Minimal tomography with entanglement witnesses

Huangjun Zhu,1,2 Yong Siah Teo,1,3 and Berthold-Georg Englert1,3

1Centre for Quantum Technologies, National University of Singapore, Singapore 117543, Singapore
2NUS Graduate School for Integrative Sciences and Engineering, Singapore 117597, Singapore
3Department of Physics, National University of Singapore, Singapore 117542, Singapore

(Dated: 22 June 2009)

We introduce informationally complete measurements whose outcomes are entanglement witnesses and so answer the question of how many witnesses need to be measured to decide whether an arbitrary state is entangled or not: as many as the dimension of the state space. The optimized witness-based measurement can provide exponential improvement with respect to witness efficiency in high-dimensional Hilbert spaces, at the price of a reduction in the tomographic efficiency. We describe a systematic construction, and illustrate the matter at the example of two qubits.

PACS numbers: 03.65.Ud, 03.65.Wj, 03.67.-a

Quantum entanglement is a useful resource with a wide range of applications such as quantum teleportation [1-3], quantum key distribution [4], and quantum computation [5]. Crucial for the implementation of all these nonclassical tasks are the detection and characterization of entanglement in experiments. Entanglement can be detected by measuring entanglement witnesses [6, 7]. How many witnesses do we have to measure to determine whether a generic unknown quantum state is entangled or separable? [8] If we were to rely on each witness separately, we would have to measure an infinite number of them even in the case of two qubits, as we will see below.

On the other hand, state tomography with an informationally complete (IC) probability operator measurement (POM) [9, 10, 11, 12], which may consist of no more than $d^2$ outcomes ($d$ is the dimension of the Hilbert space, a minimal IC-POM has $d^2$ outcomes) can provide accurate information about an unknown input state, if sufficiently many input states are available. With this tomographic information at hand, we can reconstruct the unknown input state and then determine its separability, possibly exploiting well known criteria, such as the PPT criterion [6, 13], the range criterion [14], the matrix realignment criterion [15, 16], the covariance matrix criterion [17], or perhaps others, or making use of available algorithms [18, 19]. If we can design a minimal IC-POM such that every outcome is a witness, $d^2$ witnesses will suffice to determine the separability of any unknown input state.

We establish that such witness operator measurements (WOMs) do exist and show how to construct WOMs with optimal witnesses [20] as outcomes from rank-one POMs — POMs in which each outcome is a subnormalized projector onto a pure state. These WOMs can provide exponential improvement of the witness efficiency at the price of a much lower tomographic efficiency. The trade-off between witness efficiency and tomographic efficiency turns out to be quite common, and it is impossible to construct a minimal IC-POM which achieves both the best witness efficiency and optimal tomographic efficiency.

We shall be concerned with a bipartite system whose parts have subsystem dimensions $d_1$, $d_2$ with $d_1 \leq d_2$, and the total dimension is $d = d_1 d_2$. Usually, a witness is a Hermitian operator with nonnegative mean values for all separable states, and negative mean values for some entangled states [6], but this convention of the threshold at zero is not expedient here. For us, a witness is a positive operator with mean values less than or equal to some threshold for all separable states, and mean values above this threshold for some entangled states. A simple example of such a witness in the two-qubit case is a projector onto a Bell state with the threshold at $\frac{1}{2}$.

All unit-trace positive operators can serve as statistical operators. The largest mean value of a statistical operator $\rho_w$ is its largest eigenvalue $\lambda_{\text{max}}$, and if the largest mean value $\mu$ of $\rho_w$ with all separable states satisfies $\mu < \lambda_{\text{max}}$, then $\rho_w$ is a witness with the threshold at $\mu$. Accordingly, $\rho_w$ can serve as a witness if its eigenvalue to the largest eigenvalue does not contain any product state, and only then. As a consequence, every entangled pure state is a witness, and because almost all pure states are entangled, it is easy to construct an IC-POM with rank-one witnesses as outcomes.

To improve the witness efficiency (the probability of detecting a random entangled state), it would be favorable to have optimal witnesses [20] as outcomes. Since rank-one POMs are the best choice for tomographic purposes, it is of much concern whether a pure-state witness can be an optimal witness. As we shall see shortly, the efficiency of pure-state witnesses is poor, and there are more efficient witnesses for the construction of WOMs.

