Necessary Conditions for Extended Noncontextuality in General Sets of Random Variables

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We explore the graph approach to contextuality to restate the extended definition of noncontextuality as given by J. Kujala et. al. in Ref1 in using graph-theoretical terms. This extended definition avoids the assumption of the pre-sheaf or non-disturbance condition, which states that if two contexts overlap, then the marginal distribution obtained for the intersection must be the same, a restriction that will never be perfectly satisfied in real experiments. With this we are able to derive necessary conditions for extended noncontextuality for any set of random variables based on the geometrical aspects of the graph approach, which can be tested directly with experimental data in any contextuality experiment and which reduce to traditional necessary conditions for noncontextuality if the non-disturbance condition is satisfied.
I. INTRODUCTION

Quantum theory assigns probabilities to subsets of possible measurements of a physical system. The phenomenon of contextuality states that there may be no global probability distribution that is consistent with these subsets, which are also called contexts\textsuperscript{2–6}.

A key consequence of contextuality is that the statistical predictions of quantum theory cannot be obtained from models where the measurement outcomes reveal pre-existent properties that are independent on which, or whether, other compatible measurements are jointly performed. This fundamental limitation follows from the existence of incompatible measurements in quantum systems. It thus represents an exotic, intrinsically non-classical phenomenon, that leads to a more fundamental understanding of many aspects of quantum theory\textsuperscript{7–12}. In addition, contextuality has been recognized as a potential resource for quantum computing,\textsuperscript{13–15} random number certification\textsuperscript{16}, and several other information processing tasks in the specific case of space-like separated systems\textsuperscript{17}.

As a consequence, experimental verifications of contextuality have received much attention\textsuperscript{18–22}. It is thus of utmost importance to develop a robust theoretical framework for contextuality that can be efficiently applied to real experiments. In particular, it is important to include the treatment of sets of random variables that do not satisfy the assumption of the so called pre-sheaf\textsuperscript{6,12} or non-disturbance\textsuperscript{7} condition. This assumption states that if the intersection of two contexts is non-empty, then the marginal probability distributions at the intersection must be the same, a restriction that will never be perfectly satisfied in real experiments. This problem was considered in Refs.\textsuperscript{23,24}, but the methods proposed there to take into account the context-dependent change in a random variable involve quantities that cannot be directly measured.

In Ref.\textsuperscript{1}, the authors propose an alternative definition of noncontextuality that can be applied to any set of random variables. Such a treatment reduces to the traditional definition of noncontextuality if the non-disturbance property is satisfied and, in addition, it can be verified directly from experimental data. In this alternative definition, a set of random variables is said to be noncontextual (in the extended sense) if there is a joint probability distribution which is consistent with the joint distribution for each context and maximizes the probability of two realizations of the same set of random variables present in different contexts being equal. Then the authors provide necessary and sufficient conditions for
contextuality in a broad class of scenarios, namely the so called $n$-cycle scenario.

In this contribution, we explore the graph approach to contextuality, developed in Refs.\textsuperscript{10,25,26} and further explored in Refs.\textsuperscript{27–29}, to rewrite the definition of extended noncontextuality in graph theoretical terms. To this end, from the compatibility graph $G$ of a scenario $\Gamma$, we define another graph $\mathcal{G}$, which we call the extended compatibility graph of the scenario, and show that noncontextuality in the extended sense is equivalent to noncontextuality in the traditional sense with respect to the extended graph $\mathcal{G}$.

With this graph-theoretical perspective, the problem of characterizing extended noncontextuality reduces to characterizing traditional noncontextuality for the scenario defined by $\mathcal{G}$, a difficult problem for general graphs\textsuperscript{26,30–32}. Nevertheless, we can explore the connection between the noncontextual set and the cut polytope $\text{CUT}(G)$\textsuperscript{26,29} of the corresponding compatibility graph $G$ to derive necessary conditions for extended contextuality in any scenario, which can be tested directly with experimental data in any contextuality experiment and reduces to traditional necessary conditions for noncontextuality if the non-disturbance condition is satisfied.

To derive these conditions, we first prove that $\mathcal{G}$ can be obtained from $G$ combining the graph operations known as triangular elimination, vertex splitting and edge contraction\textsuperscript{32–34}. From valid inequalities for $\text{CUT}(G)$ it is possible to derive valid inequalities for any graph obtained from $G$ using a sequence of such operations. In particular, for any valid inequality for $\text{CUT}(G)$ we can derive valid inequalities for $\text{CUT}(\mathcal{G})$, among which there is one that reduces to the original inequality if the non-disturbance condition is satisfied.

As applications of our framework, we recover the characterization of extended noncontextuality for the $n$-cycle scenarios of Ref.\textsuperscript{1} and provide necessary conditions for noncontextuality exploring the $I_{3322}$\textsuperscript{35,36} and Chained inequalities\textsuperscript{37}. Finally, we use the Peres-Mermin square\textsuperscript{38,39} to illustrate that similar ideas can be used even in scenarios where the cut polytope does not provide a complete characterization of the noncontextual set.

The paper is organized as follows: in Sec. II we review the definition of a compatibility scenario and of noncontextuality in the traditional sense; in Sec. III, we review the definition of extended noncontextuality of Ref.\textsuperscript{1}, stating it in graph-theoretical terms; in Sec. IV we maximize the probability of two realizations of the same random variables in different contexts being equal; in Sec. V focusing on scenarios with two outcomes per measurement, we introduce the cut polytope and the extended compatibility hypergraph for a scenario and
show a complete characterization of the extended contextuality for the $n$–cycle scenario; In Sec. VI using the introduced cut polytope we provide necessary conditions for the existence of noncontextual behaviours in any given scenario, although the complete characterization is an extremely difficult problem; In Sec. VII and Sec. VIII we apply our methods for important families of contextuality inequalities; We discuss scenarios with more than three measurements in Sec. IX and close this work with a discussion in Sec. XI.

II. COMPATIBILITY SCENARIOS

Definition 1. A compatibility scenario is defined by a triple $\Gamma := (X, C, O)$, where $O$ is a finite set, $X$ is a finite set of random variables taking values in $O$, and $C$ is a family of subsets of $X$ such that

1. $\cup_{C \in C} C = X$;
2. $C, C' \in C$ and $C \subseteq C'$ implies $C = C'$.

The elements $C \in C$ are called contexts and the set $C$ is called the compatibility cover of the scenario.

One may think of the random variables in $X$ as representing measurements in a physical system, with possible outcomes labeled by the elements in $O$, while the sets in $C$ may be thought as encoding the compatibility relations among the measurements in $X$, that is, each set $C \in C$ consists of a maximal set of compatible, jointly measurable random variables. Equivalently, the compatibility relations among the elements of $X$ can be represented by an hypergraph.

Definition 2. The compatibility hypergraph of a scenario $(X, C, O)$ is an hypergraph $H = (X, C)$ whose vertices are the random variables in $X$ and hyperedges are the contexts $C \in C$. The compatibility graph of the scenario is the 2-section of $H$, that is, the graph $G$ has the same vertices of the hypergraph $H$ and edges between all pairs of vertices contained in the some hyperedge of $H$.

In an experiment, characterized by a compatibility scenario $\Gamma = (X, C, O)$, when compatible measurements, represented by the random variables belonging to a context $C =
\{x_1, x_2, ..., x_{|C|}\} \in \mathcal{C}, \text{ are performed jointly, a list } s = (a_1, a_2, ..., a_{|C|}) \text{ of outcomes in the Cartesian product}
\[ O^C := O \times O \times ... \times O \]
is observed. Moreover, the collection of well-defined joint probability distributions for the random variables associated with \( C \in \mathcal{C} \) receives special attention:

**Definition 3.** A behavior \( B \) for the scenario \((X, \mathcal{C}, O)\) is a family of probability distributions over \( O^C \), one for each context \( C \in \mathcal{C} \), that is,
\[ B = \left\{ p_C : O^C \to [0, 1] \mid \sum_{s \in O^C} p_C(s) = 1, C \in \mathcal{C} \right\}. \tag{2} \]

This means that for each context \( C \), \( p_C(s) \) gives the probability of obtaining outcomes \( s \) in a joint measurement of the elements of \( C \). Following standard notation in the community, given a context \( C = \{x_1, \ldots, x_{|C|}\} \) and \( s = (a_1, \ldots, a_{|C|}) \) a particular list of outcomes for those measurements in \( C \), we will from now on represent \( p_C(s) \) as
\[ p \left( a_1, \ldots, a_{|C|} \mid x_1, \ldots, x_{|C|} \right). \tag{3} \]

**Remark:** Despite of being absolutely standard using the above notation for representing an element \( p_C \) in a behaviour \( B \), to avoid misunderstanding within the mathematical community, and to make our work more readable for those from other communities who might become interested in this topic, we note that the mathematical object we are using here is the joint probability \( \mathbb{P}(x_1 = a_1, x_2 = a_2, ..., x_{|C|} = a_{|C|}) \), defined on the finite set \( O^C \).

