Certifying dimension of quantum systems by sequential projective measurements

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This work analyses correlations arising from quantum systems subjected to sequential projective measurements to certify that the system in question necessarily has a quantum dimension greater than some dimension d. We refine previous known methods and show that dimension greater than two can be certified in scenarios which are considerably simpler than the ones presented before and, for the first time in this sequential projective scenario, we certify quantum systems with dimension strictly greater than three. We also perform a systematic numerical analysis in terms of robustness and conclude that performing random projective measurements on random pure qutrit states allows a robust certification of quantum dimensions with very high probability.

1 Introduction

With the recent development of quantum technologies and the different promising applications, it is primordial to guarantee the good functioning of the used apparatus through certification or benchmarking methods [1, 2]. Such methods can rely on fundamental properties of quantum physics to assert properties of quantum systems such as self-testing [3, 4, 5, 6], randomness certification [7, 8, 9], dimension witness [10, 11, 12, 13, 14, 15].

The notion of dimension can be defined in abstract ways such as "the maximal number of perfectly distinguishable states" or as in this paper we denote by the term dimension the dimension of a quantum system, $\mathcal{H}_d \cong \mathbb{C}_d$. It has been proved that the usage of qudits instead of qubits is beneficial in a large range of applications in quantum information such as fault-tolerant quantum computation [16, 17, 18], quantum algorithms [19, 20, 21], quantum error correction [22, 23, 24], quantum simulation [25], universal optics-based quantum computation [26] and quantum communication [27, 28].

In order to certify dimension of single quantum systems, one can use outcomes statistics from a realized experiment in a specific scenario relying on sequential measurements [12, 29, 30, 31] or contextuality [13, 32]. However, the dimension witnesses in [12, 13] are particular cases that are difficult to extend to general cases due to their complexity. Another direction is to use the so-called NPA hierarchy [33, 34] which is a numerical method that gives an arbitrary close approximation to the measurement statistics of quantum systems. Such method has been used to characterize temporal correlations [35], generalized contextuality [36, 37] and in particular to characterize dimension [38, 39]. However, the method introduced in [38, 39] is computationally expensive and does not provide insights about what scenario to use to certify what dimension.

In this work we are interested in addressing both issues at the same time. We show that for dimension certification, it is not necessary to have a good measurement statistics approximation when using the NPA hierarchy. This give a substantial reduction of the computational cost.

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We also identify a way to classify scenarios and which permit to identify good scenario for dimension certification. We finally identify the different advantages to use more experimentally challenging scenarios in order to have a more accurate and robust dimension certifying.

This paper is structured as follows. In Sec. 2, we present some preliminary notions on the numerical methods used to certify dimension of quantum systems by sequential projective measurements. In Sec. 3, we propose a method to classify scenarios based on their approximation in the NPA hierarchy and make a proposal to determine what scenario can be used based on this classification. We introduce the notion of robustness that is used to provide a certificate for the dimension. In Sec. 4, we study different scenarios compare them to each other in the perspective of dimension certification. In particular we identify a trade off between the experimental challenges to perform a scenario and a more robust dimension certification. We finally show how dimension witness can be computed from our method and provide numerical examples.

2 Bounding Finite Dimension in a Sequential Measurements Scenario

2.1 Sequential Measurements Scenario

Consider a quantum state ρ in a finite Hilbert space $\mathcal{H}_d \cong \mathbb{C}_d$ which will be subjected to sequential projective measurements described by the projectors $\Pi_{s_i|r_j}$. Each measurement has an input (or *setting*) $s \in S$ and an output (or *result*) $r \in R$ and the input and output of the i-th measurement will be denoted by s_i and r_i.

We call an *event* a representation of an output for a specific input. For instance for a single measurement, an event is $r_i|s_i$ which represents obtaining the output r_i for the input s_i for the i-th measurement. Each event is associated to a projector and for the event $r_i|s_i$ the associated projector is $\Pi_{r_i|s_i}$. Such projectors verify the following conditions, the *normalization* condition: $\sum_{r_i} \Pi_{r_i|s_i} = \mathbb{1}$, where $\mathbb{1}$ is the identity matrix and the *orthogonality* condition $\Pi_{r_i|s_i}\Pi_{r'_i|s_i} = 0$ when $r_i \neq r'_i$.

For events with multiple measurements the ordering is important as it forms a sequence, for instance, the event $r_i, r_j|s_i, s_j$ which represents obtaining the output r_i for the input s_i for the i-th measurement, then obtaining the output r_j for the input s_j for the j-th measurement.

After the first measurement on the state ρ, the post-measured state is denoted by

$$\rho_{r_1|s_1} := \Pi_{r_1|s_1}\rho\Pi^\dagger_{r_1|s_1}/\mathrm{Tr}[\Pi_{r_1|s_1}\rho\Pi^\dagger_{r_1|s_1}] \tag{1}$$

where Tr[.] denotes the trace and † is the complex conjugate. After a second measurement, the state is denoted as

$$\rho_{r_1,r_2|s_1,s_2} := \Pi_{r_2|s_2}\rho_{r_1|s_1}\Pi^\dagger_{r_2|s_2}/\mathrm{Tr}[\Pi_{r_2|s_2}\rho_{r_1|s_1}\Pi^\dagger_{r_2|s_2}]. \tag{2}$$

Fig. 1 illustrates the case of three sequential measurements on the state ρ.

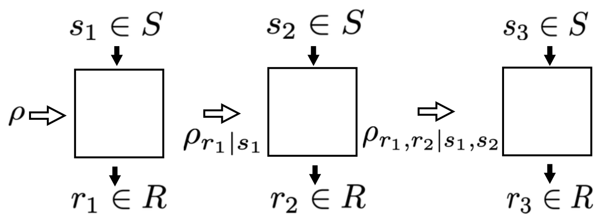

Figure 1: Sequential measurements scenario. Each measurement has an input (or *setting*) $s \in S$ and an output (or *result*) $r \in R$ and the input and output of the i-th measurement will be denoted by s_i and r_i.

For simplicity we denote the sequence of outputs $\mathbf{r} = (r_1, \ldots, r_n)$ and the sequence of settings $\mathbf{s} = (s_1, \ldots, s_n)$. The measurement operato (composition of projectors is not a projector) associated to the event $\mathbf{r}|\mathbf{s}$ is $\Pi_{\mathbf{r}|\mathbf{s}} = \Pi_{r_n|s_n} \ldots \Pi_{r_1|s_1}$.

The probability to have the event $\mathbf{r}|\mathbf{s}$ is given by the Born's rule:

$$P(\mathbf{r}|\mathbf{s}) = \mathrm{Tr}[\Pi_{\mathbf{r}|\mathbf{s}}\rho\Pi^\dagger_{\mathbf{r}|\mathbf{s}}], \tag{3}$$

In what follows, we consider the case where the set of measurements to choose from is the same for each measurement through the sequence. Moreover, we consider the case where all measurements have the same number of outcomes. Under such assumption, a scenario is characterized by three following parameters:

- The number of measurements: m.
- The maximum length of sequence of measurements: l.
- The number of outcomes for each measurements: o.

We call the MLO (Measurement, Length, Outcomes) representation of a scenario the triplet: m-l-o. As an example the Leggett-Garg scenario [40] correspond to the 3-2-2 scenario.

