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RESEARCH ARTICLE

Decision problems with quantum black boxes

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(September 22, 2011)

We examine how to distinguish between unitary operators, when the exact form of the possible operators is not known. Instead we are supplied with “programs” in the form of unitary transforms, which can be used as references for identifying the unknown unitary transform. All unitary transforms should be used as few times as possible. This situation is analogous to programmable state discrimination. One difference, however, is that the quantum state to which we apply the unitary transforms may be entangled, leading to a richer variety of possible strategies. By suitable selection of an input state and generalized measurement of the output state, both unambiguous and minimum-error discrimination can be achieved. Pairwise comparison of operators, comparing each transform to be identified with a program transform, is often a useful strategy. There are, however, situations in which more complicated strategies perform better. This is the case especially when the number of allowed applications of program operations is different from the number of the transforms to be identified.

Keywords: unambiguous discrimination; optimum discrimination; operator comparison; generalized measurements

1. Introduction

The problem of discriminating between operators in quantum mechanics is closely related to that of discriminating between quantum states (1). In order to distinguish between operators, a reference state is transformed by the different operators, and then measurements are performed on the result, so that one is ultimately distinguishing between the possible output states. Discriminating between two \textit{known} operators has already been treated (2–6). Reconstructing a single unknown operator from measurements on a series of states that have been transformed by it is known as operator, channel, or quantum process tomography (7). A final problem, operator comparison, which determines whether two unknown unitary operators are the same or different (8, 9), is closely related to the problems considered here.

Recently state discrimination problems have been considered in which not all of the states are known (10–13). One may know some of the states, but is only provided with examples of the others. For example, one is given a particle that is guaranteed to be in one of the states $|\psi_1\rangle$ or $|\psi_2\rangle$. The states $|\psi_1\rangle$ and $|\psi_2\rangle$ are unknown, but instead, an example of each of these states is provided. The object is to use the reference states to best determine whether the given particle in the

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unknown state is either $|\psi_1\rangle$ or $|\psi_2\rangle$. Another scenario is that $|\psi_1\rangle$ is known, but $|\psi_2\rangle$ is represented by a reference particle, and one is presented with a particle guaranteed to be in either $|\psi_1\rangle$ or $|\psi_2\rangle$. Again the task is to determine the state of the latter unknown particle.

In this paper we address problems in the realm of operator discrimination, which are the natural analogues of those described above, for quantum state discrimination. Instead of having a physical description of the operations, they are given as actual operations (boxes) which we are allowed to apply to input states. The situation is reminiscent of oracle quantum computation (14), in which a key component is a device that carries out one of a number of possible transformations. Generally, we would like to decide which particular unlabelled boxes match/correspond to labelled reference boxes or in which order the unlabelled boxes are placed. The problem can be viewed as programmable pattern matching, “programmable” because we do not know the actual operations as they are only supplied as reference “programs”.

We shall consider both minimum error, and unambiguous discrimination tasks. In minimum-error discrimination, the object is to always make a guess and to minimize the probability of making a mistake. In unambiguous discrimination, the procedure is allowed to fail sometimes (that is, we are allowed sometimes to refuse to make a guess) but we never want to make a mistake if we do decide to make a determination. The object is to minimize the probability of failure.

We wish to examine whether good procedures for these decision problems can be constructed from pairwise operator comparison. The task is to compare two unknown operators in order to determine whether or not they are the same. This problem was considered in (8), and the best procedure found there was to use a singlet state (8). Each operator is applied to one of the two qubits in the singlet and the result is then measured to see if it has a component in the symmetric subspace, upon which the operators must have been different. We would like to see if this procedure can be used as a basic unit for more complicated operator comparisons as discussed above. We shall see that there are cases where singlet-based pairwise comparison strategies are not optimal.

2. Pattern matching for unitary operators

The general scenario which we consider is as follows: Alice/Bob are given reference boxes, labelled either $U$ or $V$, which implement unitary operations on single qubits. The forms of these two unitary operators are not known to any of the parties. Charlie is given a number of boxes which are unlabelled, but each is guaranteed to perform either $U$ or $V$. Our task is to determine what boxes Charlie possesses by applying these boxes to a multi-qubit reference state and then measuring the results. We shall assume that each box can only be applied once and that $U$ and $V$ are equally and independently likely to be any qubit unitary. A variety of scenarios is possible, depending on which boxes are available for Alice, Bob and Charlie.

2.1. One reference box and one unlabelled box

We begin with the simplest case of one reference box and one unlabelled box which may of may not match the reference (Fig. 1a). Alice has a box that performs an unknown operation $U$ and Charlie has one that either performs $U$ or an unknown operator $V$. This is similar to operator comparison (8) where it was found that making use of the two-qubit singlet state, $|\psi^-\rangle_{AB} = (|0\rangle_A|1\rangle_B - |0\rangle_A|1\rangle_B)/\sqrt{2}$, by
Figure 1. One unlabelled box. a) Alice has a reference box $U$, and Charlie has an unlabelled box which either performs $U$ or a different unknown unitary $V$. b) Alice and Bob each have a different reference box implementing $U$ and $V$ respectively, and Charlie either has a box which performs $U$ or $V$. We prepare a test state $|\Psi\rangle$ which is acted upon by the operators and is finally measured leading to an outcome $\Pi_j$.

Sending one qubit through each box is a good strategy. After the qubits have been acted upon by the boxes, we measure the result to see if it lies in the symmetric or antisymmetric subspace. If the state is found to be symmetric, then the two unitary transforms must have been different.