In an ideal situation, one generally assumes that behaviors are non-disturbing.

**Definition 4.** The non-disturbance set \( \mathcal{X}(\Gamma) \) of a compatibility scenario \( \Gamma \) is the set of behaviors that satisfy the consistency relation
\[ \sum_{a_{|C|}' \notin C_i \cap C_j} p \left( a_1' a_2' ... a_{|C|}' \mid x_1 x_2 ... x_{|C|} \right) = \sum_{a_{|C|}' \notin C_i \cap C_j} p \left( a_1' a_2' ... a_{|C|}' \mid x_1 x_2 ... x_{|C|} \right) \tag{4} \]
for any two intersecting contexts \( C_i \) and \( C_j \) in \( \mathcal{C} \), when considering at both sides the same sets of outcomes for those measurements in \( C_i \cap C_j \).

**Remark:** Eq. (4) above says that when the non-disturbance relation is satisfied in those contexts which share some common random variables, it does not matter the way one takes
the marginalization to these variables into account. Both marginalizations, either starting from $C_i$ or starting from $C_j$, must coincide.

In an hypothetical situation where all measurements in $X$ are compatible, it would be possible to define a global probability distribution $p(a_1 a_2 \ldots a_{|X|} | x_1 x_2 \ldots x_{|X|})$, or

$$p(a_1 a_2 \ldots a_{|X|})$$

for short, that would give the probability of obtaining outcomes $a_1 a_2 \ldots a_{|X|}$ as though all measurements in $X$ were jointly performed.

**Definition 5.** A behavior $B \subset X(\Gamma)$ is noncontextual if there is a global probability distribution (5) such that for each $C \in C$

$$p(a_1 a_2 \ldots a_{|C|} | x_1 x_2 \ldots x_{|C|}) = \sum_{a_l \in \Gamma \not\in C} p(a_1 a_2 \ldots a_n),$$

where the sum is taken over the outcomes $a_l$ of the measurements $l \not\in C$ and $a_l = a_k$ for each $l = x_k \in C$.

In other words, B is noncontextual if the probability distribution assigned by B to each context can be recovered as marginal from the global probability distribution $p(a_1 a_2 \ldots a_n)^{5,6}$.

### III. Extended Contextuality

To define noncontextuality in a scenario where the non-disturbance property (4) is not valid, we first must change the definition of noncontextual behaviors given by Eq. (6). We will consider extended global probability distributions of the form

$$p\left(\begin{matrix} a_1^1 \ldots a_{|C_1|}^1 & a_1^2 \ldots a_{|C_2|}^2 & \ldots & a_{|m|}^m \mid x_1^1 \ldots x_{|C_1|}^1 & x_1^2 \ldots x_{|C_2|}^2 & \ldots & x_{|m|}^m \end{matrix}\right),$$

where $m = |C|$, that gives joint probability of obtaining outcomes $a_i^1, \ldots, a_i^{|C_i|}$ for each context $C_i = \{x_i^1, \ldots, x_i^{|C_i|}\}$. Notice that this extended global probability distribution is, in general, not equal to the probability distribution defined in Eq. (5), since the same random variable could appear in more than one context, and hence, in the list

$$x_1^1 \ldots x_{|C_1|}^1 x_1^2 \ldots x_{|C_2|}^2 \ldots x_{|m|}^1 \ldots x_{|m|}^m$$
the same random variable would be repeated several times.

To make definitions in Eqs. (5) and (7) equivalent in the case of non-disturbing behaviors, we demand that, if in different contexts $C_i, C_i, \ldots, C_i$, there exist coincident random variables $x_i^1, x_i^2, \ldots, x_i^i$, then

$$p \left( a_{k_1}^i \ldots a_{k_i}^i | x_{k_1}^i \ldots x_{k_i}^i \right) = \sum_{a_s^r \neq (i,j)} p \left( a_1^1 \ldots a_{|C_i|}^1 \ldots a_{|C_m|}^m | x_1^1 \ldots x_{|C_i|}^1 \ldots x_{|C_m|}^m \right)$$

(9)

$$= \begin{cases} 1 & \text{if } a_{k_1}^i = a_{k_2}^i = \ldots = a_{k_1}^i \\ 0 & \text{otherwise,} \end{cases}$$

(10)

that is, marginal probability distributions for $x_i^1, x_i^2, \ldots, x_i^i$, representing the same random variable in different contexts, are perfectly correlated. Hence, it is equivalent to say that B is a noncontextual behavior if there is a extended global probability distribution satisfying condition (10) such that

$$p \left( a_1^1 a_2^1 \ldots a_{|C_i|}^i | x_1^1 x_2^1 \ldots x_{|C_i|}^i \right) = \sum_{a_s^r \neq i} p \left( a_1^1 \ldots a_{|C_i|}^1 \ldots a_{|C_m|}^m | x_1^1 \ldots x_{|C_i|}^1 \ldots x_{|C_m|}^m \right)$$

(11)

A simple example of this situation is shown in Fig. 1. There, a simple compatibility scenario with three measurements 0, 1, 2 and two contexts, \{0, 1\} and \{1, 2\} is shown. A behaviour for such a scenario consists of two probability distributions $p(ab|01)$ and $p(bc|12)$. Traditionally, one says that a non-disturbing behavior for this scenario is noncontextual if there is a global probability distribution $p(abc)$ such that $p(ab|01) = \sum_c p(abc)$ and $p(bc|12) = \sum_a p(abc)$. For our purposes it will be convenient to consider an extended global probability distribution $p(abb'c|011'2)$ such that $p(bb'|11') = \sum_{a,c} p(abb'c|0112) = 1$ iff $b = b'$, and zero otherwise. Then, in this situation, we say that a behavior is noncontextual if there is an extended global probability distribution satisfying this condition such that $p(ab|01) = \sum_{b',c} p(abb'c|011'2)$ and $p(b'c|12) = \sum_{a,b} p(abb'c|011'2)$. For non-disturbing behaviors, these two notions of noncontextuality are equivalent.

To define noncontextuality in a scenario where the non-disturbance property does not hold, we adopt the strategy of Ref. 1. We relax the requirement that marginals for
FIG. 1: A simple compatibility scenario with three measurements 0, 1, 2 and two contexts, \{0, 1\} and \{1, 2\}. Here the compatibility hypergraph associated with the scenario already coincides with its compatibility graph.

\[ x_{k_1}^{i_1}, x_{k_2}^{i_2}, \ldots, x_{k_l}^{i_l}\] be perfectly correlated when they represent the same random variable. Instead of Eq. (10), we require that the probability of \( x_{k_1}^{i_1}, x_{k_2}^{i_2}, \ldots, x_{k_l}^{i_l}\) being equal is the maximum allowed by the individual probability distributions of each \( x_{k_l}^{i_l}\).

**Definition 6.** We say that a behavior has a maximally noncontextual description if there is an extended global distribution (7) such that the distribution of each context is obtained as a marginal, according to Eq. (11), and such that if \( x_{k_1}^{i_1}, x_{k_2}^{i_2}, \ldots, x_{k_l}^{i_l}\) represent the same random variable, the marginals for \( x_{k_1}^{i_1}, x_{k_2}^{i_2}, \ldots, x_{k_l}^{i_l}\) defined by Eq. (9) are such that

\[
p(x_{k_1}^{i_1} = \ldots = x_{k_l}^{i_l}) = \sum_a p(a \ldots a | x_{k_1}^{i_1} \ldots x_{k_l}^{i_l})
\]

is the maximum consistent with the marginal distributions \( p(a_{k_j}^{i_j} | x_{k_j}^{i_j})\). That is, a behavior is noncontextual in the extended sense if there is an extended global distribution that gives the correct marginal in each context and that maximizes the probability of \( x_{k_1}^{i_1}, x_{k_2}^{i_2}, \ldots, x_{k_l}^{i_l}\) being equal if they represent the same random variable in different contexts.

