Exclusivity graph approach to Instrumental inequalities

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INTRODUCTION

The existence of causal relationships between events is one of the basic principle that makes scientific investigation possible. Nonetheless extracting informations about these relationships only from experimental observations is not always feasible and can be a tricky task. In this context causal models are a indispensable tool to formalize causal assumptions and to produce falsifiable statements causal relations.

A causal model is tipically represented by a directed acyclic graph (DAG), where the nodes represent observed events, which are described by random variables, and the edges the cause-effect relationship between them. From some causal DAGs it is possible to derive constraints on the statistical distribution of the variables which allow one to reject or accept a causal assumption.

It is known, since Bell theorem, that quantum mechanics allows for statistical behavior which are impossible to reproduce in a classical context, so it is reasonable to suppose that the constraints derived from classical causal assumptions could be violated by quantum systems. Indeed Bell experiment can be modelled using a causal DAG, as shown in fig 2, and the Bell inequality obtained as a consequence of causal assumptions. More recently it has been proved and experimentally demonstrated that the well-known "instrumental" causal structure (see fig. 1) posses classical constraints that are violated by quantum mechanics.

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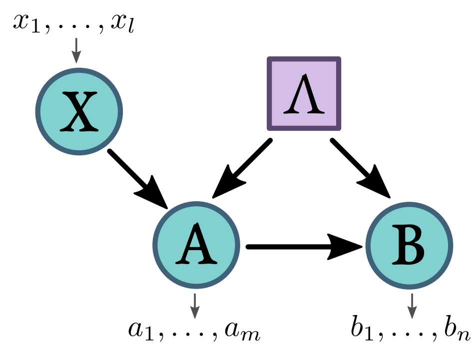

FIG. 1. The DAG representing a general Instrumental scenario.

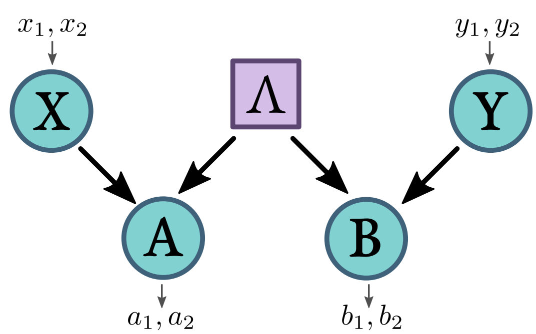

FIG. 2. The DAG representing the CHSH scenario.

INSTRUMENTAL CAUSAL STRUCTURE

The Instrumental causal structure is a widely studied structure both for its simplicity and commonness. It can be described by four random variables Λ, X, A, B where X and Λ are independent from the others while B depends on X only via the node A, as graphically depicted in Fig. 1.

The consequences of these causal relations on the distributions of the four variables have been throughly studied in previous works [1, 2]. Suppose that X, A, B take l, m, n different values and call $P(a_i b_j|x_k)$ the probability that A and B take, respectively, values a_i and b_j, given that X reads x_k. Such system respects the following inequalities, named *Pearl's inequalities* [1]:

$$\sum_{j=0}^{n} P(a_i b_j|x_{k(i,j)}) \leq 1 \tag{1}$$

for all $i \in 1, \ldots, m$ and for all the possible functions $k(i,j)$.

In [2] Bonet showed that the polytope of allowed correlation is not tightly bounded by *Pearl's inequalities.* For instance for $(l, m, n) = (3, 2, 2)$ the following inequality must also be satisfied:

$$P(a_1 b_1|x_1) + P(a_2 b_2|x_1) + P(a_1 b_1|x_2) + \\ + P(a_2 b_1|x_2) + P(a_1 b_2|x_3) \leq 2 \tag{2}$$

along with other similar inequalities obtained by permuting the labels of a_i, b_j and x_k.

These inequalities are related to the one introduced in [3]:

$$-\langle B\rangle_{x_1} + 2\langle B\rangle_{x_2} + \langle A\rangle_{x_1} - \langle AB\rangle_{x_1} + 2\langle AB\rangle_{x_3} \leq 3 \tag{3}$$

which was experimentally violated in the same work, with a value of 3.790±0.013. As one can expect, with the same data it is also possible to violate inequality (2) with a value of 2.159 ± 0.005.

EXCLUSIVITY GRAPH METHOD

The exclusivity graph method was primarily developed to study non-contextual inequalities and obtain their quantum violation [5] as well as for non-locality scenarios. In this formalism every possible event, i.e. every possible set of outcomes $a_1 \dots, a_n$ of measurements $A_1, \dots, A_n$ given settings $x_1, \dots, x_n$, is associated to a vertex in a (undirected) graph $G = (V, E)$. Two vertices $u, v \in V$ are then connected by an edge $uv \in E$ if and only if they are exclusive, i.e. if exists a measurement that can distinguish between them.

A linear constraint can be expressed as a linear function

$$I_w(p) = \sum_{\substack{a_1,\dots,a_n \\ x_1,\dots,x_n}} w_{\substack{a_1,\dots,a_n \\ x_1,\dots,x_n}} p(a_1, \dots, a_n | x_1, \dots, x_n) \quad (4)$$

on the probabilities for each possible event. In this framework this can be represented by weighted exclusivity graph G, and it is possible to relate classical bound and quantum violation to well-known graph invariants: the independence number $\alpha(G, w)$ and the Lovász theta $\theta(G, w)$.

Here we briefly introduce these concepts and their relationships, a more extensive and general treatment can be found in [5, 6]

Consider a graph $G(V, E)$ with vertex weights w, and $|V| = n$. We call a *characteristic labelling* for $U \subseteq V$ a vector $x_v \in \{0, 1\}^n$ such that $x_v = 1$ if $v \in U$ and $x_v = 0$ otherwise.

