On geometrical aspects of the graph approach to contextuality

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The connection between contextuality and graph theory has paved the way for numerous advancements in the field. One notable development is the realization that sets of probability distributions in many contextuality scenarios can be effectively described using well-established convex sets from graph theory. This geometric approach allows for a beautiful characterization of these sets. The application of geometry is not limited to the description of contextuality sets alone; it also plays a crucial role in defining contextuality quantifiers based on geometric distances. These quantifiers are particularly significant in the context of the resource theory of contextuality, which emerged following the recognition of contextuality as a valuable resource for quantum computation. In this paper, we provide a comprehensive review of the geometric aspects of contextuality. Additionally, we use this geometry to define several quantifiers, offering the advantage...
of applicability to other approaches to contextuality where previously defined quantifiers may not be suitable.

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1. Introduction

Interesting discrepancies arise between quantum and classical probability theories when dealing with finite sets of measurements that are divided among multiple jointly measurable sets with non-empty intersections. One particular discrepancy is associated with quantum contextuality. This term refers to the unexpected observation that the statistical predictions of quantum theory cannot be explained by models where measurement outcomes reflect pre-existing properties independent of the choice or order of other compatible measurements [1–3]. Quantum contextuality is closely tied to the incompatibility of measurements, highlighting a peculiar and intrinsically non-classical phenomenon. It has the potential to provide a deeper and more fundamental understanding of the entire theory [4–9].

Contextuality represents a significant advancement in the foundations of quantum theory, and both its theoretical and experimental aspects have garnered considerable attention in recent times [10–14]. A powerful framework for investigating contextuality, known as the graph approach, was introduced in [8,15] and subsequently expanded upon in [16,17]. This framework has yielded remarkable results, stemming from the recognition that insights from graph theory can be directly applied to the field of contextuality. Specifically, in numerous contextuality scenarios, the sets of probability distributions can be effectively described using familiar convex sets from graph theory, leading to an elegant geometric characterization of such sets.

In addition to its significance in the foundations of physics, contextuality has been recognized not just as an intriguing feature of quantum theory but also as a vital resource for quantum computing in specific models [18–20], random number certification [21] and several other information processing tasks, especially in the case of space-like separated systems [22]. This recognition has spurred the development of a resource theory of contextuality [23–26], analogous to the well-established resource-theoretic approaches to quantum non-locality [27–34].

Resource theories provide powerful frameworks for formally treating a physical property as an operational resource. These frameworks are well suited for characterizing, quantifying and manipulating the said resource [35,36]. Resource theories comprise three key components. Firstly, there is the set of objects, defining the physical entities capable of possessing the resource. Secondly, there exists a distinct class of transformations known as the free operations. These operations possess the crucial property of mapping every resourceless object in the theory to another resourceless object. Lastly, resource quantifiers play a role in quantitatively assessing the amount of the resource contained within a given object, providing a means of characterizing the quantity or degree of the resource present.

In [25,26], an abstract characterization of the axiomatic structure of a resource theory of contextuality is presented. The authors introduce the concept of the relative entropy of contextuality as a quantifier for contextuality, derived from the notion of relative entropy distance, also known as the Kullback–Leibler divergence. Additionally, the authors briefly mention another quantifier called the robustness of contextuality, based on the convexity of the non-contextual set. Another quantifier based on convexity, the contextual fraction, was introduced in [37,38] and further investigated in [23]. Contextuality can also be quantified using the relation between quasi-probabilities and the non-disturbance set, a problem investigated in [37,39]. A natural class of contextuality-free operations with a clear operational interpretation and an explicit parametrization, the non-contextual wirings, was introduced in [24].

In this contribution, we offer a comprehensive review of the geometric aspects of quantum contextuality that arise from the graph approach. We analyse these features within the framework
of the compatibility-hypergraph approach, where a contextuality scenario is defined by the compatibility relations among measurements. Furthermore, we explore the convex sets of probability distributions that stem from classical, quantum and general probabilistic theories. We delve into their relationships with graph invariants, shedding light on the connections between these sets and the underlying graphs.

In the compatibility-hypergraph approach, the non-contextual set is related to the cut polytope \( \text{CUT}(G) \) of the corresponding compatibility graph \( G \) and, for a special class of scenarios, to the metric polytope \( M(G) \) of \( G \). The quantum set is related to the eliptope \( E(G) \), and the non-disturbance set is related to the rooted semimetric polytope \( \text{RCMET}(G) \). Using the geometry of these sets, we generalize the contextuality quantifier introduced in [25] by employing symmetric distances in the space of probabilities. This approach offers two distinct advantages. Firstly, it enables us to use both graph invariants and non-contextuality inequalities to compute this quantifier, thereby enhancing our understanding of its properties. Secondly, this approach allows us to define a contextuality quantifier within other frameworks for contextuality where the quantifier proposed in [25] is not applicable. Additionally, we outline some important features of the convexity-based contextuality quantifiers, providing valuable insights into their nature and utility.

2. The compatibility-hypergraph approach

**Definition 2.1.** A compatibility scenario is defined by a triple \( \Upsilon := (\mathcal{M}, \mathcal{C}, O) \), where \( O \) is a finite set, \( \mathcal{M} \) represents measurements in a physical system taking values in \( O \), and \( \mathcal{C} \) is a family of subsets of \( \mathcal{M} \) such that \( \cup_{C \in \mathcal{C}} C = \mathcal{M} \) and \( C, C' \in \mathcal{C} \) and \( C \subseteq C' \) imply \( C = C' \). The elements \( C \in \mathcal{C} \) are called (maximal) contexts, and the set \( \mathcal{C} \) is referred to as the compatibility cover of the scenario.

The sets in \( \mathcal{C} \) encode the compatibility relations among the elements of \( \mathcal{M} \); that is, each \( C \in \mathcal{C} \) consists of a maximal set of measurements that can be jointly performed.

**Definition 2.2.** The compatibility hypergraph of \( (\mathcal{M}, \mathcal{C}, O) \) is denoted by \( H = (\mathcal{M}, \mathcal{C}) \), where its vertex-set is \( \mathcal{M} \) and its edge-set is \( \mathcal{C} \). The compatibility graph of the scenario is the 2-section of \( H \), the graph \( G \) with vertex-set of \( \mathcal{M} \) and edge-set of \( E(G) = \{(M_i, M_j) | \exists e \in E(H); M_i, M_j \in e\} \).

Since pairwise compatibility of a set of measurements does not guarantee their joint compatibility, the compatibility hypergraph is more subtle than its 2-section counterpart. However, in the context of quantum contextuality with projective measurements specifically, pairwise compatibility does imply joint compatibility. In this case, the maximal contexts within this compatibility cover correspond to the maximal cliques of the compatibility graph.

For a given context \( C \in \mathcal{C} \), the set of possible tuples of outcomes for a joint measurement of the elements of \( C \) is the Cartesian product of \( |C| \) copies of \( O \), denoted by \( O^C \). When the measurements in \( C \) are jointly performed, a set of outcomes in \( O^C \) will be observed. This individual run of the experiment will be referred to as a measurement event.

**Definition 2.3.** A behaviour \( B \) for the scenario \( (\mathcal{M}, \mathcal{C}, O) \) comprises a set \( \{p_C : O^C \rightarrow [0, 1] | C \in \mathcal{C}\} \) of probability distributions \( p_C \) on \( O_C \) (i.e. \( p_C(s) \geq 0 \) and \( \sum_{s \in O_C} p_C(s) = 1 \)) for each \( C \in \mathcal{C} \).

For each \( C \), \( p_C(s) \) gives the probability of obtaining outcomes \( s \) in a joint measurement of the elements of \( C \).

Given a probability distribution in \( C \in \mathcal{C} \), we can also naturally define marginal distributions for each \( U \subset C \): \( p_U^C(s) = \sum_{s' \in O^C | s'|_U = s} p_C(s') \) where \( s'|_U \) is the restriction of \( s \) to \( U \). The superscript \( C \) in \( p_U^C \) is necessary because, without further restrictions, the marginals may depend on the context \( C \).

