

Optimal Quantum Tomography of States, Measurements, and Transformations

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We present the first complete optimization of quantum tomography, for states, positive operator value measures, and various classes of transformations, for arbitrary prior ensemble and arbitrary representation, giving corresponding feasible experimental schemes in terms of random Bell measurements.

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A crucial task in quantum-information theory is the precise determination of states and processes using a finite amount of measurement data. Achieving this task is the aim of *quantum tomography* [1–3], whose framework can be briefly summarized as follows. A quantum measurement is generally described by a positive operator value measure (POVM), i.e., a collection of positive operators $P_i \in \mathcal{B}(\mathcal{H})$ satisfying the normalization $\sum_i P_i = I$ [4]. The probability of measurement outcome i is given by the Born statistical formula

$$p_i = \text{Tr}[\rho P_i]. \quad (1)$$

Tomographing an unknown state ρ of a quantum system means performing a suitable POVM $\{P_i\}$ such that the expectation value of an arbitrary operator A can be evaluated from the probability distribution $p_i = \text{Tr}[\rho P_i]$. The expectation value of A can be obtained when it is possible to expand A over the POVM as follows:

$$A = \sum_i f_i[A] P_i, \quad (2)$$

$f_i[A]$ denoting suitable expansion coefficients. The expectation $\langle A \rangle = \text{Tr}[\rho A]$ is then given by $\langle A \rangle = \sum_i f_i[A] \langle P_i \rangle$. For tomography expansion (2) must hold for all operators in $\mathcal{B}(\mathcal{H})$ —i.e., $\mathcal{B}(\mathcal{H}) = \text{span}\{P_i\}$ —and the POVM $\{P_i\}$ is called *informationally complete* [5,6].

It is convenient to associate every operator $A \in \mathcal{B}(\mathcal{H})$ to a bipartite vector in $\mathcal{H} \otimes \mathcal{H}$ in the following way:

$$A = \sum_{m,n=1}^d A_{mn} |m\rangle\langle n| \leftrightarrow |A\rangle\rangle = \sum_{m,n=1}^d A_{mn} |m\rangle|n\rangle. \quad (3)$$

Information completeness of the POVM along with convergence of the series (2) are equivalent to the condition $a\|A\|_2^2 \leq \sum_i |\langle P_i | A \rangle|^2 \leq b\|A\|_2^2$, $\forall A \in \mathcal{B}(\mathcal{H})$, with $0 < a \leq b < \infty$. Sets of vectors $|P_i\rangle\rangle$ satisfying this condition are known as *frames* [7]. This condition is equivalent to invertibility of the *frame operator* $F = \sum_i |P_i\rangle\rangle\langle\langle P_i|$. The expansion in Eq. (2) can be written as follows:

$$|A\rangle\rangle = \sum_i \langle\langle D_i | A \rangle\rangle |P_i\rangle\rangle, \quad (4)$$

where $\{D_i\}$ is a *dual frame*, namely, a set of operators

satisfying the identity $\sum_i |P_i\rangle\rangle\langle\langle D_i| = I$. For linearly dependent frame $\{P_i\}$ the dual $\{D_i\}$ is not unique.

The request for the POVM $\{P_i\}$ to be informationally complete can be relaxed if we have some prior information about the state ρ . If we know that the state belongs to a given subspace $\mathcal{V} \subseteq \mathcal{B}(\mathcal{H})$ the expectation value is

$$\langle A \rangle = \text{Tr}[\rho A] = \langle\langle \rho | A \rangle\rangle = \langle\langle \rho | Q_{\mathcal{V}} | A \rangle\rangle, \quad (5)$$

$Q_{\mathcal{V}}$ orthogonal projector on \mathcal{V} , whence the set $\{P_i\}$ is required to span only \mathcal{V} .

