Lifting noncontextuality inequalities

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Kochen-Specker contextuality is a fundamental feature of quantum mechanics and a crucial resource for quantum computational advantage and reduction of communication complexity. Its presence is witnessed in empirical data by the violation of noncontextuality inequalities. However, all known noncontextuality inequalities corresponding to facets of noncontextual polytopes are either Bell inequalities or refer to cyclic or state-independent KS contextuality scenarios. We introduce a general method for lifting noncontextuality inequalities, deriving facets of noncontextual polytopes for more complex scenarios from known facets of simpler sub-scenarios. Concretely, starting from an arbitrary scenario, the addition of a new measurement or a new outcome preserves the facet-defining nature of any noncontextuality inequality. This extends the results of Pironio [J. Math. Phys. **46**, 062112 (2005)] from Bell nonlocality scenarios to contextuality scenarios and unifies liftings of Bell and noncontextuality inequalities. We show that our method produces facet-defining noncontextuality inequalities in all scenarios with contextual correlations, and we present examples of facet-defining noncontextuality inequalities for scenarios where no examples were known. Our results shed light on the structure of noncontextuality polytopes and the relationship between such polytopes across different scenarios.

Motivation

Kochen–Specker (KS) contextuality [15, 7], i.e. the impossibility of explaining with a single global probability distribution the marginal probability distributions produced by either ideal measurements of compatible observables [14, 8] or by measurements on spatially separated systems [4, 9], is a characteristic signature of quantum mechanics, and a crucial informational or computational resource [13, 19, 6, 11, 12, 23]. Contextuality is typically witnessed by the violation of linear constraints called noncontextuality (NC) inequalities. However, all known facet-defining NC inequalities, which provide a minimal set of conditions for deciding whether measurement statistics are contextual, are either for Bell scenarios [9] or refer to cyclic [14] or state-independent [8, 3, 22] contextuality scenarios.

The set of noncontextual correlations for a given measurement scenario forms a convex polytope. Characterising all its facet-defining inequalities is a notoriously hard problem (NP-complete [2]) to solve in general. As such, there are few fully characterised scenarios, for which all facet-defining NC inequalities are known: non-Bell scenarios include two-outcome k-cycle ($k \geq 5$) scenarios [1], Bell scenarios include the $(2, 2, 2)$ CHSH scenario [9], and various classes generalising it such as $(2, m, 2)$ [16, 5], $(n, 2, 2)$ [20], and $(2, 2, k)$ [10] scenarios, where (n, m, k) stands for n parties, each with m measurement settings, each with k possible outcomes. Furthermore, there are many Bell scenarios for which a partial characterisation of their Bell inequalities has been carried out.

Despite the demoralising hardness of characterising arbitrary scenarios, some non-trivial work has been done linking simpler Bell scenarios with more complex ones. In Ref. [17], Pironio proposed a method to derive (some of the) facet-defining Bell inequalities of complex Bell polytopes starting from known inequalities of simpler Bell polytopes. It employed the idea of *lifting*, a commonly used technique in convex polyhedral theory to derive facet-defining inequalities of a polytope in $\mathbb{R}^n$ from facet-defining inequalities of a related polytope in $\mathbb{R}^m$ where $m < n$. The upshot is that once the facets of a simpler polytope have been fully or partially identified, one need not start from scratch when searching for the facets of certain more complex polytopes. One may instead concentrate efforts on finding the facet-defining inequalities that are absent in or do not arise from simpler cases.

Aiming to foster facet characterisation for general Bell scenarios, Pironio showed that any facet-defining inequality of an arbitrary Bell polytope can be lifted to one or more facet-defining inequalities of any more complex Bell polytope, where by 'more complex' we mean a Bell scenario with more parties, more local measurements for a party, or more outcomes for a measurement (or a combination of all three) than in the original scenario. Building on this work, in Ref. [18] Pironio characterised Bell scenarios whose only facets are given by liftings of the CHSH inequality. These include e.g. the bipartite scenarios where one party has a binary choice of dichotomic measurements, irrespective of the number of measurement settings and outcomes for the other party.