We call a *behavior*, $\mathbf{P} := \{P(\mathbf{r}|\mathbf{s})\}_{\mathbf{rs}}$, the probability distribution over all the possible events in given sequential measurement scenario. In what follow, we address the issue of certifying dimension by their behaviors. In other words, we are interested to know whether for a behaviour represented by an outcomes statistic $P(\mathbf{r}|\mathbf{s})$, there exist a d-dimensional state $\rho \in \mathcal{H}_d$ and a set of projective measurements $\{\Pi_{r_i|s_j}\}_{ij}$ such that $P(\mathbf{r}|\mathbf{s}) = \mathrm{Tr}(\Pi_{\mathbf{r}|\mathbf{s}}\rho\Pi^\dagger_{\mathbf{r}|\mathbf{s}})$.

2.1.1 Unrestricted Dimensional case

We first present the study of behaviors of quantum systems in a sequential measurements scenario without dimensional constraints [35]. To this end we introduce the so-called moment matrix representation. A moment matrix M is a symmetric square matrix which entries, in this case, are all the expectation values of the product of pairs of $\Pi_{\mathbf{r}|\mathbf{s}}$. We adopted the specific representation used in [33, 35], where in the set of projectors, for each setting $\mathbf{s}$, one of the result $\mathbf{r}$ is left out and we add the identity matrix to the list of projectors. The matrix elements of the moment matrix M are:

$$M_{\mathbf{r}|\mathbf{s},\mathbf{r}'|\mathbf{s}'} := \mathrm{Tr}[\Pi^\dagger_{\mathbf{r}|\mathbf{s}}\Pi_{\mathbf{r}'|\mathbf{s}'}\rho], \tag{4}$$

where we use the notation $\Pi_{\mathbf{0}|\mathbf{0}} = \mathbb{1}$ to include the identity matrix. Note that $M_{\mathbf{0}|\mathbf{0},\mathbf{r}|\mathbf{s}} = M_{\mathbf{r}|\mathbf{s},\mathbf{0}|\mathbf{0}} = M_{\mathbf{r}|\mathbf{s},\mathbf{r}|\mathbf{s}} = P(\mathbf{r}|\mathbf{s})$.

It follows from Born's rule that the moment matrix from a behaviour with a quantum realization is positive semidefinite ($M \geq 0$), and satisfies

$$M_{\mathbf{r}|\mathbf{s},\mathbf{r}'|\mathbf{s}'} = M_{\mathbf{r}''|\mathbf{s}'',\mathbf{r}'''|\mathbf{s}'''} \tag{5}$$

when $\Pi^\dagger_{\mathbf{r}|\mathbf{s}}\Pi_{\mathbf{r}'|\mathbf{s}'} = \Pi^\dagger_{\mathbf{r}''|\mathbf{s}''}\Pi_{\mathbf{r}'''|\mathbf{s}'''}$. Moreover, when no constraints on the dimension are imposed, Ref. [35] exploited the methods of [33, 34] to prove a *completness* relation, that is, every positive semidefinite operator M respecting the conditions of (5) and $M_{\mathbf{0}|\mathbf{0},\mathbf{0}|\mathbf{0}} = 1$ have a quantum realization. Note that this simple completeness relation does not hold when dimensional constraints are imposed [39], this point is discussed in details in Sec. 2.1.2.

From here that are two types of problem that we will encounter in what follows:

- *Feasibility problem*: For a given behavior $P(\mathbf{r}|\mathbf{s})$, there exists a d-dimensional quantum realization. This problem will be further described in Sec. 3.3.
- *Optimization problem*: Given a set of real coefficient, $\gamma_{\mathbf{r}|\mathbf{s}}$ what is the maximum value of $\sum_{\mathbf{r},\mathbf{s}}\gamma_{\mathbf{r}|\mathbf{s}}P(\mathbf{r}|\mathbf{s})$. For such optimization it is convinient to use moment matrices with linear objective function as shown in Eq. 6a which is given by a semidefinite program (SDP).

When the dimension is unrestricted the *optimization problem* can be written as follows:

$$\begin{aligned} p^* := \max_{M} \quad & \sum_{\mathbf{r},\mathbf{s}} \gamma_{\mathbf{r}|\mathbf{s}} M_{\mathbf{r}|\mathbf{s},\mathbf{r}|\mathbf{s}} && \text{(6a)}\\ \text{s.t.} \quad & M_{\mathbf{0}|\mathbf{0},\mathbf{0}|\mathbf{0}} = 1, && \text{(6b)}\\ & M \succeq 0, && \text{(6c)}\\ & M_{\mathbf{r}|\mathbf{s},\mathbf{r}'|\mathbf{s}'} = M_{\mathbf{r}''|\mathbf{s}'',\mathbf{r}'''|\mathbf{s}'''}, \\ & \text{if } \Pi^\dagger_{\mathbf{r}|\mathbf{s}}\Pi_{\mathbf{r}'|\mathbf{s}'} = \Pi^\dagger_{\mathbf{r}''|\mathbf{s}''}\Pi_{\mathbf{r}'''|\mathbf{s}'''}. && \text{(6d)} \end{aligned}$$

This becomes useful to characterize behaviors via inequalities as shown in [35]. This approach can be used to verify the possible quantumness of a behavior regardless of the dimensionality of its quantum realization.

2.1.2 Finite Dimensional case

We present the case of certifying the dimension of a quantum system via its behavior in a sequential measurements scenario. Using the Peres-Mermin square [41, 42] it is possible to derive a state-independent quantum dimension witnesses to separate qubits' behaviors from the above dimensions [12]. However, this method can only be used to separate qubits from the above dimension and is only based on a specific *optimization problem* or witness. Generally, the *optimization problem* can be represented by what follows

$$\begin{aligned} p^*_d := \max_{\mathcal{H},\mathbf{X},\rho} \quad & \mathrm{Tr}[p(\mathbf{X})\rho] && \text{(7a)}\\ \text{s.t.} \quad & \dim(\mathcal{H}) \leq d, && \text{(7b)}\\ & q_i(\mathbf{X}) \succeq 0, \forall i \in \{1,\ldots,q\}, && \text{(7c)} \end{aligned}$$

where $\mathbf{X}$ is a set of observables, $p(.)$ and $q_i(.)$ are polynomial functions and d and q are both integers.

This is more general than the case we actually need to consider here as we might not impose any constraints represented by the $q_i(.)$ polynomials. However, the optimization problem described in Eq. 8 is regularly encountered in quantum information. For instance, in contextuality, one of the simplest known inequality is the so-called KCBS inequality [43]. It resembles very much to a sequential measurement scenario as we consider with an MLO of 5-2-2, where we impose commutation relationships as $[X_i, X_{i+1}] = 0$.

$$
\begin{aligned}
p^*_{d,KCBS} :=& \max_{\mathcal{H},\mathbf{X},\rho} && \mathrm{Tr}[\sum_{i=1}^{5} X_i X_{i+1} \rho] && \text{(8a)}\\
& \text{s.t.} && \dim(\mathcal{H}) \leq d, && \text{(8b)}\\
& && [X_i, X_{i+1}] = 0, \forall i \in \{1, \ldots, 5\}. && \text{(8c)}
\end{aligned}
$$

While this optimization program has a clear interpretation it is not straight forward to solve it. However, it is possible to re-express it using the moment matrix representation to solve the optimization problem via a hierarchy of semidefinite programming relaxations [38, 39]. The k-th level of the hierarchy has the following SDP formulation:

$$
\begin{aligned}
p^*_{d,k} :=& \max_{M} && \sum_{\mathbf{r},\mathbf{s}} \gamma_{\mathbf{r}|\mathbf{s}} M_{\mathbf{r}|\mathbf{s},\mathbf{r}|\mathbf{s}} && \text{(9a)}\\
& \text{s.t.} && M_{\mathbf{0}|\mathbf{0},\mathbf{0}|\mathbf{0}} = 1, && \text{(9b)}\\
& && M \in \mathcal{M}^k_d, && \text{(9c)}\\
& && M \succeq 0, && \text{(9d)}
\end{aligned}
$$

where the set $\mathcal{M}^k_d$ represents the linear span of the space of moment matrices with a quantum realization satisfying the constrains in Eq. 7c with a quantum system of dimension d and where k indicates that the moment matrices correspond to a maximum length of sequence given by the one define in the scenario (see the MLO scenario representation in Sec. 2.1) increased by the value $k-1$. hence the first level of the hierarchy correspond to the scenario and the second level correspond to the set of moment matrices with the maximum length of sequences is increased by one.