**Definition 2.4.** The non-disturbance set \( \chi(\Upsilon) \) is the set of behaviours such that for any two intersecting contexts \( C \) and \( C' \) the consistency relation \( p_{O_C|O_{C'}}^C = p_{O_C|O_{C'}^C}^{C'} \) holds.

The non-disturbance set is a polytope, defined by a finite number of linear inequalities and equalities.
Now, we inquire whether it is feasible to extend the distributions $p_C$ consistently to larger sets that include $C$. The ideal goal would be to define a distribution on the set $O^M$ specifying the assignment of outcomes to all measurements, such that the restrictions of this distribution yield the probabilities specified by the behaviour within all contexts in $C$. However, a more refined and appropriate question arises: under what circumstances is it possible to achieve this goal?

This question was initially explored by Fine [40], focusing on the restricted case of Bell scenarios. It was subsequently generalized by Brandenburger and Abramsky [37]. The concept of contextuality is intimately linked to the possibility of extending elements from $O^C$ to global sections within $O^M$.

**Definition 2.5.** A global section for $M$ is a probability distribution $p_M : O^M \rightarrow [0, 1]$, where $O^M$ denotes the Cartesian product of $|M|$ copies of $O$. A global section for a behaviour $B \in X(\Upsilon)$ is a global section for $M$ such that the restriction of $p_M$ to each context $C \in C$ is equal to $p_C$. The behaviours with a global section are called non-contextual.

Behaviours with global section are deeply connected with non-contextual completions of quantum theory, also known as non-contextual hidden variable models [37,41].

(a) Classical realizations and non-contextuality

**Definition 2.6.** A classical realization for the scenario $\Upsilon = (M, C, O)$ is given by a probability space $(\Omega, \Sigma, \mu)$, where $\Omega$ is a sample space, $\Sigma$ a $\sigma$-algebra and $\mu$ a probability measure in $\Sigma$, and for each $M \in M$ a partition of $\Omega$ into $|O|$ disjoint subsets $A^M_j \in \Sigma$, $j \in O$. For each context $C = \{M_1, \ldots, M_m\}$, the probability of the outcome $s = (a_1, \ldots, a_m)$ for a joint measurement of the elements of $C$ is

$$p_C(s) = \mu \left( \bigcap_{k=1}^m A^M_{a_k} \right). \quad (2.1)$$

The behaviours that can be obtained in this form are called classical behaviours. The set of all classical behaviours will be denoted by $C(\Upsilon)$.

The set $C(\Upsilon)$ is a polytope with $|O^M|$ vertices. If a behaviour $B$ is classical, we have that

$$p_C^B(s|U) = \mu \left( \bigcap_{k \in M \in U} A^M_{a_k} \right), \quad (2.2)$$

is independent of the context $C$, for all $C \in C$ such that $U \subset C$ and hence $B \in X(\Upsilon)$.

**Theorem 2.7.** A behaviour has a global section if and only if it is classical.

For a proof of this result, see corollary 2.1 in [41]. This proves that classical behaviours and non-contextual behaviours are equivalent concepts.

(b) Quasi-probabilities and the set of non-disturbing behaviours

A quasi-probability distribution is a set of real numbers $p_i$ such that $\sum_i p_i = 1$. If we relax the restriction that $p_M$ be a probability distribution and require only that it is a quasi-probability distribution, then every non-disturbing behaviour has a global quasi-probability distribution consistent with it [37].

**Theorem 2.8.** A behaviour is non-disturbing if, and only if, it has a quasi-probability global section $p_M$.

*Proof.* The sets $C(\Upsilon)$ and $X(\Upsilon)$ are polytopes with the same dimension, with $C(\Upsilon) \subseteq X(\Upsilon)$. Hence $X(\Upsilon)$ is contained in the subspace generated by $C(\Upsilon)$. Given a behaviour $B \in X(\Upsilon)$ it can
then be written as a linear combination of elements of $C(\mathcal{Y})$:

$$B = \sum_i \lambda_i B_i^C, \quad \lambda_i \in \mathbb{R}, \ B_i^C \in C(\mathcal{Y}). \quad (2.3)$$

Let $p^i_M$ be a global section for $B_i^C$. Then $p_M = \sum_i \lambda_i p^i_M$ is a quasi-probability global section for $B$.

Non-contextuality can be characterized in terms of quasi-probability global sections. A behaviour $B$ is non-contextual if and only if a quasi-probability global section for $B$ exists with non-negative entries.

### (c) Quantum realizations

**Definition 2.9.** A quantum realization for the scenario $\mathcal{Y} = (\mathcal{M}, C, O)$ is defined by a Hilbert space $\mathcal{H}$, where for each $M \in \mathcal{M}$ there exists a partition of the identity operator acting on $\mathcal{H}$ into $|O|$ projectors $P^M_i$ $(i \in O)$, and a density matrix $\rho$ acting on $\mathcal{H}$. In a given context $C = M_1, \ldots, M_m \in C$, the compatibility condition demands that

$$[P^M_i, P^M_j] = 0, \forall i, j, k, l. \quad (2.4)$$

The probability of the outcome $s = (a_1, \ldots, a_m)$ for a joint measurement of $C$ is given by

$$p_C(s) = \text{Tr} \left( \prod_{k=1}^m P^M_k \rho \right). \quad (2.5)$$

Behaviours that can be expressed in this form are termed quantum behaviours. The set of all quantum behaviours will be denoted by $Q(\mathcal{Y})$.

It is a known fact that $Q(\mathcal{Y})$ is convex, and $C(\mathcal{Y}) \subseteq Q(\mathcal{Y}) \subseteq X(\mathcal{Y})$. However, it is not a polytope in general. Notice that the Hilbert space is not fixed, and the set $Q(\mathcal{Y})$ contains realizations in all dimensions.

### 3. The geometry of scenarios with $H = G$ and $|O| = 2$

Since there are many constraints in the definition of $X(\mathcal{Y})$, this set can be described in various equivalent ways. The same is true for $C(\mathcal{Y})$. If $\mathcal{Y}$ is a scenario in which every context consists of at most two measurements, that is, $H = G$, and additionally each measurement has two outcomes, denoted as $\pm 1$; these descriptions lead to well-known polytopes from graph theory.

In this type of scenario, the non-disturbance set $X(\mathcal{Y})$ is a subset of $\mathbb{R}^{4|E|}$. Given a context $\{M_i, M_j\} \in C$, we denote by $p_{ij}(ab)$ the probability of obtaining outcome $a$ for measurement $M_i$ and outcome $b$ for measurement $M_j$. We denote by $p_i(a) = \sum_b p_{ij}(ab)$ the marginal probability for measurement $M_i$ and similar for measurement $M_j$.

The normalization and non-disturbance conditions imposed on the behaviour allow us to determine all its entries knowing only $p_{ij}(-1 - 1)$ and $p_i(-1)$. We define

$$\phi : \mathbb{R}^{4|E|} \rightarrow \mathbb{R}^{|V(G)|+|E(G)|}$$

$$p = (p_{ij}(ab))_{(i,j) \in E(G), a=\pm 1, b=\pm 1} \mapsto q = (q_i, q_{jk})_{i \in V(G), (j,k) \in E(G)} \quad (3.1)$$

such that $q_i = p_i(-1)$ and $q_{jk} = p_{jk}(-1 - 1)$. The image of all non-contextual behaviours for this scenario under the action of transformation is equal to a well-known convex polytope from graph theory, the correlation polytope of $G$.

**Definition 3.1.** Given $S \subset V(G)$, we define the correlation vector $v(S) \in \mathbb{R}^{|V(G)|+|E(G)|}$

$$v(S)_i = \begin{cases} 1 & \text{if } i \in S; \\ 0 & \text{otherwise, } i \in V(G) \end{cases} \quad \text{and} \quad v(S)_{jk} = \begin{cases} 1 & \text{if } j, k \in S; \\ 0 & \text{otherwise, } (j, k) \in E(G). \end{cases} \quad (3.2)$$

The correlation polytope $\text{COR}(G)$ is the convex hull of all correlation vectors.
Notice that the correlation vectors correspond to the image of the extremal behaviours in $C(G)$ under the action of $\phi$, which proves the following result:

**Theorem 3.2.** If $Y$ is a scenario for which $H = G$ and $|O| = 2$, then $\phi(C(Y)) = COR(G)$.

The image of the non-disturbance polytope is also a well-known polytope from graph theory.

