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Letter

Tight conic approximation of testing regions for quantum statistical models and measurements

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ABSTRACT

Quantum statistical models (i.e., families of normalized density matrices) and quantum measurements (i.e., positive operator-valued measures) can be regarded as linear maps: the former, mapping the space of effects to the space of probability distributions; the latter, mapping the space of states to the space of probability distributions. The images of such linear maps are called the testing regions of the corresponding model or measurement. Testing regions are notoriously impractical to treat analytically in the quantum case. Our first result is to provide an implicit outer approximation of the testing region of any given quantum statistical model or measurement in any finite dimension: namely, a region in probability space that contains the desired image, but is defined implicitly, using a formula that depends only on the given model or measurement. The outer approximation that we construct is *minimal* among all such outer approximations, and *close*, in the sense that it becomes the *maximal inner* approximation up to a constant scaling factor. Finally, we apply our approximation to provide sufficient conditions, that can be tested in a semi-device-independent way, for the ability to transform one quantum statistical model or measurement into another.

1. Introduction

In statistics, information theory, and mathematical economics one is often faced with the problem of comparing two setups in terms of their expected performances on a particular task of interest. For example, one might compare two statistical models by comparing their informativeness in a given parameter estimation problem, or two noisy channels with respect to a given communication figure of merit, or again two portfolios with respect to their expected utility in a given betting scenario. The comparison could also be extended, so to ask when a given setup is *always* better than another one, i.e., independent of any particular task at hand. Such "global" comparisons, generally described by a preorder relation, play a crucial role in the formulation of mathematical statistics.

The simplest example of one such preorder in statistics is given by the *majorization preorder* of probability distributions [1–4]. Generalizing this, we find the comparison of families comprising two or more probability distributions. The case of pairs of probability distributions (i.e., *dichotomies*) is also known as *relative* majorization [5–8], whereas the case of multiple elements is usually referred to as comparison of statistical *experiments* or *models* [5–7,9].

The relevance of such preorder relations is epitomized by Blackwell's theorem [5,6], which establishes the equivalence between the above mentioned statistical comparisons, and the existence of a suitable stochastic map that transforms one setup (the "always better" one) into the other (the "always worse" one). For this reason, Blackwell's theorem and its variants provide a powerful framework for general resource theories [10], and indeed recent quantum extensions of Blackwell's theorem [11–13] have found fruitful application in the study of quantum entanglement [14], quantum thermodynamics [15,16], and quantum measurement theory [17–19], for example.

Mathematically, equivalence theorems *à la* Blackwell start from the characterization of suitably defined *testing regions*, corresponding to the statistical models at hand. In the simplest scenario, the testing region of a statistical model $\{\rho_i : 1 \leq i \leq n\}$ is constructed as follows: for any effect $0 \leq \pi \leq \mathbb{1}$, one computes the n-dimensional real vector whose i-th component is $\mathrm{Tr}[\pi\, \rho_i]$; the collection of all such vectors, for varying effect π, constitute the testing region of $\{\rho_i\}_i$.[1] In other words, the testing region

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[1] The definition of testing region can be straightforwardly extended also to families of effects $\boldsymbol{\pi} = \{\pi_i : 1 \leq i \leq n\}$. In this case the region in $\mathbb{R}^n$ to consider is the collection of vectors whose components are given by $\mathrm{Tr}[\pi_i\, \rho]$, for varying ρ in the set of all states.

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of a statistical model is the *image* of the set of effect through the linear map induced by the former. For this reason, in what follows we will use the terms "testing region" and "image" interchangeably. Two statistical models with the same number of elements can then be compared by looking at their testing regions. A particularly relevant condition occurs when the testing region of one statistical model contains that of the other one. In the case of dichotomies, the inclusion relation for testing regions corresponds exactly with the preorder of relative majorization [8,13].

Unfortunately, due to the non-commutativity of the underlying algebra, the quantum version of Blackwell's equivalence [11] turns out to be more convoluted than its original classical variant. One reason for this is that testing regions quickly become impractical to treat analytically.[2] This is particularly evident already in the case of relative majorization: while classical relative majorization can be summarized in a finite collection of easily computable inequalities [5,8], in the quantum case (with the notable exceptions of qubits [20,21]) an infinite number of scalar inequalities must be evaluated [13]. The situation becomes even more cumbersome in the case of quantum statistical models [11].

In this paper, in order to shed more light on the structure of quantum testing regions, we provide techniques to construct implicit approximations of the testing region of arbitrary quantum statistical models and measurements, in any finite dimension. More precisely, we construct conic regions in probability space that contain (outer approximations), or are contained (inner approximations) by, the desired testing region. Such approximations, unlike the testing region, can be defined implicitly, using a formula that depends only on the given setup (i.e., quantum statistical model or measurement). The approximations that we construct are *optimal* among all such approximations, that is, we prove that they are the minimal outer and the maximal inner conic approximations. They are moreover *close*, in the sense that the minimal outer approximation becomes the maximal inner approximation up to a constant scaling factor. Our approximation techniques thus generalize the bounding recently provided in Ref. [22] by Xu, Schwonnek, and Winter: first, the extension is from Pauli strings to arbitrary measurements; second, the optimization is not restricted to the radius of fixed-axis ellipsoids, but it is a *global* optimization over all the parameters of the ellipsoid.

As an application, we utilize our approximation formulas to provide sufficient conditions, that can be tested in a semi-device independent way, for the ability to transform one quantum measurement into another, or one quantum statistical model into another. Other fields of applications of our approximation formulas include the contexts of the accessible information [31] of quantum ensembles, the informational power [32] of quantum measurements, and the observational entropy [33] of quantum measurements, as well as other related optimization tasks. In these tasks, given a measurement or statistical model, the goal consists of optimizing an operationally relevant payoff function (in the cases above, a relative entropy) over its domain; our approximations thus provide a more tractable domain of optimization that can lead e.g. to bounds on the desired quantities.

2. Main results

2.1. Quantum measurements

Given a d-dimensional quantum measurement $\boldsymbol{\pi} = \{\pi_i : 1 \le i \le n\}$, $\pi_i \ge 0$, $\sum_i \pi_i = \mathbb{1}$, its testing region is defined as the image $\boldsymbol{\pi}(\mathbb{S}_d)$ of the set $\mathbb{S}_d$ of d-dimensional states through $\boldsymbol{\pi}$. By definition, this is given in parametric form, that is, it is a body in the probability space parameterized by states in the state space. Ideally, one would aim at implicitizing it, that is, writing it in the form $f(p) \le 1$, for probability distributions p. However, due to intractability of the structure of the state space, we resort here to providing inclusion conditions in terms of implicit bodies.