Each level of the hierarchy in Eq. 9 gives an approximation of the problem defined in Eq. 9 such that $p^*_{d,k} \geq p^*_d$. We denote by $\mathcal{Q}^k_d$ the set of behaviors from a specific level k of the hierarchy and for a specific dimension d and we called $\mathcal{Q}_d$ the set of behavior corresponding to Eq. 9.

For any level k we are ensured to have and outer approximation $\mathcal{Q}_d \subseteq \mathcal{Q}^k_d$ (as illustrated in Fig. 2). Also, in [39] it is shown that for sufficiently large k, the hierarchy converges to the set of quantum d-dimension correlations, that is, there exist a K such that $\mathcal{Q}^{k>K}_d = \mathcal{Q}_d$.

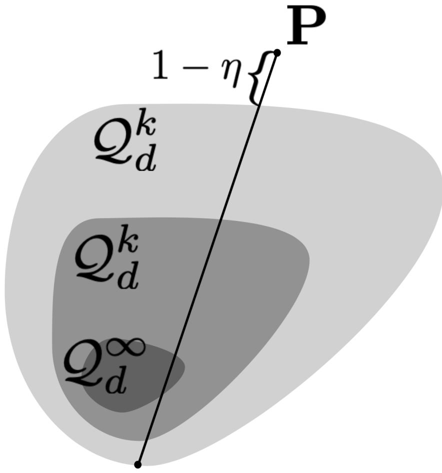

Figure 2: Schematic representation of the sets of behaviors in the different level of the hierarchy such that $\mathcal{Q}^\infty_d \subseteq \mathcal{Q}^k_d \subseteq \mathcal{Q}^1_d$. A behavior $\mathbf{P}$ is given, with $\mathbf{P} \notin \mathcal{Q}^1_d$. We have represented the visibility η computed with the generalized robustness (see Sec. 3.3).

In [39], it was shown that for some fixed level k of the hierarchy the set $\mathcal{Q}^k_d$ may be strictly larger than $\mathcal{Q}_d$. Here we illustrate this fact by presenting a different example. In the the guess-your-neighbor's-input inequality [44], in particular in its sequential measurement scenario [35]. It is a sequential scenario with a MLO of 2-3-2. The inequality is:

$$
P(000|000) + P(110|011) + P(011|101) + P(101|110) \leq 1. \quad (10)
$$

Reference [35] evaluated the SDP in Eq. 6 to find the maximum value $p^* \approx 1.0225$ when the dimension is unrestricted. Here we have used the methods discussed in [39] to obtain $p^*_{2,1} \approx 1.1588$ for the maximum value for the first level of the hierarchy for a qubit system. This show that in the scenario 2-3-2, in the first level of the hierarchy for qubit, and provides a direct proof that completeness is not satisfied in the restricted dimension case. This also shows that in the scenario 2-3-2, in the first level of the hierarchy for qubit, some behavior do not admit quantum realization. Hence, the first level of the hierarchy is not enough to fully characterize the set $\mathcal{Q}_d$ of sequential quantum correlations. This example is further discussed in the Appendix A and the code is provided in [45].

3 Methods and Proposal

As discussed in Eq. 9, one way to characterize the set $\mathcal{M}_d^k$ involves finding a basis for its linear span. In this section we provide a refinement of the random method proposed in Ref. [38, 39] to obtain such basis. Our refinement consists in a systematic method to ensure that the random procedure has obtained the desired basis.

3.1 Building a Basis of Moment Matrices

By using the randomized method described in Append. B, it is possible to construct multiple moment matrices from which a basis can be constructed. One way is to find the highest number of linearly independent (LI) moment matrices or by using the Gram-Schmidt process on a set of moment matrices until the zero matrix is left through the process. We use the second method while keeping the number of linearly independent moment matrices to characterizecheterize a scenario for a specific dimension and level in the hierarchy.

An efficient way to build a basis using the Gram Schmidt process is to generate a random moment matrix and using the standard Gram Schmidt process on this matrix with the previously generated moment matrices. By checking the norm of the matrix after removing the 'projections' from the previous moment matrices and at each iteration we can find when only the null matrix is left and decide to stop the process. Due to numerical precision the resulting matrix will be non zero but small enough to be detected. In Fig. 3 we show the norm of the resulted moment matrices after each iteration in the scenario. We clearly see a drop of the norms through the iterations. Hence the number of LI moment matrices is the number of iteration just before such drop. We can clearly see that such drop does not appear at the same position depending on the dimension considered. Further detail on that is presented in Sec. 3.2.

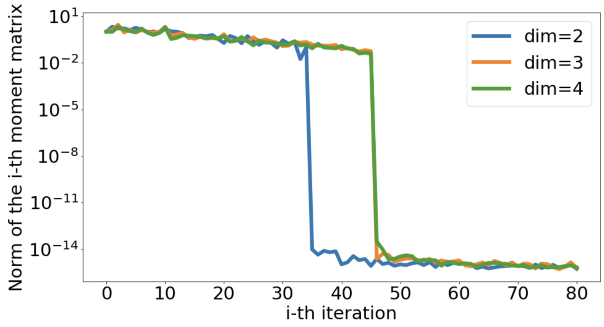

Figure 3: Norm (in log scale) of the i-th moment matrix during the Gram Schmidt process in the 3-2-2 scenario at the first level of the hierarchy and for $d \in \{2, 3, 4\}$. We can see that for all considered cases we observe a clear drop of the norm to zero (up to numerical artefacts) indicating when to stop the Gram Schmidt Process.

3.2 Classification via Basis Cardinal

A basis of the set of the moment matrices, $\mathcal{M}_d^k$, can be constructed following the randomized method described in Sec.3.1. The number of elements in the basis depends on the scenario (the MLO), the level of the hierarchy k and the dimension of the Hilbert space d.

In Fig. 4 is represented the number of elements of the basis as a function of the dimension in different scenarios. In the tested scenarios with MLO m-l-2 with $m \in \{2, 3, 4, 5, 6\}$ for $l = 2$ and $m \in \{2, 3, 4, 5\}$ for $l = 3$ the number of elements in the basis is the same for $d = \{3, 4, 5\}$ and smaller for $d = 2$. This already tell us the following important information, in these considered scenarios we have $\mathcal{Q}_{d=2}^{k=1} \subset \mathcal{Q}_{d>2}^{k=1}$.

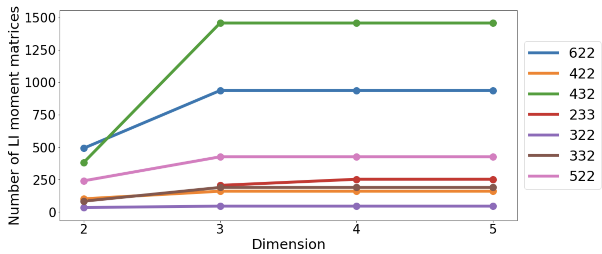

Figure 4: Maximal number of linearly independent (LI) moment matrices in the sets $\mathcal{M}_{d\in[2,3,4,5]}^{k=1}$.