Non-Bell-type contextuality scenarios, on the other hand, have not received as much attention in terms of facet characterisation. Our work aims to address this gap.

Contributions

We introduce a method for producing facet-defining NC inequalities in arbitrary KS contextuality scenarios. This is based on – and strictly extends – the lifting techniques used by Pironio [17] for Bell scenarios. The method allows us to identify facet-defining NC inequalities for *any* scenario which admits contextual correlations and thus provides a key to explore an infinity of as-of-yet unexplored scenarios. This is ensured by Vorob'ev's theorem [21], which guarantees that any contextuality-witnessing scenario contains an induced k-cycle sub-scenario (for some $k \geq 4$), and by the complete characterisation of the noncontextual polytopes for all such cycle scenarios [1].

We first give a concise, high-level summary of our main results; please refer to the full paper for definitions and details. A scenario $\mathbf{S}$ can be extended to a more complex scenario $\mathbf{T}$ by adding more measurements and/or

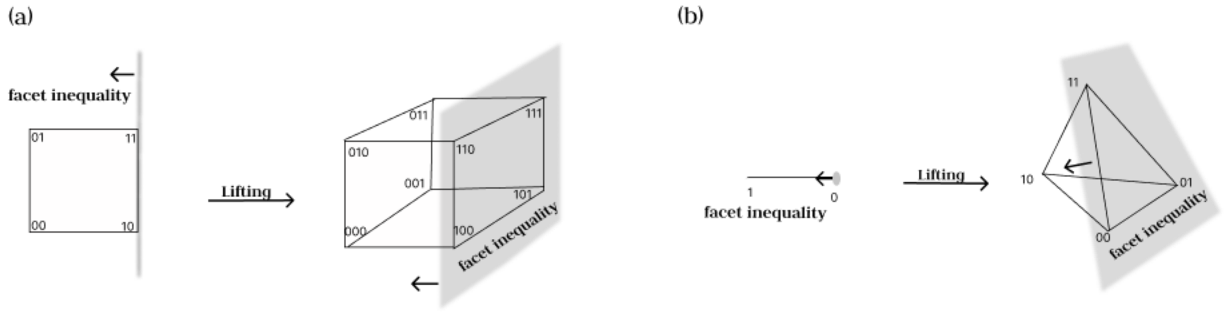

Figure 1: Measurement lifting in simple scenarios with dichotomic measurements: (a) Case I from the scenario with two incompatible measurements to the scenario with three pairwise incompatible measurements; (b) Case II from the scenario with a single measurement to the scenario with two compatible measurements.

more outcomes. We focus on one such step at a time: either adding *one* measurement or adding *one* outcome for an already existing measurement. An arbitrary extension can be seen as a sequence of such single-step extensions. We fix an initial facet-defining NC inequality for **S** which we aim to lift to (one or more) facet-defining NC inequalities for **T**. We achieve this in both situations, but the specifics differ somewhat.

Measurement lifting. When **T** is obtained from **S** by adjoining a new measurement A, the method of lifting depends both on the compatibility relations between A and the pre-existing measurements and on the facet-defining inequality being lifted, namely on the set of measurements that *effectively contribute* (see Sec. IV C 2 in paper for a precise definition) to that inequality. We distinguish two cases:

I. If A is incompatible with some measurement that contributes to the initial inequality, then the inequality lifts unchanged to a facet-defining inequality for the scenario **T**. The new measurement A is traced out and does not effectively contribute to the lifted inequality, thus it need not be performed for testing the inequality.

II. If A is compatible with all the measurements that contribute to the initial inequality, then the inequality lifts to a facet-defining inequality of **T** for each outcome a_k of A. Each such lifted inequality can be tested by first measuring A, post-selecting on obtaining the outcome a_k, and then testing the initial inequality.