[2] Another reason is that the requirement of *complete positivity* demands an extended comparison [11].

Definition 1. For any d-dimensional, n-outcome measurement $\boldsymbol{\pi} = \{\pi_i\}_{i=1}^n$, we define the family $\{\mathcal{E}_r(\boldsymbol{\pi})\}_{r\in\mathbb{R}}$ of hyper-ellipsoids given by:

$$\mathcal{E}_r(\boldsymbol{\pi}) := \left\{ \mathbf{p} \in \boldsymbol{\pi}\left(\mathbb{C}^d\right) \,\middle|\, \left|\sqrt{Q^+}\left(\mathbf{p}-\mathbf{t}\right)\right|_2^2 \le \frac{1}{r^2} \right\},$$

where $Q^+ \in \mathbb{R}^{n\times n}$ is the pseudo-inverse of the symmetric positive semi-definite covariance matrix given by

$$Q_{ij} = \frac{d-1}{d}\left(\mathrm{Tr}\left[\pi_i\pi_j\right] - \frac{\mathrm{Tr}\left[\pi_i\right]\mathrm{Tr}[\pi_j]}{d}\right),$$

for any $0 \le i, j \le n$, and $\mathbf{t} \in \mathbb{R}^n$ is the vector

$$t_i = \frac{1}{d}\,\mathrm{Tr}\left[\pi_i\right], \qquad 1 \le i \le n.$$

Theorem 1. *For any d-dimensional, n-outcome informationally complete measurement $\boldsymbol{\pi}$, one has that $\mathcal{E}_{d-1}(\boldsymbol{\pi})$ is the maximum volume ellipsoid enclosed in $\boldsymbol{\pi}(\mathbb{S}_d)$ and $\mathcal{E}_1(\boldsymbol{\pi})$ is the minimum volume ellipsoid enclosing $\boldsymbol{\pi}(\mathbb{S}_d)$.*

If measurement $\boldsymbol{\pi}$ is not informationally complete, ellipsoids $\mathcal{E}_{d-1}(\boldsymbol{\pi})$ and $\mathcal{E}_1(\boldsymbol{\pi})$ still are inner and outer approximations of $\boldsymbol{\pi}(\mathbb{S}_d)$, although not necessarily maximal and minimal in volume, respectively.

We postpone the proof of Theorem 1 to Section 3.2.

As examples, let us consider symmetric, informationally complete (SIC) and mutually unbiased basis (MUB) measurements.

A d-dimensional measurement $\boldsymbol{\pi}$ is SIC if and only if it has $n = d^2$ effects satisfying the condition $\mathrm{Tr}\,\pi_i\pi_j = (d\delta_{i,j}+1)/(d^2(d+1))$. By explicit computation one has

$$Q = \frac{d-1}{d^2\,(d+1)}\left(\mathbb{1}_{d^2} - \hat{\mathbf{u}}\hat{\mathbf{u}}^T\right),$$

where $\hat{\mathbf{u}}$ denotes the unit vector with all equal entries. As expected, Q is a $d^2\times d^2$ matrix of rank d^2-1, and it is proportional to a projector [23]. Its pseudo-inverse is then given by

$$Q^+ = \frac{d^2\,(d+1)}{d-1}\left(\mathbb{1}_{d^2} - \hat{\mathbf{u}}\hat{\mathbf{u}}^T\right).$$

A d-dimensional measurement $\boldsymbol{\pi}$ is a complete MUB if and only if it has $n = d(d+1)$ effects satisfying the condition $\mathrm{Tr}[\pi_{i,j}\pi_{k,l}] = (\delta_{i,k}\delta j,l + (1-\delta_{i,k})/d)/(d+1)^2$, where indices i,k denote the basis and indices j,l denote the effect within the basis. By explicit computation one has

$$Q = \frac{d-1}{d\,(d+1)^2}\left(\mathbb{1}_{d(d+1)} - \oplus_{i=1}^{d+1}\,\hat{\mathbf{u}}_d^i\hat{\mathbf{u}}_d^{iT}\right),$$

where $\mathbf{u}_d^i$ is the vector with ones for the entries corresponding to basis i and zero otherwise. As expected, Q is a $d(d+1)\times d(d+1)$ matrix of rank d^2-1, and it is proportional to a projector [23]. Its pseudo-inverse is then given by

$$Q^+ = \frac{d\,(d+1)^2}{d-1}\left(\mathbb{1}_{d(d+1)} - \oplus_{i=1}^{d+1}\,\hat{\mathbf{u}}_d^i\hat{\mathbf{u}}_d^{iT}\right).$$

Now that we have a close approximation of the image of the set of states through any given measurement, we turn our attention to applying it to semi-device independent tests of simulability. A test is semi-device independent if it only assumes the dimension of the devices involved, but does not otherwise assume their mathematical description. We say that a d_1-dimensional, n-outcome measurement $\boldsymbol{\pi}_1$ simulates a d_0-dimensional, n-outcome measurement $\boldsymbol{\pi}_0$ if and only if there exists a completely positive map $\mathcal{C} : \mathcal{L}(\mathbb{C}^{d_0}) \to \mathcal{L}(\mathbb{C}^{d_1})$ such that

$$\boldsymbol{\pi}_1 \circ \mathcal{C} = \boldsymbol{\pi}_0. \tag{1}$$

In Corollary 2 of Ref. [21] the following sufficient condition, that can in principle be tested in a semi-device-independent way, was given

$$\boldsymbol{\pi}_0\left(\mathbb{S}_d\right) \subseteq \mathrm{conv}\,\mathcal{P},$$

for any uncharacterized qubit or qutrit measurement $\boldsymbol{\pi}_0$ to be simulable by whatever three-outcomes qubit measurement $\boldsymbol{\pi}_1$ generated a given a set $\mathcal{P}$ of probability distributions. However, when $\boldsymbol{\pi}_0$ is a qutrit measurement, its range $\boldsymbol{\pi}_0(\mathbb{S}_d)$ is challenging to characterize, rendering such a test impractical; in this case, the tight conic approximation is much more convenient to work with. The following corollary addresses this issue, providing a practical semi-device independent test of Eq. (1).