To quantify this gap, in Fig. 5 is represented the ratio between the number of elements of the basis for $d = \{3, 4, 5\}$ and $d = 2$ as a function of the number of measurements in the m-2-2 scenario.

Another curve in Fig. 4 corresponds to the scenario 2-3-3 for $d = \{3, 4, 5\}$. In this scenario we

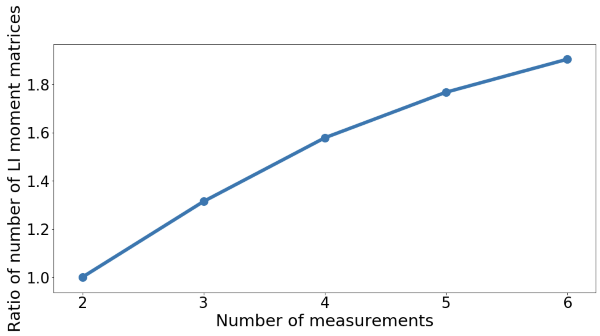

Figure 5: Ratio between the number of elements of the basis for $d = \{3, 4, 5\}$ (they are all equal in this case) and $d = 2$ as a function of the number of measurements in the m-2-2 scenario.

see that the number of linearly independent moment matrices for $d = 3$ is smaller than the one for $d = \{4, 5\}$. Hence in the 2-3-3 scenario, we have $\mathcal{Q}^{k=1}_{d=3} \subset \mathcal{Q}^{k=1}_{d>3}$.

3.3 Proposal

Comparing the numbers of elements in the basis of moment matrices in a way that has been presented in Sec. 3.2 only gives insights about the geometry of sets with different dimensions at the same level of the hierarchy. With this method and in order to certify a minimum dimension of a quantum system from its behavior, one could try to derive the basis for higher level of the hierarchy until its convergence. However, deriving the method is indeed computationally expensive and potentially subject to error due to numerical precisions.

The other option is to use that the fact that $\mathcal{Q}_d \subset \mathcal{Q}^k_d$. In this case if we could test whether a given behavior $\mathbf{P}$ is not in $\mathcal{Q}^k_d$. If it is the case then we know that $\mathbf{P} \notin \mathcal{Q}_d$. But if one find that $\mathbf{P} \in \mathcal{Q}^k_d$ this does not imply $\mathbf{P} \notin \mathcal{Q}_d$. In this method one can certify a minimum dimension of quantum system by its behavior without the need to characterize moment matrices sets at a computationally challenging level of the hierarchy.

In addition of simply testing if a given behavior $\mathbf{P}$ belongs to $\mathcal{Q}^k_d$, we are also going to quantify "how much" the behavior is outside the set $\mathcal{Q}^k_d$. This will be done by means of robustness, which is analogous to the robustness of entanglement [46] and have also been used to quantify quantum EPR-steering [47], measurement incompatibility [48, 49], indefinite causality [50], coherence [51, 52],and other quantities in quantum information theory. Given a behavior $\mathbf{P}$, the general robustness visibility is

$$\begin{aligned} & \text{given } \mathbf{P} := \{P(\mathbf{r}|\mathbf{s})\}_{\mathbf{r},\mathbf{s}} \\ \nu := \quad & \max_{\eta, \mathbf{P}_{d,k}} \eta \\ & \text{s.t. } \eta\mathbf{P} + (1-\eta)\mathbf{P}_{d,k} \in \mathcal{Q}^k_d \\ & \mathbf{P}_{d,k} \in \mathcal{Q}^k_d, \end{aligned} \tag{11}$$

we can then see that when $\nu < 1$, we have $\mathbf{P} \notin \mathcal{Q}^k_d$. In Fig. 2 is represented this quantity. Also, if the quantum system describing the experiment is given by ρ, we can ensure that there exists a quantum state σ such that for every visibility $\eta > \nu$, the noisy state $\eta\rho + (1-\eta)\sigma$ can generate behaviors which are not inside $\mathcal{Q}^k_d$. Interestingly, when solving the robustness optimization problem presented in Eq. (11), one also obtains a dimension witness to certify the dimensionality of the given behavior, this topic will be discussed in Sec. 4.2.1. Further details and a reformulation of this problem simpler for computer codes can be found at the Appendix C.

4 Main Results

4.1 Certifying Dimension in the m-l-2 Scenario

4.1.1 3-2-2 Scenario

In order to make a step further in the understandings of the geometry of the sets, we focus here on the specific 3-2-2 scenario, namely the Leggett-Garg scenario [40] which is the simplest known sequential measurement scenario to observe quantum features. In particular, with an eye toward certifying dimensions, a legitimate question is wheter in the 3-2-2 scenario there exists a behavior given by a qutrit system that cannot be reproduce by any qubit system. In other words, is there a behavior $\mathbf{P} \in \mathcal{Q}_3$ such that $\mathbf{P} \notin \mathcal{Q}_2$. We show that the answer is yes and using our method, this question can be addressed without the need to fully characterize the set of qubit's behavior, $\mathcal{Q}_2$, as the first level of the SDP hierarchy [38, 39], $\mathcal{Q}^1_2$, turns out to be sufficient.

To go even further, we estimate the probability $P(\mathbf{P} \notin \mathcal{Q}^k_2 | \mathbf{P} \in \mathcal{Q}_3)$, the probability for a qutrit's behavior, $\mathbf{P} \in \mathcal{Q}_3$, to be outside the set $\mathcal{Q}^k_2$ for a given k characterizing the level of the hierarchy. From a geometrical perspective, this probability is related to the following volume ratio:

$$P(\mathbf{P} \notin \mathcal{Q}_2^k|\mathbf{P} \in \mathcal{Q}_3) = \frac{V(\overline{\mathcal{Q}_3 \cap \mathcal{Q}_2^k})}{V(\mathcal{Q}_3)}, \qquad (12)$$

where $V(.)$ denotes the volume of the set.

We evaluate the probability $P(\mathbf{P} \notin \mathcal{Q}_2^k|\mathbf{P} \in \mathcal{Q}_d)$ for $d \in \{3,4,5\}$ and $k \in \{1,2\}$. In order to evaluate this probability, we first build the basis of moment matrices $\mathcal{M}_2^{k\in\{1,2\}}$ for the sets $\mathcal{Q}_2^{k\in\{1,2\}}$ with the method described in Sec. 3.1. Then, with the same method, we also sample the sets $\mathcal{Q}_{d\in\{3,4,5\}}$ and compute the visibilities (defined in Eq.11) for each sampled data point. For that purpose we used CVXPY [53, 54] with the solver MOSEK [55]. We used about 10000 points to evaluate each probability. Note that the evaluation of the volume depends on the measure used to sample the space of states and quantum measurements and corresponds to the *Haar measure* in our case (see Sec. B). The code is available in [45].

The probability is evaluated in the following way:

$$P(\mathbf{P} \notin \mathcal{Q}_2^k|\mathbf{P} \in \mathcal{Q}_3) \approx \frac{N(\nu < 1)}{N_{tot}}, \qquad (13)$$

where $N(\nu > 1)$ represents the number of data points with a visibility $\nu > 1$ and N_{tot} is the total number of data points. This ratio gives an approximation of the ratio of the volumes in Eq. 12.