This is in fact the optimal strategy also for the situation we are now considering, if we confine ourselves to two qubits and demand an unambiguous result. We have to apply both transforms to a test state $|\Psi\rangle$, giving two possible cases

$$|\Psi_1\rangle_{AC} = U \otimes U |\Psi\rangle_{AC} \quad \text{and} \quad |\Psi_2\rangle_{AC} = U \otimes V |\Psi\rangle_{AC}. \quad (1)$$

The forms of the single-qubit operators, $U$ and $V$, are unknown, and so we must average over $U$ and $V$ to obtain the possible output states

$$\rho_1 = \int du |\Psi_1\rangle_{AC} \langle \Psi_1| \quad \text{and} \quad \rho_2 = \int dv |\Psi_2\rangle_{AC} \langle \Psi_2|, \quad (2)$$

between which we should distinguish. The integrals are Haar integrals over $SU(2)$, and can be performed using the following parameterization. We first set $U = \exp(-i\theta \hat{e} \cdot \vec{\sigma}/2)$, where $\hat{e}$ is a unit vector equal to $(\sin \mu \cos \phi, \sin \mu \sin \phi, \cos \mu)$, with $0 \leq \theta \leq 2\pi$, $0 \leq \phi \leq 2\pi$, and $0 \leq \mu \leq \pi$, and $\vec{\sigma} = \{\sigma_x, \sigma_y, \sigma_z\}$ is a vector of the usual Pauli matrices. The second operator, $V$, is parametrized similarly. We then have that

$$du = \frac{1}{4\pi^2} \sin^2 \left(\frac{\theta}{2}\right) \sin \mu d\theta d\phi d\mu. \quad (3)$$

A general 2-qubit test state can be written

$$|\Psi\rangle_{AC} = a|\psi^-\rangle + b|\psi^+\rangle + c|\phi^-\rangle + d|\phi^+\rangle, \quad (4)$$

where $|\psi^\pm\rangle = (|01\rangle \pm |10\rangle)/\sqrt{2}$ and $|\phi^\pm\rangle = (|00\rangle \pm |11\rangle)/\sqrt{2}$ are the usual Bell states, and $|a|^2 + |b|^2 + |c|^2 + |d|^2 = 1$. Performing the integrals for this initial test state, we find that

$$\rho_1 = |a|^2 P^a + \frac{1}{3}(|b|^2 + |c|^2 + |d|^2) P^a$$

$$\rho_2 = \frac{1}{4} I_A \otimes I_C. \quad (5)$$
Here $P^a$ and $P^s$ are the projectors onto the antisymmetric and symmetric subspaces respectively. As the support of $\rho_2$ is all of the two-qubit space, $\rho_1$ can never be unambiguously identified, as its support will always be contained in that of $\rho_2$. To unambiguously identify the state $\rho_2$, the initial test state should lie entirely either in the antisymmetric or in the symmetric subspace, and we look for a component of the final state in the symmetric or antisymmetric subspace, respectively.

It is straightforward to check that starting with a singlet state by choosing $|a|^2 = 1$ will give a higher success probability than starting in the symmetric subspace. The positive operator valued measure (POVM) elements for the optimal measurement are the projections $\Pi_0 = P^a$, corresponding to the inconclusive result (failure), and $\Pi_2 = P^s$, corresponding to identifying the state as $\rho_2$. Therefore, assuming that $\rho_1$ and $\rho_2$ are equally probable, the probability of the measurement failing is

$$p_f = \frac{1}{2} [\text{Tr}(\Pi_0 \rho_1) + \text{Tr}(\Pi_0 \rho_2)] = \frac{5}{8},$$

so that the success probability is $p_s = 3/8$. An initial test state in the symmetric subspace would give a success probability of $p_s = 1/8$.

Now let us consider the minimum-error strategy. The optimal minimum-error measurement for distinguishing between two states $\rho_1$ and $\rho_2$, with prior probabilities $p_1$ and $p_2$, has the error probability ($15$)

$$p_e = \frac{1}{2} \left[ 1 - \text{Tr} \sqrt{(p_1 \rho_1 - p_2 \rho_2)^2} \right],$$

where we shall consider the case $p_1 = p_2 = 1/2$. Substituting in the density matrices from Eq. (5), we find that

$$\text{Tr} \sqrt{(\rho_1 - \rho_2)^2} = 2 \left| \frac{1}{4} - |a|^2 \right|. \quad (8)$$

This is clearly maximized, and the error probability minimized, when $|a|^2 = 1$, which occurs when the input state is a singlet. In that case we have that $\Pi_1 = P^a$ corresponds to Bob’s box being $U$, and $\Pi_2 = P^s$ corresponds to Bob’s box being $V$, and the probability of error is 1/8. For the singlet test state, this is the optimal measurement, as the optimal minimum-error measurement.

Note that the unambiguous discrimination strategy only gives us an answer when Charlie’s unknown box is $V$. If Alice instead has a reference box $V$, we can get an answer only when Bob’s box is $U$. The measurement and success probability stays the same.

2.2. Two reference boxes and one unlabelled box

Let us now consider a decision problem where Alice has a reference box $U$, Bob has reference box $V$, and Charlie has an unlabelled box guaranteed to be either $U$ or $V$ (Fig. 1b). First let us look at a three-qubit test state $|\Psi\rangle_{ABC}$ and apply the boxes held by Alice, Bob and Charlie to their respective qubits. A general pure three-qubit state can be written as

$$|\Psi\rangle_{ABC} = a_0|000\rangle + a_1|001\rangle + \ldots + a_7|111\rangle,$$  \quad (9)
with $\sum |a_i|^2 = 1$. This means that we are trying to discriminate between the states

\[
|\Psi_1\rangle_{ABC} = U \otimes V \otimes U|\Psi\rangle_{ABC} \\
|\Psi_2\rangle_{ABC} = U \otimes V \otimes V|\Psi\rangle_{ABC}.
\]