Corollary 1 *(Semi-device independent simulability test). Given a set $\mathcal{P}$ of n-element probability distributions generated by a d_1-dimensional (otherwise unspecified) measurement $\boldsymbol{\pi}_1$, for any d_0 and for any d_0-dimensional n-outcome measurement $\boldsymbol{\pi}_0$ such that*

$$\mathcal{E}_1\left(\boldsymbol{\pi}_0\right) \subseteq \operatorname{conv} \mathcal{P},$$

there exists a trace preserving map C that is positive on the orthogonal complement to the kernel of $\boldsymbol{\pi}_0$ such that Eq. (1) holds. Moreover, if $d_1 = 2$, $n \leq 3$, and $d_0 \leq 3$, map C in Eq. (1) is completely positive, that is, measurement $\boldsymbol{\pi}_1$ simulates measurement $\boldsymbol{\pi}_0$.

Proof. The first part of the statement follows from Theorem 1 and from Proposition 7.1 of Ref. [24]. The second part of the statement follows from Theorem 1 and from Theorem 2 of Ref. [21]. □

2.2. Quantum statistical models

Given a d-dimensional quantum statistical model $\boldsymbol{\rho} = \{\rho_i : 1 \leq i \leq n\}$, $\rho_i \geq 0$, $\operatorname{Tr}[\rho_i] = 1$, its testing region is defined as the image $\boldsymbol{\rho}(\mathbb{E})$ of the cone $\mathbb{E}$ of effects through $\boldsymbol{\rho}$, seen as a classical-quantum (c-q for short) channel. By definition, the testing region $\boldsymbol{\rho}(\mathbb{E})$ is given in parametric form, that is, it is a body in the probability space parameterized by effects in the effect space. Ideally, one would aim at implicitizing it, that is, write it in the form $f(q) \leq 1$, for vectors of probabilities q. However, due to the intractability of the structure of the effect space, we resort here to providing inclusion conditions in terms of implicit bodies.

Definition 2. For any d-dimensional family $\boldsymbol{\rho} = \{\rho_i\}_{i=1}^n$ of n states, let $\{\mathcal{E}_r^k(\boldsymbol{\rho})\}_{r\in\mathbb{R}}^{k=0,\dots d}$ be the following family of hyper-ellipsoids:

$$\mathcal{E}_r^k(\boldsymbol{\rho}) = \left\{ \mathbf{q} \in \boldsymbol{\rho}\left(\mathbb{C}^d\right) \,\middle|\, \left|\sqrt{Q_k^+}\left(\mathbf{q} - \frac{k}{d}\mathbf{u}\right)\right|_2^2 \leq \frac{1}{r^2} \right\},$$

where $Q_k^+ \in \mathbb{R}^{n\times n}$ is the pseudo-inverse of the symmetric positive semi-definite covariance matrix given by

$$\left(Q_k\right)_{ij} = \left(k - \frac{k^2}{d}\right)\left(\operatorname{Tr}\left[\rho_i\rho_j\right] - \frac{1}{d}\right),$$

for any $0 \leq i, j \leq n$, and $\mathbf{u} \in \mathbb{R}^n$ is the vector with all unit entries.

We introduce a d-cone as a generalization of the bicone. A d-cone in $\mathbb{R}^n$ is the convex hull of the origin and d arbitrary $(n-1)$-balls with aligned and equidistant centers lying on hyperplanes orthogonal to the line of the centers (hence, including the origin, the d-cone is the convex hull of $(d+1)$ balls). Let $r(x)$ be the radius of the ball at distance x from the origin and L be the distance of the furthest ball. If $r(x)$ is symmetric, that is $r(x) = r(L-x)$ for any $0 \leq x \leq L$, then we say that the d-cone is symmetric. In this case, symmetry imposes that the ball lying further from the origin is itself a point, as the origin is. The usual bicone is recovered as the symmetric 2-cone. A pictorial representation of d-cones is given in Fig. 1. An elliptical d-cone is the image of a d-cone through a linear transformation that preserves the line joining the centers of the balls.

Theorem 2. *For any d-dimensional, n-outcome informationally complete family $\boldsymbol{\rho}$ of states, one has that $\operatorname{conv}\cup_{k=0}^d \mathcal{E}_{\eta(k,d)}^k(\boldsymbol{\rho})$ is the maximum volume elliptical d-cone enclosed in $\boldsymbol{\rho}(\mathbb{E})$ and $\operatorname{conv}\cup_{k=0}^d \mathcal{E}_1^k(\boldsymbol{\rho})$ is the minimum volume elliptical d-cone enclosing $\boldsymbol{\rho}(\mathbb{E})$, where*

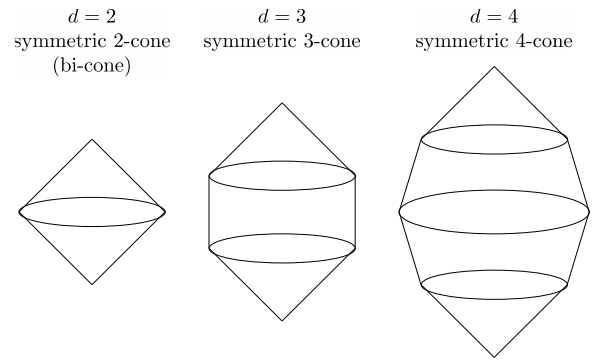

Fig. 1. A pictorial representation of symmetric d-cones in $\mathbb{R}^3$, for $d = 2, 3, 4$.

$$\eta(k,d)^2 = (d-1)\frac{k(d-k)}{\min\left(k^2, (d-k)^2\right)}.$$

If family $\boldsymbol{\rho}$ of states is not informationally complete, elliptical d-cones $\operatorname{conv}\cup_{k=0}^d \mathcal{E}_{d-1}^k(\boldsymbol{\rho})$ and $\operatorname{conv}\cup_{k=0}^d \mathcal{E}_1^k(\boldsymbol{\rho})$ still are inner and outer approximations of $\boldsymbol{\rho}(\mathbb{E})$, although not necessarily maximal and minimal in volume, respectively.

We postpone the proof of Theorem 2 to Section 3.3.

As examples, let us consider symmetric, informationally complete (SIC) and mutually unbiased basis (MUB) families of states.