Finally all the computed probabilities are represented in the Tab. 1. As these probabilities are non zero, there are possibilities to find qutrit's behaviors in the 3-2-2 scenario that cannot be reproduce by any qubit's behavior. To obtain this information it is not necessary to characterize the set of qubit's behavior $\mathcal{Q}_2$ directly. This is because the probability $P(\mathbf{P} \notin \mathcal{Q}_2^1|\mathbf{P} \in \mathcal{Q}_3) \approx 0.37$ and $\mathcal{Q}_2 \subset \cdots \subset \mathcal{Q}_2^2 \subset \mathcal{Q}_2^1$.

d	$k=1$	$k=2$
3	0.365198	0.392267
4	0.268526	0.317939
5	0.215904	0.247898

Table 1: Probability, $P(\mathbf{P} \notin \mathcal{Q}_2^k|\mathbf{P} \in \mathcal{Q}_d)$, for a behavior in $\mathcal{Q}_{d\in\{3,4,5\}}$ to be outside $\mathcal{Q}_2^{k\in\{1,2\}}$.

Moreover, we have $P(\mathbf{P} \notin \mathcal{Q}_2^1|\mathbf{P} \in \mathcal{Q}_3) < P(\mathbf{P} \notin \mathcal{Q}_2^2|\mathbf{P} \in \mathcal{Q}_3) \approx 0.39$. Hence, a behavior $\mathbf{P} \in \mathcal{Q}_3$ has more chance to be outside the second level of the hierachy than the first level. This corresponds well to $\mathcal{Q}_2^2 \subset \mathcal{Q}_2^1$. For all the dimension $d \in \{3,4,5\}$, we have $P(\mathbf{P} \notin \mathcal{Q}_2^1|\mathbf{P} \in \mathcal{Q}_d) < P(\mathbf{P} \notin \mathcal{Q}_2^2|\mathbf{P} \in \mathcal{Q}_d)$ as shown in Tab. 1.

A result that could seem counterintuitive is when we compare the probabilities for different dimension for the same level of the hierarchy. We find that $P(\mathbf{P} \notin \mathcal{Q}_2^k|\mathbf{P} \in \mathcal{Q}_d) < P(\mathbf{P} \notin \mathcal{Q}_2^k|\mathbf{P} \in \mathcal{Q}_{d'})$ for $d < d'$ with $d, d' \in \{3,4,5\}$. This could sound counterintuitive as we would expect that higher dimension could at least perform as good as the lower dimensions.

The source of these differences is related to the sampling method. Following the discussion in Append. B, larger dimension means larger number of options for binning for the projectors and the use of the Haar measure to sample unitary matrices does not necessarily guarantee uniformity at the behaviors level as well. Moreover, this is related to the so-called Bertrand's Paradox [56], which shows that probabilities may not be well defined as they rely on the method used to produce random variables. In the Bertrand's Paradox, the method used to sample through a circle affects the probabilities. We make the analogy here, where sampling behaviors from different Hilbert spaces of different dimensions impacts the resulted probabilities. For that reasons the values presented in Tab. 1 are not absolut and the different dimension are not comparable. However, within a dimension, as the sampling is the same, the order relationship is not affected: $P(\mathbf{P} \notin \mathcal{Q}_2^1|\mathbf{P} \in \mathcal{Q}_3) < P(\mathbf{P} \notin \mathcal{Q}_2^2|\mathbf{P} \in \mathcal{Q}_3)$.

The results showed in Tab. 1 has two main consequences on our understandings of certifying dimensions of quantum systems via their behaviors. First, in the 3-2-2 scenario, the Leggett-Garg inequality [40] is already maximally violated by a qubit's behavior. However, our results implies that the 3-2-2 scenario is sufficient and inequalities based certification could be build (see Sec. 4.2.1). Secondly, the only know way to certify qubit from the above dimensions is through the Peres-Mermin square [12], which corresponds to the 9-3-2 scenario. Our results provide a reduction of the previously known results by six measurements and shorten the length of the sequence of measurements by one which is much more favorable to experimental perspectives.

4.1.2 Advantage to certify dimension in the m-l-2 Scenario

In the previous section, in Sec. 4.1.1, we show that the scenario 3-2-2 can be used to certify some qutrit (and above dimension) behaviors from qubit's behaviors by only using the first level of the hierarchy. Moreover, as shown in Tab. 1 using to the second level increases the chance of success. In what follow we show what are the advantage to either increase the number of measurements (m-2-2 scenarios) or to increase the maximum length of the sequence of measurements (3-l-2 scenarios).

Following the method explained in Sec. 4.1.1 we evaluate the probability for a random qutrit behavior, $\mathbf{P} \in \mathcal{Q}_3$, not to be explained by the approximation of any qubit behavior at the first level of the hierarchy. In other words, we want to evaluate $P(\mathbf{P} \notin \mathcal{Q}_2^1 | \mathbf{P} \in \mathcal{Q}_3)$ in the scenario $m-2-2$ for $m \in \{3, \dots, 8\}$.

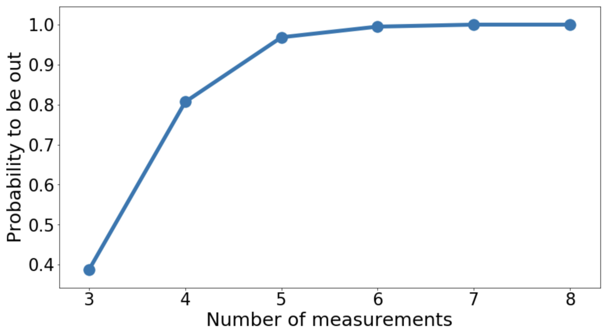

Figure 6: Probability of a random qutrit behavior not to be reproduce by a behavior in the first level of the hierachy of qubit behaviors in the m-2-2 scenario.

In Fig 6, we show that such probability increases in a log-like manner until it reaches the value of 1 in our numerical analysis. Because of numerical precision, we obtain the value 1 but it is most likely that this log-like curve actually converges to 1 instead. Regardless of how close to the value 1 it is, it seems that using more than 5 or 6 measurements do not bring any critical advantage when trying to certify dimension in this scenario. However, compared to the 3-2-2 scenario, with a probability approximately 0.37, by using one additional measurement (4-2-2 scenario), this probability increases to approximately 0.81, which is about the double and by using two additional measurements (5-2-2 scenario), this probability increases to approximately 0.96, which is about the 2.6 times larger than in the 3-2-2 scenario.

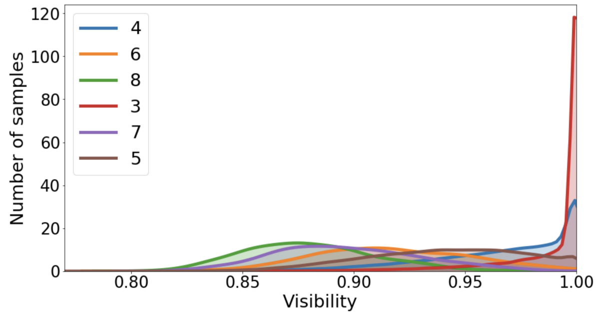

Figure 7: Critical visibility to ensure that a random qutrit behaviors is outside of the first level of the hierarchy of qubit behavior in the m-2-2 scenario.

As explained in Sec. 4.1.1 and in particular in Eq.13, the probabilities are evaluated by using the visibility. Looking at the distribution of the visibility provides also a very good insight as the visibility has a good geometrical interpretation and gives a more fine grain level of information. In Fig 7, we show the distribution of the visibilities of random qutrit behaviors, $\mathbf{P} \in \mathcal{Q}_3$ compared to the set $\mathcal{Q}_2^1$ in the scenario $m-2-2$ for $m \in \{3, \dots, 8\}$. Interestingly all the distributions are different in way that when the number of measurement increases in the scenario m-2-2, the distribution's mean value becomes smaller. From a geometric perspective, one can say that the behaviors are farer to qubit behaviors when the number of measurement increases.