First we show that among the pure-state witnesses, the only candidates for optimal witnesses are maximally entangled states in the case of $d_1 = d_2$. The optimality of a pure-state witness is determined by its Schmidt coefficients, and without loss of generality we can assume $\rho_w = |\Psi\rangle\langle \Psi|$, $|\Psi\rangle = \sum_{i=1}^{d_1} |ii\rangle \sqrt{\lambda_i}$ with the Schmidt coefficients $\sqrt{\lambda_i}$ in nonincreasing order. The eigenvalues of the partial transpose $\rho_w^{T_2}$ are

$$\lambda_i (i = 1, \ldots, d_1), \pm \sqrt{\lambda_i \lambda_j} (i, j = 1, \ldots, d_1, i < j). (1)$$

It follows that, for separable states $\rho_{\text{sep}}$,

$$\text{Tr} \{ \rho_{\text{sep}} \rho_w \} = \text{Tr} \{ \rho_{\text{sep}}^{T_2} \rho_w^{T_2} \} \leq \lambda_1, (2)$$
and $\rho_{\text{sep}} = |11\rangle\langle 11|$ achieves this bound, so the threshold of the pure-state witness $\rho_w$ can be set at $\lambda_1$. To determine the optimality of such a witness, we construct the corresponding witness in the usual sense, that is: with the threshold at zero, $W = \lambda_1 1 - |\Psi\rangle\langle \Psi|$, where $1$ denotes the identity operator. Its partial transpose $Q = W_{T2}$, which is a positive operator, is

\[
Q = \sum_{i=1}^{d_1} |ii\rangle\langle ii| + \sum_{i,j=1,i\neq j}^{d_1} \left(\lambda_1 - \lambda_j\right) P_{ij}^{(+)} + \lambda_1 P_{ij}^{(-)}\]

with

\[
P_{ij}^{(\pm)} = \frac{1}{2}(|ij\rangle \pm |ji\rangle)(|ij\rangle \pm |ji\rangle),
\]

\[
P_{ij}^{+} = \sum_{i=1}^{d_1} \sum_{j=d_1+1}^{d_2} |ij\rangle\langle ij|.
\]

If $d_2 > d_1$ or $|\Psi\rangle$ is not maximally entangled, the range of $Q$ always contains some product vector and, according to Theorem 2 of [21], $W$ is not optimal. If $d_1 = d_2$, and $|\Psi\rangle$ is a maximally entangled state, then $Q$ is proportional to the projector onto the antisymmetrical subspace which contains no product vector in its range, and $W$ could be an optimal witness.

The probability that a random pure state is detected by a pure-state witness decreases exponentially with the dimension of the Hilbert space. To demonstrate this point we note that pure states $|\Phi\rangle$ can be represented as points on a $2d_1d_2 - 1$ dimensional unit sphere (many points may correspond to the same state, but it doesn’t matter, as we are only concerned with the ratio), and the set of pure product states is of measure zero. The states detected by $\rho_w$ form a spherical cap determined by $|\Phi\rangle|\rho_w|\Phi\rangle > \lambda_1$. The detection probability is equal to the hyper-area of the spherical cap to that of the sphere, which is given by

\[
(1 - \lambda_1)^{d_1d_2-1}\text{ with } \lambda_1 \geq 1/d_1,
\]

where $\lambda_1$ is the square of the largest Schmidt coefficient of $\rho_w = |\Psi\rangle\langle \Psi|$. The maximum detection probability of $(1 - 1/d_1)^{d_1d_2-1}$ is achieved when $|\Psi\rangle$ is maximally entangled. This maximum detection probability approaches $e^{-d_2}$ for $d_1 \gg 1$. So, even for the best pure-state witnesses, the detection probability decreases exponentially with the dimension, and it is desirable to find more efficient witnesses.