Outcome lifting. When **T** is obtained from **S** by adding a new outcome a_0 for an already existing measurement A, the original inequality lifts to a facet-defining inequality on **T** for each choice of outcome $a_k \neq a_0$ of A. The choice indicates the outcome a_k of A with which a_0 is being 'clubbed together'. When testing the inequality, any occurrence of the new outcome a_0 for A is treated as if it were an a_k in the original scenario. An exception is that the initial inequality cannot itself be the result of case II measurement lifting with the *same* choice of outcome a_k, as intuitively this would entail post-selecting on two different outcomes for A.

Overview of key ideas

We offer an accessible, intuitive sketch of the main ingredients of our lifting method using small – trivial yet visualisable – examples to convey the flavour of the various forms of lifting. The noncontextual polytope for the simplest contextuality-witnessing scenario is 8-dimensional. It is thus impossible to visualise lifting starting from this polytope. Nonetheless, there are simple visualisable NC polytopes – albeit for scenarios unable to witness contextuality – which aptly capture the idea of lifting. We use these examples to provide an intuition for the idea behind our lifting method. Despite being thoroughly uninteresting from the point of view of contextuality, these examples are indeed special cases of our lifting results which 'contain all the germs of generality'.

Case I Measurement lifting This applies when the new measurement added to **S** is not simultaneously compatible with all the measurements contributing to the facet-defining inequality being lifted, i.e. it is incompatible with at least one such measurement. We illustrate this case with an example that serves as a proxy for *all* such situations. Consider **S** the scenario with two dichotomic measurements, A and B, that are incompatible with each other. Its NC polytope S is two-dimensional (embedded in a four-dimensional ambient vector space) and is shown on the left-hand side of Fig. 1(a). Its four vertices correspond to the deterministic assignments – 00, 01, 10, 11 – to measurements A and B, in that order. Observe that the fact that A and B are incompatible induces an affine dependency among the vertices of the polytope,

$$v_{00} - v_{01} - v_{10} + v_{11} = 0, \tag{1}$$

which would not hold were A and B compatible; cf. the simplex on the right-hand side of Fig. 1(b). This kind of affine relation induced by measurement incompatibility is the cornerstone of our proofs; see e.g. Eq. (17) in the full paper. Since S is a two-dimensional polytope, its facets are one-dimensional. One of its facet-defining inequalities is depicted in the figure; it supports the facet containing the vertices v_{10} and v_{11}.

Now consider extending **S** to **T** by introducing a new measurement C incompatible with both A and B. The NC polytope T is three-dimensional (embedded in a six-dimensional ambient vector space), and is shown on the right-hand side of Fig. 1(a). Notice that each outcome of C determines an extension of each deterministic assignment in **S** (hence, vertex of S) to a deterministic assignment in **T** (vertex of T); e.g. v_{010} and v_{011} in T are the two extensions of v_{01} in S. One can think of this as captured by a polytope projection from T to S which 'forgets' the outcome of C. The polytope T has a facet with vertices v_{100}, v_{101}, v_{110}, and v_{111}, whose supporting inequality is depicted on the right of Fig. 1(a). These four vertices of T are precisely the extensions of the vertices v_{01} and v_{11} of S, which saturate the initial inequality depicted on the left. The inequality shown on the right of Fig. 1(a) is thus the *lifting* of the inequality on the left. One can similarly obtain three other facet-defining inequalities of T from the remaining three facets of S.

In general, case I measurement lifting maps a facet F of S to the facet of T whose set of vertices is exactly the set of all extensions of vertices in the original facet F. The explicit form of the lifted inequality turns out to be, in a sense, the same as that of the initial inequality, since the outcome of the new measurement is ignored and thus 'traced out'; see Sec. IV C in the full paper.