A d-dimensional family $\boldsymbol{\rho}$ of states is SIC if and only if it has $n = d^2$ states satisfying the condition $\operatorname{Tr}\rho_i\rho_j = (d\delta_{i,j} + 1)/(d+1)$. By explicit computation one has

$$Q_k = \frac{kd - k^2}{d^2(d+1)}\left(\mathbb{1}_{d^2} - \hat{\mathbf{u}}\hat{\mathbf{u}}^T\right),$$

where $\hat{\mathbf{u}}$ denotes the unit vector with all equal entries. As expected, Q_k are $d^2 \times d^2$ matrix of rank $d^2 - 1$, and they are proportional to a projector. Their pseudo-inverses are then given by

$$Q_k^+ = \frac{d^2(d+1)}{kd - k^2}\left(\mathbb{1}_{d^2} - \hat{\mathbf{u}}\hat{\mathbf{u}}^T\right).$$

A d-dimensional family $\boldsymbol{\rho}$ of states is a complete MUB if and only if it has $n = d(d+1)$ states satisfying the condition $\operatorname{Tr}[\rho_{i,j}\rho_{k,l}] = (\delta_{i,k}\delta j, l + (1-\delta_{i,k})/d)$, where indices i, k denote the basis and indices j, l denote the effect within the basis. By explicit computation one has

$$Q_k = \frac{kd - k^2}{d(d+1)^2}\left(\mathbb{1}_{d(d+1)} - \oplus_{i=1}^{d+1}\hat{\mathbf{u}}_d^i\hat{\mathbf{u}}_d^{iT}\right),$$

where $\mathbf{u}_d^i$ is the vector with ones for the entries corresponding to basis i and zero otherwise. As expected, Q_k are $d(d+1) \times d(d+1)$ matrices of rank $d^2 - 1$, and they are proportional to a projector. Their pseudo-inverses are then given by

$$Q_k^+ = \frac{d(d+1)^2}{kd - k^2}\left(\mathbb{1}_{d(d+1)} - \oplus_{i=1}^{d+1}\hat{\mathbf{u}}_d^i\hat{\mathbf{u}}_d^{iT}\right).$$

Now that we have a close approximation of the image of the set of effects through any given family of states, we turn our attention to applying it to semi-device independent tests of simulability. We say that a d_1-dimensional, n-outcome family of states $\boldsymbol{\rho}$ simulates a d_0-dimensional, n-outcome measurement $\boldsymbol{\rho}_0$ if and only if there exists a completely positive trace preserving map (a quantum channel) $\mathcal{C} : \mathcal{L}(\mathbb{C}^{d_1}) \to \mathcal{L}(\mathbb{C}^{d_0})$ such that

$$\mathcal{C} \circ \boldsymbol{\rho}_1 = \boldsymbol{\rho}_0. \tag{2}$$

The following corollary generalizes Corollary 1 of Ref. [21] to the arbitrary dimensional case, providing a semi-device independent test of Eq. (2).

Corollary 2 *(Semi-device independent simulability test). Given a set $\mathcal{Q}$ of n-element vectors of probabilities generated by a d_1-dimensional (otherwise unspecified) family of n states $\boldsymbol{\rho}_1$, for any d_0 and for any d_0-dimensional family of n states $\boldsymbol{\rho}_0$ such that*

$$\operatorname{conv} \cup_{k=0}^{d} \mathcal{E}_1^k\left(\boldsymbol{\rho}_0\right) \subseteq \operatorname{conv} \mathcal{Q},$$

there exists a (not necessarily trace preserving) map C that is positive on the orthogonal complement to the kernel of $\boldsymbol{\rho}_0$ such that Eq. (1) holds. Moreover, if $d_1 = 2$, $n = 2$, and $d_0 = 2$, map C in Eq. (1) is completely positive trace preserving, that is, family $\boldsymbol{\rho}_1$ of states simulates family $\boldsymbol{\rho}_0$ of states.

Proof. The first part of the statement follows from Theorem 2. The second part of the statement follows from Theorem 2 and from Theorem 1 of Ref. [21]. □

3. Proofs

3.1. Formalization

For any positive integer d, let $\mathcal{L}(\mathbb{C}^d)$ denote the space of Hermitian operators on $\mathbb{C}^d$ equipped with the Hilbert-Schmidt product, that is, for any $\rho, \pi \in \mathcal{L}(\mathbb{C}^d)$ we have $\rho \cdot \pi = \operatorname{Tr}[\rho\pi]$. For any positive integer n, let $\mathbb{R}^n$ denote the space of n-dimensional real vectors equipped with the usual inner product, that is, for any $p, q \in \mathbb{R}^n$ we have $p \cdot q = \sum_{i=1}^n p_i^\dagger q_i$.

A d-dimensional, n-outcome measurement is a map

$$\boldsymbol{\pi} : \mathcal{L}\left(\mathbb{C}^d\right) \to \mathbb{R}^n.$$

Any measurement $\boldsymbol{\pi}$ can be represented as an indexed family $\{\pi_i \in \mathcal{L}(\mathbb{C}^d)\}_{i=1}^n$ of operators as follows. Recalling that the space $\mathcal{L}(\mathbb{C}^d)$ is equipped with the Hilbert-Schmidt product, the action of $\boldsymbol{\pi}$ on an operator $\rho \in \mathcal{L}(\mathbb{C}^d)$ is naturally given by

$$\boldsymbol{\pi}(\rho) := \begin{bmatrix} \langle\langle \pi_1 | \\ \vdots \\ \langle\langle \pi_n | \end{bmatrix} |\rho\rangle\rangle = \begin{bmatrix} \operatorname{Tr}\left[\pi_1 \rho\right] \\ \vdots \\ \operatorname{Tr}\left[\pi_n \rho\right] \end{bmatrix} \in \mathbb{R}^n,$$

where $\langle\langle \pi | : \mathcal{L}(\mathbb{C}^d) \to \mathbb{R}$ is given by $\langle\langle \pi | \rho \rangle\rangle = \operatorname{Tr}[\pi\rho]$.