We restrict our attention to decomposable witnesses. An optimal decomposable witness $W$ can be written as the partial transpose of some positive operator $Q$ whose range contains no product vector [20]. We take a probabilistic approach in the study of detection efficiency of a generic witness constructed from the partial transpose of a statistical operator $Q$, see also [21], because the method used in the calculation of detection efficiency of a pure-state witnesses is generally difficult to carry out and may not give an intuitive result. When $\Phi$ is distributed according to the normalized unitarily invariant Haar measure $d\mu(\Phi)$, the expectation value and variance of the random variable $\langle \Phi|Q_{T2}|\Phi\rangle$ are

\[
E[\langle \Phi|Q_{T2}|\Phi\rangle] = \frac{1}{d},
\]

\[
\text{Var}[\langle \Phi|Q_{T2}|\Phi\rangle] = \frac{1}{d(d+1)}.
\]

(6)

We note that the variance is proportional to the squared Hilbert–Schmidt (HS) distance between $Q$ and the maximally mixed state.

In high dimension, there are generally many positive and negative eigenvalues of $Q_{T2}$ distributed randomly for a generic $Q$, and as a consequence of the central-limit theorem, the distribution of the random variable $\langle \Phi|Q_{T2}|\Phi\rangle$ will approximate a Gaussian distribution, so that the probability of obtaining a negative value is mainly determined by the ratio of the expectation value to the standard deviation.

It would be favorable to maximize the standard deviation in order to increase the detection efficiency. Recall that the expectation value of the purity $\text{Tr}(Q^2)$ with respect to the HS measure and Bures measure are $2\pi$ and $5d^2 + 1/2d(d^2 + 2)$, respectively, which both scale $\propto 1/d$ for $d \gg 1$. So, if we choose $Q$ randomly according to either of these two measures, or other measures commonly used, the ratio of $E[\langle \Phi|Q_{T2}|\Phi\rangle]^2$ to $\text{Var}[\langle \Phi|Q_{T2}|\Phi\rangle]$ is on the order of $d$ with high probability, and the detection probability decreases exponentially with growing $d$. It is now clear why a pure-state witness can only detect a very small fraction of entangled states in high dimension: because, when turned into a witness $W$ in the usual sense, the positive operator $Q = W_{T2}$ is highly mixed, see Eq. [3].

However, if $Q$ is a pure entangled state, the witness $W$ is optimal [24], and the ratio is of order $1$. Also, in high dimension, a randomly chosen pure state is approximately a maximally entangled state with high probability. For a maximally entangled state $Q$, the detection probability of $W$ can be calculated similarly to the case of pure-state witnesses, with the result

\[
\int_0^{\pi/4} d\cos\alpha \int_0^{\pi/2} d\sin\alpha \sum_{k=0}^{d_1} \frac{\Gamma(d_1/2)^2}{\Gamma((d_1+k)/2)^2} \sum_{k=0}^{d_1} \frac{\Gamma(d_1/2)^2}{\Gamma((d_1+k)/2)^2} \sum_{k=0}^{d_1} \frac{\Gamma(d_1/2)^2}{\Gamma((d_1+k)/2)^2}.
\]

(8)

This ratio becomes $(2\pi)^{-1} \int_0^\infty e^{-x^2} dx \approx 0.1573$ in the limit $d_1 \to \infty$; see also [21]. Numerical calculation shows
that when \( d_1 \geq 7 \), the deviation of the ratio from the limit is within 1%, the largest deviation occurs when \( d_1 = 2 \), where the ratio is \( \frac{1}{7} \). In conclusion, in high dimension, a witness constructed from the partial transpose of a randomly chosen pure state will, with high probability, detect about 15.7% of pure entangled states, thus achieving exponential improvement over a pure-state witness.

We can now construct WOMs with optimal witnesses as outcomes. Given a rank-one POM with outcomes \( \sum_i w_i \rho_i = 1 \), where \( w_i > 0 \) and the \( \rho_i \)'s are projectors to pure entangled states, we can construct a WOM with outcomes \( \propto w_i \rho_i w_i \), where \( \rho_{\text{w}} = \lambda_{\text{max}} \mathbf{1} - \rho_{T_2}^2 \) with \( \lambda_{\text{max}} \) the maximum of the largest eigenvalues of \( \rho_{T_2}^2 \). This WOM can achieve exponential improvement with respect to witness efficiency, and if the POM is IC, so is the WOM.