**Definition 3.3.** The rooted correlation semimetric polytope $RCMET(G)$ of a graph $G$ is the set of vectors $q = (q_i, q_j) \in \mathbb{R}^{(V(G) + 1) |E(G)|}$ such that

$$q_{ij} \geq 0, \quad q_i - q_j \geq 0, \quad 1 - q_i - q_j + q_{ij} \geq 0. \quad (3.3)$$

**Theorem 3.4.** If $Y$ is a scenario for which $H = G$ and $|O| = 2$, then $\phi(\mathcal{X}(Y)) = RCMET(G)$.

For a proof of this result, see theorem 2.9 of [41].

(a) The cut polytope

**Definition 3.5.** Given a graph $G$ and $c \in \{-1, 1\}^{|V(G)|}$, the cut vector of $G$ defined by $c$ is the vector $x(c) \in \mathbb{R}^{|E(G)|}$ such that $x(c)_{ij} = c_i c_j, (i, j) \in E(G)$. The cut polytope of $G$, $CUT^{\pm 1}(G)$, is the convex hull of all cut vectors of $G$.

There exists a relation between the polytopes $CUT$ and $COR$.

**Definition 3.6.** The suspension graph $\nabla G$ of $G$ is the graph with vertex-set $V(G) \cup \{e\}$ and edge-set $E(G) \cup \{(e, i), i \in V(G)\}$.

Intuitively, $\nabla G$ is the graph obtained from $G$ by adding an extra vertex and connecting it to all vertices of $G$.

**Theorem 3.7.** $CUT^{\pm 1}(\nabla G) = \psi(COR(G))$, in which $x = \psi(q)$ is given by

$$x_{ij} = 1 - 2q_i - 2q_j + 4q_{ij}, (i, j) \in E(G) \quad x_{ei} = 1 - 2q_i, i \in V(G). \quad (3.4)$$

For a proof of this result, see §26.1 of [42].

We can interpret $x$ in terms of expectation values of the measurements $M_i$ in the scenario:

$$x_{ij} = \langle M_i M_j \rangle = p_{ij}(1) + p_{ij}(-1 - 1) - p_{ij}(-1) - p_{ij}(1 - 1) \quad (3.5)$$

and

$$x_{ei} = \langle M_i \rangle = p_i(1) - p_i(-1). \quad (3.6)$$

We can also define the cut polytope using the outcome values 0 and 1 instead of $\pm 1$.

**Definition 3.8.** Given a graph $G$ and $c \in \{0, 1\}^{|V(G)|}$, the 01-cut vector of $G$ defined by $c$ is the vector $y(c) \in \mathbb{R}^{|E(G)|}$ such that $y(c)_{ij} = c_i c_j, (i, j) \in E(G)$. The 01-cut polytope of $G$, $CUT^{01}(G)$, is the convex hull of all 01-cut vectors of $G$.

The two definitions $CUT^{\pm 1}$ and $CUT^{01}$ are related by a bijective linear map $\alpha$ that maps $x$ to $y = 1 - 2x$.

Characterizing these polytopes for general scenarios is challenging due to the exponential growth in the number of extremal points as the number of vertices in the compatibility graph increases. However, we can seek connections between these polytopes and other simpler polytopes, even if these connections are only valid for a restricted class of graphs. In line with this approach, for certain graphs, it is possible to establish a relationship between $CUT^{01}(G)$ and the metric polytope of $G$, denoted as $MET(G)$.

**Definition 3.9.** A graph $G'$ is called a minor of the graph $G$ if $G'$ can be obtained from $G$ by deleting edges, vertices and by contracting edges, that is, identifying vertices that are connected by an edge in $G$. 


Definition 3.10. Let $d$ be a semimetric on $n$ points, i.e. a function $d: \{1, \ldots, n\}^2 \rightarrow \mathbb{R}^+$, satisfying the triangle inequalities $d(i, j) + d(i, k) - d(j, k) \geq 0$. Let $y \in \mathbb{R}^{|E(G)|}$ be such that $y_{ij} = d(i, j), (i, j) \in E(G)$. The set of all $y$ satisfying this condition is the metric polytope of $G$.

Let $K_n$ be the complete graph on $n$ vertices, that is, $|V(G)| = n$ and $(i, j) \in E(G)$ for every $i \neq j$.

Theorem 3.11. $\text{CUT}^{01}(G) = \text{MET}(G)$ if, and only if, $G$ has no $K_5$ minor.

A proof of this result can be found in §27.3 of [42]. It is extremely useful since MET$(G)$ is easily characterized. Given $F \subseteq E(G)$ and $v \in \mathbb{R}^{|E(G)|}$, let $v(F) = \sum_{(i,j) \in F} v_{ij}$.

Definition 3.12. The $n$-cycle graph $C_n$ is the graph with vertices $\{0, \ldots, n - 1\}$ such that vertices $i$ and $j$ are connected if $i - j = 1$ modulo $n$.

Theorem 3.13. The following are true for MET$(G)$:

(i) $\text{MET}(G) = \{ y \in \mathbb{R}^{|E(G)|} \mid y_{ij} \leq 1, y(F) - y(C \setminus F) \leq |F| - 1, C$ cycle of $G, F \subseteq C, |F|$ odd $\}$;

(ii) The inequality $y(F) - y(C \setminus F) \leq |F| - 1$ defines a facet of MET$(G)$ if, and only if, $C$ is a chordless cycle;

(iii) The inequality $y_{ij} \leq 1$ defines a facet of MET$(G)$ if, and only if, the edge $(i, j)$ does not belong to a triangle of $G$.

Theorems 3.11 and 3.13 can be used to find all facets of CUT$^{01}(G)$ if $G$ has no $K_5$-minor. In this case, the facets are defined by the so-called $n$-cycle inequalities:

$$y(F) - y(C \setminus F) \leq |F| - 1,$$

(3.7)

for $C$ a cycle of $G$, $F \subseteq C$ and $|F|$ odd. We can use these inequalities and the map $\alpha$ to find the facet-defining inequalities of CUT$^{\pm 1}(G)$, if $G$ has no $K_5$-minor, which are given by

$$x(F) - x(C \setminus F) \leq |C| - 2,$$

(3.8)

for $C$ a cycle of $G$, $F \subseteq C$, and $|F|$ odd. This is the same set of inequalities found for the special case $G = C_n$ in [43].

A similar result is valid for RCMET$(G)$.

Theorem 3.14. The image of RCMET$(G)$ under $\psi$ is the rooted semimetric polytope of $\nabla G$, $\text{RMET}(\nabla G)$.

The proofs of theorems 3.11, 3.13, 3.14 and many other properties of these polytopes can be found in §27.3 of [42]. As a corollary, we have:

Corollary 3.15. If $\Upsilon$ is a scenario for which $H = G$, then $\psi \circ \phi(C(\Upsilon)) = \text{CUT}^{\pm 1}(\nabla G)$, $\alpha \circ \psi \circ \phi(C(\Upsilon)) = \text{CUT}^{01}(\nabla G)$, and $\psi \circ \phi(\chi(\Upsilon)) = \text{RMET}(\nabla G)$.

(b) Correlation functions

To describe completely the sets $\chi(\Upsilon)$, $Q(\Upsilon)$ and $C(\Upsilon)$ for scenarios with at most two measurements per context using the convex bodies defined in the previous sections, we have to use vectors in $\mathbb{R}^{\|\nabla(G)\| + |E(G)|}$. In some situations, it might be useful to consider a projection $\Pi$ of these vectors in $\mathbb{R}^{|E(G)|}$ obtained by eliminating the coordinates relative to the edges $(e, i)$. The vectors in $\Pi(\text{RMET}(G))$ are called correlation vectors.

Theorem 3.16. Given a graph $G$, $\Pi(\text{RMET}(G)) = [-1, 1]^{|E(G)|}$ and $\Pi(\text{CUT}^{\pm 1}(\nabla G)) = \text{CUT}^{\pm 1}(G)$.