Averaging over $U$ and $V$ means that we have to distinguish between the states

\[
\rho_1 = \int dudvU \otimes V \otimes U|\Psi\rangle_{ABC}\langle U| \otimes V \otimes U^\dagger \\
\rho_2 = \int dudvU \otimes V \otimes V|\Psi\rangle_{ABC}\langle U| \otimes V \otimes V^\dagger.
\]

Again using the results in Appendix A, we get

\[
\rho_1 = \frac{1}{4} P_{AC}^a \otimes I_B (|a_1 - a_4|^2 + |a_3 - a_6|^2) \\
+ \frac{1}{6} P_{AC}^a \otimes I_B (|a_0|^2 + |a_2|^2 + |a_1 + a_4|^2 + |a_3 + a_6|^2 + |a_5|^2 + |a_7|^2) \\
\rho_2 = \frac{1}{4} P_{BC}^a \otimes I_A (|a_1 - a_2|^2 + |a_5 - a_6|^2) \\
+ \frac{1}{6} P_{BC}^a \otimes I_A (|a_0|^2 + |a_3|^2 + |a_1 + a_2|^2 + |a_5 + a_6|^2 + |a_4|^2 + |a_7|^2).
\]

For unambiguous discrimination to be possible, the support of either $\rho_1$ or $\rho_2$ or both has to be less than all of the three-qubit space. Without loss of generality, let us assume that $\rho_1$ has support in either $P_{AC}^a \otimes I_B$ or $P_{AC}^a \otimes I_B$, but not in both. The first possibility clearly corresponds to a test state which is a singlet in qubits $A$ and $C$, tensored with any state for qubit $B$. This strategy has an overall success probability of $3/8$. The optimal measurement tests whether or not we have a singlet in qubits $A$ and $C$, and if not, this unambiguously identifies the state as $\rho_2$. We could also start with a singlet state in qubits $B$ and $C$, and test whether we still have a singlet in these qubits after application of the unitary transforms.

The other possibility is that $\rho_1$ has support in the space symmetric in qubits $A$ and $C$. In this case $\rho_2$ either has support in all of Hilbert space, or only in the space symmetric in qubits $B$ and $C$. The latter alternative gives a higher success probability, as we then have a nonzero probability to unambiguously identify both $\rho_1$ and $\rho_2$. We then have

\[
\rho_1 = \frac{1}{6} P_{AC}^a \otimes I_B \quad \text{and} \quad \rho_2 = \frac{1}{6} P_{BC}^a \otimes I_A.
\]

The POVM that unambiguously discriminates between these two density matrices must have the element that detects $\rho_1$ be proportional to $P_{BC}^a \otimes I_A$, because the only vectors orthogonal to $\rho_2$ are of the form $|\psi^-\rangle_{BC} \otimes |\eta\rangle_A$, where $|\eta\rangle_A$ is an arbitrary state in the space of qubit $A$, and by symmetry, this POVM element should treat all vectors in the space of qubit $A$ equally. Similar considerations apply to the element that detects $\rho_2$. The only remaining task is to determine the constant of proportionality that is allowed by the requirement that the third POVM element, which correspond to the failure of the measurement, be positive. Doing so, we find
that the optimal measurement in this case has measurement operators \((10, 13)\)

\[
\begin{align*}
\Pi_1 &= \frac{2}{3} P_{BC} \otimes I_A \\
\Pi_2 &= \frac{2}{3} P_{AC} \otimes I_B \\
\Pi_? &= I - \Pi_1 - \Pi_2,
\end{align*}
\]

and the overall success probability is \(1/6\). This is higher than \(1/8\), which is the result if we choose to randomly test for a singlet either in qubits \(AC\) or qubits \(BC\). But it is still much lower than \(3/8\), which we achieve if we start with a singlet state either in qubits \(AC\) or qubits \(BC\).

For the minimum-error task, we can also try to use a state that approximates a singlet state in qubits \(AC\) and \(BC\) as well as possible, without obeying the strict symmetry rules necessary for the unambiguous discrimination strategy. The state

\[
|\Psi\rangle_{ABC} = \frac{1}{2\sqrt{3}} (|100\rangle + |010\rangle + |111\rangle + |101\rangle) - \frac{1}{\sqrt{3}} (|001\rangle + |110\rangle)
\]

has the property that its reduced density operators \(\rho_{AC}\) and \(\rho_{BC}\) have overlap with the singlet state

\[
\langle \psi^- | \rho_{AC} | \psi^- \rangle = \langle \psi^- | \rho_{BC} | \psi^- \rangle = 3/4
\]

where \(|\psi^-\rangle\) is a singlet. It is straightforward to prove that the fidelity of \(3/4\) is the best possible if one demands that the fidelities in qubit pairs \(AC\) and \(BC\) should be equal. After Alice, Bob, and Charlie have applied their boxes to obtain (10) and (11), and then averaging over \(U\) and \(V\), the two possible output states are

\[
\rho_1 = \left( \frac{3}{8} P_{AC}^a + \frac{1}{24} P_{AC}^s \right) \otimes I_B, \quad \rho_2 = \left( \frac{3}{8} P_{BC}^a + \frac{1}{24} P_{BC}^s \right) \otimes I_A,
\]

which then have to be distinguished. The optimum minimum error (Helstrom) strategy for distinguishing between two density operators \(\rho_1\) and \(\rho_2\) has the error probability

\[
P_e = \frac{1}{2} \left\{ 1 - \text{Tr} \left[ (p_1 \rho_1 - p_2 \rho_2)^2 \right] \right\}^{1/2} = \frac{1}{2} \left( 1 - \sum |\lambda_i| \right),
\]

where \(\lambda_i\) are the eigenvalues of \(p_1 \rho_1 - p_2 \rho_2\). In our case \(p_1 = p_2 = 1/2\), and