Recalling that the space $\mathbb{R}^n$ is instead equipped with the usual inner product, the action of the Hermitian conjugate $\boldsymbol{\pi}^\dagger$ on a vector $\mathbf{p} \in \mathbb{R}^n$ is naturally given by

$$\begin{aligned} \boldsymbol{\pi}^\dagger \mathbf{p} &= \begin{bmatrix} |\pi_1\rangle\rangle & \dots & |\pi_n\rangle\rangle \end{bmatrix} \begin{bmatrix} p_1 \\ \vdots \\ p_n \end{bmatrix} \\ &= \sum_{i=1}^n p_i |\pi_i\rangle\rangle \in \mathcal{L}\left(\mathbb{C}^d\right). \end{aligned}$$

Finally, for any measurements $\boldsymbol{\pi}$ and $\boldsymbol{\tau}$, the compositions $\boldsymbol{\tau}^\dagger \boldsymbol{\pi}$ and $\boldsymbol{\pi}\boldsymbol{\tau}^\dagger$ are given by

$$\begin{aligned} \boldsymbol{\tau}^\dagger \boldsymbol{\pi} &= \begin{bmatrix} |\tau_1\rangle\rangle & \dots & |\tau_n\rangle\rangle \end{bmatrix} \begin{bmatrix} \langle\langle \pi_1 | \\ \vdots \\ \langle\langle \pi_n | \end{bmatrix} \\ &= \sum_{i=1}^n |\tau_i\rangle\rangle\langle\langle \pi_i | \in \mathcal{L}\left(\mathbb{C}^d\right) \to \mathcal{L}\left(\mathbb{C}^d\right), \end{aligned}$$

and

$$\begin{aligned} \boldsymbol{\pi}\boldsymbol{\tau}^\dagger &= \begin{bmatrix} \langle\langle \pi_1 | \\ \vdots \\ \langle\langle \pi_n | \end{bmatrix} \begin{bmatrix} |\tau_1\rangle\rangle & \dots & |\tau_n\rangle\rangle \end{bmatrix} \\ &= \begin{bmatrix} \operatorname{Tr}\left[\pi_1 \tau_1\right] & \dots & \operatorname{Tr}\left[\pi_1 \tau_n\right] \\ \vdots & & \vdots \\ \operatorname{Tr}\left[\pi_n \tau_1\right] & \dots & \operatorname{Tr}\left[\pi_n \tau_n\right] \end{bmatrix} \in \mathbb{R}^n \to \mathbb{R}^n. \end{aligned}$$

For any d-dimensional, n-outcome measurement $\boldsymbol{\pi}$, its pseudo-inverse $\boldsymbol{\pi}^+$ is the unique n-elements row vector of operators in $\mathcal{L}(\mathbb{C}^d)$ such that

$$\begin{aligned} \boldsymbol{\pi}\boldsymbol{\pi}^+\boldsymbol{\pi} &= \boldsymbol{\pi}, \\ \boldsymbol{\pi}^+\boldsymbol{\pi}\boldsymbol{\pi}^+ &= \boldsymbol{\pi}^+, \\ \boldsymbol{\pi}^+\boldsymbol{\pi} &= \left(\boldsymbol{\pi}^+\boldsymbol{\pi}\right)^\dagger, \\ \boldsymbol{\pi}\boldsymbol{\pi}^+ &= \left(\boldsymbol{\pi}\boldsymbol{\pi}^+\right)^\dagger. \end{aligned}$$

3.2. Quantum measurements

Leveraging on the formalism introduced in Section 3.1, for any d-dimensional, n-outcome measurement $\boldsymbol{\pi}$ we can provide the following definitions of covariance matrix Q and probability distribution $\mathbf{t}$:

$$Q := \frac{d-1}{d} (\boldsymbol{\pi} - \boldsymbol{\tau})(\boldsymbol{\pi} - \boldsymbol{\tau})^\dagger,$$

and

$$\mathbf{t} := \boldsymbol{\tau} \frac{|\mathbb{1}\rangle\rangle}{d},$$

where $\boldsymbol{\tau}$ is the d-dimensional, n-outcome measurement given by

$$\boldsymbol{\tau} := \frac{1}{d} \begin{bmatrix} \operatorname{Tr}\left[\pi_1\right] \langle\langle \mathbb{1} | \\ \vdots \\ \operatorname{Tr}\left[\pi_n\right] \langle\langle \mathbb{1} | \end{bmatrix}.$$

Notice that these definitions are consistent with those in Definition 1.

For any dimension d we denote with $\mathbb{B}_d$ the ball whose extremal points include all pure states, that is

$$\mathbb{B}_d := \left\{ \rho \in \mathcal{L}\left(\mathbb{C}^d\right) \middle| \operatorname{Tr}[\rho] = 1,\ \operatorname{Tr}\left[\rho^2\right] \le 1 \right\}.$$

Consider the image $\boldsymbol{\pi}(\mathbb{B}_d)$ of the ball $\mathbb{B}_d$ through a measurement $\boldsymbol{\pi}$. Again, this expression describes a body in the probability space parameterized by a body in the state space. The following lemma makes implicit this parametric equation by removing the dependence on the states and expressing the image of $\mathbb{B}_d$ in the form $f(\mathbf{p}) \le 0$. The lemma generalizes Theorem 1 of Ref. [25] from the qubit case to the arbitrary dimensional case.

Lemma 1 *(Implicitization of $\boldsymbol{\pi}(\mathbb{B}_d)$). For any d-dimensional, n-outcome measurement $\boldsymbol{\pi}$, the image $\boldsymbol{\pi}(\mathbb{B}_d)$ is given by the following hyper-ellipsoid:*

$$\boldsymbol{\pi}\left(\mathbb{B}_d\right) := \mathcal{E}_1(\boldsymbol{\pi}).$$

Proof. One has

$$\begin{aligned} \mathbf{p} &= \boldsymbol{\pi}|\rho\rangle\rangle \\ &= (\boldsymbol{\pi} - \boldsymbol{\tau} + \boldsymbol{\tau})|\rho\rangle\rangle \\ &= (\boldsymbol{\pi} - \boldsymbol{\tau})|\rho\rangle\rangle + \boldsymbol{\tau}|\rho\rangle\rangle \\ &= (\boldsymbol{\pi} - \boldsymbol{\tau})|\rho\rangle\rangle + \mathbf{t}. \end{aligned}$$

Hence

$$\boldsymbol{\pi}\left(\mathbb{B}_d\right) = \left\{ \mathbf{p} = (\boldsymbol{\pi} - \boldsymbol{\tau})|\rho\rangle\rangle + \mathbf{t} \middle| \operatorname{Tr}\rho = 1, \operatorname{Tr}\rho^2 \le 1 \right\}.$$