The outcomes of this WOM are highly mixed, and this decreases the tomographic efficiency. To compare the tomographic efficiencies of the WOM and the POM, we consider an example in which the POM is a symmetric IC-POM (SIC-POM), which was conjectured to exist in finite dimensions \([23, 29, 28]\). The mean square errors (according to the HS distance) achieved by the SIC-POM and the optimal WOM are given by \([23, 24]\):

\[
E(\|\hat{\rho} - \rho_{\text{HS}}^2\|_{\text{POM}}) = \frac{1}{N}(d^2 + d - 1 - \text{Tr}\{\rho^2\}) \sim \frac{d^2}{N},
\]

\[
E(\|\hat{\rho} - \rho_{\text{HS}}^2\|_{\text{WOM}}) = \frac{1}{N}(\frac{1}{d}(d + 1)^2(d - 1) - (d\lambda_{\text{max}} - 1)^2 + 1) - \text{Tr}\{\rho^2\}) \sim \frac{\lambda_{\text{max}}^2 d^4}{N},
\]

where \( \hat{\rho} \) is an estimate of the input state \( \rho \) in accordance with the measurement results, and \( N \) is the number of copies of the input state available for state tomography. Note that \( \lambda_{\text{max}} \geq 1/d_1 \) (if every fiducial vector of the SIC-POM is approximately maximally entangled, \( \lambda_{\text{max}} \sim 1/d_1 \)), so in high dimension, to achieve the same mean square error, the number of copies of an input state required in the WOM is at least \( d_1^2 \) times larger. For different rank-one POMs, the specific reduction of the tomographic efficiency may be different, but the order of magnitude should be similar. The trade-off between the tomographic efficiency and the witness efficiency is not restricted to this specific example, as we have seen that rank-one outcomes, which are best for tomographic purposes, are generally very poor as witnesses, the more so in high dimension. Generally speaking, positive operators with high purity tend to be poor witnesses, and those with low purity are not desirable for tomography.

Detection of entanglement of mixed states turns out to be much more difficult \([21]\), even if \( Q \) is a pure state. For \( W = |\Psi\rangle\langle\Psi|_{T_2} \), the distribution of the random variable \( \text{Tr}\{\rho W\} = \langle\Psi|\rho_{T_2}^2|\Psi\rangle \) is the same in form as that of the random variable \( \langle\Phi|Q_{T_2}^2|\Phi\rangle \) discussed above, provided \( \rho \) varies among all unitarily equivalent statistical operators according to the Haar measure. In particular, the expectation value and variance of the random variable is the same as in Eq. (6) after replacing \( Q \) by \( \rho \). As the fraction of separable states approaches zero in high dimension, by similar arguments as before, we can conclude that the probability of detecting entanglement of a random mixed state will generally decrease exponentially as the purity of the input state decreases.

Despite exponential improvement with respect to witness efficiency, the WOM with optimal witnesses as outcomes is still not efficient enough to detect highly mixed entangled states. In that case, entanglement detection through state tomography may be a better choice. To estimate the number of copies required in state tomography to reach sufficient accuracy for determining the separability of an input state, we recall that the radius of the largest separable ball in the space of statistical operators is \( \sqrt{1/(d - 1)d} \approx 1/d \) \([30]\), the dimension of the state space is \( d^2 - 1 \approx d^2 \), and a reasonable estimate of accuracy requirement would be \( E(\|\hat{\rho} - \rho_{\text{HS}}^2\|) \sim 1/d^3 \), \( E(\|\hat{\rho} - \rho_{\text{HS}}^2\|) \sim 1/d^6 \); for state tomography with a SIC-POM this would mean \( N \sim d^6 \).

For illustration, we now turn to the situation of two qubits, and analyze the difference between rank-one POMs and WOMs with optimal witnesses. In the case of two qubits, there are only decomposable witnesses \([20]\). Since every rank-two subspace contains at least one product vector \([31, 32]\), the only candidates of optimal witnesses (in the usual sense) are the partial transposes of some entangled pure states, and they are indeed optimal \([20]\). We first compare pure-state witnesses and witnesses constructed from their partial transposes.