According Ref\(^1\) we define maximal coupling as follows:

**Definition 7.** Given \( \{x_{i_1}^{k_1}, x_{i_2}^{k_2}, \ldots, x_{i_l}^{k_l}\}\) a set of random variables representing the same measurement, we call a distribution \( p(a_{i_1}^{k_1} a_{i_2}^{k_2} \ldots a_{i_l}^{k_l} | x_{i_1}^{k_1} x_{i_2}^{k_2} \ldots x_{i_l}^{k_l})\) that gives the correct marginals \( p(a_{i_j}^{k_j} | x_{i_j}^{k_j})\) a coupling for \( x_{i_1}^{k_1}, x_{i_2}^{k_2}, \ldots, x_{i_l}^{k_l}\). We say that such a coupling is maximal if \( p(x_{i_1}^{k_1} = x_{i_2}^{k_2} = \ldots = x_{i_l}^{k_l})\) achieves the maximum value consistent with the marginals \( p(a_{i_j}^{k_j} | x_{i_j}^{k_j})\).
IV. EXISTENCE OF MAXIMAL COUPLINGS

It could be the case that a maximal coupling, as in Def. 7 did not exist for a given set of random variables which represents the same measurement. It turns out that it would never happen. Here we constructively show that a maximal coupling is a well-defined notion. i.e. under certain assumptions there always exists at least one maximal coupling for a given set of random variables.

**Theorem 1.** Given a set of random variables $x_{i_1}^{k_1}, x_{i_2}^{k_2}, \ldots, x_{i_l}^{k_l}$ with distributions $p(a_{i_j}^{k_j} | x_{i_j}^{k_j})$ it is always possible to construct a maximal coupling for this set with

$$p(x_{i_1}^{k_1} = x_{i_2}^{k_2} = \ldots = x_{i_l}^{k_l}) = \sum_a \min_j \left\{ p(a^{k_j} | x_{i_j}^{k_j}) \right\}.$$  \hfill (13)

**Proof.** Let

$$p_-(a) = \min_j \left\{ p(a^{k_j} | x_{i_j}^{k_j}) \right\}.$$  \hfill (14)

Then

$$p(x_{i_1}^{k_1} = x_{i_2}^{k_2} = \ldots = x_{i_l}^{k_l} = a) \leq p_-(a)$$  \hfill (15)

and hence,

$$p(x_{i_1}^{k_1} = \ldots = x_{i_l}^{k_l}) = \sum_a p(x_{i_1}^{k_1} = \ldots = x_{i_l}^{k_l} = a) \leq \sum_a p_-(a).$$  \hfill (16)

Construct the coupling as follows: if $a_{i_1}^{k_1} = a_{i_2}^{k_2} = \ldots = a_{i_l}^{k_l} = a$, we define

$$p(a \ldots a | x_{i_1}^{k_1}, x_{i_2}^{k_2} \ldots x_{i_l}^{k_l}) = p_-(a);$$  \hfill (17)

if not, we define

$$p(a_{i_1}^{k_1} a_{i_2}^{k_2} \ldots a_{i_l}^{k_l} | x_{i_1}^{k_1}, x_{i_2}^{k_2} \ldots x_{i_l}^{k_l}) = \prod_j p'(a_{i_j}^{k_j} | x_{i_j}^{k_j}),$$

where

$$p'(a_{i_j}^{k_j} | x_{i_j}^{k_j}) = p(a_{i_j}^{k_j} | x_{i_j}^{k_j}) - p_-(a).$$  \hfill (18)

This defines a maximal coupling for $x_{i_1}^{k_1}, x_{i_2}^{k_2}, \ldots, x_{i_l}^{k_l}$. \hfill \(\blacksquare\)

One should notice that although the method we have applied in the proof above provides a maximal coupling for the considered set of random variables, there is no guarantee that such a coupling is the unique consistent with Def. 7 when treating with the general case.
Actually, it turns out that in some specific situations the coupling constructed above is indeed unique. This is always the case, for example, for two variables with any number of outcomes and three variables each of which with two outcomes.

**Theorem 2** (Sufficient condition for extended contextuality). *If there is an extended global distribution, as in Eq. (7), such that the marginals in each context are equal to the distributions of the behavior \( B \), according to Eq. (11), and such that the corresponding couplings for each set \( x_{i_1}^{k_1}, x_{i_2}^{k_2}, \ldots, x_{i_l}^{k_l} \) representing the same random variable, defined by Eq. (9), are equal to the ones given in Thm. 1, then the behavior \( B \) is noncontextual in the extended sense.*

The condition stated in Thm. 2 is also necessary when the coupling constructed in the proof of Thm. 1 is unique.

When the coupling given in Thm. 1 is not unique, the difference between any other coupling and the one constructed in the proof of this theorem can only appear in the terms

\[
p(a_{i_1}^{k_1} a_{i_2}^{k_2} \ldots a_{i_l}^{k_l} | x_{i_1}^{k_1} x_{i_2}^{k_2} \ldots x_{i_l}^{k_l})
\]

for which the outcomes \( a_{i_1}^{k_1}, a_{i_2}^{k_2}, \ldots, a_{i_l}^{k_l} \) are not all equal. Otherwise this would contradict the hypotheses that the coupling is maximal. Then for any maximal coupling we can at least say that for each pair \( x_{i_m}^{k_m} \) and \( x_{i_n}^{k_n} \) we have

\[
p_-(a) = p(x_{i_1}^{k_1} = \ldots = x_{i_l}^{k_l}) \leq p(x_{i_m}^{k_m} = x_{i_n}^{k_n} = a) \leq \min_{m,n} \{ p(a | x_{i_m}^{k_m}), p(a | x_{i_n}^{k_n}) \}.
\]

This relation will be used to construct necessary condition for extended noncontextuality in Sec. VI.

**Theorem 3** (Necessary condition for maximal coupling). *If \( p(a_{i_1}^{k_1} a_{i_2}^{k_2} \ldots a_{i_l}^{k_l} | x_{i_1}^{k_1} x_{i_2}^{k_2} \ldots x_{i_l}^{k_l}) \) is a maximal coupling for the random variables \( x_{i_1}^{k_1}, x_{i_2}^{k_2}, \ldots, x_{i_l}^{k_l} \), then

\[
p_-(a) = p(x_{i_1}^{k_1} = \ldots = x_{i_l}^{k_l}) \leq p \left( \{ x_{i_j}^{k_j} = a \} \right) \leq \min_{j \in S} \{ p(a | x_{i_j}^{k_j}) \}
\]

for any subset \( S \subset [l] \).

V. **TWO OUTCOMES**

When \( O = \{-1, 1\} \) we can use a powerful tool from graph theory to find necessary conditions for noncontextuality: the *cut polytope*.12,31,41
FIG. 2: An example of a suspension graph. On the right hand side we depicted a 7-cycle, whereas on the left it is depicted its suspension graph, with a new vertex $u$ added to the vertex set, and connected to each other vertex already belonging to the 7-cycle.

Definition 8 (Cut Polytope). The cut polytope of a graph $G = (V, E)$, denoted by $\text{CUT}(G)$, is the convex hull of the set $V = \{\delta_G(S) \in \mathbb{R}^E; S \subset V\}$ which contains all cut vectors of $G$. Given $S \subset V$, the cut vector $\delta_G(S) \in \mathbb{R}^E$ associated with $S$ is defined as:

$$
\delta_{u,v} := \begin{cases} 
1, & \text{if } |S \cap \{u,v\}| = 1 \\
0, & \text{otherwise.} 
\end{cases}
$$

(22)

Let $G = (X, E)$ be the compatibility graph of a scenario $\Gamma = (X, C, \{-1, 1\})$. Given a behaviour $B$, let $P_B \in \mathbb{R}^X \times \mathbb{R}^E$ be the vector whose first $|X|$ entries are the expectation values of the random variables in $X$

$$
P_x := \langle x \rangle = p(1|x) - p(-1|x), \ x \in X
$$

(23)

and whose $|E|$ subsequent entries are the expectation values of product of pairs of compatible random variables in $X$

$$
P_{xy} := \langle xy \rangle = p(x = y) - p(x \neq y), \ (x, y) \in E.
$$

(24)

Let $\nabla G$ be the suspension graph of $G$, obtained from $G$ by adding one new vertex $u$ to $X$ which is adjacent to all the other vertices (see Fig. 2).
Proposition 4. Let $\Gamma = (X, C, \{-1, 1\})$ be a compatibility scenario, and let $G$ be the compatibility graph associated with $\Gamma$. If a behavior $B$ is noncontextual, the vector $P_B$ belongs to the cut polytope of $\nabla G$.