The other parameter that is possible to change experimentally is the length of the sequence of measurement used in the experimental setup. It is important to clarify that this is different compare to changing the level of the hierarchy. In the case where we increase the length experimentally we need to collect data for the right length of sequence, while by increasing the level of the hierarchy these data would not be given. In Fig 8 we show the distribution of the visibility of random qutrit behaviors, $\mathbf{P} \in \mathcal{Q}_3$, compared to the set of qubit behavior at the first level of the hierarchy in the scenario $3-l-2$ for $l \in \{3, 4\}$. Similarly to the number of measurements, increasing the length of the sequence of measurements makes the behavior farer to the set of qubit behaviors.

Our analysis shows that there are advantages to either increase the number of measurements (m-2-2 scenarios) or to increase the maximum length of the sequence of measurement (3-l-2 scenarios) to increase the change to certify qutrit behaviors from qubit behaviors. These two pa-

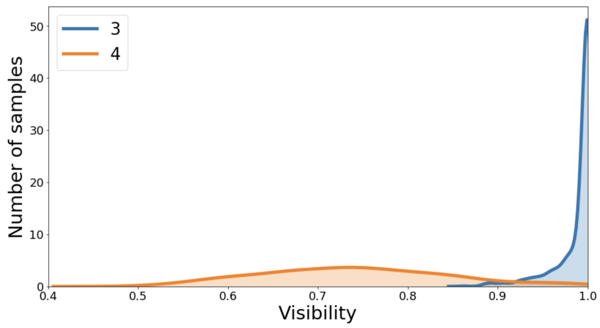

Figure 8: Critical visibility to ensure that a random qutrit behaviors is outside of the second level of the hierarchy of qubit behavior in the 3-l-2 scenario.

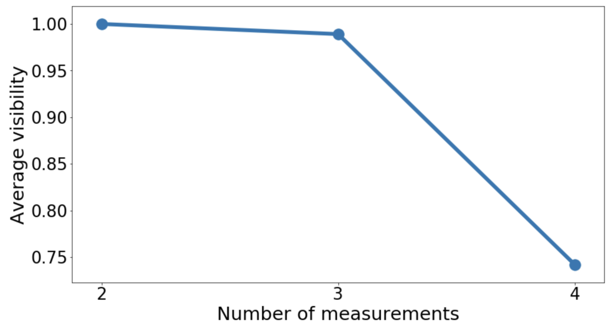

Figure 10: Average visibility of random qutrit behaviors compared to the first level of the hierarchy of qubit behavior in the 3-l-2 scenario for $l \in \{2, 3, 4\}$.

rameters require a change in the experimental setup when collecting data while when by increasing the level of the hierarchy it is only about the data processing on a classical computer. While we show that increasing the number of measurements or increasing the maximum length of the sequence of measurement, there are also noticeable differences. Indeed, in the scenario 8-2-2 the average visibility is 0.88 (see Fig. 9) while in the 3-4-2 scenario the average visibility is about 0.75. (see Fig. 10) Hence, increasing the length of the sequence of measurements seems more effective. However, this could be more challenging from an experimental point of view.

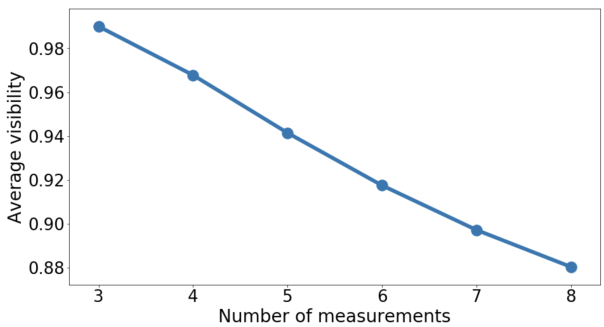

Figure 9: Average visibility of random qutrit behaviors compared to the first level of the hierarchy of qubit behavior in the m-2-2 scenario for $m \in \{3, \dots, 8\}$.

Our analysis on the distribution of the visibility also shows that increasing one of these parameters, could make an experiment more robust to noise. Because of experimental precisions it might sometimes not be clear whether a qutrit behavior could be obtained with a qubit system. A solution to this issue is to prefer a scenario where behaviors are not likely to be close (in a geometrical way) to qubit behaviors. Another important result, is when increasing these parameters, even with random measurements, it becomes possible to certify almost all genuine qutrit behaviors from any qubit behavior. This is promising for applications where dimension is critical.

4.2 Dimension Witnesses from the Robustness' Dual

4.2.1 Building Dimension Witness for qubits

Witnesses are simple to use and commonly used to test quantum properties in an experimental setup. From a geometric perspective, they correspond to hyperplanes in the probability space. In Sec. 2.1.1 we present what we call the *feasability problem* to test whether a given behavior admits a quantum realization with a specific dimension d. A partial answer to this decision problem could be done by using the hyperplane in an inequality form when one ensures that all the behaviors from quantum realizations with a specific dimension d do not violate the inequality as a consequence of the hyperplane separation theorem. Hence, when the inequality is violated we can infer that the behavior does not admit a quantum realization of dimension d.

When a behavior $\mathbf{P}'$ does not belong to the set $\mathcal{Q}_d^k$, one can always find a set of real coefficients $\{\gamma_{\mathbf{r}|\mathbf{s}}\}_{\mathbf{rs}}$ and a real number x such that

$$\sum_{\mathbf{r},\mathbf{s}} \gamma_{\mathbf{r}|\mathbf{s}} P_{d,k}(\mathbf{r}|\mathbf{s}) \geq -x, \forall \mathbf{P}_{d,k} \in \mathcal{Q}_d^k, \quad (14)$$

but

$$\sum_{\mathbf{r},\mathbf{s}} \gamma_{\mathbf{r}|\mathbf{s}} P'(\mathbf{r}|\mathbf{s}) < -x. \quad (15)$$

Moreover such inequality can be explicitly obtained by means of the dual formulation of the robustness optimization problem presented in

Eq. (11). We present the details on the dual formulation and how to construct such inequalities on the Appendix C. Also, to demonstrate this technique, we provide an explicit example (available at the github repository [45]) in the scenario 3-2-2, where we obtained a randomly generated behavior from a qutrit and solve the generalized robustness problem. The inequality we obtain can be used in any experiment in the scenario 3-2-2 to test if the experimentally obtained behavior does not admit a a quantum realization with a qubit.

4.3 Higher Dimension Witness

As it has been shown in Sec. 3.2 and in Fig. 4, in the 2-3-3 scenario, we have $\mathcal{Q}^{k=1}_{d=3} \subset \mathcal{Q}^{k=1}_{d>3}$. This suggests that there might be ququart behaviors that cannot be obtain via qutrit behaviors as we have seen it is the case to certify dimension higher than two in the m-l-2 scenario presented in Sec.4.1.2. Following the same method used in Sec.4.2.1, we provide an explicit example of an dimension witness and a ququart quantum state and quantum measurements (available at the github repository [45]) which behavior cannot be reproduced by qutrit behaviors. This is done by generating a random ququart behavior in the 2-3-3 scenario and computing its visibility regarding the set $\mathcal{Q}^{1}_{d=3}$. Once such behavior is found we can find the dimension witness by using the dual problem of the generalized robustness.

5 Conclusion

In this work we have refined the known methods that analyze correlations arising from quantum systems subjected to sequential projective measurements to certify that the system in question necessarily has a quantum dimension greater than some dimension d. We showed that, in the context of dimension certification, it is not necessary to go at high level in the NPA hierarchy and in all the examples we have treated the first level of the hierarchy was already sufficient to certify dimensions.