Please refer to proposition 4 of [42] for a proof. It is important to note that solely knowing the correlation functions is insufficient to fully reconstruct the behaviour, as the information on the marginals is lost during the projection $\Pi$. Nevertheless, these correlation vectors can still be valuable for two reasons. Firstly, they offer a simpler representation of the behaviours, which can provide insights in scenarios where dealing with the complexity of $\nabla G$ becomes challenging.
Secondly, although correlation vectors do not provide complete information about the behaviour, they can be adequate to determine whether the corresponding behaviours are contextual or not. For instance, in the case of \( G = C_n \), the knowledge of \( \Pi(X) \) is sufficient to determine membership in \( \mathcal{C}(\Upsilon) \), as demonstrated in Theorem 1 of [43].\(^1\) However, characterizing the set \( \Pi(Q(\Upsilon)) \) is significantly more challenging.

(c) The eliptope and the set of quantum behaviours

**Definition 3.17.** A complete bipartite graph is a graph whose vertices can be partitioned into two subsets \( V_1 \) and \( V_2 \) such that no edge has both endpoints in the same subset, and every possible edge that could connect vertices in different subsets is part of the graph. A complete bipartite graph with partitions of size \( |V_1| = m \) and \( |V_2| = n \) is denoted \( K_{m,n} \).

In Bell scenarios involving two parties, where one party has \( n \) measurements available and the other party has \( m \) measurements available, the associated graph is the complete bipartite graph \( K_{m,n} \). In this specific scenario, the set \( \Pi(Q(\Upsilon)) \) is connected to the eliptope of the graph \( G \).

**Theorem 3.18.** The following are true

(i) \( z \in \Pi(Q(\Upsilon)) \);
(ii) There are vectors \( u_i, v_j \in \mathbb{R}^d \), \( 1 \leq i \leq m, 1 \leq j \leq n, d \leq m + n \), such that \( z_{ij} = \{ u_i \mid v_j \} \).

For a proof of this result, see Theorem 2.1 of [44].

**Definition 3.19.** The eliptope \( \mathcal{E}(G) \) of a graph \( G \) is the set of vectors \( x \in \mathbb{R}^{|E(G)|} \) such that for each \( i \in V(G) \) exists a unit vector \( u_i \in \mathbb{R}^{|V(G)|} \) such that \( x_{ij} = \{ u_i \mid u_j \} \).

With this definition, theorem 3.18 asserts that the set of quantum correlation vectors in a bipartite Bell scenario corresponds to the eliptope of \( K_{m,n} \) [45]. The natural question arises as to whether this also holds for general contextuality scenarios. In other words, we want to determine whether, for any given graph \( G \), the equality \( \Pi(Q(\Upsilon)) = \mathcal{E}(G) \) holds. It is true that the inclusion \( \Pi(Q(\Upsilon)) \subset \mathcal{E}(G) \) always holds.

**Theorem 3.20.** \( \Pi(Q(\Upsilon)) \subset \mathcal{E}(G) \).

Refer to electronic supplementary material, section I for a proof of this result. However, for certain graphs, the inclusion \( \mathcal{E}(G) \subset \Pi(Q(\Upsilon)) \) does not hold. This is the case for the \( n \)-cycle \( C_n \) for any odd \( n \). It can be demonstrated that the violation of the \( n \)-cycle inequalities for certain points in the eliptope can exceed the maximum violation achievable with quantum behaviours.

**Theorem 3.21.** There is a point \( z \in \mathcal{E}(C_n) \) for which

\[
\sum_{i=0}^{n-2} z_{i+1} - z_{0n-1} = n \cos \left( \frac{\pi}{n} \right) .
\tag{3.9}
\]

This result is proved in electronic supplementary material, section II. Its presence serves as evidence that, in general, \( \Pi(Q(\Upsilon)) \neq \mathcal{E}(G) \). For any odd \( n \), theorem 3.21 demonstrates the existence of an element where \( \sum_{i=0}^{n-2} z_{i+1} - z_{0n-1} = n \cos(\pi/n) \), while the maximum value achievable with quantum behaviours for the same quantity, computed in theorem 3 of [43] is

\[
\frac{3n \cos(\pi/n) - n}{1 + \cos(\pi/n)} \leq n \cos \left( \frac{\pi}{n} \right) .
\tag{3.10}
\]

Another family of graphs where \( \mathcal{E}(G) \) differs from the quantum set is the complete graph \( K_n \). In this case, all measurements are compatible, resulting in the quantum set being equal to the classical set, which is a polytope. However, \( \mathcal{E}(G) \) forms a polytope only when \( G \) is a

\(^1\)This also follows as a corollary of theorem 3.11.
In such cases, \( \text{CUT}^{\pm}(G) = \mathcal{E}(G) = \Pi(\text{RMET}(G)) = [-1,1]^{|E|} \). For \( n \)-cycles with even \( n \), \( \mathcal{E}(C_n) = \Pi(Q(Y)) \). This is due to the fact that in this case, \( C_n \) is a subgraph of the complete bipartite graph \( K_{n/2,n/2} \), and the eliptope of \( C_n \) is a projection of the eliptope of \( K_{n/2,n/2} \).

4. Contextuality quantifiers

In the continuous pursuit of understanding and exploring various applications of physical phenomena, the approach of resource theories has emerged as a highly powerful tool. These theories provide a unique perspective that transcends the traditional boundaries of physics and information theory. They not only facilitate the quantification of resources available in physical systems but also offer profound insights into how these resources can be explored and manipulated to achieve specific tasks. These theories establish robust frameworks for the formal treatment of properties considered as operational resources, proving ideal for the characterization, quantification and manipulation of these resources. Moreover, they present a general approach whose concept accommodates a wide variety of situations, including those in which resources are not strictly physical states or processes but also logical entities [36].

The key elements of this approach are the objects, which may or may not possess the resource in question, and a special class of transformations between these objects [36]. Resourceless objects are called free objects, and transformations that map free objects into free objects are called free operations. Thus, the central questions of a resource theory can be expressed as: which resources can be converted into others using free operations? And how can this conversion be accomplished?

For contextuality, the set of objects is \( \mathcal{X}(\mathcal{Y}) \) and an object is free if it belongs to \( \mathcal{C}(\mathcal{Y}) \). Many classes of free operations for contextuality have been studied in the literature, but a detailed analysis of these is out of the scope of this text. A comprehensive discussion of resource theories of contextuality can be found in [46].

**Definition 4.1.** A resource theory for contextuality is defined by a set \( \mathcal{F} \) of linear free operations, that is, \( T : \mathcal{X}(\mathcal{Y}) \to \mathcal{X}(\mathcal{Y}) \) such that \( T[C(\mathcal{Y})] \subseteq C(\mathcal{Y}) \). A function \( X : \mathcal{X}(\mathcal{Y}) \to \mathbb{R} \) is a contextuality monotone for this resource theory of contextuality if \( X(T(B)) \leq X(B) \) for every \( T \in \mathcal{F} \).

Besides monotonicity under free operations, other properties of a monotone \( X \) are also desirable [23,26]:

(i) **Faithfullness:** for all \( B \in C(\mathcal{Y}), X(B) = 0 \).

(ii) **Preservation under reversible operations:** if \( T \in \mathcal{F} \) is reversible, then \( X(T(B)) = X(B) \).

(iii) **(Sub)Additivity:** we consider two kinds of (sub)additivity. First we consider a scenario \( \mathcal{Y} \) such that its compatibility hypergraph \( H \) consists of two disconnected components \( H_1 \) and \( H_2 \). The behaviours for \( \mathcal{Y} \) are formed by the list of probabilities for the scenario given by \( H_1 \) followed by the list of probabilities for the scenario given by \( H_2 \). It follows that any behaviour \( B \) in \( H \) is the juxtaposition of a behaviour \( B_1 \) for \( H_1 \) and a behaviour \( B_2 \) for \( H_2 \), which we denote by \( B_1 \& B_2 \). The quantifier \( X \) should be such that \( X(B_1 \& B_2) \leq X(B_1) + X(B_2) \). One may also require that equality holds. Another kind of operation we can apply to two scenarios is considering that all measurements in \( H_1 \) are compatible with all measurements in \( H_2 \), but with the restriction that they should be independent. This implies that a behaviour for \( H \) is the tensor product of one behaviour for \( H_1 \) with a behaviour for \( H_2 \). For this kind of operation, subadditivity of \( X \) should hold: \( X(B_1 \otimes B_2) \leq X(B_1) + X(B_2) \).