For a proof of this result, see Refs.\textsuperscript{26,29,40}. It implies that characterizing completely the cut polytope $\text{CUT}(\nabla G)$ gives a strong necessary condition for noncontextuality. However, as shown in references\textsuperscript{26,30–32}, such a characterization is unlikely, since membership testing in this polytope is a NP-complete problem\textsuperscript{42} for general graphs. To do so requires one to find all linear inequalities that define the facets of $\text{CUT}(\nabla G)$, which is only feasible for limited, although important, scenarios. Nevertheless, one can generally find necessary conditions for membership in $\text{CUT}(\nabla G)$, which can be used to witness contextuality in scenarios where a complete characterization of $\text{CUT}(\nabla G)$ is still missing.

Definition 9. Given $A \in \mathbb{R}^{|X|+|E|}$ and $b \in \mathbb{R}$ we say that the linear inequality
\[
A \cdot P \leq b, \tag{25}
\]
on $P \in \mathbb{R}^{|X|+|E|}$ is a noncontextuality inequality if it is satisfied for all $P \in \text{CUT}(\nabla G)$. We say that this inequality is tight if $A \cdot P = b$ for some $P \in \text{CUT}(\nabla G)$ and we say that this inequality is facet-defining if the set
\[
\{P \in \text{CUT}(\nabla G) | A \cdot P = b \} \tag{26}
\]
is a facet of $\text{CUT}(\nabla G)$.

Every noncontextuality inequality gives a necessary condition for noncontextuality in the corresponding scenario. What we do next is to use known inequalities valid for $\text{CUT}(\nabla G)$ to find necessary conditions for noncontextuality in the extended sense.

A. Extended compatibility hypergraph

Definition 10. Let $H$ be the compatibility hypergraph for a compatibility scenario $\Gamma = (X, C, \{-1, 1\})$. Construct the extended compatibility hypergraph $\mathcal{H}$ of this scenario in the following way. Given a vertex $x \in X$, let $C_{i_1}, \ldots, C_{i_l}$ be all hyperedges containing it. We add to the vertex set of $\mathcal{H}$ the vertices $x^{i_1}, \ldots, x^{i_l}$, which form a hyperedge in $\mathcal{H}$. The other hyperedges of $\mathcal{H}$ are in one-to-one correspondence with the hyperedges of $H$: to each hyperedge $C_i = \{x_1, x_2, \ldots, x_{|C_i|}\}$ in $H$ corresponds the hyperedge $\{x_1^{i_1}, x_2^{i_2}, \ldots, x_{|C_i|}^{i_l}\}$ in $\mathcal{H}$.
Fig. 3 illustrates this construction for a simple example.

Definition 11. Given a behavior $B$ for the compatibility scenario defined by hypergraph $H$, we construct an extended behavior $B'$ for $B$ in the following way: for context $\{x_1^i x_2^i \ldots x_n^i\}$ of $H$ corresponding to context $C_i = \{x_1 x_2 \ldots x_n\}$ of $H$ the probability distribution assigned by behavior $B$ is equal to the probability distribution assigned to $C_i$ by behavior $B'$; for context $x_1^i, \ldots, x_n^i$ of $H$ corresponding to a vertex $x \in X$ of $H$, the probability distribution assigned by behavior $B$ is any maximal coupling for the variables $x_1^i, \ldots, x_n^i$.

Since, in general, maximal couplings are not unique, for a given behaviour $B$, there might exist more than only one extended behaviour $B'$ associated with it. In other words, $B'$ will also not be unique. With these definitions, we can rewrite Dfn. 6 as the following theorem:

Theorem 5. A behavior $B$ for the compatibility scenario defined by the hypergraph $H$ has a maximally noncontextual description if, and only if, there is an extended behavior $B'$ for $B$ which is noncontextual with respect to the compatibility scenario defined by the extended compatibility hypergraph $H$.

Thus, the problem of deciding if a behavior $B$ is noncontextual in the extended sense is equivalent to the problem of finding a noncontextual extended behavior $B'$ which is noncon-
textual in the extended scenario $\mathcal{H}$. This gives, as a corollary, a complete characterization of extended contextuality for the $n$-cycle scenario.

**B. The $n$-cycle scenario**

In the $n$-cycle scenario, $X = \{0, \ldots, n-1\}$ and two measurements $i$ and $j$ are compatible iff $j = i + 1 \mod n$. The corresponding hypergraph $H$ is a cycle with $n$ vertices. The extended hypergraph $H$ is a $2n$-cycle, with vertices $i$, $i+1$ and edges $\{i, (i+1)\}$, $\{i, i-1\}$, $i = 0, \ldots, n-1$ (see Fig. 4).

![Diagram](image)

**FIG. 4:** (a) The compatibility hypergraph $H$ of the 5-cycle scenario, which consists of five measurements $0, \ldots, 4$ and five contexts $\{i, i+1\}$, $i = 0, \ldots, 4$, the sum being taken mod 5. (b) The extended compatibility hypergraph $H$ of the 5-cycle scenario, which is a 10-cycle with vertices $i-1, i$ and edges $\{i, (i+1)\}$, $\{i, i-1\}$, $i = 0, \ldots, 4$.

**Corollary 6.** A behavior $B$ for the $n$-cycle scenario is noncontextual in the extended sense iff

$$s \left( \langle i^i (i+1)^i \rangle, 1 - \langle i^i \rangle - \langle i^{i-1} \rangle \right)_{i=0, \ldots, n-1} \leq 2n - 2,$$

where

$$s \left( z_1, \ldots, z_k \right) = \max_{\gamma_i = \pm 1, \prod \gamma_i = -1} \sum_{i=1}^{k} \gamma_i z_i.$$

**Proof.** In this case the extended behavior $H$ is unique and, as shown in Ref.1, for every context $\{i^{i-1}, i^i\}$ corresponding to $i \in X$ we have that maximal couplings satisfy:

$$\langle i^{i-1}i^i \rangle = 1 - \langle i^{i-1} \rangle - \langle i^i \rangle.$$
Hence,  
\[ P_{\mathcal{B}} = (\langle i^i(i+1)^i \rangle, 1 - \langle i^{i-1} \rangle - \langle i^i \rangle)_{i=0, \ldots, n-1}. \] (30)

As shown in Ref.\textsuperscript{43}, Eq. (27) is a necessary and sufficient condition for membership in \( \text{CUT}(\nabla C_{2n}) \). Thm. 5 implies the result. \( \blacksquare \)

VI. FROM VALID INEQUALITIES FOR \( \nabla G \) TO VALID INEQUALITIES FOR \( \nabla \mathcal{G} \)

The problem of deciding if a given behavior is noncontextual in the extended sense is, in general, extremely difficult (see, for instance Ref.\textsuperscript{42}). To completely solve it we need, first, to characterize the set of all extended behaviors \( \mathcal{B} \) and, second, characterize the set of noncontextual behaviors in the extended scenario, which is, as we mentioned before, a complex task. Although we cannot solve the problem completely, except for very special situations as in Sub. VB, we are able to find necessary conditions for the existence of a noncontextual extended behavior in any scenario using the cut polytope. The first step in this direction consists in defining a useful and important graph, associated with a given scenario, which is going to be recurrently utilized from now on:

**Definition 12.** Given a scenario \( \Gamma = (X, \mathcal{C}, O) \), let \( \mathcal{H} \) be the extended hypergraph associated with it. We call the 2-section of \( \mathcal{H} \) the extended compatibility graph associated with \( \Gamma \), and denote it by \( \mathcal{G} \).