\[
p_1 \rho_1 - p_2 \rho_2 = \frac{1}{2} \left[ \left( \frac{3}{8} P_{AC}^a + \frac{1}{24} P_{AC}^s \right) \otimes I_B - \left( \frac{3}{8} P_{BC}^a + \frac{1}{24} P_{BC}^s \right) \otimes I_A \right]
\]

\[
= \frac{1}{2} \left[ \left( \frac{1}{3} P_{AC}^a + \frac{1}{24} I_{AC} \right) \otimes I_B - \left( \frac{1}{3} P_{BC}^a + \frac{1}{24} I_{BC} \right) \otimes I_A \right]
\]

\[
= \frac{1}{6} \left[ P_{AC}^a \otimes I_B - P_{BC}^a \otimes I_A \right]
\]

\[
= \frac{1}{12} \left( |100\rangle\langle 100| + |011\rangle\langle 011| - |010\rangle\langle 010| - |101\rangle\langle 101| - |001\rangle\langle 001| + |110\rangle\langle 110| + |110\rangle\langle 110| + h.c. \right).
\]
This operator is six-dimensional, but happens to be block diagonal with two blocks of size $3 \times 3$. This is easily seen since the off-diagonal elements only couple states with an equal number of 0’s and 1’s. Ordering the basis vectors within the blocks \{$|010\rangle, |100\rangle, |001\rangle$\} and \{$|101\rangle, |011\rangle, |110\rangle$\}, each of the blocks takes the form

$$\frac{1}{12} \begin{pmatrix} -1 & 0 & 1 \\ 0 & 1 & -1 \\ 1 & -1 & 0 \end{pmatrix}.$$ 

The blocks have eigenvalues $\pm 1/(4\sqrt{3})$ and zero, and the sum of the absolute values of all eigenvalues is therefore $1/\sqrt{3}$. This gives an error probability of $P_e = (1 - 1/\sqrt{3})/2 \approx 0.211325$ which is higher than $1/8$. Therefore, the simple singlet strategy (a singlet either in pair $AB$ or $AC$) does better.

### 2.2.1. Doing better than pairwise operator comparison

So far, the best strategies we have found are based on pairwise operator comparison. Can we do better? It turns out that if we use a four-qubit state then we can. In particular, we shall show that it is possible to improve the success probabilities for unambiguous discrimination. We first note that we can get distinct signals for both operators in the case of unambiguous discrimination if we use four qubits. Let

$$|\Psi\rangle_{ABCD} = \frac{1}{\sqrt{2}}(|\psi^-\rangle_{AC}|0\rangle_B|0\rangle_D + |\psi^-\rangle_{BC}|0\rangle_A|1\rangle_D).$$ (16)

As usual, Alice, Bob and Charlie apply their respective boxes but no operation is applied to the fourth qubit $D$. It is best to express the resulting states as density matrices. If Charlie’s box performs $U$, the operator $U \otimes V \otimes U \otimes I$ is applied to $|\Psi\rangle_{ABCD}$, and after averaging over both $U$ and $V$ we obtain

$$\rho_1 = \frac{1}{4} P_{AC}^s \otimes I_B \otimes \left(|0\rangle_D + \frac{1}{2}|1\rangle_D\right) \left(D\langle 0| + \frac{1}{2} D\langle 1|\right)$$

$$+ \frac{1}{16} P_{AC}^s \otimes I_B \otimes |1\rangle_D|1|.$$ (17)

If Charlie’s box performs $V$, the operator $U \otimes V \otimes V \otimes I$ is applied to $|\Psi\rangle_{ABCD}$, and after averaging over both $U$ and $V$ we obtain

$$\rho_2 = \frac{1}{4} P_{BC}^s \otimes I_A \otimes \left(|1\rangle_D + \frac{1}{2}|0\rangle_D\right) \left(D\langle 1| + \frac{1}{2} D\langle 0|\right)$$

$$+ \frac{1}{16} P_{BC}^s \otimes I_A \otimes |0\rangle_D|0|.$$ (18)

We will consider only the case of unambiguous discrimination and first choose the POVM elements to be

$$\Pi_1 = P_{BC}^s \otimes I_A \otimes |1\rangle_D|1|$$

$$\Pi_2 = P_{AC}^s \otimes I_B \otimes |0\rangle_D|0|$$

$$\Pi_0 = I - \Pi_1 - \Pi_2 = P_{BC}^s \otimes I_A \otimes |1\rangle_D|1| + P_{AC}^s \otimes I_B \otimes |0\rangle_D|0|.$$ (19)

The element $\Pi_1$ corresponds to Charlie’s box being $U$, $\Pi_2$ corresponds to it being $V$, and $\Pi_0$ corresponds to the indeterminate result. We find that $\text{Tr}(\Pi_1 \rho_2) =$
This page continues the discussion of the discrimination of density matrices using a four-qubit test state. The authors start by considering the case of two references and two unlabelled boxes (Fig. 2). They introduce a strategy using four-qubits in the form of two singlet states, \(|\Psi^{\pm}_{ABC_1C_2}\rangle = |\psi^{\pm}_{AC_1}\rangle |\psi^{\pm}_{BC_2}\rangle\) and \(|\Psi^{\pm}_{ABC_1C_2}\rangle\), which allows for the discrimination of the ranges of the two possible density matrices with a success probability of \(\frac{3}{8}\). This success probability is greater than that of the simpler two-qubit procedure, but the authors note that this does not guarantee an unambiguous identification of both boxes.