(iv) **Convexity:** if a behaviour can be written as \( B = \sum_i \pi_i B_i \), where \( \pi_i \in [0,1] \) and each \( B_i \) is a behaviour for the same scenario, then

\[
X(B) \leq \sum_i \pi_i X(B_i). \tag{4.1}
\]

\(^2\)A tree is a graph in which any two vertices are connected by exactly one path. A forest is a disjoint union of trees.
Continuity: \( X(B) \) should be a continuous function of \( B \).

In what follows we exhibit a number of monotones for different resource theories of contextuality and list which of the properties above they satisfy.

(a) Entropic contextuality quantifiers

Grudka et al. [25] introduce two measures of contextuality based on the notion of relative entropy distance, also called the Kullback–Leibler divergence. Given two probability distributions \( p \) and \( q \) in a sample space \( \Omega \), the Kullback–Leibler divergence between \( p \) and \( q \)

\[
D_{\text{KL}}(p||q) = \sum_{i \in \Omega} p(i) \log \frac{p(i)}{q(i)},
\]

is a measure of the difference between the two probability distributions \( p \) and \( q \).

**Definition 4.2.** The relative entropy of contextuality of a behaviour \( B \) is defined as

\[
E_{\text{max}}(B) = \min_{B^{\text{NC}} \in C(\Upsilon)} \max_{\pi} \sum_{C \in C} \pi(C) D_{\text{KL}}(p_C||p_C^{\text{NC}}),
\]

where the minimum is taken over all non-contextual behaviours \( B^{\text{NC}} = \{p_C^{\text{NC}}\} \) and the maximum is taken over all probability distributions \( \pi \) defined on the set of contexts \( C \). The uniform relative entropy of contextuality of \( B \) is defined as

\[
E_u(B) = \frac{1}{N} \min_{B^{\text{NC}} \in C(\Upsilon)} \sum_{C \in C} D_{\text{KL}}(p_C||p_C^{\text{NC}}),
\]

where \( N = |C| \) is the number of contexts in \( C \) and, once more, the minimum is taken over all non-contextual behaviours \( B^{\text{NC}} = \{p_C^{\text{NC}}\} \).

Both \( E_{\text{max}} \) and \( E_u \) can be interpreted as a ‘distance’ of the behaviour \( B \) to the set of non-contextual behaviours \( C(\Upsilon) \). In [24], it is shown that \( E_{\text{max}} \) is a monotone under the free operations of contextuality known as non-contextual wirings (defined in electronic supplementary material, equation (24)). On the other hand, \( E_u \) is not a monotone under the complete class of non-contextual wirings, as demonstrated in [32] for the special class of Bell scenarios. However, it is a monotone under a broad class of such operations. Specifically, it is monotone under post-processing operations and under a subclass of pre-processing operations, as discussed in electronic supplementary material, subsection IIIa.

(b) Geometric contextuality quantifiers

We now introduce contextuality monotones based on geometric distances, in contrast with the previous defined quantifiers which are based on entropic distances. Let \( D \) be any distance defined in the real vector space \( \mathbb{R}^K \), where \( K = \sum_C |O^C| \) is the number of entries in a behaviour \( B \).

**Definition 4.3.** The \( D \)-contextuality of a behaviour \( B \) is defined as

\[
D(B) = \min_{B^{\text{NC}} \in C(\Upsilon)} D(B, B^{\text{NC}}).
\]

We can also calculate the distance between the behaviours \( B \) and \( B^{\text{NC}} \) for each context \( C \) and then averaging over the contexts. When the choice of context is uniform, we have:

**Definition 4.4.** The \( D \)-uniform contextuality of a behaviour \( B \) is defined as

\[
D_u(B) = \frac{1}{N} \min_{B^{\text{NC}} \in C(\Upsilon)} \sum_{C \in C} D(p_C, p_C^{\text{NC}}),
\]

where \( N = |C| \) is the number of contexts in \( C \).
If we allow a non-uniform choice of context, the natural way of quantifying contextuality will be:

**Definition 4.5.** The $D$-*max contextuality* of a behaviour $B$ is defined as

$$D_{\text{max}}(B) = \min_{B^{\text{NC}} \in C(\Upsilon)} \max_{\pi \in \mathcal{C}} \pi(C) \cdot D(p_C, p^{\text{NC}}_C),$$

(4.7)

where the minimum is taken over all non-contextual behaviours $B^{\text{NC}} = \{p^{\text{NC}}_C\}$ and the maximum is taken over all probability distributions $\pi$ defined over the set of contexts $\mathcal{C}$.

The quantifiers $D_u$ and $D_{\text{max}}$ are just special cases of $D$, since we obtain them using a proper choice of distance in Equation (4.5). Nevertheless, we stress these definitions because of their physical meaning and special mathematical properties (see theorem 4.8).

This contextuality quantifier was generalized for disturbing systems within the framework of contextuality-by-default (CbD) in [47,48], where it is denoted by $\text{CNT}_2$. These references also discuss another contextuality quantifier based on geometric distances, the measure $\text{CNT}_1$, but a discussion of this quantity would require a proper introduction to the CbD framework that is outside the scope of this text. The interested reader is referred to [39,49] for a proper introduction to CbD and to [47,48,50] for a discussion of contextuality quantifiers within this framework.

Calculating exact values for these quantifiers is generally a challenging computational problem. For instance, if we consider the distances obtained with the $\ell_1$ and $\ell_2$ norms, the minimization can be efficiently performed using linear and quadratic programming, respectively, based on the number of vertices of the set of non-contextual behaviours. However, as the compatibility graph becomes more complex, the number of vertices grows exponentially, rendering the problem intractable for a large number of vertices. Nevertheless, we can compute these distances for specific examples of interest (see §4h and, for the special class of Bell scenarios, [51]).

The properties exhibited by the quantities defined in equations (4.5)--(4.7) will depend on the chosen distance $D$ in the definition. In this context, we focus our attention on distances defined by $\ell_p$ norms.

(c) **Contextual fraction**

A contextuality quantifier based on the intuitive notion of what fraction of a given behaviour admits a non-contextual description was introduced in [37,38]. Several properties of this quantifier were further discussed in [23].

**Definition 4.6.** The contextual fraction of a behaviour $B$ is defined as

$$\mathcal{C}F(B) = \min\{\lambda | B = \lambda B' + (1 - \lambda)B^{\text{NC}}\},$$

(4.8)

where $B^{\text{NC}}$ is an arbitrary non-contextual behaviour and $B'$ is an arbitrary non-disturbing behaviour.

(d) **Robustness of contextuality**

The robustness of contextuality is a quantifier based on the intuitive notion of how much non-contextual noise a given behaviour can sustain before becoming non-contextual [26].

**Definition 4.7.** The robustness of a behaviour $B$ is defined as

$$\mathcal{R}(B) = \min\{\lambda | (1 - \lambda)B + \lambda B^{\text{NC}} \in C(\Upsilon)\},$$

(4.9)

where $B^{\text{NC}}$ is an arbitrary non-contextual behaviour.
(e) Negativity of quasi-probability global sections

We can also use the quasi-probability global sections defined in §2b to derive a contextuality quantifier

$$\mathcal{N}(B) = \min \sum_s |p_M(s)| - 1$$

(4.10)

where the minimum is taken over all global quasi-probability distributions $p_M$ consistent with $B$ and the sum is taken over all possible outcomes $s \in O^M$. We have that $\mathcal{N}(B) = 0$ if and only if there is a global section consistent with $B$. As a consequence, $B$ is non-contextual if and only if $\mathcal{N}(B) = 0$.

This contextuality quantifier was also generalized for disturbing systems within the framework CbD in [47,48], where it is denoted by CNT\textsubscript{3}.