In estimating the expectation $\langle A \rangle$, optimality means minimum variance $\delta(A)$ of the random variable $f_i[A] = \langle\langle D_i | A \rangle\rangle$ with probability distribution $p_i = \text{Tr}[\rho P_i]$, i.e.,

$$\delta(A) := \sum_i |\langle\langle D_i | A \rangle\rangle|^2 \text{Tr}[\rho P_i] - |\text{Tr}[\rho A]|^2. \quad (6)$$

In a Bayesian scheme the state ρ is randomly drawn from an ensemble $\mathcal{S} = \{\rho_k, p_k\}$ of states ρ_k with prior probability p_k , with the variance averaged over \mathcal{S} , leading to

$$\delta_{\mathcal{S}}(A) := \sum_i |\langle\langle D_i | A \rangle\rangle|^2 \text{Tr}[\rho_{\mathcal{S}} P_i] - \sum_k p_k |\text{Tr}[\rho_k A]|^2, \quad (7)$$

where $\rho_{\mathcal{S}} = \sum_k p_k \rho_k$. Moreover, *a priori* we can be interested in some observables more than other ones, and this can be specified in terms of a weighted set of observables $\mathcal{G} = \{A_n, q_n\}$, with weight $q_n > 0$ for the observable A_n . Averaging over \mathcal{G} we have

$$\delta_{\mathcal{S}, \mathcal{G}} := \sum_i \langle\langle D_i | G | D_i \rangle\rangle \text{Tr}[\rho_{\mathcal{S}} P_i] - \sum_{k,n} p_k q_n |\text{Tr}[\rho_k A_n]|^2, \quad (8)$$

where $G = \sum_n q_n |A_n\rangle\rangle\langle\langle A_n|$. The weighted set \mathcal{G} yields a *representation of the state*, given in terms of the expectation values $\langle A_n \rangle$. The representation is faithful when $\{A_n\}$ is an operator frame, e.g., when it is made of the dyads $|i\rangle\langle j|$ corresponding to the matrix elements $\langle j | \rho | i \rangle$.

Notice that only the first term of $\delta_{\mathcal{S}, \mathcal{G}}$ depends on $\{P_i\}$ and $\{D_i\}$. If $\rho_i \in \mathcal{V}$ for all states $\rho_i \in \mathcal{S}$, by making use of Eq. (5) the first term of Eq. (8) becomes

$$\eta = \sum_i \langle\langle D_i | Q_{\mathcal{V}} G Q_{\mathcal{V}} | D_i \rangle\rangle \text{Tr}[\rho_{\mathcal{S}} P_i]. \quad (9)$$

We now generalize this approach to tomography of quantum operations, keeping generally different input and output Hilbert spaces \mathcal{H}_{in} and \mathcal{H}_{out} , respectively. This has the remarkable advantage that the usual tomography of states comes as the special case of one-dimensional \mathcal{H}_{in} , whereas tomography of POVMs corresponds to one-dimensional \mathcal{H}_{out} .

A quantum operation is a trace nonincreasing completely positive (CP) map $\mathcal{T} : \mathcal{B}(\mathcal{H}_{\text{in}}) \rightarrow \mathcal{B}(\mathcal{H}_{\text{out}})$. In order to gather information about a quantum operation \mathcal{T} , the most general procedure consists in (i) preparing a state $\rho \in \mathcal{B}(\mathcal{H}_{\text{in}} \otimes \mathcal{H}_A)$ where \mathcal{H}_A is an ancillary system with the same dimension of \mathcal{H}_{in} , (ii) performing a POVM $\{P_i\}$ on the state $(\mathcal{T} \otimes I_A)(\rho)$. The probability of obtaining a generic outcome i is given by

$$p_i = \text{Tr}[(\mathcal{T} \otimes I_A)(\rho)P_i], \quad (10)$$

which, using the Choi-Jamiołkowski isomorphism [8]

$$R_{\mathcal{T}} = \mathcal{T} \otimes I(|I\rangle\rangle\langle\langle I|), \quad \mathcal{T}(\rho) = \text{Tr}_{\text{in}}[(I_{\text{out}} \otimes \rho^T)R_{\mathcal{T}}], \quad (11)$$

becomes

$$p_i = \text{Tr}\{P_i \text{Tr}_{\text{in}}[(I_{\text{out}} \otimes \rho^{\theta_{\text{in}}})(R_{\mathcal{T}} \otimes I_A)]\} = \text{Tr}[R_{\mathcal{T}} \Pi_i^{(\rho)}], \quad (12)$$

where θ_{in} denotes partial transposition on \mathcal{H}_{in} , and

$$\Pi_i^{(\rho)} = \text{Tr}_A[(P_i \otimes I_{\text{in}})(I_{\text{out}} \otimes \rho^{\theta_{\text{in}}})]. \quad (13)$$