The authors then discuss the case of two reference boxes and two unlabelled boxes, which they divide into two subcases: two reference boxes and two of the same unlabelled box. In the first subcase, where Charlie has identical boxes, the authors propose using four-qubits as mentioned above to discriminate the density matrices. In the second subcase, where Charlie has different unlabelled boxes, they consider the order in which the reference boxes and the unlabelled boxes appear. The authors conclude that there are better procedures than simple pairwise operator comparison for solving their three-box decision problem.
apply the boxes. If both boxes $C_1$ and $C_2$ are $V$, then the output state is

$$|\Psi_1\rangle_{ABC_1C_2} = (U \otimes V)|\psi^-\rangle_{AC_1} (V \otimes V)|\psi^-\rangle_{BC_2},$$

and if both $C_1$ and $C_2$ are $U$, then we have

$$|\Psi_2\rangle_{ABC_1C_2} = (U \otimes U)|\psi^-\rangle_{AC_1} (V \otimes U)|\psi^-\rangle_{BC_2}. \quad (21)$$

If we now average over both $U$ and $V$, we obtain the possible output density operators

$$\rho_1 = \frac{1}{4} I_{AC_1} \otimes P_{BC_2}^a \quad \rho_2 = \frac{1}{4} P_{AC_1}^a \otimes I_{BC_2}, \quad (22)$$

between which we must distinguish.

Let us first consider unambiguous discrimination. The best POVM elements are

$$\Pi_1 = P_{AC_1}^s \otimes P_{BC_2}^a \quad \Pi_2 = P_{AC_1}^a \otimes P_{BC_2}^s \quad \Pi_0 = P_{AC_1}^s \otimes P_{BC_2}^a + P_{AC_1}^a \otimes P_{BC_2}^s, \quad (23)$$

where $\Pi_0$ is associated with the failure outcome. We find that, as is necessary, $\text{Tr}(\Pi_1 \rho_2) = \text{Tr}(\Pi_2 \rho_1) = 0$, and that $\text{Tr}(\Pi_1 \rho_1) = \text{Tr}(\Pi_2 \rho_2) = 3/4$. With both situations being equally likely, our overall success probability is then $3/4$.

For minimum-error discrimination, we always need a result; the measurement is not allowed to fail. This means that we have to do something with the operators appearing in $\Pi_0$. We first note that the outcome corresponding to $P_{AC_1}^s \otimes P_{BC_2}^a$ never occurs, so it can be added to either $\Pi_1$ or $\Pi_2$ without any effect. The outcome corresponding to $P_{AC_1}^a \otimes P_{BC_2}^a$ can occur, and for either density matrix does so with a probability $1/4$. When it does, we have no idea which density matrix we have, so we have to guess. One way of guessing is that we can always guess $\rho_2$, and we shall be wrong half the time. This corresponds to adding $P_{AC_1}^a \otimes P_{BC_2}^{(2)}$ to $\Pi_2$. (For equal prior probabilities of $\rho_1$ and $\rho_2$, it does not matter how we guess, but if the probabilities are unequal, we should always guess the more likely one.) Therefore, for minimum-error discrimination we can choose for our POVM operators

$$\Pi_1 = P_{AC_1}^s \otimes P_{BC_2}^a + P_{AC_1}^a \otimes P_{BC_2}^s \quad \Pi_2 = P_{AC_1}^a \otimes P_{BC_2}^a + P_{AC_1}^s \otimes P_{BC_2}^s, \quad (24)$$

and the probability of error will be $1/8$.

### 3.2. Two reference boxes and two different unlabelled boxes

We now turn our attention to a variant of our decision problem in which the object is to determine which box corresponds to which operator. Charlie has two boxes $C_1$ and $C_2$, and either box $C_1$ performs $U$ and box $C_2$ performs $V$, or vice versa. Our object is to determine which of these two situations holds. This version of the problem is sometimes equivalent to the version with one unknown box considered in previous sections. For example, if in addition to Charlie’s boxes, there is only
one program box $U$, we now have to distinguish between $U \otimes V \otimes U$ and $V \otimes U \otimes U$. As we are averaging over $U$ and $V$, we can however interchange these in the second density matrix, so that $V \otimes U \otimes U$ becomes $U \otimes V \otimes V$. This scenario is equivalent, therefore, to the third box being unlabelled, with one reference box each of $U$ and $V$. All the strategies we have discussed above that apply to this three-box situation can therefore be carried over to the order-finding version. It remains, therefore, to consider the four-box situations, in which Alice and Bob both have reference boxes.

3.2.2. One reference box of $U$ and one reference box of $V$

In the case in which Alice and Bob both have the same reference box, say $U$, and Charlie has either $C_1 = U$ and $C_2 = V$, or vice versa ((Fig. 2b)), we can map this case directly onto the case in Section 3.1. We note that the two possibilities for $ABC_1C_2$ are either $U \otimes U \otimes U \otimes V$ or $U \otimes U \otimes V \otimes U$. As we have to average over all possible $U$ and $V$, this is equivalent to trying to distinguish between $U \otimes U \otimes U \otimes U$ and $U \otimes V \otimes U \otimes U$ where we have simply re-ordered the boxes ($C_1C_2AB$) and interchanged $U$ and $V$ in the second case.

3.2.2. One reference box of $U$ and one reference box of $V$

One might wonder if replacing one of the $U$ operators by a $V$ in this scheme would improve the results. That is, suppose that Bob has a box that performs $V$ instead of $U$ (Fig. 2c). If box $C_1$ is $U$ and box $C_2$ is $V$, then we now have the state

$$|\Psi_1\rangle_{ABC_1C_2} = (U \otimes U)|\psi^-\rangle_{AC_1} (V \otimes V)|\psi^-\rangle_{BC_2},$$

(25)

and if box $C_1$ is $V$ and box $C_2$ is $U$, we have

$$|\Psi_2\rangle_{ABC_1C_2} = (U \otimes V)|\psi^-\rangle_{AC_1} (V \otimes U)|\psi^-\rangle_{BC_2}.$$  

(26)