By some local unitary transformation, any entangled two-qubit state can be turned into the form,

\[
|\Psi\rangle = |00\rangle \cos \alpha + |11\rangle \sin \alpha ,
\]

\[
0 < \alpha = \frac{1}{2} \arcsin(q) \leq \frac{\pi}{4} ,
\]

\[
p = \sqrt{1 - q^2} , \quad (10)
\]

where \( q \) is the concurrence of the pure state, \( p \) is the length of the Bloch vector of each reduced density matrix, and \( \alpha \) is introduced for convenience. Because either one of the parameters \( q, p, \alpha \) specifies \( |\Psi\rangle \), we will use them interchangeably to denote a pure state with given concurrence. Two pure states are aligned if there exists a local unitary transformation which turns both of them into the form of Eq. (10), possibly with different parameters \( \alpha_1, \alpha_2 \) or, equivalently, if the Bloch vectors of their reduced statistical operators are parallel, and the fidelity between them is equal to that between their reduced statistical operators. The fidelity between two pure states with given concurrences obtains the maximum value of \( \cos(\alpha_1 - \alpha_2)^2 \) when they are aligned.

If \( \alpha < \frac{\pi}{4} \), the witness constructed from the pure state is not optimal, and Lemma 2 of \([20]\) implies that the witnesses constructed from its aligned pure states with larger concurrences are finer. The probability that a random pure entangled state is detected by a pure-state witness with concurrence \( q \) is \( \frac{1}{2} (1 - q^2) \) as follows from Eq. (5), with the maximum \( \frac{1}{8} \) achieved for a Bell state. For two
aligned pure states $\rho(\alpha_1)$ and $\rho(\alpha_2)$, state $\rho(\alpha_2)$ can
detect state $\rho(\alpha_1)$ if

$$0 < \text{Tr}(\rho(\alpha_1)\rho(\alpha_2)) - \cos(\alpha_2)^2 = \sin(\alpha_1)\sin(2\alpha_2 - \alpha_1),$$

(11)

which means $2\alpha_2 > \alpha_1$. A counterintuitive consequence
of this observation is that, when $\alpha \leq \frac{\pi}{4}$ or $q \leq \frac{1}{2}\sqrt{2}$, $\rho(\alpha)$
cannot detect any Bell states. An analogous phenomenon
also exists in high dimension: if one Schmidt coefficient
of an entangled pure state is particularly large, then it
cannot detect any maximally entangled states.

The four eigenvalues of $\rho(\alpha)^T P$ are \(\frac{1}{2}(1 \pm p)\), \(\pm q\) [22],
so that statistical operators, which are also optimal wit-
nesses related to $\rho(\alpha)$, can be constructed as

$$\rho_w(\alpha) = \frac{1 \pm \sqrt{2} - \rho(\alpha)^T P}{1 + 2p},$$

(12)

Such a $\rho_w(\alpha)$ has concurrence $q/(1 + 2p)$ and negativ-
ity $(1 - p)/(1 + 2p)$, and $\mu = (1 + p)/(2 + 4p)$ is its
witness threshold. These states are quite special, they are
Bell states if $\alpha = \frac{\pi}{4}$, and are maximally entangled mixed
states for other values of $\alpha$, those states whose concurrence
cannot be increased by any global unitary transformation [23]. When $\rho_w(\alpha_1), \rho_w(\alpha_2)$ are aligned—we
call $\rho_w(\alpha_1), \rho_w(\alpha_2)$ aligned if $\rho(\alpha_1), \rho(\alpha_2)$ are aligned—
$\rho_w(\alpha_2)$ can detect $\rho_w(\alpha_1)$ if

$$0 > \text{Tr}\{\rho(\alpha_1)\rho(\alpha_2)^T P\} = \frac{\sin(\alpha_2)\sin(\alpha_2 - 2\alpha_1)}{1 + 2p},$$