Now, as another corollary of Thm. 5, we have:

**Corollary 7.** If a behavior \( B \) is noncontextual in the extended sense, then there is an extended behavior \( \mathcal{B} \) for \( B \) such that \( P_{\mathcal{B}} \) belongs to the cut polytope of \( \nabla \mathcal{G} \), where \( \mathcal{G} \) is the extended compatibility graph of the scenario.

A. Triangular elimination

From valid inequalities for \( \text{CUT}(\nabla G) \) it is possible to derive valid inequalities for \( \text{CUT}(\nabla \mathcal{G}) \) using the operation of triangular elimination.

**Definition 13** (Triangular Elimination for Graphs). Let \( G = (V, E) \) be a graph, \( t \) an integer, and let \( F = \{u_i v_i \mid i = 1, \ldots, t\} \) be any subset of \( E \). The graph \( G' = (V', E') \) is a triangular
elimination of $G$ with respect to $F$ if $V' = V \cup \{w_1, w_2, \ldots, w_t\}$, where $w_1, w_2, \ldots, w_t$ are new vertices not in $V$, and $E' \supseteq \{w_iu_i, w_iv_i \mid i = 1, \ldots, t\}$ and $E' \cap E = E \setminus F$.

The graph $G'$ is obtained from $G$ by removing each edge $u_iv_i$ in $F$ from $E$ and replacing it with a new vertex $w_i$, which is connected to $u_i$ and $v_i$. Other edges connecting $w_i$ with other vertices other then $u_i$ and $v_i$ may or may not be added. A simple example is shown in Fig. 5.

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{example}
\caption{A triangular elimination of graph $G$ with respect to the edge $\{1, 2\}$. This edge is removed, and a new vertex, labelled vertex 3, is added. This new vertex is connected to both 1 and 2. The dashed edge connecting 0 and 3 may or may not be added. In both cases one ends with a valid triangular elimination for the graph $G$.}
\end{figure}

**Definition 14** (Triangular elimination for inequalities). Let $G' = (V', E')$ be a triangular elimination of $G = (V, E)$ with respect to $F = \{u_iv_i \mid i = 1, \ldots, t\}$, and suppose $A \in \mathbb{R}^E$, $A' \in \mathbb{R}^{E'}$, $b, b' \in \mathbb{R}$. The inequality $A' \cdot P' \leq b'$ is a triangular elimination of inequality $A \cdot P \leq b$ if it can be obtained from this last inequality by summing positive multiples of inequalities

$$-P_{u_iw_i} - P_{v_iw_i} - P_{u_iv_i} \leq 1,$$

$$P_{u_iw_i} + P_{v_iw_i} - P_{u_iv_i} \leq 1$$

or the other two inequalities obtained from (32) by permuting $u_i, v_i$ and $w_i$. 
**Proposition 8.** Let $G' = (V', E')$ be a triangular elimination of $G = (V, E)$. Let $A \cdot P \leq b$ be a valid inequality for $CUT(G)$ and $A' \cdot P' \leq b'$ be a triangular elimination of $A \cdot P \leq b$. Then $A' \cdot P' \leq b'$ is valid for $CUT(G')$.

**Remark:** We should remark that for our own purposes the content of Prop. 8 above is enough (see Corollary 10). Nonetheless, in Ref. [41] the authors have shown that the other implication in Prop. 8 is also true. It means that if $A' \cdot P' \leq b'$ is a valid inequality for $CUT(G')$, then $A \cdot P \leq b$ is valid for $CUT(G)$, provided that $G'$ and $A' \cdot P' \leq b'$ be triangular eliminations of $G$ and $A \cdot P \leq b$ respectively.

**B. Triangular elimination and extexted contextuality**

**Theorem 9.** Let $\Gamma$ be a compatibility scenario. If the compatibility hypergraph of $\Gamma$ coincides with its 2-section, i.e. if $H = G$, then the extended compatibility graph $\mathcal{G}$ is a triangular elimination of the compatibility graph $G$. Moreover, $\nabla \mathcal{G}$ is a triangular elimination of $\nabla G$.

**Proof.** We start with $G = (X, E(G))$ and $x_1 \in X$. Let $E_{x_1} = \{x_1y_1, x_1y_2, \ldots, x_1y_n\} \subset E(G)$ be the set of all edges incident to $x_1$ and let $G_1 = (V(G_1), E(G_1))$ be the graph obtained from $G$ in the following way: remove from $E(G)$ all edges in $E_{x_1}$, from $X$ remove the vertex $x_1$, add vertices $x_1, x_1, x_1, \ldots, x_1$, edges $\{x_1y_1, x_1y_2, \ldots, x_1y_n\}$ and all edges $x_1x_1$ with $1 \leq k < l \leq n$. The graph $G_1$ is a triangular elimination of $G$. Take now $x_2 \in V(G_1) \setminus \{x_1, x_1, x_1, \ldots, x_1\}$ and repeat the same procedure, obtaining graph $G_2$. Proceeding analogously for every vertex in $X$, and since it is finite, we get $\mathcal{G}$ in the last step. Similar argument can be used with $\nabla G$.

As a direct consequence of Prop. 8 and Thm. 9, we have:

**Corollary 10.** Given a compatibility scenario $\Gamma$, suppose that $H = G$. A necessary condition for the behavior $B$ to be noncontextual in the extended sense is that for every extended behavior $\mathcal{B}$ and for every inequality valid for $CUT(\nabla G)$, its triangular eliminations are satisfied by the vector $P_\mathcal{B}$ corresponding to $\mathcal{B}$.

It is important to notice that terms of the form of inequality (32) added to $A \cdot P \leq b$ will be satisfied at equality if the behaviors are perfectly non-disturbing. Hence, there is one
FIG. 6: The extended compatibility graph $\mathcal{G}$ is a triangular elimination of $G$. In this case, after relabelling vertex 0 as $0_1$, we remove edges $\{0, 2\}$, $\{0, 3\}$ and $\{0, 4\}$. We add vertex $0_2$, connected to $0_1$ and 2, vertex $0_3$, connected to $0_1$ and 3 and vertex 4, connected to $0_1$ and 0_4. We also add all edges between the vertices $0_i$ that are missing.

triangular elimination of $A \cdot P \leq b$ that is tight and reduces to the original inequality for non-disturbing behaviors.

When $\mathcal{B}$ is unique, we obtain a simple necessary condition for noncontextuality in the extended sense. We calculate $P_\mathcal{B}$ and substitute its entries in the inequalities for $\text{CUT} (\nabla \mathcal{G})$ obtained from the inequalities for $\text{CUT} (\nabla G)$ via triangular elimination. If we find that some of them are not satisfied, we can conclude that $B$ is contextual in the extended sense.

In the case $\mathcal{B}$ is not unique, it may be impractical to determine all possible $P_\mathcal{B}$ so we can not test directly if these vectors satisfy all triangular eliminations of a given inequality for $\text{CUT} (\nabla G)$ or not. Nevertheless, Thm. 3 will help us circumvent this difficulty.

If $A' \cdot P' \leq b'$ is a triangular elimination of $A \cdot P \leq b$, then the left-hand-side can be written as a sum of two terms $A' \cdot P' = A_1 \cdot P_1 + A_2 \cdot P_2$, where $P_1$ is the projection of $P'$ that contains the entries depending only on the contexts in $\mathcal{H}$ that come from the contexts in $H$ and $P_2$ is the projection of $P'$ that contains the terms depending only on the contexts consisting on random variables that represent the same measurement. From $P_\mathcal{B}$ we calculate $P_1$. To calculate $P_2$ explicitly we have to determine the maximal couplings for each pair of variables.
that represent the same measurement, which can be a hard task. Instead of doing this, we use the necessary condition satisfied for all maximal couplings presented in theorem 3 to calculate which value of \( A_2 \cdot P_2 \) is the worst, respecting the condition of maximal couplings. This proves the following:

**Theorem 11.** Let \( A' \cdot P' = A_1 \cdot P_1 + A_2 \cdot P_2 \leq b' \) be a valid inequality for \( \text{CUT} (\nabla G) \). Let \( m \) be the minimum of \( A_2 \cdot P_2 \) over all possible values of \( P_2 \) satisfying conditions given in Thm. 3. If

\[
A_1 \cdot P_B + m > b'
\]

\( P_B \) is contextual in the extended sense.