It is convenient to use here the notion of a *tester* along with the theoretical framework introduced in [9]. A tester is the natural generalization of the concept of POVM from states to transformations, and is represented by a set of positive operators $\Pi_i \in \mathcal{B}(\mathcal{H}_{\text{out}} \otimes \mathcal{H}_{\text{in}})$ with

$$\sum_i \Pi_i = I_{\text{out}} \otimes \sigma, \quad \text{Tr}[\sigma] = 1. \quad (14)$$

As one can see from Eq. (12), the probability distribution gets the form of a new kind of Born rule, with the tester $\{\Pi_i\}$ in place of $\{P_i\}$, and the operator $R_{\mathcal{T}}$ in place of ρ . On the other hand, it is possible to prove [9] that the generalized Born rule $p_i = \text{Tr}[R_{\mathcal{T}} \Pi_i]$ always arises from a physical scheme of measurement on the state $(\mathcal{T} \otimes I_A)(\nu)$:

$$p_i = \text{Tr}[R_{\mathcal{T}} \Pi_i] = \text{Tr}[\mathcal{T} \otimes I_A(\nu)P_i], \quad (15)$$

with entangled state ν and POVM $\{P_i\}$ given by

$$\nu = |\sqrt{\sigma}\rangle\rangle\langle\langle\sqrt{\sigma}|, \quad P_i = (I_{\text{out}} \otimes \sigma^{-1/2})\Pi_i(I_{\text{out}} \otimes \sigma^{-1/2}). \quad (16)$$

This method allows a straightforward generalization of tomography from states to transformations. Now tomographing a quantum operation means using a suitable tester $\{\Pi_i\}$ such that the expectation value of any other possible measurement can be inferred by the probability distribution $p_i = \text{Tr}[R_{\mathcal{T}} \Pi_i]$. To achieve this task we have to

require that $\{\Pi_i\}$ is an operator frame for $\mathcal{B}(\mathcal{H}_{\text{out}} \otimes \mathcal{H}_{\text{in}})$, i.e., any operator A can be expanded as

$$A = \sum_i \langle\langle \Delta_i | A \rangle\rangle \Pi_i, \quad A \in \mathcal{B}(\mathcal{H}_{\text{out}} \otimes \mathcal{H}_{\text{in}}), \quad (17)$$

where $\{\Delta_i\}$ is a possible dual of the frame $\{\Pi_i\}$; that is, the condition $\sum_i |\Pi_i\rangle\rangle\langle\langle \Delta_i| = I_{\text{out}} \otimes I_{\text{in}}$ holds.

Optimizing the tomography of quantum operations means minimizing the statistical error $\delta(A)$ in the determination of the expectation $\langle A \rangle = \text{Tr}[R_{\mathcal{T}} A]$ of an arbitrary operator A as in Eq. (17), given by

$$\delta(A) = \sum_i \langle\langle \Delta_i | A \rangle\rangle^2 \text{Tr}[R_{\mathcal{T}} \Pi_i] - |\text{Tr}[R_{\mathcal{T}} A]|^2. \quad (18)$$

Averaging $\delta(A)$ over an ensemble $\mathcal{E} = \{R_k, p_k\}$ of possible transformations and a weighted set $\mathcal{G} = \{A_n, q_n\}$ of possible observables, we then obtain

$$\delta_{\mathcal{E}, \mathcal{A}} := \sum_i \langle\langle \Delta_i | G | \Delta_i \rangle\rangle \text{Tr}[R_{\mathcal{E}} \Pi_i] - \sum_{k,n} p_k q_n |\text{Tr}[R_k A_n]|^2. \quad (19)$$

Optimizing this figure of merit means (i) optimizing the choice of the dual frame $\{\Delta_i\}$, (ii) optimizing the choice of the tester $\{\Pi_i\}$. The optimization of the tester $\{\Pi_i\}$ amounts to both choosing the best input state for the quantum operation and the best final measurement.