Solutions of $(\boldsymbol{\pi} - \boldsymbol{\tau})|\rho\rangle\rangle = \mathbf{p} - \mathbf{t}$ in ρ exist if and only if $\mathbf{p} - \mathbf{t}$ belongs to the range of $\boldsymbol{\pi} - \boldsymbol{\tau}$. Solutions are given by

$$|\rho\rangle\rangle = (\boldsymbol{\pi} - \boldsymbol{\tau})^+ (\mathbf{p} - \mathbf{t}) + (\mathbb{1} - \Pi)|\sigma\rangle\rangle, \tag{3}$$

where $\Pi := (\boldsymbol{\pi} - \boldsymbol{\tau})^+(\boldsymbol{\pi} - \boldsymbol{\tau})$, for any $\sigma \in \mathcal{L}(\mathbb{C}^d)$. Notice that $\Pi|\mathbb{1}\rangle\rangle = 0$ since $(\boldsymbol{\pi} - \boldsymbol{\tau})|\mathbb{1}\rangle\rangle = \mathbf{t} - \mathbf{t}$. Hence Eq. (3) is equivalent to

$$|\rho\rangle\rangle = (\boldsymbol{\pi}-\boldsymbol{\tau})^{+}(\mathbf{p}-\mathbf{t}) + \lambda\frac{|\mathbb{1}\rangle\rangle}{d} + \left(\mathbb{1}-\frac{1}{d}|\mathbb{1}\rangle\rangle\langle\langle\mathbb{1}| - \Pi\right)|\sigma\rangle\rangle,$$

again for any $\sigma \in \mathcal{L}(\mathbb{C}^d)$.

The condition $\mathrm{Tr}\,\rho = 1$ immediately implies $\lambda = 1$. Moreover, due to the Hilbert-Schmidt orthogonality of $(\boldsymbol{\pi}-\boldsymbol{\tau})^{+}(\mathbf{p}-\mathbf{t})$ and $(\mathbb{1}-|\mathbb{1}\rangle\rangle\langle\langle\mathbb{1}|/d - \Pi)|\sigma\rangle\rangle$, one has that for any σ such that $\mathrm{Tr}\,\rho^2 \le 1$, the same condition is also verified for $\sigma = 0$. Hence, without loss of generality we take $\sigma = 0$. Thus we have

$$|\rho\rangle\rangle = (\boldsymbol{\pi}-\boldsymbol{\tau})^{+}(\mathbf{p}-\mathbf{t}) + \frac{|\mathbb{1}\rangle\rangle}{d}.$$

Hence,

$$\mathrm{Tr}\,\rho^2 = (\mathbf{p}-\mathbf{t})^T(\boldsymbol{\pi}-\boldsymbol{\tau})^{+\dagger}(\boldsymbol{\pi}-\boldsymbol{\tau})^{+}(\mathbf{p}-\mathbf{t}) + \frac{1}{d}.$$

Thus, condition $\mathrm{Tr}\,\rho^2 \le 1$ becomes

$$(\mathbf{p}-\mathbf{t})^T(\boldsymbol{\pi}-\boldsymbol{\tau})^{+\dagger}(\boldsymbol{\pi}-\boldsymbol{\tau})^{+}(\mathbf{p}-\mathbf{t}) \le 1 - \frac{1}{d}.$$

Hence the statement follows. □

We are now in a position to prove Theorem 1, that we rewrite here for convenience.

Theorem 3. *For any d-dimensional, n-outcome informationally complete measurement $\boldsymbol{\pi}$, one has that $\mathcal{E}_{d-1}(\boldsymbol{\pi})$ is the maximum volume ellipsoid enclosed in $\boldsymbol{\pi}(\mathbb{S}_d)$ and $\mathcal{E}_1(\boldsymbol{\pi})$ is the minimum volume ellipsoid enclosing $\boldsymbol{\pi}(\mathbb{S}_d)$.*

Proof. First, we prove that the image $\boldsymbol{\pi}(\mathbb{B}_d)$ coincides with the minimum volume ellipsoid $\mathcal{E}(\boldsymbol{\pi}(\mathbb{S}_d))$ enclosing the image of $\mathbb{S}_d$. This can be shown as follows. First, we show that any 2-design $\{\lambda_k, \rho_k\}_k$ is a scalable frame, that is, a family of weights over states such that

$$\sum_k \lambda_k |\rho_k - \tfrac{\mathbb{1}}{d}\rangle\rangle\langle\langle\rho_k - \tfrac{\mathbb{1}}{d}| = \left(\mathbb{1} - \frac{1}{d}|\mathbb{1}\rangle\rangle\langle\langle\mathbb{1}|\right).$$

Indeed, for any state ρ we have

$$\begin{aligned}
&\sum_k \lambda_k \left(\rho_k - \tfrac{\mathbb{1}}{d}\right)\mathrm{Tr}\left[\left(\rho_k - \tfrac{\mathbb{1}}{d}\right)\left(\rho - \tfrac{\mathbb{1}}{d}\right)\right] \\
&= \sum_k \lambda_k \rho_k \,\mathrm{Tr}\left[\rho_k\left(\rho - \tfrac{\mathbb{1}}{d}\right)\right] \\
&= \mathrm{Tr}_2\left[\sum_k \lambda_k \rho_k^{\otimes 2}\left(\mathbb{1}\otimes\left(\rho - \tfrac{\mathbb{1}}{d}\right)\right)\right] \\
&= \mathrm{Tr}_2\left[(\mathbb{1}+S)\left(\mathbb{1}\otimes\left(\rho - \tfrac{\mathbb{1}}{d}\right)\right)\right] \\
&= \mathrm{Tr}_2\left[S\left(\mathbb{1}\otimes\left(\rho - \tfrac{\mathbb{1}}{d}\right)\right)\right] \\
&= \left(\rho - \tfrac{\mathbb{1}}{d}\right),
\end{aligned}$$

where S denotes the swap operator. Notice that, from Sections 6.9 and 6.11 of Ref. [26] it immediately follows that finite 2-designs exist in any dimension d, hence the existence of scalable frames in any dimension d. Then, the statement immediately follows from Theorem 2.11 of Ref. [27].

Notice that, if rescaled by constant factor $d^2 - 1$, minimum volume enclosing ellipsoids are enclosed in the convex body (see e.g. Section 8.4.1 of Ref. [28]). However, the lower bound in Theorem 1 is tighter than this, hence the need for the following independent proof.