This gives a necessary condition for extended contextuality that can be applied in any compatibility scenario.

**VII. THE I_{3322} INEQUALITY**

Our first example is the \((3, 3, 2, 2)\) Bell scenario\(^{35,36}\), where two distinct parties perform three measurements each, each measurement with two outcomes. In this case each context has exactly two measurements, one form each party. With our notation, it means that this scenario is described by

\[
\Gamma = \{\{A_1, A_2, A_3, B_1, B_2, B_3\}, \{A_i B_j\}_{i \neq j}, \{-1, 1\}\}
\]

and \( H = G \). The compatibility graph of this scenario is the complete bipartite graph \( K_{3,3} \), shown in Fig. 7.

One of the facets of \( \text{CUT} (\nabla G) \) is given by the so called \( I_{3322} \) inequality\(^{35,36}\):

\[
\langle A_1 \rangle + \langle A_2 \rangle + \langle B_1 \rangle + \langle B_2 \rangle - \langle A_1 B_1 \rangle - \langle A_1 B_2 \rangle - \langle A_2 B_1 \rangle - \langle A_2 B_2 \rangle - \langle A_1 B_3 \rangle - \langle A_2 B_3 \rangle - \langle A_3 B_1 \rangle - \langle A_3 B_2 \rangle \leq 4
\]

The extended compatibility graph \( G \) of this scenario is shown in Fig. 8. Each vertex \( A_i \) becomes three new vertices \( A_i^1, A_i^2, A_i^3 \) in \( G \), and similar for each \( B_i \). Vertices \( A_i^j \) and \( B_j^i \) are connected. The vertices \( A_i^1, A_i^2, A_i^3 \) are connected for each \( i \) and similar for \( B_i^1, B_i^2, B_i^3 \).

Applying triangular elimination in the \( I_{3322} \) inequality, we can derive the following valid inequality for \( \text{CUT} (\nabla G) \).
FIG. 7: Compatibility graph $G$ of the $(3, 3, 2, 2)$ Bell scenario. Measurements of first party are labeled $A_1, A_2, A_3$ and measurements of the second party are labelled $B_1, B_2, B_3$.

FIG. 8: Extended compatibility graph $\mathcal{G}$.

\[
\langle A_1^1 \rangle + \langle A_2^1 \rangle + \langle B_1^1 \rangle + \langle B_2^1 \rangle - \langle A_1^1 B_1^1 \rangle - \langle A_2^2 B_2^1 \rangle - \langle A_3^3 B_3^1 \rangle - \langle A_2^1 B_1^2 \rangle \\
- \langle A_2^2 B_2^2 \rangle + \langle A_3^3 B_3^2 \rangle - \langle A_3^1 B_3^1 \rangle + \langle A_3^2 B_2^2 \rangle + \langle A_1^1 A_1^2 \rangle + \langle A_1^3 A_1^3 \rangle + \langle A_2^2 A_2^2 \rangle \\
+ \langle A_2^1 A_3^3 \rangle + \langle A_3^1 A_3^2 \rangle + \langle B_1^1 B_1^2 \rangle + \langle B_1^3 B_3^1 \rangle + \langle B_2^1 B_2^2 \rangle + \langle B_1^3 B_3^2 \rangle + \langle B_1^1 B_3^1 \rangle + \langle B_3^1 B_3^2 \rangle \leq 14 \quad (36)
\]

This inequality is tight and reduces to Ineq. (35) for non-disturbing behaviors, since in this particular case we have that $\langle A_i^j A_i^k \rangle = 1$ and $\langle B_i^j B_i^k \rangle = 1$ for every $i, j, k$.

In this scenario, each measurement has two outcomes and belongs to three contexts, therefore each behavior $B$ has a unique extended behavior $\mathcal{B}$ corresponding to it. This, in turn, implies the following result:

**Corollary 12.** A necessary condition for extended noncontextuality of a behavior $B$ in the
Bell scenario is that the unique extended behavior of $B$ satisfies the triangular elimination of the $I_{3322}$ inequality given by Eq. (36).

VIII. CHAINED INEQUALITIES

We consider now the $(n, n, 2, 2)$ Bell scenario with 2 parties, $n$ measurements per party, each measurements with 2 outcomes. Also in this case each context has exactly two measurements, one from each party, and $H = G$. Once again, sticking to our notation, we describe such a scenario with

$$\Gamma = \{\{A_1, ..., A_n, B_1, ..., B_n\}, \{A_i A_j\}_{i \neq j}, \{-1, 1\}\}$$  \hfill (37)

The compatibility graph $G$ is the complete bipartite graph $K_{n,n}$. A family of noncontextuality inequalities for these scenarios consists of the so called Chained Inequalities$^{37}$, given by

$$\langle A_1 B_2 \rangle + \langle B_1 A_2 \rangle + \ldots + \langle B_{n-1} A_n \rangle + \langle A_n B_n \rangle - \langle B_n A_1 \rangle \leq 2n - 2.$$  \hfill (38)

Each vertex $A_i$ becomes $n$ new vertices $A_i^1, A_i^2, \ldots, A_i^n$ in the extended compatibility graph $\mathcal{G}$, and similar for each $B_i$. Vertices $A_i^j$ and $B_i^j$ are connected. The vertices $A_i^1, A_i^2, \ldots, A_i^n$ are connected for each $i$ and similar for $B_i^1, B_i^2, \ldots, B_i^n$.

Applying triangular elimination in the inequality (38), we can derive the following valid inequality for CUT $\langle \nabla \mathcal{G} \rangle$, which is tight and reduces to Ineq. (38) for no-disturbing behaviors:

$$\langle A_1^1 B_2^1 \rangle + \langle B_1^1 A_2^1 \rangle + \ldots + \langle B_{n-1}^n A_n^n \rangle + \langle A_n^n B_n^n \rangle - \langle B_n^1 A_1^1 \rangle + \langle A_1^1 A_1^n \rangle + \langle A_1^2 A_2^2 \rangle + \ldots + \langle A_1^{n-1} A_n^n \rangle + \langle B_1^1 B_1^2 \rangle + \langle B_2^2 B_2^3 \rangle + \ldots + \langle B_n^1 B_n^n \rangle \leq 4n - 2.$$  \hfill (39)

In this scenario, each measurement belongs to $n$ contexts, therefore each behavior $B$ may have several extended behaviors $\mathcal{B}$ corresponding to it. Given such $\mathcal{B}$, we construct the vector $P_{\mathcal{B}}$. Let $P_1$ be the projection of $P_{\mathcal{B}}$ over the entries corresponding to contexts $A_i^j B_j^i$ and $P_2$ be the projection of $P_{\mathcal{B}}$ over the entries corresponding to contexts $A_i^j A_k^i$ and $B_j^i B_k^i$. $P_1$ depends only in $P_B$ and hence is the same for all extended behaviors $P_{\mathcal{B}}$. The projection $P_2$ depends on the choice of maximal coupling for each pair $A_i^j A_k^i$ and $B_j^i B_k^i$. 

21
The left-hand side of inequality (39) can be divided in two parts. The first part contains the terms

$$\langle A_1^2 B_2^1 \rangle + \langle B_1^2 A_2^1 \rangle + \ldots + \langle B_{n-1}^n A_n^{n-1} \rangle + \langle A_n^n B_n^n \rangle - \langle B_1^n A_1^n \rangle$$

(40)

and depends only on $P_1$, and hence only on $P_B$. The second part contains the terms

$$\langle A_1^n A_1^n \rangle + \langle A_1^n A_2^n \rangle + \ldots + \langle A_{n-1}^n A_n^n \rangle + \langle B_1^1 B_1^1 \rangle + \langle B_1^2 B_2^2 \rangle + \ldots + \langle B_n^n B_n^n \rangle$$

(41)

and depends only on $P_2$. No matter which extended behavior we have, the projection $P_2$ must necessarily satisfy the constraint given in Thm. 3. Let $m$ be the minimum of the second term (41) over all vectors $P_2$ satisfying Thm. 3.

**Corollary 13.** A necessary condition for extended noncontextuality of a behavior $B$ in the $(n, n, 2, 2)$ Bell scenario is that the inequality

$$\langle A_1^2 B_2^1 \rangle + \langle B_1^2 A_2^1 \rangle + \ldots + \langle B_{n-1}^n A_n^{n-1} \rangle + \langle A_n^n B_n^n \rangle - \langle B_1^n A_1^n \rangle + m \leq 2(2n - 1)$$

(42)

is satisfied by the projection $P_1$ of the extended behaviors $\mathcal{B}$ for $B$.