In the following, for the sake of clarity we will consider $\dim(\mathcal{H}_{\text{in}}) = \dim(\mathcal{H}_{\text{out}}) := d$ and focus on the ‘‘symmetric’’ case $G = I$; this happens, for example, when the set $\{A_n\}$ is an orthonormal basis, whose elements are equally weighted. Moreover, we assume that the averaged channel of the ensemble \mathcal{E} is the maximally depolarizing channel, whose Choi operator is $R_{\mathcal{E}} = d^{-1}I \otimes I$. With these assumptions the relevant term in $\delta_{\mathcal{E}, \mathcal{A}}$ becomes

$$\eta = \sum_i \langle\langle \Delta_i | \Delta_i \rangle\rangle d^{-1} \text{Tr}[\Pi_i]. \quad (20)$$

Since $R_{\mathcal{E}}$ is invariant under the action of $SU(d) \times SU(d)$ we now show that it is possible to impose covariance on the tester without increasing the value of η . Let us define

$$\Pi_{i,g,h} := (U_g \otimes V_h) \Pi_i (U_g^\dagger \otimes V_h^\dagger), \quad (21)$$

$$\Delta_{i,g,h} := (U_g \otimes V_h) \Delta_i (U_g^\dagger \otimes V_h^\dagger). \quad (22)$$

It is easy to check that $\Delta_{i,g,h}$ is a dual of $\Pi_{i,g,h}$ by evaluating the group average after the sum over i . Then we observe that the normalization of $\Pi_{i,g,h}$ gives

$$\sum_i \int dg dh \Pi_{i,g,h} = d^{-1}I \otimes I, \quad (23)$$

corresponding to $\sigma = d^{-1}I$ in Eqs. (14) and (16); namely, one can choose $\nu = d^{-1}|I\rangle\rangle\langle\langle I|$. In the last identity dg and dh are invariant measures normalized to unit. Moreover, the figure of merit for $\{\Pi_{i,g,h}\}$ is the same as for $\{\Pi_i\}$,

whence without loss of generality we optimize the covariant tester $\{\Pi_{i,g,h}\}$. The condition that the covariant tester is informationally complete with respect to the subspace of transformations to be tomographed will be verified after the optimization.

A generic covariant tester is obtained by Eq. (21), with the operators Π_i becoming “seeds” of the covariant POVM, and the normalization condition (14) becoming

$$\sum_i \text{Tr}[\Pi_i] = d \quad (24)$$

[analogous of covariant POVM normalization in [4,10]]. The problem of optimization of the dual frame has been solved in [11]. With the optimal dual, the figure of merit simplifies as

$$\eta = \text{Tr}[\tilde{X}^{-1}], \quad (25)$$

where

$$\begin{aligned} \tilde{X} &= \sum_i \int dg dh \frac{d|\Pi_{i,g,h}\rangle\langle\Pi_{i,g,h}|}{\text{Tr}[\Pi_{i,g,h}]} \\ &= \int dg dh W_{g,h} X W_{g,h}^\dagger \end{aligned} \quad (26)$$

with $W_{g,h} = U_g \otimes U_g^* \otimes V_h \otimes V_h^*$ and $X = \sum_i d|\Pi_i\rangle\langle\Pi_i|/\text{Tr}[\Pi_i]$. Using Schur’s lemma we have [12]

$$\begin{aligned} \tilde{X} &= P_1 + AP_2 + BP_3 + CP_4, & P_1 &= \Omega_{13} \otimes \Omega_{24}, \\ P_2 &= (I_{13} - \Omega_{13}) \otimes \Omega_{24}, & P_3 &= \Omega_{13} \otimes (I_{24} - \Omega_{24}), \\ P_4 &= (I_{13} - \Omega_{13}) \otimes (I_{24} - \Omega_{24}), \end{aligned} \quad (27)$$

having posed $\Omega = |I\rangle\langle I|/d$ and

$$\begin{aligned} A &= \frac{1}{d^2 - 1} \left\{ \sum_i \frac{\text{Tr}[(\text{Tr}_2[\Pi_i])^2]}{\text{Tr}[\Pi_i]} - 1 \right\}, \\ B &= \frac{1}{d^2 - 1} \left\{ \sum_i \frac{\text{Tr}[(\text{Tr}_1[\Pi_i])^2]}{\text{Tr}[\Pi_i]} - 1 \right\}, \\ C &= \frac{1}{(d^2 - 1)^2} \left\{ \sum_i \frac{d\text{Tr}[\Pi_i^2]}{\text{Tr}[\Pi_i]} - (d^2 - 1)(A + B) - 1 \right\}. \end{aligned} \quad (28)$$

One has

$$\text{Tr}[\tilde{X}^{-1}] = 1 + (d^2 - 1) \left[\frac{1}{A} + \frac{1}{B} + \frac{(d^2 - 1)}{C} \right]. \quad (29)$$