(f) Properties of the contextuality quantifiers

**Theorem 4.8.** The quantities defined previously satisfy the following properties:

(i) $\mathcal{C}$ and $\mathcal{R}$ are monotonies under all linear operations that preserve the classical set $C(\Upsilon)$;

(ii) $E_{\text{max}}, D_{\text{max}}$ and $\mathcal{N}$ are contextuality monotonies for the resource theory of contextuality defined by non-contextual wirings;

(iii) $E_{\text{u}}, D_{\text{u}}$ are contextuality monotonies for the resource theory of contextuality defined by post-processing operations and a subclass of pre-processing operations;

(iv) $E_{\text{max}}, E_{\text{u}}, D_{\text{max}}, D_{\text{u}}$ are faithful, additive, convex, continuous and preserved under relabellings of inputs and outputs;

(v) $\mathcal{C}, \mathcal{R}$ and $\mathcal{N}$ are faithful, convex, continuous and preserved under relabellings of inputs and outputs;

(vi) $\mathcal{C}(B_1&B_2) \leq \max_i \mathcal{C}(B_i)$;

(vii) $\mathcal{C}(B_1 \otimes B_2) \leq \mathcal{C}(B_1) + \mathcal{C}(B_2) - \mathcal{C}(B_1)C\mathcal{C}(B_2)$;

(viii) $\mathcal{R}(B_1&B_2) \leq \max_i \mathcal{R}(B_i)$;

(ix) $\mathcal{R}(B_1 \otimes B_2) \leq \mathcal{R}(B_1) + \mathcal{R}(B_2) - \mathcal{R}(B_1)\mathcal{R}(B_2)$;

(c) $\mathcal{C}$, $\mathcal{R}$ and $\mathcal{N}$ can be calculated via linear programming.

The proof of this result is given in electronic supplementary material, section III.

(g) Contextuality monotonies for scenarios with $H = G$ and $|O| = 2$

In §3, we demonstrated that it is possible to employ different polytopes to characterize the set of behaviours in the specific case where contexts consist of at most two measurements, and each measurement has two outcomes. Regardless of the chosen representation, the non-disturbance, quantum and non-contextual sets are convex sets in $\mathbb{R}^{(|V(G)|+|E(G)|}$ with full dimension. We can explore this fact to rewrite the contextuality quantifiers defined above.

Previously, we have defined contextuality monotonies using distances in real vector spaces when behaviours are described by the vector $p_{ij}(ab)$. Following the same approach, we can define contextuality quantifiers using distances in the following scenarios:

(i) When behaviours are described by vectors $q = \phi(p) \in \phi[\mathcal{X}(\Upsilon)] = \text{RCMET}(G)$, using a distance $D(q, q_{\text{NC}})$.

(ii) When behaviours are described by vectors $x \in \psi \circ \phi[\mathcal{X}(\Upsilon)] = \text{RMET}(G)$, using a distance $D(x, x_{\text{NC}})$.

(iii) When behaviours are described by vectors $y \in \alpha \circ \psi \circ \phi[\mathcal{X}(\Upsilon)]$, using a distance $D(y, y_{\text{NC}})$.

In each of these cases, we can define the contextual fraction and the robustness of contextuality in a similar manner as described in §4c and (d). In any case, we have a contextuality quantifier
that satisfies all the properties listed in §4f. However, computing these quantities for general graphs is not a trivial task due to the complexity of the polytopes \( \text{COR}(G) \), \( \text{CUT}^{\pm 1}(VG) \), and \( \text{CUT}^{01}(VG) \). Nonetheless, these polytopes have full dimension of \( |V(G)| + |E(G)| \), and their facets are hyperplanes with maximum dimension, making the computation of these quantifiers possible in certain scenarios. In §4h, we provide an analytical expression for \( D(x) \) in the \( n \)-cycle scenario when the distance function \( D \) is defined by an \( \ell_p \) norm.

(h) The \( n \)-cycle

When the compatibility graph of the scenario is the \( n \)-cycle \( G = C_n \), the conditions of theorem 3.13 are satisfied, and therefore, the facets of the cut polytope \( \text{CUT}^{\pm 1}(V C_n) \) are defined by the \( n \)-cycle inequalities:

\[
x(F) - x(C_n \setminus F) \leq n - 2, \quad F \subset C_n, \quad |F| \text{ odd}.
\]

(4.11)

In this case, the contextuality quantifier \( D \) can be easily computed. Each contextual behaviour violates only one of these inequalities, so the distance of such a point to the set of non-contextual behaviours is equal to the distance of this behaviour to the hyperplane defining the facet [43].

Given \( x \notin \text{CUT}^{\pm 1}(V C_n) \), suppose \( x(F) - x(C_n \setminus F) \leq n - 2 \) is the inequality which \( x \) violates. If the distance \( D \) is defined by any \( \ell_p \)-norm in \( \mathbb{R}^{|V(G)| + |E(G)|} = \mathbb{R}^{2n} \), the distance from \( x \) to \( \text{CUT}^{\pm 1}(VG) \) is given by

\[
\frac{x(F) - x(C_n \setminus F) - n + 2}{\sqrt{n}},
\]

(4.12)

where \( q \in \mathbb{N} \) is such that \( (1/p) + (1/q) = 1 \). Hence, we have an expression for the \( D \)-contextuality of a behaviour in terms of the violation of an non-contextuality inequality.

The same argument applies whenever a contextual behaviour violates only one facet-defining inequality for \( \text{CUT}^{\pm 1}(VG) \). To calculate \( D \), it is sufficient to identify which inequality the behaviour violates and calculate the distance from the corresponding point to the facet defined by that inequality. However, in the general case, the structure of \( \text{CUT}^{\pm 1}(VG) \) can be intricate, and the behaviour may violate more than one facet-defining inequality. For example, in the \((3,3,2,2)\) Bell scenario, there exists a behaviour that violates both the CHSH inequality and the \( I_{3322} \) inequality, which are both facet-defining. An example can be found in electronic supplementary material, section IV.

(i) Connection to graph invariants

To each scenario, we can associate a graph \( G \) in which the vertices represent the measurement events, and the edges connect exclusive events [4,8,41]. Two events are considered exclusive if they correspond to the same measurement but have different outcomes. We refer to \( G \) as the exclusivity graph of the scenario [8,41]. The exclusivity graph \( G_I \) of a non-contextuality inequality is the induced subgraph of \( G \) that includes only the vertices corresponding to the events appearing in the inequality.

It turns out that when a non-contextuality inequality is formulated in terms of probabilities \( p_C(s) \), the classical and quantum maximum values for this inequality are connected to graph invariants of \( G_I \) [8]. This implies that we can use graph invariants to compute the distances \( D \) as defined earlier, or at the very least, obtain upper bounds for them in the worst-case scenario.

**Definition 4.9.** The independence number \( \alpha(G) \) of a graph \( G \) is the cardinality of a maximum independent set of \( G \).

**Definition 4.10.** Let \( \{1, \ldots, n\} \) be the set of vertices of a graph \( G \). An orthonormal representation for \( G \) in a finite-dimensional vector space with inner product \( V \) is a set of unit vectors \( \{u_1, \ldots, u_n\} \) such that \( u_i \) and \( u_j \) are orthogonal whenever \( i \) and \( j \) are not connected in \( G \).
Definition 4.11. The Lovász number of a graph $G$ is

$$\vartheta(G) = \sup \sum_i |\langle u_i | \psi \rangle|^2$$

(4.13)

where the supremum is taken over all vector spaces $V$, all orthogonal representations \{\ket{u_1}, \ldots, \ket{u_n}\} for $G$ and all unit vectors $|\psi\rangle \in V$.

Theorem 4.12 (Cabello et al. [8]). The maximum value for the sum $\sum_{i} \gamma(Y_{i} C(s_{i}))$ attained with classical behaviours is the vertex-weighted independence number $\alpha(G_{l}, \gamma)$. The maximum value attained with quantum behaviours is upper bounded by the vertex-weighted Lovász number $\vartheta(G_{l}, \gamma)$ of the exclusivity graph $G_{l}$ of the inequality with vertex weights given by the coefficients $\gamma_{i}$ of the sum.

We also consider post-quantum behaviours obtained when we use generalized probability theories, but satisfying the following principle:

Principle 4.13 (The exclusivity principle). Given a set \{\upsilon_{k}\} of pairwise exclusive events, the corresponding probabilities $p_{k}$ satisfy $\sum_{k} p_{k} \leq 1$.

