Applying lemma 4.3, one first expands the given tetrahedron until it is maximal in the Bloch sphere; one then rotates the maximal one such that the optimality condition in equation (26) is fulfilled. The resulting tetrahedron $C_1C_2C_3C_4$ defines the polytope of complementary states, from which it is clear that the optimal POVM elements are $\{M_x = OM_x\}_{x=1}^4$ such that $OM_x = -OC_x$.

To find complementary states, one has to rotate the obtained maximal quadrilateral so that the optimality condition in equation (19) is fulfilled. The resulting quadrilateral from which complementary states can be found is then, $C_1C_2C_3C_4$, where $OC_x$ for $x = 1, 2, 3, 4$ are complementary states. It can happen that, since a given quadrilateral $X_1X_2X_3X_4$ is arbitrarily shaped, some vertices may not be on the surface of the Bloch sphere. As is depicted in figure 6, suppose that $OC_1$ cannot lie at the surface of the sphere. This means that complementary state $\sigma_1$ is not pure; thus the POVM element for state $\rho_1$ corresponds to the null measurement, $M_1 = 0$. This follows from the optimality condition in lemma 4.2 to fulfill equation (9). The optimal discrimination strategy for these states is thus to prepare measurement such that there are three kinds of outcomes from $M_x$ with $x = 2, 3, 4$. Note also that, as the convex hull of the POVM elements $M_1M_2M_3$ contains the origin, one can also construct a complement measurement.

4.3.3. Four-state example III: tetrahedron. We now consider four qubit states $\{\rho_x\}_{x=1}^4$ which form a polytope having a volume in the Bloch sphere, see figure 7. Suppose that they are given with probability $1/4$ for each and for convenience we assume that the tetrahedron constructed by four states is covered by a sphere. Later, this can be relaxed and generalized to cases where all vertices of the tetrahedron are not touched by a sphere. Here, since the tetrahedron is covered by a sphere, the four states have the same purity, which we denote by $f$.

Referring to figure 7, let us show how to find the guessing probability, complementary states and optimal measurement. The guessing probability immediately follows by applying lemma 4.3. The ratio $r$ can be computed by finding the ratio of two diameters of two spheres: one
is the sphere covering the given tetrahedron and the other the Bloch sphere covering a maximal tetrahedron similar to the given one. As the purity is given by $f$, the guessing probability is given by

$$P_{\text{guess}} = \frac{1}{4} + \frac{1}{4}f,$$

which does not depend on detailed relations among given states, such as angles between given states. The above holds true for any four states whose tetrahedron in the Bloch sphere can be covered by a single sphere.

Then, one rotates the maximal tetrahedron within the Bloch sphere such that the resulting one satisfies the optimality condition in equation (19). Since the tetrahedron already fully occupies the Bloch sphere, it is not difficult to see that the resulting tetrahedron has the reflection symmetry to the given tetrahedron, with respect to the origin of the Bloch sphere, see figure 7. Each vertex $OC_x$ for $x = 1, 2, 3, 4$ corresponds to complementary states; optimal POVM elements are found to be those rank-one operators orthogonal to complementary states.

4.4. Etc

So far, we have considered discrimination of two, three and four qubit states. In this way, for any number of qubit states given, one can apply the geometric formulation and then find the guessing probability, complementary states and optimal measurement. The framework can be summarized as follows. The first stage is to construct a polytope of given states; then one has to search for the polytope of complementary states such that the optimality condition in equation (19), or equivalently equation (8), is fulfilled. The two resulting polytopes must be congruent and the corresponding labeled lines from the respective polytopes are anti-parallel. For cases when measurement is applied, its POVM element is of rank-one and also corresponding complementary states must be of rank-one, that is, pure states. If it is found that complementary states are not of rank-one, then their POVM elements are the null operator and thus the optimal strategy for those states is to apply no-measurement. For implementation in the experiment, this means that no output port is needed for those states.

As we have also shown, there is a further simplification in optimal discrimination when the polytope of quantum states given with equal prior probabilities is tightly covered by a sphere, such that all vertices of the polytope touch the sphere. Then, the guessing probability simply follows from the ratio between diameters of two spheres, one from the sphere covering a given polytope and the other the Bloch sphere. In this case, it is explicitly shown that the guessing probability does not depend on detailed relations of given states, such as the angles between any two given states.

**Remark 4.3.** For $N$ qubit states given with equal prior probabilities $1/N$, if their polytope in the Bloch sphere is covered by a smaller sphere of radius $r$ such that each vertex touches the sphere and contains the origin of the Bloch sphere, the guessing probability for those states is given by $P_{\text{guess}} = 1/N + r$ independently to detailed relations among given states.

For high-dimensional quantum systems, a general geometric expression is lacking and therefore the geometric formation shown in section 2.3 cannot be further applied in general. Once given states give an underlying geometry in which the convex polytope picture is clear, one can apply and formalize the method of geometric formulation.
In this paper, we have considered the problem of ME state discrimination and have shown the general structure of the problem. The main idea of the development is to view the problem from various approaches. Finally, it turns out that the general structure can be summarized in the formulation of the so-called complementarity problem that generalizes convex optimization. The key element in the structure is a single positive operator, called the symmetry operator, which gives the complete characterization of optimal discrimination. Then, one can exploit the symmetry operator to find the optimal parameters in the ME discrimination, such as the guessing probability, complementary states and optimal measurement. The symmetry operator also allows an interpretation of the guessing probability as the averaged distance of given states being deviated from the symmetry operator in terms of the trace norm. The interpretation is in accordance with cases when classical systems are employed, where the guessing probability is interpreted as the deviation from the uniform distribution.

It is shown that in ME discrimination of quantum states, the symmetry operator is uniquely determined whereas optimal measurement is not. This means, rather than optimal measurement, a symmetry operator can characterize the ME discrimination. Symmetry operators are therefore exploited to define equivalence classes among sets of quantum states, such that for those sets in the same class, ME discrimination is completely characterized by an identical symmetry operator. This provides an alternative approach to ME discrimination: by checking whether two given sets are in the same class, one can find the optimal discrimination. Conversely, given a symmetry operator, we have shown how one can construct a set of quantum states for which the ME discrimination is characterized by the operator.

From general structures found from the optimality conditions, we have provided a geometric formulation of ME state discrimination. In the formulation, the geometry of quantum states is exploited to find the guessing probability, instead of optimization over measurement. More precisely, the polytope of given states in the state space is linked to the guessing probability, without directly referring to measurement operators via the measurement postulate. It is clear that the method can be applied once the underlying geometry of given states is well-defined. Conversely, we have also argued that, from cases where the optimal discrimination is known, the guessing probability is useful to find the underlying geometry of high-dimensional quantum states. We have applied the geometric formulation to qubit states and solved ME discrimination: (i) the complete solution is provided for any set of qubit states when prior probabilities are equal, (ii) this gives an upper bound to cases when prior probabilities are not equal, (iii) solutions are obtained even if given states do not contain any symmetry among them, (iv) it is shown that the guessing probability does not depend on detailed relations among given states but a geometric property assigned by the set itself. The conclusion (iv) is along the conclusion in [31] that distinguishability within an ensemble of quantum states is assigned as a global property that cannot be reduced to properties of pairs of states. We arrive here at the conclusion by quantifying the distinguishability with the guessing probability, while it is with von Neumann entropy in [31].

Discrimination of quantum states poses a simple question connected to the fundamental and profound limitations in various contexts of quantum information theory. The results presented here not only provide a useful method of solving optimal discrimination, but also give a general, unique and fresh understanding to ME quantum state discrimination.
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