(13)

which means $2\alpha_1 > \alpha_2$, a condition that is dual to the
condition of Eq. (11). If $\alpha_1 > \frac{\pi}{4}$, so that $\rho_w(\alpha_1)$ could
be any Bell state, then $\rho_w(\alpha_1)$ can be detected by any
aligned optimal witness $\rho_w(\alpha_2)$. On the other hand, an
optimal witness $\rho_w(\alpha_2)$ cannot detect any state $\rho_w(\alpha_1)$
with $\alpha_1 \leq \alpha_2/2$; in particular, Bell states cannot detect
any states $\rho_w(\alpha_1)$ with $\alpha_1 \leq \frac{\pi}{4}$. As $\alpha, q \to 0$, the $\rho_w(\alpha)$s
approach separable states, and they can detect fewer and
fewer entangled states but, surprisingly, they are still the
best witnesses for detecting even more weakly entangled
states $\rho_w(\alpha')$ with $\alpha' \leq \alpha$. As a consequence, an infinite
number of witnesses are needed to detect all entangled
states, if we rely on each witness separately.

Taking a SIC-POM [22, 26, 27] as example, we shall now
show the sharp difference between a rank-one POM
and a WOM consisting of optimal witnesses. Most known
examples of SIC-POMs are constructed from fiducial
states under the action of the generalized Pauli group,
or Heisenberg–Weyl group. In four dimensions, one such
fiducial state is given in Eq. (147) of [27]. In the case
of two qubits, if we choose the standard product basis
$|00\rangle, |01\rangle, |10\rangle, |11\rangle$ for Appleby’s $|e_0\rangle, |e_1\rangle, |e_2\rangle, |e_3\rangle$, then
the SIC-POM thus constructed has the very peculiar property
that the concurrence of all fiducial states are the
same, namely $\sqrt{2/5}$ [24]. We note that these fiducial
states are typical in the sense that their squared concurrence
equals the average squared concurrence of all pure
two-qubit states [22].

According to the general procedure presented above,
we can construct a WOM with optimal witnesses as out-
comes. Moreover, the WOM is literally also SIC, ex-
cept that the outcomes are not pure. Figure 1 shows the
entanglement detection ratio for the SIC-POM and the
WOM for both pure and mixed states, with each witness
acting separately. There is a huge improvement of the
WOM over the SIC-POM with respect to witness efficiency
especially for the detection of mixed states. The
SIC-POM cannot detect any Bell states, because the
concurrence of each fiducial vector is less than $\sqrt{1/2}$; yet, the
detection ratio of the WOM approaches 1 as the concur-
rence of the input state approaches 1. If mixed states are
distributed according to the HS measure, the overall
detection probability of the WOM is about 13%, for states
with concurrence larger than $\frac{1}{2}$, the probability is about
84%.

The improvement in the witness efficiency comes at the
price of a much lower tomographic efficiency, the mean
square error achieved by the SIC-POM and the WOM
given in Eq. (9) now reads,

$$E(|\hat{\rho} - \rho|_{\text{HS}}^2) = \frac{1}{N}(19 - \text{Tr}(\rho^2)),$$

$$E(|\hat{\rho} - \rho|_{\text{WOM}}^2) = \frac{1}{N}(64 + 15\sqrt{15} - \text{Tr}(\rho^2)),$$

(14)

where we have inserted the value $\lambda_{\text{max}} = \frac{1}{2}(1 + \sqrt{3/5})$.

The reduction in the tomographic efficiency of the WOM
compared to the SIC-POM is roughly by a factor of $\sqrt{4/3}$.

In summary, we have introduced WOMs, and devel-
oped a systematic method of constructing a WOM with
optimal witnesses as outcomes from a rank-one POM.
This WOM can provide exponential improvement with respect to the witness efficiency in high dimension, at the price of a reduction in the tomographic efficiency by a factor of order $d^{-2}$. The trade-off between the witness efficiency and the tomographic efficiency is quite common — this reflects the intrinsic difficulty of entanglement detection.

We are grateful for valuable discussions with Artur Ekert and Karol Życzkowski. HJZ thanks Maciej Lewenstein and Lin Chen for assistance and advice. Centre for Quantum Technologies is a Research Centre of Excellence funded by Ministry of Education and National Research Foundation of Singapore.

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