**IX. SCENARIOS WITH CONTEXTS WITH MORE THAN THREE MEASUREMENTS**

When there are contexts with more than three measurements, $H \neq G$ and $\mathcal{B}$ is not a triangular elimination of $G$. Nevertheless we can still generate valid inequalities for CUT ($\nabla \mathcal{B}$) from valid inequalities for CUT ($\nabla G$) using two strategies: the first one is to use a graph operation called *vertex splitting* [31,33,41]; the second one is to use triangular elimination combined with a graph operation called *edge contraction* [31,33,41].

**A. Vertex splitting**

**Definition 15** (Vertex splitting for graphs). Let $G = (V, E)$ be a graph, $w \in V$ and $(S, T, B)$ be a partition of the neighbors of $w$. The graph $G' = (V', E')$ is obtained from $G$ by splitting vertex $w$ into $s$ and $t$, for $s, t \notin V$, with respect to the partition $(S, T, B)$ if

$V' = (V \setminus \{w\}) \cup \{s, t\}$
and
\[ E' = (E \setminus \delta(w)) \cup (s : S \cup B) \cup (t : T \cup B) \cup \{st\}, \] (43)
where \( \delta(w) \) is the set of neighbours of \( w \), \( (s : S \cup B) \) is the set of all edges connecting \( s \) to the vertices in \( S \cup B \) and \( (t : T \cup B) \) is the set of all edges connecting \( t \) to the vertices in \( T \cup B \).

In other words, the graph \( G' \) is the graph obtained from \( G \) removing the vertex \( w \) and replacing it by vertices \( s \) and \( t \), which are connected. The vertices in \( S \) are connected only to \( s \), the vertices in \( T \) are connected only to \( t \) and the vertices in \( B \) are connected to both \( s \) and \( t \). Figures 9a-9b illustrate a simple example of this operation.

Definition 16 (Vertex splitting for inequalities). Let \( G = (V, E) \) be a graph, \( w \in V \), \( (S, T, B) \) be a partition of the neighbours of \( w \) and \( A \cdot P \leq b \) be an inequality valid for \( \text{CUT} \ (G) \). Assume without loss of generality that \( \sum_{v \in T} |A_{wv}| \leq \sum_{v \in S} |A_{wv}| \). Define \( A' \) in the following way:

\[
A'_{st} = -\sum_{v \in T} |A_{wv}| \quad \text{(44)}
\]
\[
A'_{tv} = 0, \ v \in B \quad \text{(45)}
\]
\[
A'_{tv} = A_{wv}, \ v \in T \quad \text{(46)}
\]
\[
A'_{sv} = A_{wv}, \ v \in S \cup B \quad \text{(47)}
\]
\[
A'_{uv} = A_{uv}, \ uv \in E' \setminus [\delta(s) \cup \delta(t)] \quad \text{(48)}
\]
The inequality \( A' \cdot P' \leq b \) is called the vertex splitting of \( A \cdot P \leq b \) with respect to \( w \in V \) and \( (S, T, B) \).
Proposition 14. Let graph $G'$ and inequality $A' \cdot P' \leq b$ be vertex splittings of $G$ and $A \cdot P \leq b$ (resp.) with respect to $w \in V$ and $(S, T, B)$. If $A \cdot P \leq b$ is a valid inequality for CUT ($G$), then $A' \cdot P' \leq b$ is a valid inequality for CUT ($G'$).

Theorem 15. The extended compatibility graph $G$ and its suspension graph $\nabla G$ can be obtained from the compatibility graph $G$ and $\nabla G$, respectively, using a sequence of vertex splitting operations.

Proof. Choose $x \in X$ and let $C_1, \ldots, C_n$ be the contexts containing $x$. Then $\delta(x)$ contains the measurements in $\cup C_i \setminus C_1$. Starting with $G$, the first operation is splitting $x$ into $x_1$ and $x_1'$ with respect to the partition

$$
(S_1 = C_1 \setminus \cup_{i>1} C_i, T_1 = \cup_{i>1} C_i \setminus C_1, B_1 = \cup_{i>1} C_i \cap C_1).
$$

Vertex $x_1$ is connected to $S_1$, vertex $x_1'$ is connected to $T_1$ and both $x_1$ and $x_1'$ are connected to $B_1$. With this operation, we set $x_1$ as the copy of $x$ in $G$ corresponding to context $C_1$. The next operation is split $x_1'$ into vertices $x_2$ and $x_2'$ with respect to partition

$$
(S_2 = C_2 \setminus \cup_{i>2} C_i, T_2 = \cup_{i>2} C_i \setminus C_2, B_2 = \cup_{i=2}^n C_i \cap C_2 \cup \{x_1\}).
$$

With this operation, we set $x_2$ as the copy of $x$ in $G$ corresponding to context $C_2$. We proceed analogously, in each step splitting vertex $x_k'$ into $x_{k+1}$ and $x_{k+1}'$ with respect to the partition

$$
(S_{k+1} = C_{k+1} \setminus \cup_{i>k+1} C_i, T_{k+1} = \cup_{i>k+1} C_i \setminus C_{k+1}, B_{k+1} = \cup_{i=k+1}^n C_i \cap C_{k+1} \cup \{x_1, \ldots, x_k\}).
$$

With this chain of operations we eliminate vertex $x$ and add the clique $x_1, \ldots, x_n$, each $x_i$ connected only to the vertices in context $C_i$ and the other $x_j$. Applying the same procedure to the other vertices in $X$ we recover $G$. A similar argument can be used for $\nabla G$. ■

A simple example of the procedure described in the previous proof is shown in Fig. 10.

Combining Prop. 14 and Thm. 15, we have:

Corollary 16. From valid inequalities for CUT ($\nabla G$) we can generate necessary conditions for extended noncontextuality using vertex splitting.
FIG. 10: (a) The compatibility graph of the scenario with measurements 0, . . . , 5 and contexts $C_1 = \{0, 1, 2\}$, $C_2 = \{0, 3, 5\}$ and $C_3 = \{0, 4, 5\}$. (b) Applying vertex splitting to vertex 0 with respect to the partition $S_1 = \{1, 2\}$, $T_1 = \{3, 4, 5\}$, $B_1 = \emptyset$. Vertex $0_1$ is the copy of 0 in $G$ corresponding to context $C_1$. (c) Applying vertex splitting to vertex $0_1'$ with respect to the partition $S_2 = \{3\}$, $T_1 = \{4\}$, $B_1 = \{0, 1, 5\}$. This step generates vertices $0_2$ and $0_2' = 0_3$, corresponding to contexts $C_2$ and $C_3$ respectively. Applying a similar procedure to vertex 5 we get $G$.

B. Triangular Elimination and Edge Contraction

Definition 17 (Edge contraction for graphs). Let $G = (V, E)$ be a graph, $w \notin V$, and $uv \in E$. The graph $G' = (V', E')$ is a contraction of $G$ at edge $uv$ if $V' = [V \setminus \{u, v\}] \cup \{w\}$ and $E' = [E \setminus \{(uv) \cup \{wx | x \in \delta(u)\} \cup \{vx | x \in \delta(v)\}\}] \cup \{wx | x \in \delta(u) \cup \delta(v)\}$.

A simple example of this operation is shown in Fig. 11.

FIG. 11: Contraction of graph $G$ at the edge connecting vertices 0 and 1.
Definition 18 (Edge contraction for inequalities). Let $G = (V, E)$ be a graph, $uv \in E$ and $A \cdot P \leq b$ be an inequality valid for CUT $(G)$. Define $A'$ in the following way:

\[
A'_{xy} = A_{xy}, \quad x, y \neq w \tag{52}
\]
\[
A'_{ux} = A_{ux}, \quad x \in \delta(u) \setminus \delta(v) \tag{53}
\]
\[
A'_{ux} = A_{ux}, \quad x \in \delta(v) \setminus \delta(u) \tag{54}
\]
\[
A'_{ux} = A_{ux} + A_{ux}, \quad x \in \delta(u) \cap \delta(v). \tag{55}
\]

The inequality $A' \cdot P \leq b$ is called the contraction of $A \cdot P \leq b$ at the edge $uv$.