From now on, we refer to the exclusivity principle simply as the E-principle. From the graph theoretical point of view, this restriction is equivalent to imposing the condition that whenever the set of vertices \{\upsilon_{k}\} is a clique in $G_{l}$, the sum of the corresponding probabilities $p_{k}$ cannot exceed one.

A detailed discussion of the E-principle and its consequences can be found in [41]. The maximum value of this sum for models satisfying the E-principle is also related to the graph $G_{l}$.

Definition 4.14. The fractional packing number $\alpha^*(G)$ of a graph $G$ is defined as

$$\alpha^*(G) = \sup \left\{ \sum_{i} p_{i} \mid 0 \leq p_{i} \leq 1 \text{ and } \sum_{i} p_{i} \leq 1 \text{ Q any clique of } G \right\}.$$  

(4.14)

Theorem 4.15 (Cabello et al. [8]). The maximum value for the sum $\sum_{i} \gamma(Y_{i} C(s_{i}))$ attained with behaviours satisfying the E-principle is equal to the vertex-weighted fractional packing number $\alpha^*(G_{l}, \gamma)$ of the exclusivity graph $G_{l}$ of the inequality.

Notice that $\langle M_{i} M_{j} \rangle = 2(p_{ij}(11) + p_{ij}(-1)(1)) - 1$ and $-\langle M_{i} M_{j} \rangle = 2(p_{ij}(p(1)(1) + p_{ij}(-1)) - 1$. Hence, there are $2n$ events in each non-contextuality inequality for the $n$-cycle scenario, $11|ij_1$, $-11|ij_1$ if $\langle M_{i} M_{j} \rangle$ appears with positive sign and $-11|ij_1$, $11|ij_1$ if $\langle M_{i} M_{j} \rangle$ appears with negative sign in the inequality. If $n$ is odd, the corresponding exclusivity graph is the prism graph of order $n, Y_{n}$ and if $n$ is even, the exclusivity graph is the Möbius ladder of order $2n, M_{2n}$ [43].

The observation that

$$\vartheta(Y_{n}) = \frac{3n \cos \left( \frac{\pi}{n} \right) - n}{1 + \cos \left( \frac{\pi}{n} \right)}.$$

$$\vartheta(M_{2n}) = n \cos \left( \frac{\pi}{n} \right),$$

(4.15)

and theorem 4.12 were used in [43] to find the quantum maximum violation of the $n$-cycle inequalities, which in this case coincides with the Lovász number of the exclusivity graph. The classical bound is equal to $n$ for $n$ even and $n - 1$ for $n$ odd, while the E-principle bound is equal to $2n$ for every $n$. This allows us to compute the maximum value of $D$ in this scenario, which gives us the following result:

Theorem 4.16. The maximum values of $D$ for the $n$-cycle scenarios attainable with quantum behaviours are

$$\frac{\vartheta(Y_{n}) - \alpha(Y_{n})}{\sqrt{n}}, \quad \frac{\vartheta(M_{2n}) - \alpha(M_{2n})}{\sqrt{n}}$$

(4.16)

for $n$ odd and for $n$ even, respectively. The maximum values of $D$ for the $n$-cycle scenario attainable with E-principle behaviours are

$$\frac{\alpha^*(Y_{n}) - \alpha(Y_{n})}{\sqrt{n}} \quad \text{and} \quad \frac{\alpha^*(M_{2n}) - \alpha(M_{2n})}{\sqrt{n}}$$

(4.17)

for $n$ odd and for $n$ even, respectively.
5. Conclusion

The complete characterization of a contextuality scenario is generally challenging due to the exponential growth in the complexity of the set of distributions as the number of available measurements increases. However, we can leverage various geometric features of this set to assist us in tackling this problem. The graph-based approach to contextuality is a fundamental tool as it allows us to map several contextuality problems to well-studied problems in graph theory. As a result, we can establish connections between several convex sets that appear in contextuality and well-known convex sets from the literature of graph theory.

The identification of these sets provides us with a captivating geometry that can be further explored. One application of this geometry is the definition of contextuality quantifiers based on the geometric distances within these convex sets. This definition is particularly significant in the context of the resource theory of contextuality.

There are three notable advantages to the definition of contextuality quantifiers based on geometric distances:

(i) It is possible to establish connections between these quantifiers and graph invariants, leveraging existing knowledge from graph theory in the calculation of these quantities.
(ii) These quantifiers can be computed more efficiently than quantifiers based on relative entropy, resulting in computational advantages.
(iii) These quantifiers are applicable to the other approaches to contextuality, such as the exclusivity graph approach, where previous quantifiers based on entropies are not suitable or applicable.

Overall, this approach offers a promising avenue for understanding and quantifying contextuality, enabling us to exploit the rich geometric structure of convex sets associated with contextuality scenarios.

Data accessibility. The data are provided in the electronic supplementary material [52].

Declaration of AI use. We have not used AI-assisted technologies in creating this article.

Authors’ contributions. B.A.: conceptualization, formal analysis, investigation, writing—original draft; M.T.C.: conceptualization, investigation.

Both authors gave final approval for publication and agreed to be held accountable for the work performed therein.

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References

1. Bell JS. 1966 On the problem of hidden variables in quantum mechanics. Rev. Mod. Phys. 38, 447–452. (doi:10.1103/RevModPhys.38.447)
2. Kochen S, Specker E. 1967 The problem of hidden variables in quantum mechanics. J. Math. Mech. 17, 59–87. (doi:10.1512/iumj.1968.17.17004)
3. Specker EP. 1960 Die Logik nicht gleichzeitig entscheidbarer Aussagen. Dialectica 14, 239. (doi:10.1111/j.1746-8361.1960.tb00422.x)
4. Amaral B. 2014 The Exclusivity principle and the set of quantum distributions. PhD thesis, Universidade Federal de Minas Gerais.
5. Amaral B, Terra Cunha M, Cabello A. 2014 Exclusivity principle forbids sets of correlations larger than the quantum set. Phys. Rev. A 89, 030101. (doi:10.1103/PhysRevA.89.030101)
6. Cabello A. 2013 New scenarios in which Specker’s principle explains the maximum quantum contextuality. Submitted (28 February 2013) to Proc. of the 2013 Biennial Meeting of the Spanish Royal Society of Physics, Valencia, Spain, 15–19 June 2013.
7. Cabello A. 2013 Simple explanation of the quantum violation of a fundamental inequality. *Phys. Rev. Lett.* **110**, 060402. (doi:10.1103/PhysRevLett.110.060402)

8. Cabello A, Severini S, Winter A. 2014 Graph-theoretic approach to quantum correlations. *Phys. Rev. Lett.* **112**, 040401. (doi:10.1103/PhysRevLett.112.040401)

9. Nawareg M, Bisesto F, D’Ambrosio V, Amselem E, Scarrino F, Bourennane M, Cabello A. 2013 Bonding quantum theory with the exclusivity principle in a two-city experiment. (http://arxiv.org/abs/quant-ph/1311.3495)

10. Amselem E, Rådmark M, Bourennane M, Cabello A. 2009 State-independent quantum contextuality with single photons. *Phys. Rev. Lett.* **103**, 160405. (doi:10.1103/PhysRevLett.103.160405)

11. Borges G, Carvalho M, de Assis PL, Ferraz J, Araújo M, Cabello A, Cunha MT, Pádua S. 2014 Experimental test of the quantum violation of the noncontextuality inequalities for the $n$-cycle scenario. *Phys. Rev. A* **89**, 052106. (doi:10.1103/PhysRevA.89.052106)

12. Hasegawa Y, Loidl R, Badurek G, Baron M, Rauch H. 2006 Quantum contextuality in a single-neutron optical experiment. *Phys. Rev. Lett.* **96**, 230401. (doi:10.1103/PhysRevLett.97.230401)

13. Kirchmair G, Zähringer F, Gerritsma R, Kleinmann M, Gühne O, Cabello A, Blatt R, Roos CF. 2009 State-independent experimental test of quantum contextuality. *Nature* **460**, 494. (doi:10.1038/nature08172)

14. Lapkiewicz R, Li P, Schaeff C, Langford N, Ramelow S, Wiesniak M, Zeilinger A. 2011 Experimental non-classicality of an indivisible quantum system. *Nature* **460**, 494. (doi:10.1038/nature08172)