We average these two states over $U$ and $V$ giving us the two density matrices

$$\rho_1 = |\Psi_1\rangle_{ABC_1C_2} \langle \Psi_1|$$

$$\rho_2 = \frac{1}{4} \left( P^a_{BC_1} \otimes P^s_{AC_2} + P^s_{BC_1} \otimes P^a_{AC_2} \right).$$

(27)

In comparing these two density matrices, it is useful to express $|\Psi\rangle_{ABC_1C_2}$ as

$$|\Psi\rangle_{ABC_1C_2} = \frac{1}{2} (|\psi^+\rangle_{BC_1}|\psi^+\rangle_{AC_2} + |\psi^-\rangle_{BC_1}|\psi^-\rangle_{AC_2} - |00\rangle_{BC_1}|11\rangle_{AC_2} - |11\rangle_{BC_1}|00\rangle_{AC_2}).$$

(28)

The first thing to notice is that the support of $\rho_1$ is contained in the support of $\rho_2$, so that if we are considering unambiguous discrimination, we will be able to positively identify $\rho_2$, but we will never be able to positively identify $\rho_1$.

We choose $\Pi_2$, the POVM element corresponding to $\rho_2$, to be the sum of three projection operators. The first is the projection onto the part of $\mathcal{H}_{BC_1} \otimes \mathcal{H}_{AC_2}$ that is orthogonal to the vector

$$|q\rangle = |\psi^+\rangle_{BC_1}|\psi^+\rangle_{AC_2} - |00\rangle_{BC_1}|11\rangle_{AC_2} - |11\rangle_{BC_1}|00\rangle_{AC_2},$$

(29)

the second is the projection onto $\mathcal{H}_{BC_1}^a \otimes \mathcal{H}_{AC_2}^a$, and the third is the projection onto $\mathcal{H}_{BC_1} \otimes \mathcal{H}_{AC_2}^a$. The notation here is that $\mathcal{H}_j^a$ is the symmetric subspace of qubits $j$ and $k$, while $\mathcal{H}_j^a$ is the antisymmetric subspace of qubits $j$ and $k$. The POVM element corresponding to failure is $\Pi_0 = I - \Pi_2$. We find that $\text{Tr}(\Pi_2\rho_2) = 2/3$, which means the our overall success rate is $1/3$; we succeed with a probability...
of $2/3$ if we have $\rho_2$, which happens with a probability of $1/2$, and we get an indeterminate answer if we are given $\rho_1$.

We have found that replacing one of the $U$ operators by $V$ has made the situation worse. This makes sense as detecting a difference in either the pair $AC_1$ or $BC_2$ will identify the order of $U$ and $V$ for boxes $C_1$ and $C_2$. If we match up identical operations in both singlet pairs, then we have no chance of unambiguously identifying the order of boxes $C_1$ and $C_2$. Matching different transforms up in both pairs gives a higher probability to detect a difference, as opposed to when there is a difference in only one singlet pair. This cannot, however, make up for our inability to detect a difference when identical transforms were matched up. It may be that in this situation, a strategy with more than four qubits would help. This is because the situation is somewhat similar to the three-box situation in Section 2.2.1. There, we would like to compare the unlabelled box against a reference box which does not match it, in order to unambiguously identify the unlabelled box. We cannot know which reference box to choose, however, and half the time we will choose to compare the unlabelled box against an identical reference box. The four-qubit strategy somehow helps us beat the odds. Here, we would like to compare both unlabelled boxes with reference boxes which do not match, but half the time we make the wrong choice and match the unlabelled boxes up with matching reference boxes. A strategy with more qubits might do better, but this is still an open problem.

4. Conclusion

We have discussed a number of operator decision problems. In each we are set the task of determining whether boxes perform the same or different unitary transformations, $U$ or $V$. We have no prior information of the forms of the transformations, but, instead, we have reference boxes that are known to perform the transformations $U$ or $V$.

We began by considering one reference box and one unknown box. This situation reduced to operator comparison, and for both unambiguous discrimination and minimum-error discrimination it is best to send into each box one of the particles from a singlet state. We then went on to examine the situation where one has two reference boxes and one unknown box. This can be thought of as a kind of pattern matching. Each of the reference operators represents a pattern, and we are trying to determine which of the two patterns the unknown operator matches. We studied both unambiguous and minimum-error strategies based on pairwise operator comparison. We also studied a minimum-error strategy based on an entangled three-qubit state that best approximates two singlet states. This strategy was not as good as pairwise operator comparison. Using subspace discrimination, we found an unambiguous strategy that is better than pairwise operator comparison, which demonstrates that the pairwise comparison strategy is not optimal. Finally, we studied situations with two reference boxes and two unknown boxes. For these cases, we only studied strategies based on pairwise operator comparison.

Our objective was not to present a comprehensive theory of operator comparison problems, but to to gain some idea of the issues involved and to present some strategies that will work for specific problems. One conclusion is that pairwise operator comparison works well, but is not always optimal. Finding optimal strategies is a subject that deserves further study.

Acknowledgments
Appendix A.

Here we present some additional information on the Haar integrals that were used extensively throughout the paper. As was noted, for $SU(2)$ these integrals can be performed using the following parameterization. We first set $U = \exp(-i\theta \hat{e} \cdot \hat{\sigma}/2)$, where $\hat{e}$ is a unit vector equal to $(\sin \mu \cos \phi, \sin \mu \sin \phi, \cos \mu)$, with $0 \leq \theta \leq 2\pi$, $0 \leq \phi \leq 2\pi$, and $0 \leq \mu \leq \pi$, and $\hat{\sigma} = \{\sigma_x, \sigma_y, \sigma_z\}$ is a vector of the usual Pauli matrices. We then have that

$$du = \frac{1}{4\pi^2} \sin^2 \left(\frac{\theta}{2}\right) \sin \mu d\theta d\phi d\mu. \quad (A1)$$

By explicit integration we find that

$$\int du U|0\rangle\langle 0| U^\dagger = \int du U|1\rangle\langle 1| U^\dagger = \frac{1}{2} I,$$
$$\int du U|0\rangle\langle 1| U^\dagger = \int du U|1\rangle\langle 0| U^\dagger = 0. \quad (A2)$$

The unitary invariance of the measure then implies that for any qubit state $|\psi\rangle$

$$\int du U|\psi\rangle\langle \psi| U^\dagger = \frac{1}{2} I,$$
$$\int du U|\psi\rangle\langle \psi_\perp| U^\dagger = 0,$$  
where $\langle \psi|\psi_\perp \rangle = 0$.