Proposition 17 (Edge contraction lemma\textsuperscript{31,41}). If $G'$ and $A' \cdot P \leq b$ are contractions of $G$ and $A \cdot P \leq b$, respectively, at edge $uv$ and $A \cdot P \leq b$ is a valid for CUT $(G)$, the inequality $A' \cdot P \leq b$ is valid for CUT $(G')$.

Theorem 18. The extended compatibility graph $G$ and its suspension graph $\nabla G$ can be obtained from $G$ and $\nabla G$, respectively, using triangular elimination and edge contraction.

Proof. When some contexts have three elements or more, the problem with the construction of Thm. 9 is that we have a copy for $v \in X$ for each vertex in $\delta(v)$ instead of one copy for each context containing $v$. From this graph we can obtain $G$ identifying these extra copies contracting the corresponding edges. A similar argument can be used for $\nabla G$. □

A simple example of this procedure is shown in Fig. 12. As an corollary, we have the following:

Corollary 19. Valid inequalities for $G$ can be generated combining triangular elimination and edge contraction of valid inequalities for $G$.

This provides another tool to derive necessary conditions for extended noncontextuality in any scenario.

X. THE PERES-MERMIN INEQUALITY

Although the cut polytope provides a powerful tool to derive necessary conditions for contextuality, both in the standard and in the extended sense, it is not enough to characterize completely the set of noncontextual distributions in scenarios with contexts containing more then two random variables, since there are contextual behaviors that can not be detected...
FIG. 12: (a) Compatibility graph of the scenario with measurements 0, \ldots, 4 and contexts $C_1 = \{0, 1, 2\}$ and $C_2 = \{0, 3, 4\}$. (b) The graph $G'$ obtained from $G$ after applying the procedure described in Thm. 9. Notice that this is not the extended compatibility graph of the scenario, since there are four copies of 0 instead of two. (c) The extended compatibility graph of the scenario is obtained contracting the edges $0^10^2$, which gives vertex $0_1$ (the copy of vertex 0 corresponding to context $C_1$), and $0^30^4$, which gives vertex $0_2$ (the copy of vertex 0 corresponding to context $C_2$).

when we look only to the binary expectation values of Eq. (24), that is, there are contextual behaviors $B$ for which $P_B \in \text{CUT} (\nabla G)$.

With this in mind, it would be useful to find strategies to derive necessary conditions for extended contextuality from inequalities that involve expectation values with more than two random variables. In what follows, we show that this is possible with a simple procedure, similar to triangular elimination, using the Peres-Mermin inequality as an example.

The Peres-Mermin square is a contextuality scenario with nine measurements $A_i$, $i = 1, \ldots, 9$, with outcomes ±1, and compatibility hypergraph shown in Fig. (13). These measurements can be chosen in quantum theory in such a way that the product of the three measurements in each line and in the first two columns is equal to the identity operator $I$, while the product of the measurements in the last column is equal to $-I$.

For this scenario, every noncontextual behavior must satisfy the inequality

$$\langle A_1A_2A_3 \rangle + \langle A_4A_5A_6 \rangle + \langle A_7A_8A_9 \rangle + \langle A_1A_4A_7 \rangle + \langle A_2A_5A_8 \rangle - \langle A_3A_6A_9 \rangle \leq 4$$

while for all quantum behaviors the left hand side is equal to 6. This is one of the famous examples of state independent contextuality: for this choice of measurements, all quantum
states yield noncontextual behaviors.

The extended compatibility hypergraph for this scenario is shown in Fig. 14. Labeling the hyperedges of H defined by the rows in Fig. 13 as 1, 2, 3 and the hyperedges defined by the columns as 4, 5, 6, each measurement $A_i$ is divided in two new vertices of $\mathcal{H}$ $A_i^j$ and $A_i^k$, where $j \in \{1, 2, 3\}$ and $k \in \{4, 5, 6\}$ according to the row and column $A_i$ belongs to. Although the tools provided by the CUT polytope can not be used in this case, since the inequality (56) involves mean values of the product of three measurements instead of two, some ideas of Sec. VI can be used in similar way to derive valid inequalities for the extended scenario from it.
We start with the Ineq. 56, substituting each $A_i$ with its copy $A_i^j$ with $j \in \{1, 2, 3\}$:

\[
\langle A_1^1 A_2^1 A_3^1 \rangle + \langle A_2^2 A_5^2 A_6^2 \rangle + \langle A_3^3 A_8^3 A_9^3 \rangle + \langle A_1^1 A_4^1 A_7^1 \rangle + \langle A_2^2 A_5^2 A_8^2 \rangle - \langle A_3^3 A_6^3 A_9^3 \rangle \leq 4 \tag{57}
\]

valid for all noncontextual extended behaviors.

To eliminate the term $\langle A_1^1 A_2^2 A_3^3 \rangle$ we use

\[
A_1^1 A_2^2 A_3^3 = A_1^4 A_2^4 A_3^4 - \Delta A_1 A_4 A_2^4 + A_1^4 A_2^1 A_4^1 A_7^1 + A_1^4 A_2^1 A_4^1 A_7^1 + A_1^4 A_2^1 A_4^1 A_7^1 \tag{58}
\]

where $\Delta A_1 = A_1^1 - A_1^4$ and similar for $\Delta A_4$ and $\Delta A_7$. From this we get

\[
\langle A_1^1 A_2^1 A_3^3 \rangle + \langle A_2^2 A_5^2 A_6^2 \rangle + \langle A_3^3 A_8^3 A_9^3 \rangle + \langle A_1^1 A_4^1 A_7^1 \rangle + \langle A_2^2 A_5^2 A_8^2 \rangle - \langle A_3^3 A_6^3 A_9^3 \rangle \leq 4 - \langle \Delta A_1 A_4 A_2^4 \rangle - \langle A_1^4 A_2^1 A_4^1 A_7^1 \rangle - \langle A_1^4 A_2^1 A_4^1 A_7^1 \rangle \tag{59}
\]

\[
4 + \sum_{i=1}^{4} |\Delta A_i| \tag{60}
\]

Proceeding analogously with the other terms, we get the inequality

\[
\langle A_1^1 A_2^1 A_3^3 \rangle + \langle A_2^2 A_5^2 A_6^2 \rangle + \langle A_3^3 A_8^3 A_9^3 \rangle + \langle A_4^4 A_4^1 A_4^1 \rangle + \langle A_5^5 A_5^5 A_5^5 \rangle - \langle A_6^6 A_6^6 A_6^6 \rangle \leq 4 + \sum_{i=1}^{9} |\Delta A_i| \tag{61}
\]

valid for all noncontextual extended behaviors. This inequality is tight and reduces to the original Peres-Mermin Ineq. (56) for non-disturbing behaviors.

**XI. DISCUSSION**

Apart from its primal importance in the foundations of quantum physics, contextuality has been discovered as a potential resource for quantum computing\textsuperscript{13–15}, random number certification\textsuperscript{16}, and several other tasks in the particular case of Bell scenarios\textsuperscript{17}. Within these both fundamental and applied perspectives, certifying contextuality experimentally is undoubtedly an important primitive. It is then crucial to develop a robust theoretical framework for contextuality that can be easily applied to real experiments. This should include the possibility of treating sets of random variables that do not satisfy the assumption of *non-disturbance*, which will be hardly satisfied in experimental implementations\textsuperscript{1}.

Here we have further developed the extended definition of noncontextuality of Ref.\textsuperscript{1}, which can be applied in situations where the non-disturbance condition does not hold,
rewriting it in graph-theoretical terms. We then explore the geometrical aspects of the graph approach to contextuality to derive necessary conditions for extended contextuality that can be tested directly with experimental data in any contextuality experiment and which reduce to traditional necessary conditions for noncontextuality if the non-disturbance condition is satisfied.

It would be interesting to give a characterization of which of these inequalities are facet-defining. In Ref.\textsuperscript{41}, several results regarding this issue were proved, but unfortunately our scenarios do not satisfy the hypotheses needed for the validity of such results. A more ambitious problem would be to identify which scenarios can be completely characterized with these procedures, the $n$-cycle scenarios being an important example. We leave these inquiries for future work, hoping that our results might motivate further research in these directions.

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