15. Cabello A, Severini S, Winter A. 2010 (Non-)contextuality of physical theories as an axiom. (http://arxiv.org/abs/quant-ph/1010.2163)

16. Cabello A, Severini S, Winter A. 2014 Graph-theoretic approach to quantum correlations. *Phys. Rev. Lett.* **112**, 040401. (doi:10.1103/PhysRevLett.112.040401)

17. Rabelo R, Duarte C, López-Tarrida AJ, Cunha MT, Cabello A. 2014 Multigraph approach to quantum non-locality. *J. Phys. A: Math. Theor.* **47**, 424021. (doi:10.1088/1751-8113/47/42/424021)

18. Delfosse N, Allard Guerin P, Bian J, Raussendorf R. 2015 Wigner function negativity and contextuality in quantum computation on rebits. *Phys. Rev. X* **5**, 021003. (doi:10.1103/PhysRevX.5.021003)

19. Howard M, Wallman J, Veitch V, Emerson J. 2014 Contextuality supplies the `/'magic/' for quantum computation. *Nature* **510**, 351–355. (doi:10.1038/nature13460)

20. Raussendorf R. 2013 Contextuality in measurement-based quantum computation. *Phys. Rev. A* **88**, 022322. (doi:10.1103/PhysRevA.88.022322)

21. Um M, Zhang X, Zhang J, Wang Y, Yangchao S, Deng DL, Duan L, Kim K. 2013 Experimental certification of random numbers via quantum contextuality. *Sci. Rep.* **3**, 1627. (doi:10.1038/srep01627)

22. Brunner N, Cavalcanti D, Pironio S, Scarani V, Wehner S. 2014 Bell nonlocality. *Rev. Mod. Phys.* **86**, 419–478. (doi:10.1103/RevModPhys.86.419)

23. Abramsky S, Barbosa RS, Mansfield S. 2017 Contextual fraction as a measure of contextuality. *Phys. Rev. Lett.* **119**, 050504. (doi:10.1103/PhysRevLett.119.050504)

24. Amaral B, Cabello A, Cunha MT, Aolita L. 2018 Noncontextual wirings. *Phys. Rev. Lett.* **120**, 130403. (doi:10.1103/PhysRevLett.120.130403)

25. Grudka A, Horodecki K, Horodecki M, Horodecki P, Horodecki R, Joshi P, Kłosub W, Wójcik A. 2014 Quantifying contextuality. *Phys. Rev. Lett.* **112**, 120401. (doi:10.1103/PhysRevLett.112.120401)

26. Horodecki K, Grudka A, Joshi P, Kłosub W, Łodyga J. 2015 Axiomatic approach to contextuality and nonlocality. *Phys. Rev. A* **92**, 032104. (doi:10.1103/PhysRevA.92.032104)

27. Allcock J, Brunner N, Linden N, Popescu S, Skrzypczyk P, Vértesi T. 2009 Closed sets of nonlocal correlations. *Phys. Rev. A* **80**, 062107. (doi:10.1103/PhysRevA.80.062107)

28. Barrett J, Linden N, Massar S, Pironio S, Popescu S, Roberts D. 2005 Nonlocal correlations as an information-theoretic resource. *Phys. Rev. A* **71**, 022101. (doi:10.1103/PhysRevA.71.022101)

29. de Vicente JI. 2014 On nonlocality as a resource theory and nonlocality measures. *J. Phys. A: Math. Theor.* **47**, 424017. (doi:10.1088/1751-8113/47/42/424017)

30. Gallego R, Würflinger LE, Acín A, Navascués M. 2012 Operational framework for nonlocality. *Phys. Rev. Lett.* **109**, 070401. (doi:10.1103/PhysRevLett.109.070401)
31. Gallego R, Aolita L. 2015 Resource theory of steering. Phys. Rev. X 5, 041008. (doi:10.1103/PhysRevX.5.041008)
32. Gallego R, Aolita L. 2017 Nonlocality free wirings and the distinguishability between bell boxes. Phys. Rev. A 95, 032118. (doi:10.1103/PhysRevA.95.032118)
33. Joshi P, Horodecki M, Horodecki R, Grudka A, Horodecki K, Horodecki P. 2013 No-broadcasting of non-signaling boxes via operations which transform local boxes into local ones. Quant. Inf. Comput. 13, 567. (doi:10.26421/QIC13.7-8-2)
34. Lang B, Vértesi T, Navascués M. 2014 Closed sets of correlations: answers from the zoo. J. Phys. A: Math. Theor. 47, 424029. (doi:10.1088/1751-8113/47/42/424029)
35. L. Brandão FGS, Gour G. 2015 Reversible framework for quantum resource theories. Phys. Rev. Lett. 115, 070503. (doi:10.1103/PhysRevLett.115.070503)
36. Coecke B, Fritz T, Spekkens RW. 2016 A mathematical theory of resources. Inf. Comput. 250, 59–86. (doi:10.1016/j.ic.2016.02.008)
37. Abramsky A, Brandenburger A. 2011 The sheaf-theoretic structure of non-locality and contextuality. New J. Phys. 13, 113036. (doi:10.1088/1367-2630/13/11/113036)
38. Amselem E, Danielsen LE, López-Tarrida AJ, Portillo JR, Bourennane M, Cabello A. 2012 Experimental fully contextual correlations. Phys. Rev. Lett. 108, 200405. (doi:10.1103/PhysRevLett.108.200405)
39. Dzhafarov EN, Kujala JV. 2016 Context-content systems of random variables: the contextuality-by-default theory. J. Math. Psychol. 74, 11–33. (doi:10.1016/j.jmp.2016.04.010)
40. Fine A. 1982 Hidden variables, joint probability, and the Bell inequalities. Phys. Rev. Lett. 48, 291–295. (doi:10.1103/PhysRevLett.48.291)
41. Amaral B, Cunha MT. 2018 On graph approaches to contextuality and their role in quantum theory. Berlin, Germany: Springer.
42. Deza MM, Laurent M. 1997 Geometry of cuts and metrics, vol. 15. Algorithms and Combinatorics. Berlin, Germany: Springer.
43. Araújo M, Quintino MT, Budroni C, Terra Cunha M, Cabello A. 2013 All noncontextuality inequalities for the $n$-cycle scenario. Phys. Rev. A 88, 022118. (doi:10.1103/PhysRevA.88.022118)
44. Tsirel’son BS. 1987 Quantum analogues of the bell inequalities. the case of two spatially separated domains. J. Soviet Math. 36, 557–570. (doi:10.1007/BF01663472)
45. Avis D, Imai H, Ito T. 2006 On the relationship between convex bodies related to correlation experiments with dichotomic observables. J. Phys. A: Math. Gen. 39, 11283. (doi:10.1088/0305-4470/39/36/010)
46. Amaral B. 2019 Resource theory of contextuality. Phil. Trans. R. Soc. A 377, 20190010. (doi:10.1098/rsta.2019.0010)
47. Dzhafarov EN, Kujala JV, Cervantes VH. 2020 Contextuality and noncontextuality measures and generalized bell inequalities for cyclic systems. Phys. Rev. A 101, 042119. (doi:10.1103/PhysRevA.101.042119)
48. Kujala JV, Dzhafarov EN. 2019 Measures of contextuality and non-contextuality. Phil. Trans. R. Soc. A 377, 20190149. (doi:10.1098/rsta.2019.0149)
49. Dzhafarov EN, Kujala JV. 2017 Contextuality-by-default 2.0: systems with binary random variables. In Quantum interaction (eds JA de Barros, B Coecke, E Pothos), pp. 16–32. Cham, Switzerland: Springer International Publishing.
50. Amaral B, Duarte C. 2019 Characterizing and quantifying extended contextuality. Phys. Rev. A 100, 062103. (doi:10.1103/PhysRevA.100.062103)
51. Brito SGA, Amaral B, Chaves R. 2018 Quantifying bell nonlocality with the trace distance. Phys. Rev. A 97, 022111. (doi:10.1103/PhysRevA.97.022111)
52. Amaral B, Terra Cunha M. 2024 On geometrical aspects of the graph approach to contextuality. Figshare. (doi:10.6084/m9.figshare.c.7029801)