Now let us move on to two qubits. One can explicitly evaluate the integrals

$$\int du U \otimes U|00\rangle\langle 00| U^\dagger \otimes U^\dagger = \frac{1}{3} P^s,$$
$$\int du U \otimes U|00\rangle\langle 11| U^\dagger \otimes U^\dagger = 0$$
$$\int du U \otimes U|\psi^-\rangle\langle 00| U^\dagger \otimes U^\dagger = 0. \quad (A4)$$

The unitary invariance of the measure allows us to immediately extend these results

$$\int du U \otimes U|\psi_+\rangle\langle \psi_+| U^\dagger \otimes U^\dagger = \frac{1}{3} P^s,$$
$$\int du U \otimes U|\psi_\perp\rangle\langle \psi_\perp| U^\dagger \otimes U^\dagger = 0$$
$$\int du U \otimes U|\psi^-\rangle\langle \psi_\perp| U^\dagger \otimes U^\dagger = 0,$$  
where $\langle \psi_\perp|\psi_\perp \rangle = 0$.  

$(A5)$
where $|\psi_u\rangle$ and $|\psi_{s\perp}\rangle$ are in the symmetric subspace, $\langle\psi_u|\psi_{s\perp}\rangle = 0$, and $|\psi_u\rangle$ is in the antisymmetric subspace.

Appendix B.

Here we present the details of the POVM that optimally discriminates between the ranges of $\rho_1$ and $\rho_2$ in Eqs. (17) and (18). Let $S_1$ denote the range of $\rho_1$. It is spanned by the orthonormal vectors

$$|u_1\rangle = \frac{2}{\sqrt{3}}|\psi^-\rangle_{AC}|0\rangle_B \left(\frac{1}{2}|1\rangle_D + \frac{1}{2}|0\rangle_D\right), \quad |u_5\rangle = |11\rangle_{AC}|0\rangle_B|1\rangle_D$$

$$|u_2\rangle = \frac{2}{\sqrt{3}}|\psi^-\rangle_{AC}|1\rangle_B \left(\frac{1}{2}|1\rangle_D + \frac{1}{2}|0\rangle_D\right), \quad |u_6\rangle = |11\rangle_{AC}|1\rangle_B|1\rangle_D$$

$$|u_3\rangle = |00\rangle_{AC}|0\rangle_B|1\rangle_D, \quad |u_7\rangle = |\psi^+\rangle_{AC}|0\rangle_B|1\rangle_D$$

$$|u_4\rangle = |00\rangle_{AC}|1\rangle_B|1\rangle_D, \quad |u_8\rangle = |\psi^+\rangle_{AC}|1\rangle_B|1\rangle_D. \quad (B1)$$

Here, $|\psi^+\rangle = (|0\rangle|1\rangle + |1\rangle|0\rangle)/\sqrt{2}$. In this basis, we have

$$\rho_1 = \frac{5}{16}(|u_1\rangle\langle u_1| + |u_2\rangle\langle u_2|) + \frac{1}{16} \sum_{j=3}^{8} |u_j\rangle\langle u_j|. \quad (B2)$$

Now, let $S_2$ denote the range of $\rho_2$. It is spanned by the orthonormal vectors

$$|v_1\rangle = \frac{2}{\sqrt{3}}|\psi^-\rangle_{BC}|0\rangle_A \left(\frac{1}{2}|1\rangle_D + \frac{1}{2}|0\rangle_D\right), \quad |v_5\rangle = |11\rangle_{BC}|0\rangle_A|0\rangle_D$$

$$|v_2\rangle = \frac{2}{\sqrt{3}}|\psi^-\rangle_{BC}|1\rangle_A \left(\frac{1}{2}|1\rangle_D + \frac{1}{2}|0\rangle_D\right), \quad |v_6\rangle = |11\rangle_{BC}|1\rangle_A|0\rangle_D$$

$$|v_3\rangle = |00\rangle_{BC}|0\rangle_A|0\rangle_D, \quad |v_7\rangle = |\psi^+\rangle_{BC}|0\rangle_A|0\rangle_D$$

$$|v_4\rangle = |00\rangle_{BC}|1\rangle_A|0\rangle_D, \quad |v_8\rangle = |\psi^+\rangle_{BC}|1\rangle_A|0\rangle_D. \quad (B3)$$

In this basis

$$\rho_2 = \frac{5}{16}(|v_1\rangle\langle v_1| + |v_2\rangle\langle v_2|) + \frac{1}{16} \sum_{j=3}^{8} |v_j\rangle\langle v_j|. \quad (B4)$$

Examining these vectors, we see that $|u_5\rangle$ and $|u_6\rangle$ are orthogonal to $S_2$, and $|v_3\rangle$ and $|v_4\rangle$ are orthogonal to $S_1$. The remaining vectors can be arranged into two sets of overlapping subspaces. The subspaces spanned by $\{|u_1\rangle, |u_4\rangle, |u_7\rangle\}$ and by $\{|v_1\rangle, |v_4\rangle, |v_7\rangle\}$ overlap and the subspaces spanned by $\{|u_2\rangle, |u_5\rangle, |u_8\rangle\}$ and $\{|v_2\rangle, |v_5\rangle, |v_8\rangle\}$ overlap. The subspaces in the first set are orthogonal to those in the second.