We have shown that scenarios can be classified by the number of elements in the moment matrices basis at the first level of the hierarchy. For all the scenarios where different dimensions have different number of basis elements we have proved that dimension can be certified in these scenarios. While this seems convincing to say that this property is a necessary condition it is an open problem. Moreover, we demonstrated that the randomized method to build the basis of moment matrices that was previously considered as a non accurate method due to potential numerical precisions can actually be accurate if one keeps track of the moment matrices norms in the Gram Schmidt process. We showed how dimension witnesses can be obtained from our method and we have provided concrete numerical examples.

With this method we found that in the 3-2-2 scenario, while the known Leggett-Garg inequality is already maximally violated by a qubit's behavior our results implies that the 3-2-2 scenario is sufficient. So far, the only known way to certify qubit from the above dimensions was through the Peres-Mermin square, which corresponds to the 9-3-2 scenario in our notation. Our results provide a drastic simplification of the previously known results by six measurements and shorten the length of the sequence of measurements by one which is much more favorable to experimental perspectives. We provided a deep analysis and a characterization of scenarios in which dimension certification of dimension greater than two is possible. In particular, we use two metrics: the probability for a random quantum states with random measurements that does not admit any qubit quantum realization and the distribution of the visibility derived from the generalized robustness. We observed that the probability to find a behaviors with no qubit quantum realization increases when the experiment is more complex (more measurements or longer sequence of measurements). This is also possible by increasing the level of the hierarchy. When we increase the number of measurements or the length of the sequence we see that the distribution of the visibility shifts to lower values, this can be interpreted as a more robust certification. In summary, in the selection of scenarios, when the experiment is more complex there are more chances to make a successful certification which is also getting more robust.

In addition, our methods led us to certify, for the first time in this projective measurements scenario, quantum systems with dimensions strictly greater than three.

We have implemented the methods described in this paper using the language Python and all code is publicly available on the online repository [45] and free to use under the Apache License 2.0.

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Appendix

A Guess Your Neighbor's Input Inequality

In Sec. 2.1.2, we provided a specific example to show that the completeness is not necessarily verified in at any level of the hierarchy. Moreover, in this specific example there exist no quantum realization. It is in the case of the so-called guess-your-neighbor's-input inequality [44], in particular in its sequential measurement scenario [35]. It is a sequential scenario with a MLO of 2-3-2 and the inequality is:

$$P(000|000) + P(110|011) + P(011|101) + P(101|110) \leq 1. \tag{16}$$

As mentioned in Sec. 2.1.2, by solving the SDP referred in Eq. 6 one can find the maximum value $p^* \approx 1.0225$ when the dimension is unrestricted [35].

We are interested to know what is the maximum for the behaviors $\mathbf{P} \in \mathcal{Q}^{k=1}_{d=2}$. This can be done by solving the SDP in Eq. 9. In this case it is:

$$\begin{aligned}
p^*_{GYNI,d=2,k=1} := \max_{M} \quad & \sum_{\mathbf{r},\mathbf{s}} \gamma_{GYNI,\mathbf{r}|\mathbf{s}} M_{\mathbf{r}|\mathbf{s}} && \text{(17a)}\\
\text{s.t.} \quad & M_{\mathbf{0}|\mathbf{0},\mathbf{0}|\mathbf{0}} = 1, && \text{(17b)}\\
& M \in \mathcal{M}^{k=1}_{d=2}, && \text{(17c)}\\
& M \succeq 0, && \text{(17d)}
\end{aligned}$$

where

$$\gamma_{GYNI,\mathbf{r}|\mathbf{s}} = \begin{cases} 1 & \text{if } \mathbf{r}|\mathbf{s} \in E_{GYNI} \\ 0 & \text{otherwise.} \end{cases} \tag{18}$$

and $E_{GYNI} = \{(000|000), (110|011), (011|101), (101|110)\}$ is the set of events appearing in the inequality in Eq.10.

$$\begin{aligned}
p^*_{GYNI,d=2,k=1} := \max_{M} \quad & \sum_{\mathbf{r},\mathbf{s}} \gamma_{GYNI,\mathbf{r}|\mathbf{s}} M_{\mathbf{r}|\mathbf{s}} && \text{(19a)}\\
\text{s.t.} \quad & M_{\mathbf{0}|\mathbf{0},\mathbf{0}|\mathbf{0}} = 1, && \text{(19b)}\\
& M = \sum_{i=1}^{n} \alpha_i M^{k=1}_{d=2,i}, && \text{(19c)}\\
& \alpha \in \mathbb{R}^n, && \text{(19d)}\\
& M \succeq 0, && \text{(19e)}
\end{aligned}$$

where $\{M^{k=1}_{d=2,i}\}^n_{i=1}$ is a basis of $\mathcal{M}^{k=1}_{d=2}$.

We obtain $p^*_{2,1} \approx 1.1588$, showing that in the scenario 2-3-2, some behaviors $\mathbf{P} \in \mathcal{Q}^{k=1}_{d=2}$ do not admit any quantum realization. This example shows that the completeness is not verified. The code is provided in [45].

B Generating Random Moment Matrices

In what follow we refer to the randomized method used in [39]. A moment matrix, M, can be obtained by the Eq. 21 if a quantum state ρ and a set of projectors $\{\Pi_{\mathbf{r}|\mathbf{s}}\}$ is provided. In the randomized method, we randomly select a state form the space of states and each projective measurements in the set of projectors. They are multiple ways to do this and we have adopted the following one. The state ρ is prepared as follows:

$$\rho = U|0\rangle\langle 0|U^{\dagger}, \tag{20}$$

where U is a random $d \times d$ unitary matrix obtained using the *Haar measure* [57].

For the projectors, it is more subtle as we need to to satisfied normalization: $\sum_r \Pi_{\mathbf{r}|\mathbf{s}} = \mathbb{1}$. When the number of outcomes is equal to the dimension of the Hilbert space, in order to satisfy the normalization and orthogonality among projectors of different outcomes, all the projectors must be rank-1. However, when the dimension is larger than the number of outcomes some of the projectors must have higher rank. The assignment of the rank of the projectors can be done using a pseudorandom number generator such as the Mersenne Twister [58]. In other words, this corresponds to a binning method. To assign each result $r_i \in R_i$ to different dimension (to keep the orthogonality), we can define the different sets $B_{r_i|s_i}$ $\forall r_i \in R_i$ such that: $B_{r_i|s_i} \succeq \{0, \dots, d-1\}$, $B_{r_i|s_i} \cap B_{r_i'|s_i} = \emptyset$ if $r_i \neq r_i'$ and $\cup_{r_i \in R_i} B_{r_i|s_i} = \{0, \dots, d-1\}$.

The projector $\Pi_{r_i|s_i}$ is prepared as follows:

$$\Pi_{r_i|s_i} = \sum_{j \in B_{r_i|s_i}} U_{s_i}|j\rangle\langle j|U_{s_i}^{\dagger}, \tag{21}$$

where U_{s_i} is a random $d \times d$ unitary matrix obtained using the *Haar measure* [57] and characteristic of the setting s_i. It is important to keep the same unitary U_{s_i} for all the projectors with the same setting in order to keep the orthogonality. Then each projectors of sequences of measurements can be obtained as explained in Sec. 2.1 with the expression $\Pi_{\mathbf{r}|\mathbf{s}} = \Pi_{r_n|s_n} \dots \Pi_{r_1|s_1}$.

A behavior $\mathbf{P}$ can also be randomly created using the same technique as the diagonal elements of a moment matrix obtained by this technique is a behavior.