The inner ellipsoid must include boundary states, otherwise it would not be a maximizer of the volume as it could be rescaled while remaining inside the state space. It is immediate to verify that, among all boundary states, the ones that minimize the 2-norm are the projectors of rank $d-1$. The ellipsoids we are considering lie on a plane orthogonal to the maximally mixed state. Since for the 2-norm of pure states and of the maximally mixed state one has $\mathrm{Tr}[|\phi\rangle\langle\phi|]^{1/2} = 1$ and $\mathrm{Tr}[\mathbb{1}/d^2]^{1/2} = 1/\sqrt{d}$, a direct application of the Pythagorean theorem shows that the radius of the outer ellipsoid is given by $\sqrt{1-1/d} = \sqrt{(d-1)/d}$. Since for the 2-norm of rank $(d-1)$ projectors one has that $\mathrm{Tr}[(\mathbb{1}-|\phi\rangle\langle\phi|)/(d-1)^2]^{1/2} = 1/\sqrt{d-1}$, a new application of the Pythagorean theorem shows that the radius of the inner ellipsoid is given by $\sqrt{1/(d-1) - 1/d} = \sqrt{1/(d(d-1))}$. Hence, the ratio of the two radii is $\sqrt{(d-1)/d}\sqrt{(d(d-1))} = d-1$.

Using Theorem [J] of Ref. [29], we have that the lower bound in Theorem 1 holds again in any dimension in which there exists a finite scalable frame $\{\lambda_k, \rho_k\}$ of states proportional to rank-$(d-1)$ projectors. Since for any pure state ϕ one has

$$\frac{\mathbb{1}-|\phi\rangle\langle\phi|}{d-1} - \frac{\mathbb{1}}{d} = -\frac{d}{d-1}\left(|\phi\rangle\langle\phi| - \frac{\mathbb{1}}{d}\right),$$

one has that such a scalable frame exists if and only if a scalable frame of pure states exists, hence the proof of the lower bound goes along that of the upper bound. □

3.3. Quantum states

Leveraging on the formalism introduced in Section 3.1, for any d-dimensional, n-outcome family $\boldsymbol{\rho}$ of states we can provide the following definition of covariance matrix Q:

$$Q_k := \left(k - \frac{k^2}{d}\right)(\boldsymbol{\rho}-\boldsymbol{\sigma})(\boldsymbol{\rho}-\boldsymbol{\sigma})^{\dagger},$$

where $\boldsymbol{\sigma}$ is the d-dimensional, n-outcome c-q channel given by

$$\boldsymbol{\sigma} := \frac{1}{d}\begin{bmatrix}\langle\langle\mathbb{1}| \\ \vdots \\ \langle\langle\mathbb{1}|\end{bmatrix}.$$

Notice that this definition is consistent with that in Definition 2.

For any dimension d and any $0 \le k \le d$ we denote with $\mathbb{B}_d^k$ the ball whose extremal points include all extremal effects with trace k, that is

$$\mathbb{B}_d^k := \left\{\pi \in \mathcal{L}\left(\mathbb{C}^d\right) \,\middle|\, \mathrm{Tr}\left[\pi\right] = k,\ \mathrm{Tr}\left[\pi^2\right] \le k\right\}.$$

We denote with $\mathbb{D}_d$ the symmetric d-cone whose extremal points include all extremal effects, that is

$$\mathbb{D}_d := \mathrm{conv}\cup_{k=0}^{d}\mathbb{B}_d^k.$$

Consider the image $\boldsymbol{\rho}(\mathbb{D}_d)$ of the d-cone $\mathbb{D}_d$ through a c-q channel $\boldsymbol{\rho}$. Again, this expression describes a body in the probability space parameterized by a body in the effect space. The following lemma makes implicit this parametric equation by removing the dependence on the effects and expressing the image of $\mathbb{D}_d$ in the form $f(\mathbf{q}) \le 0$. The lemma generalizes Proposition 2 of Ref. [30] from the qubit case to the arbitrary dimensional case.

Lemma 2 *(Implicitization of $\boldsymbol{\rho}(\mathbb{D}_d)$). For any d-dimensional, n-outcome c-q channel $\boldsymbol{\rho}$, the image $\boldsymbol{\rho}(\mathbb{D}_d)$ is given by the following convex hull of hyperellipsoids:*

$$\boldsymbol{\rho}\left(\mathbb{D}_d\right) := \mathrm{conv}\cup_{k=0}^{d}\mathcal{E}_1^k\left(\boldsymbol{\rho}\right).$$

Proof. One has

$$\begin{aligned}
\mathbf{q} &= \boldsymbol{\rho}|\pi\rangle\rangle \\
&= (\boldsymbol{\rho}-\boldsymbol{\sigma}+\boldsymbol{\sigma})|\pi\rangle\rangle \\
&= (\boldsymbol{\rho}-\boldsymbol{\sigma})|\pi\rangle\rangle + \boldsymbol{\sigma}|\pi\rangle\rangle \\
&= (\boldsymbol{\rho}-\boldsymbol{\sigma})|\pi\rangle\rangle + \frac{k}{d}\mathbf{u}.
\end{aligned}$$

Hence

$$\boldsymbol{\rho}\left(\mathbb{B}_d^k\right) = \left\{ \mathbf{q} = (\boldsymbol{\rho}-\boldsymbol{\sigma})\,|\pi\rangle\rangle + \frac{k}{d}\mathbf{u} \,\middle|\, \operatorname{Tr}\pi = k, \operatorname{Tr}\pi^2 \le k \right\}.$$

Solutions of $(\boldsymbol{\rho}-\boldsymbol{\sigma})|\pi\rangle\rangle = \mathbf{q} - k\mathbf{u}/d$ in π exist if and only if $\mathbf{q} - k\mathbf{u}/d$ belongs to the range of $\boldsymbol{\rho}-\boldsymbol{\sigma}$. Solutions are given by

$$|\pi\rangle\rangle = (\boldsymbol{\rho}-\boldsymbol{\sigma})^+\left(\mathbf{q} - \frac{k}{d}\mathbf{u}\right) + (\mathbb{1} - \Pi)\,|\tau\rangle\rangle, \tag{4}$$

where $\Pi := (\boldsymbol{\rho}-\boldsymbol{\sigma})^+(\boldsymbol{\rho}-\boldsymbol{\sigma})$, for any $\tau \in \mathcal{L}(\mathbb{C}^d)$. Notice that $\Pi|\mathbb{1}\rangle\rangle = 0$ since $(\boldsymbol{\rho}-\boldsymbol{\sigma})|\mathbb{1}\rangle\rangle = k\mathbf{u}/d - k\mathbf{u}/d$. Hence Eq. (4) is equivalent to

$$\begin{aligned}|\pi\rangle\rangle =& (\boldsymbol{\rho}-\boldsymbol{\sigma})^+\left(\mathbf{q} - \frac{k}{d}\mathbf{u}\right) + \lambda\frac{k}{d}|\mathbb{1}\rangle\rangle \\ &+ \left(\mathbb{1} - \frac{1}{d}|\mathbb{1}\rangle\rangle\langle\langle\mathbb{1}| - \Pi\right)|\tau\rangle\rangle,\end{aligned}$$

again for any $\tau \in \mathcal{L}(\mathbb{C}^d)$.