We note that if the ensemble of transformations is contained in a subspace $\mathcal{V} \subseteq \mathcal{B}(\mathcal{H}_{\text{out}} \otimes \mathcal{H}_{\text{in}})$, the figure of merit becomes $\eta = \text{Tr}[\tilde{X}^\ddagger Q_\mathcal{V}]$, where \tilde{X}^\ddagger is the Moore-Penrose pseudoinverse. We now carry on the minimization for three relevant subspaces:

$$\begin{aligned} \mathcal{Q} &= \mathcal{B}(\mathcal{H}_{\text{out}} \otimes \mathcal{H}_{\text{in}}), & \mathcal{C} &= \{R \in \mathcal{Q}, \text{Tr}_{\text{out}}[R] = I_{\text{in}}\}, \\ \mathcal{U} &= \{R \in \mathcal{Q}, \text{Tr}_{\text{out}}[R] = I_{\text{in}}, \text{Tr}_{\text{in}}[R] = I_{\text{out}}\}, \end{aligned} \quad (30)$$

corresponding, respectively, to quantum operations, general channels, and unital channels. The subspaces \mathcal{C} and \mathcal{U} are invariant under the action of the group $\{W_{g,h}\}$, and thus the respective projectors decompose as

$$Q_\mathcal{C} = P_1 + P_2 + P_4, \quad Q_\mathcal{U} = P_1 + P_4. \quad (31)$$

Without loss of generality we can assume the operators $\{\Pi_i\}$ to be rank 1. In fact, suppose that Π_i has rank higher than 1. Then it is possible to decompose it as $\Pi_i = \sum_j \Pi_{i,j}$ with $\Pi_{i,j}$ rank 1. The statistics of Π_i can be completely achieved by $\Pi_{i,j}$ through a suitable postprocessing. For the purpose of optimization it is then not restrictive to consider rank 1 Π_i , namely, $\Pi_i = \alpha_i |\Psi_i\rangle\langle\Psi_i|$, with $\sum_i \alpha_i = d$. Notice that all multiple seeds of this form lead to testers satisfying Eq. (24).

In the three cases under examination, the figure of merit is then

$$\begin{aligned} \eta_\mathcal{Q} &= \text{Tr}[\tilde{X}^{-1}] = 1 + (d^2 - 1) \left[\frac{2}{A} + \frac{(d^2 - 1)^2}{1 - 2A} \right], \\ \eta_\mathcal{C} &= \text{Tr}[\tilde{X}^\ddagger Q_\mathcal{C}] = 1 + (d^2 - 1) \left[\frac{1}{A} + \frac{(d^2 - 1)^2}{1 - 2A} \right], \\ \eta_\mathcal{U} &= \text{Tr}[\tilde{X}^\ddagger Q_\mathcal{U}] = 1 + (d^2 - 1) \left[\frac{(d^2 - 1)^2}{1 - 2A} \right], \end{aligned} \quad (32)$$

where $0 \leq A = (d^2 - 1)^{-1} \{ \sum_i \alpha_i \text{Tr}[(\Psi_i \Psi_i^\dagger)^2] - 1 \} \leq \frac{1}{d+1} < \frac{1}{2}$. The minimum can simply be determined by derivation with respect to A , obtaining $A = 1/(d^2 + 1)$ for quantum operations, $A = 1/[\sqrt{2}(d^2 - 1) + 2]$ for general channels, and $A = 0$ for unital channels. The corresponding minimum for the figure of merit is

$$\begin{aligned} \eta_\mathcal{Q} &\geq d^6 + d^4 - d^2, \\ \eta_\mathcal{C} &\geq d^6 + (2\sqrt{2} - 3)d^4 + (5 - 4\sqrt{2})d^2 + 2(\sqrt{2} - 1), \\ \eta_\mathcal{U} &\geq (d^2 - 1)^3 + 1. \end{aligned} \quad (33)$$

The same result for quantum operations and for unital channels has been obtained in [13] in a different framework.