C Generalised Robustness

In Sec. 3.3 (in particular in Eq. 11) we have presented an optimization problem to quantify "how far" is a given behavior $\mathbf{P} := \{P(\mathbf{r}|\mathbf{s})\}_{\mathbf{r},\mathbf{s}}$ from the set $\mathcal{Q}_d^k$. This quantifier is analogous to the robust of entanglement[1] [46] and we defined it as:

$$\begin{aligned} & \text{given } \mathbf{P} := \{P(\mathbf{r}|\mathbf{s})\}_{\mathbf{r},\mathbf{s}} \\ \nu := \quad & \max_{\eta, \mathbf{P}_{d,k}} \eta \\ & \text{s.t. } \eta\mathbf{P} + (1-\eta)\mathbf{P}_{d,k} \in \mathcal{Q}_d^k \\ & \mathbf{P}_{d,k} \in \mathcal{Q}_d^k, \end{aligned} \tag{22}$$

where d is the dimension and k the level of the hierarchy.

By generating a basis $\{M_i\}_i$ for $\mathcal{Q}_d^k$ the above optimization problem can be phrased as an SDP:

[1] We recommend Ref. [47] for an introduction on robust quantifiers and SDP.

$$
\begin{aligned}
&\text{given } \{M_i\}_i, \{P(\mathbf{r}|\mathbf{s})\}_{\mathbf{r},\mathbf{s}} \\
\nu := &\max_{\eta, X, R, \{\alpha_i\}_i, \{\beta_i\}_i} \eta \\
\text{s.t. } &\eta P(\mathbf{r}|\mathbf{s}) + R_{\mathbf{r}|\mathbf{s},\mathbf{r}|\mathbf{s}} = X_{\mathbf{r}|\mathbf{s},\mathbf{r}|\mathbf{s}} \\
&X = \sum_i \alpha_i M_i \\
&R = \sum_i \beta_i M_i \\
&X_{0|0,0|0} = 1 \\
&R_{0|0,0|0} = 1 - \eta \\
&X \geq 0, \quad R \geq 0
\end{aligned} \tag{23}
$$

where α_i and β_i are real numbers and X and R are matrices of the size of M_i. Following the steps of Ref.[59], the Lagrangian of this optimization problem can then be written as

$$
L = \eta + \sum_{\mathbf{r}|\mathbf{s}} \gamma_{\mathbf{r}|\mathbf{s}} \left(R_{\mathbf{r}|\mathbf{s},\mathbf{r}|\mathbf{s}} - X_{\mathbf{r}|\mathbf{s},\mathbf{r}|\mathbf{s}} + \eta P(\mathbf{r}|\mathbf{s}) \right) + \mathrm{Tr}\left(A \left[X - \sum_i \alpha_i M_i \right] \right) \tag{24}
$$

$$
+ \mathrm{Tr}\left(B \left[R - \sum_i \beta_i M_i \right] \right) + \mathrm{Tr}(\rho X) + \mathrm{Tr}(\sigma R) + r(1 - \eta - R_{\mathbf{0}|\mathbf{0},\mathbf{0}|\mathbf{0}}) + x(1 - X_{\mathbf{0}|\mathbf{0},\mathbf{0}|\mathbf{0}})
$$

$$
= \eta \left(1 - r + \sum_{\mathbf{r}|\mathbf{s}} \gamma_{\mathbf{r}|\mathbf{s}} P(\mathbf{r}|\mathbf{s}) \right) + \mathrm{Tr}\left(X \left[\rho - x|0|0\rangle\langle 0|0| + \sum_{\mathbf{r}|\mathbf{s}} \gamma_{\mathbf{r}|\mathbf{s}} |\mathbf{r}|\mathbf{s}\rangle\langle \mathbf{r}|\mathbf{s}| \right] \right) \tag{25}
$$

$$
+ \mathrm{Tr}\left(R \left[\sigma - x|0|0\rangle\langle 0|0| + \sum_{\mathbf{r}|\mathbf{s}} \gamma_{\mathbf{r}|\mathbf{s}} |\mathbf{r}|\mathbf{s}\rangle\langle \mathbf{r}|\mathbf{s}| \right] \right) - \sum_i \alpha_i \mathrm{Tr}(M_i A) - - \sum_i \beta_i \mathrm{Tr}(M_i B) + r + x
$$

for dual variables γ, A, B, ρ, σ, r, and x. The dual program of the SDP described in Eq. 23 can then be written as

$$
\begin{aligned}
&\text{given } \{M_i\}_i, \{P(\mathbf{r}|\mathbf{s})\}_{\mathbf{r},\mathbf{s}} \\
\nu := &\min_{x, r, \{\gamma_{\mathbf{r}|\mathbf{s}}\}_{\mathbf{rs}}, A, B} x + r \\
\text{s.t. } &r = 1 + \sum_{\mathbf{r},\mathbf{s}} \gamma_{\mathbf{r}|\mathbf{s}} P(\mathbf{r}|\mathbf{s}) \\
&\sum_{\mathbf{r},\mathbf{s}} |\mathbf{r}|\mathbf{s}\rangle\langle \mathbf{r}|\mathbf{s}| \gamma_{\mathbf{r}|\mathbf{s}} \geq \quad A - x|0|0\rangle\langle 0|0| \\
&\sum_{\mathbf{r},\mathbf{s}} |\mathbf{r}|\mathbf{s}\rangle\langle \mathbf{r}|\mathbf{s}| \gamma_{\mathbf{r}|\mathbf{s}} \leq -B + r|0|0\rangle\langle 0|0| \\
&\mathrm{Tr}(M_i A) = 0, \ \forall i \\
&\mathrm{Tr}(M_i B) = 0, \ \forall i,
\end{aligned} \tag{26}
$$

where A and B are are matrices of the size of M_i, $\gamma_{\mathbf{r}|\mathbf{s}}$ x and r are real numbers, $|\mathbf{r}|\mathbf{s}\rangle\langle\mathbf{r}|\mathbf{s}|$ is a matrix of the size of M_i which has value 1 on the component $(\mathbf{r}|\mathbf{s}, \mathbf{r}|\mathbf{s})$ and zero everywhere else. Moreover, the real coefficiens $\{\gamma_{\mathbf{r}|\mathbf{s}}\}_{\mathbf{r},\mathbf{s}}$ provide an inequality that can be used to certify that the behavior. $\{P(\mathbf{r}|\mathbf{s})\}_{\mathbf{r},\mathbf{s}}$ does not admit a quantum realization of dimension d.

More precisely, after solving the optimization problem 26, the given behavior satisfies $\sum_{\mathbf{r},\mathbf{s}} \gamma_{\mathbf{r}|\mathbf{s}} P(\mathbf{r}|\mathbf{s}) = \nu - x - 1$. From the primal, we see that every behavior $\{P_{\mathbf{X}}(\mathbf{r}|\mathbf{s})\}_{\mathbf{r},\mathbf{s}} \in \mathcal{Q}_d^k$ respects $\nu \geq 1$, hence we have the witness $\sum_{\mathbf{r},\mathbf{s}} \gamma_{\mathbf{r}|\mathbf{s}} P_{\mathbf{X}}(\mathbf{r}|\mathbf{s}) \geq -x$. Note that if the given behavior is not inside $\mathcal{Q}_d^k$ the witness is always violated by this behavior. The primal formulation ensures that if $\{P(\mathbf{r}|\mathbf{s})\}_{\mathbf{r},\mathbf{s}} \notin \mathcal{Q}_d^k$ we have $\nu < 1$, hence $\sum_{\mathbf{r},\mathbf{s}} \gamma_{\mathbf{r}|\mathbf{s}} P(\mathbf{r}|\mathbf{s}) < -x$.