We can now apply the results of reference (17) to discriminate the two three-dimensional subspaces and to discriminate the two two-dimensional subspaces. These results are then combined with those of the previous paragraph to give us the two optimal POVM’s for unambiguously discrimination $S_1$ and $S_2$. In order to exhibit these POVM’s it is necessary to define a number of additional vectors.
We have in $S_1$

\[
|\tilde{u}_1\rangle = \frac{1}{\sqrt{3}}(|u_4\rangle + \sqrt{2}|u_7\rangle) \\
|\tilde{u}_2\rangle = \frac{1}{\sqrt{3}}(|u_5\rangle + \sqrt{2}|u_8\rangle)
\]  

(B5)

and in $S_2$

\[
|\tilde{v}_1\rangle = \frac{1}{\sqrt{3}}(|v_4\rangle + \sqrt{2}|v_7\rangle) \\
|\tilde{v}_2\rangle = \frac{1}{\sqrt{3}}(|v_5\rangle + \sqrt{2}|v_8\rangle).
\]  

(B6)

Both $|\tilde{u}_1\rangle$ and $|\tilde{u}_2\rangle$ are constructed so that they are orthogonal to $S_2$ and $|\tilde{v}_1\rangle$ and $|\tilde{v}_2\rangle$ are orthogonal to $S_1$. Our discrimination problem is now reduced to discriminating between two sets of two-dimensional subspaces. The first set consists of the subspaces spanned by $\{|u_1\rangle, |\tilde{u}_3\rangle\}$ and $\{|v_1\rangle, |\tilde{v}_3\rangle\}$, and the second set consists of the subspaces spanned by $\{|u_2\rangle, |\tilde{u}_4\rangle\}$ and $\{|v_2\rangle, |\tilde{v}_4\rangle\}$, where

\[
|\tilde{u}_3\rangle = \frac{1}{\sqrt{3}}(\sqrt{2}|u_4\rangle - |u_7\rangle) \\
|\tilde{u}_4\rangle = \frac{1}{\sqrt{3}}(\sqrt{2}|u_5\rangle - |u_8\rangle) \\
|\tilde{v}_3\rangle = \frac{1}{\sqrt{3}}(\sqrt{2}|v_4\rangle - |v_7\rangle) \\
|\tilde{v}_4\rangle = \frac{1}{\sqrt{3}}(\sqrt{2}|v_5\rangle - |v_8\rangle).
\]  

(B7)

The two sets are orthogonal to each other. The next step is to find the Jordan bases for each set of subspaces (17). In each case, we find that the two subspaces have a vector in common. Throwing these vectors out, because the clearly do not help discriminate the subspaces, we are left with two sets of one dimensional subspaces to discriminate; $|\tilde{u}_5\rangle$ and $|\tilde{v}_5\rangle$ on the one hand, and $|\tilde{u}_6\rangle$ and $|\tilde{v}_6\rangle$ on the other. These vectors are defined by

\[
|\tilde{u}_5\rangle = \frac{1}{2\sqrt{2}}(\sqrt{3}|u_1\rangle - \sqrt{5}|\tilde{u}_3\rangle) \\
|\tilde{u}_6\rangle = \frac{1}{2\sqrt{2}}(\sqrt{3}|u_2\rangle + \sqrt{5}|\tilde{u}_4\rangle) \\
|\tilde{v}_5\rangle = \frac{1}{2\sqrt{2}}(\sqrt{3}|v_1\rangle - \sqrt{5}|\tilde{v}_3\rangle) \\
|\tilde{v}_6\rangle = \frac{1}{2\sqrt{2}}(\sqrt{3}|v_2\rangle + \sqrt{5}|\tilde{v}_4\rangle).
\]  

(B8)

Our final step is to define the vectors

\[
|y_5\rangle = \frac{5}{4}(|\tilde{v}_5\rangle + \frac{3}{5}|\tilde{u}_5\rangle), \quad |z_5\rangle = \frac{5}{4}(|\tilde{u}_5\rangle + \frac{3}{5}|\tilde{v}_5\rangle) \\
|y_6\rangle = \frac{5}{4}(|\tilde{v}_6\rangle + \frac{3}{5}|\tilde{u}_6\rangle), \quad |z_6\rangle = \frac{5}{4}(|\tilde{u}_6\rangle + \frac{3}{5}|\tilde{v}_6\rangle).
\]  

(B9)

These vectors have the property that $\langle y_j|\tilde{u}_j\rangle = 0$ and $\langle z_j|\tilde{v}_j\rangle = 0$, for $j = 5, 6$. The POVM operators for optimally unambiguously distinguishing $S_1$ and $S_2$, and
thereby distinguishing $\rho_1$ and $\rho_2$, are
\begin{align}
\Pi_1 &= |u_3\rangle\langle u_3| + |u_6\rangle\langle u_6| + |\tilde{u}_1\rangle\langle \tilde{u}_1| + |\tilde{u}_2\rangle\langle \tilde{u}_2| \\
&\quad + \frac{5}{8} (|z_5\rangle\langle z_5| + |z_6\rangle\langle z_6|) \\
\Pi_2 &= |v_3\rangle\langle v_3| + |v_6\rangle\langle v_6| + |\tilde{v}_1\rangle\langle \tilde{v}_1| + |\tilde{v}_2\rangle\langle \tilde{v}_2| \\
&\quad + \frac{5}{8} (|y_5\rangle\langle y_5| + |y_6\rangle\langle y_6|) \tag{B10}
\end{align}

References

(1) S. M. Barnett and S. Croke, Advances in Optics and Photonics 1, 238 (2009).