These bounds are simply achieved by a single seed $\Pi_0 = d|\Psi\rangle\langle\Psi|$, with

$$\text{Tr}[(\Psi \Psi^\dagger)^2] = \frac{2d}{d^2 + 1}, \frac{\sqrt{2}(d^2 - 1) + 3}{d[\sqrt{2}(d^2 - 1) + 2]}, 1, \quad (34)$$

respectively, for quantum operations, general channels, and unital channels, namely, with

$$\Psi = [d^{-1}(1 - \beta)I + \beta|\psi\rangle\langle\psi|]^{1/2}, \quad (35)$$

where $\beta = \sqrt{(d+1)/(d^2+1)}$ for quantum operations, $\beta = \{(d-1)[2 + \sqrt{2}(d^2-1)]\}^{-1/2}$ for general channels,

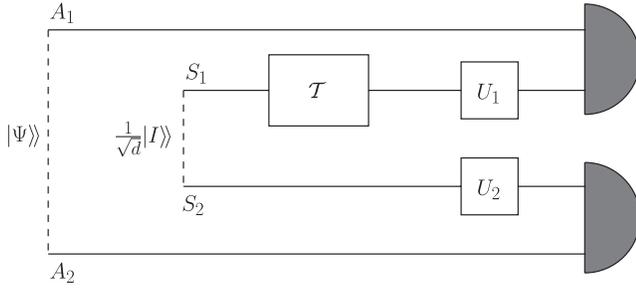


FIG. 1. Physical implementation of optimal quantum transformation tomography. The two measurements are Bell's measurements preceded by a random unitary. The state $|\Psi\rangle$ depends on the prior ensemble.

and $\beta = 0$ for unital channels, and $|\psi\rangle$ is any pure state. Informational completeness of the tester $\Pi_{g,h} = (U_g \otimes U_h)|\Psi\rangle\langle\Psi|(U_g \otimes U_h)^\dagger$ is thus verified as in [10].

The same procedure can be carried on when the operator G has the more general form $G = g_1 P_1 + g_2 P_2 + g_3 P_3 + g_4 P_4$, where P_i are the projectors defined in (27). In this case Eq. (29) becomes

$$\text{Tr}[\tilde{X}^{-1}G] = g_1 + (d^2 - 1) \left[\frac{g_2}{A} + \frac{g_3}{B} + \frac{(d^2 - 1)g_4}{C} \right], \quad (36)$$

which can be minimized along the same lines previously followed. G has this form when optimizing measuring procedures of this kind: (i) preparing an input state randomly drawn from the set $\{U_g \rho U_g^\dagger\}$, (ii) measuring an observable chosen from the set $\{U_h A U_h^\dagger\}$.

We now show how the optimal measurement can be experimentally implemented. Referring to Fig. 1, the bipartite system carrying the Choi operator of the transformation is indicated with the labels S_1 and S_2 . We prepare a pair of ancillary systems A_1 and A_2 in the joint state $|\Psi\rangle\langle\Psi|$, then we apply two random unitary transformations U_1 and U_2 to S_1 and S_2 , finally we perform a Bell measurement on the pair $A_1 S_1$ and another Bell measurement on the pair $A_2 S_2$. This experimental scheme realizes the continuous measurement by randomizing among a continuous set of discrete POVM; this is a particular application of a general result proved in [14]. The scheme proposed is feasible using, e.g., the Bell measurements experimentally realized in [15] and the pseudorandom circuits proposed in [16]. We note that choosing $|\Psi\rangle$ maximally entangled (as proposed, for example, in [17]) is generally not optimal, except for the unital case.

With the same derivation starting from Eq. (20), but keeping $\dim(\mathcal{H}_{\text{in}}) \neq \dim(\mathcal{H}_{\text{out}})$, one obtains the optimal tomography for general quantum operations. The special case of $\dim(\mathcal{H}_{\text{in}}) = 1$ [one has $P_3 = P_4 = 0$ in Eq. (27)] corresponds to optimal tomography of states, whereas case $\dim(\mathcal{H}_{\text{out}}) = 1$ ($P_2 = P_4 = 0$) gives the optimal tomog-

raphy of POVMs. The corresponding experimental schemes are obtained by removing the upper (lower) branch for POVMs (states), respectively. In the remaining branch the bipartite detector becomes a monopartite, performing a von Neumann measurement for the qudit, preceded by a random unitary in $SU(d)$. Moreover, for the case of POVM, the state $|\Psi\rangle$ is missing, whereas, for state tomography, both bipartite states are missing. The optimal η in Eq. (9) is given by $\eta = d^3 + d^2 - d$, in both cases (for state-tomography compare with Ref. [18]).

In conclusion, we presented a general method for optimizing quantum tomography, based on the new notion of *tester*. The method is very versatile, allowing one to consider arbitrary prior ensemble and representation. We provided the optimal experimental schemes for tomography of states and various kinds of process tomography, giving the corresponding performance, all schemes being feasible with the current technology.

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