The condition $\operatorname{Tr}\pi = k$ immediately implies $\lambda = 1$. Moreover, due to the Hilbert-Schmidt orthogonality of $(\boldsymbol{\rho}-\boldsymbol{\sigma})^+(\mathbf{q} - k\mathbf{u}/d)$ and $(\mathbb{1} - |\mathbb{1}\rangle\rangle\langle\langle\mathbb{1}|/d - \Pi)|\sigma\rangle\rangle$, one has that for any τ such that $\operatorname{Tr}\pi^2 \le k$, the same condition is also verified for $\tau = 0$. Hence, without loss of generality we take $\tau = 0$. Thus we have

$$|\pi\rangle\rangle = (\boldsymbol{\rho}-\boldsymbol{\sigma})^+\left(\mathbf{q} - \frac{k}{d}\mathbf{u}\right) + \frac{k}{d}|\mathbb{1}\rangle\rangle.$$

Hence,

$$\begin{aligned}&\operatorname{Tr}\pi^2 \\ &= \left(\mathbf{q} - \frac{k}{d}\mathbf{u}\right)^T (\boldsymbol{\rho}-\boldsymbol{\sigma})^{+\dagger}(\boldsymbol{\rho}-\boldsymbol{\sigma})^+\left(\mathbf{q} - \frac{k}{d}\mathbf{u}\right) + \frac{k^2}{d}.\end{aligned}$$

Thus, condition $\operatorname{Tr}\pi^2 \le k$ becomes

$$\begin{aligned}&\left(\mathbf{q} - \frac{k}{d}\mathbf{u}\right)^T (\boldsymbol{\rho}-\boldsymbol{\sigma})^{+\dagger}(\boldsymbol{\rho}-\boldsymbol{\sigma})^+\left(\mathbf{q} - \frac{k}{d}\mathbf{u}\right) \\ &\le k - \frac{k^2}{d}.\end{aligned}$$

Hence the statement follows. □

We are now in a position to prove Theorem 2, that we rewrite here for convenience.

Theorem 4. *For any d-dimensional, n-outcome informationally complete family $\boldsymbol{\rho}$ of states, one has that $\operatorname{conv}\cup_{k=0}^d \mathcal{E}^k_{\eta(k,d)}(\boldsymbol{\rho})$ is the maximum volume elliptical d-cone enclosed in $\boldsymbol{\rho}(\mathbb{E})$ and $\operatorname{conv}\cup_{k=0}^d \mathcal{E}^k_1(\boldsymbol{\rho})$ is the minimum volume elliptical d-cone enclosing $\boldsymbol{\rho}(\mathbb{E})$, where*

$$\eta(k,d)^2 = (d-1)\frac{k(d-k)}{\min\left(k^2, (d-k)^2\right)}.$$

Proof. An effect $0 \le \pi \le \mathbb{1}$ is extremal if and only if it is a projector. Hence, the set $\mathbb{E}_d$ of effects is the convex hull of projectors, that is

$$\mathbb{E}_d = \operatorname{conv}\cup_{k=0}^d \left\{ \pi \in \mathcal{L}\left(\mathbb{C}^d\right) \,\middle|\, \operatorname{Tr}[\pi] = k, \pi^2 = \pi \right\}.$$

The proof proceeds along the lines of the proof of Theorem 1. First, due to Sections 6.9 and 6.11 of Ref. [26], for any dimension there exists a finite scalable frame of k-trace projectors. Then, due to Theorem 2.11 of Ref. [27], the minimum volume ellipsoid enclosing k-trace projectors is the ball $\mathbb{B}_k^d$.

The only difference with respect to Theorem 1 is that, rather than a single ellipsoid, we have a family of ellipsoids parameterized by k. For each k, the extremal effects with trace equal to k are the projectors Π_k of rank k. The effects on the boundary (that is, with at least one non-null eigenvalue) with minimum 2-norm and trace equal to k, instead, are the subnormalized (so to satisfy the trace constraint) projectors Π_{d-1} of rank $d-1$, or their subnormalized complement $\mathbb{1} - \Pi_{d-1}$. The radii R_k and r_k of the outer and inner ellipsoids, respectively, are thus given by

$$R_k^2 = \left|\Pi_k - k\frac{\mathbb{1}}{d}\right|_2^2 = \frac{dk - k2}{d},$$

and

$$\begin{aligned}r_k^2 &= \min\left(\left|\frac{k}{d-1}\Pi_{d-1} - k\frac{\mathbb{1}}{d}\right|_2^2, \left|\left(\mathbb{1} - \frac{d-k}{d-1}\Pi_{d-1}\right) - k\frac{\mathbb{1}}{d}\right|_2^2\right) \\ &= \frac{\min\left(k^2, (d-k)^2\right)}{d(d-1)}.\end{aligned}$$

The rest of the computation proceeds as in the proof of Theorem 1. □

4. Conclusion and outlook

In this paper we provided an implicit outer approximation of the image of any given quantum measurement in any finite dimension, thus generalizing a recent result [22] by Xu, Schwonnek, and Winter on the image of Pauli strings. The outer approximation that we constructed is *minimal* among all such outer approximations, and *close*, in the sense that it becomes the *maximal inner* approximation up to a constant scaling factor. We also obtained a similar result for the dual problem of implicitizing the image of the set of effects through a family of quantum states. Finally, we applied our approximation formulas to characterize, in a semi-device independent way, the ability to transform one quantum measurement into another, or one quantum statistical model into another.

CRediT authorship contribution statement

Michele Dall'Arno: Writing – review & editing, Writing – original draft, Validation, Methodology, Investigation, Formal analysis, Conceptualization. **Francesco Buscemi:** Writing – review & editing, Writing – original draft, Validation, Conceptualization.

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: Michele Dall'Arno reports financial support was provided by Japan Society for the Promotion of Science. Francesco Buscemi reports financial support was provided by Japan Society for the Promotion of Science. If there are other authors, they declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

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