Case II Measurement lifting This applies when the newly added measurement is compatible with all the pre-existing measurements that effectively contribute to the facet-defining inequality being lifted. To visualise lifting in this case, take **S** to be the scenario with a single dichotomic measurement, say A. Its NC polytope S is a one-dimensional line segment (embedded in a two-dimensional ambient vector space), shown on the left-hand side of Fig. 1(b). It has only two facet-defining inequalities. One of them, saturated only by the vertex v_0, is depicted in the figure.

We extend this scenario to **T** by adding a dichotomic measurement B compatible with A. The resulting NC polytope T is a three-dimensional tetrahedron (embedded in a four-dimensional ambient vector space), shown on the right-hand side of Fig. 1(b). The facet-defining inequality depicted in the figure is one of two possible liftings of the initial inequality on the left. It is saturated by the vertices v_{00}, v_{01}, and v_{11}. The first two are all the extensions of v_0, the vertex that saturates the initial inequality, while the third is just one of the two possible extensions of v_1, the other, non-saturating vertex of S. The vertex of T corresponding to the other extension, v_{10}, does not saturate the inequality shown on the right of Fig. 1(b). However, a different lifting of the same initial inequality shown on the left of Fig. 1(b) would support the facet containing the vertices v_{00}, v_{01}, and v_{10}.

In general, case II measurement lifting maps a facet F of S to a facet of T whose set of vertices consists of: (i) every possible extension of the vertices in the original facet F, and (ii) every possible extension of the remaining vertices of S (not in the original facet F) except those that assign a chosen fixed outcome to the new measurement (outcome 0 for B in the example depicted above). Varying the choice of this fixed outcome for the new measurement yields different liftings to T of the same facet-defining inequality of S.

Outcome lifting In the case of outcome lifting, we consider extending a scenario **S** to **T** by adding an extra outcome a_0 to an existing measurement A. Here, unlike in the case of measurement lifting, there is no (immediate) concept of extension of assignments, and thus of vertices of S to vertices of T. In fact, the vertices of S could be seen as a strict subset of those of polytope T. These vertices behave the same way with respect to an outcome-lifted inequality in T as they do with respect to the initial facet-defining inequality of S, either saturating both or falling short by the same amount. However, there are more vertices in the larger polytope T, namely those that assign the new outcome a_0 to the measurement A. Each such vertex behaves exactly as the vertex obtained by substituting a_k for the outcome of A (while leaving the rest of the assignment intact), for some fixed choice outcome a_k of A already present in the initial scenario **S**. In other words, a facet F of S is lifted to a facet of T whose set of vertices consists of: the vertices in F plus the vertices obtained from a vertex in F by replacing (the fixed) outcome a_k by a_0 for the measurement A.

As for case II measurement lifting, there is an element of choice involved. Indeed, for each choice of k, one obtains a (possibly different) facet-defining inequality of T. There is one exception, though: choosing k fails to yield a facet of T when the initial facet of S is itself obtainable from a sub-scenario of **S** via case II measurement lifting by fixing the choice of outcome a_k when adding measurement A; in other words, when the facet-defining inequality being lifted is such that A is compatible with all the measurements effectively contributing to it and all its non-saturating vertices assign outcome a_k to A.

One may think of each such choice of k as determining a polytope projection $T \to S$ which performs a coarse-graining of the outcomes of A by clubbing together a_0 and a_k as the same outcome (see also the discussion in Sec. VI of the full paper). The lifted inequality then corresponds to 'tracing out' along this identification, much as in case I measurement lifting. This means that the form of the lifted inequality is such that it does not distinguish between the vertices with a_k and a_0 as outcomes of A, while the remaining vertices behave as they did with respect to the original inequality. Indeed, in the new scenario, the lifted inequality is still in effect testing the original inequality: the new outcome needs to be 'clubbed together' with – and thus made indistinguishable from – some pre-existing outcome so that the 'effective' number of outcomes remains the same.

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