An *independent set* or *stable set* is a set $S \subset V$ such that $uv \notin E$ for all $u, v \in S$. The independence number $\alpha(G, w)$ is defined as the maximum number of vertices (weighted with w) of an independent set of G. Is also costumary to define the set $\mathrm{STAB}(G)$ as the convex hull of all the characteristic labellings of stable sets:

$$\mathrm{STAB}(G) = \{x : x \quad \text{is a stable labelling of} \quad G\} \quad (5)$$

using this definition the independence number becomes:

$$\alpha(G, w) = \max\{w \cdot x : x \in \mathrm{STAB}(G)\} \quad (6)$$

From this definitions we can see that $\alpha(G, w)$ corresponds to the classical bound of inequality, since it is exaclty the maximum over the convex set defined by all the deterministic strategies respecting the exclusivity constraints.

We now call an *orthonormal labelling* of dimension d a map $a_v : V \to \mathbb{R}^d$ such that $a_v \cdot a_u = 0$ for all $uv \in E$ and $|a_v|^2 = 1$, and we define the set $\mathrm{TH}(G)$ as:

$$\mathrm{TH}(G) = \{x : x_v = a_v^1 \text{ where } a_v \text{ is an orthonormal labelling of } G\} \quad (7)$$

It can be proved that this set includes all the possible quantum strategies, but in general is larger as it contains also the "almost quantum correlations" described in .[**?**] Maximizing over $\mathrm{TH}(G)$ gives the Lovász theta:

$$\theta(G, w) = \{w \cdot x : x \in \mathrm{TH}(G)\} \quad (8)$$

which upper-bounds the maximum quantum value.

Moreover this approach gives a useful condition to check if a given graph G admits a quantum violation. Indeed it can be proved that $\mathrm{TH}(G) = \mathrm{STAB}(G)$ if and only if G does not contain a cycle C_n with $n \geq 5$ and odd, or its complement as an induced subgraph. This follows directly from the so called "sandwich theorem" and the "strong perfect graph theorem" [**?**].

Exclusivity graph method applied to causal models

The techniques presented in the previous section can be also employed to analyze a certain class of causal models. Suppose we have a causal scenario as in fig 3, with k observable variables, l instruments with no incoming edges, and a single unobservable latent variable Λ.

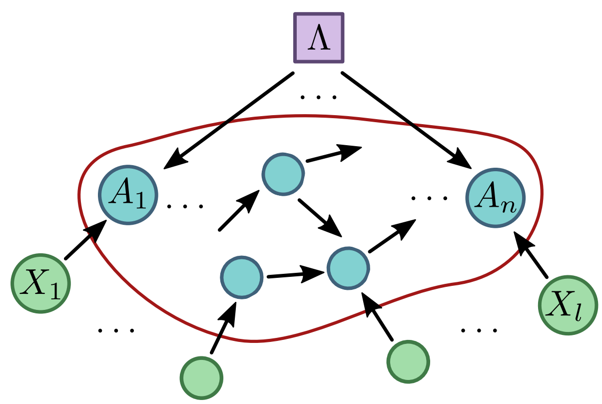

FIG. 3. A general causal graph with l instrument and a single latent variable.

In this case we can associate with such a DAG a *non-exclusivity* graph H as follows:

- Nodes are associated to events like $a|x$, where $a = (a_1, \dots, a_k)$ and $x = (x_1, \dots, x_l)$.
- Two nodes $a|x$, and $a'|x'$ are linked by an edge if and only if
  1. for all $i, j \in \{1, \dots, k\}$ if $A_i \to A_j$ then $\exists g_{ij} : g_{ij}(a_i) = a_j$ and $g_{ij}(a'_i) = a'_j$.

2. for all $i \in \{1, \ldots, l\}$ and $j \in \{1, \ldots, k\}$ if $X_i \rightarrow A_j$ then $\exists f_{ij} : f_{ij}(x_i) = a_j$ and $f_{ij}(x'_i) = a'_j$.

To the complement of this graph, $G = \bar{H}$, and its subgraphs, the previous methods can be applied to obtain inequalities with their respective quantum and classical bounds.

The Instrumental exclusivity graph

Many known results about the instrumental scenario, including the inequality (2), can also be obtained using this formalism. Restricting for the moment to the case of of dichotomic observables ($n = m = 2$), we label as $p(ab|x)$ with $a, b \in \mathcal{A} = \mathcal{B} = \{0, 1\}$ and $x \in \mathcal{X} = \{0, \ldots, l\}$, the probability of having outcomes a and b with setting x. As explained in the previous section we obtain the non-exclusivity graph for the instrumental scenario by linking two events $ab|x$ and $a'b'|x'$ if exist two functions $f : \mathcal{X} \rightarrow \mathcal{A}$ and $g : \mathcal{A} \rightarrow \mathcal{B}$ such that:

$$a = f(x) \quad \text{and} \quad a' = f(x') \tag{9}$$

$$b = g(a) \quad \text{and} \quad b' = g(a') \tag{10}$$

Using this method we can construct the graph for various l, as shown in figure 4, and use the methods described earlier to obtain classical and quantum bounds for several inequalities in the instrumental scenario.

First, we immediately obtain the result that there is no quantum violation in the case of $l = 2$, since the corresponding exclusivity graph (and its complement) does not contain any odd cyclic graph with more than 5 vertices.

For $l \geq 3$ instead we see that there is a violation for the inequality (2), since it forms a C_5 cyclic graph, i.e. the pentagon depicted in fig. 5. Knowing that $\alpha(C_n) = \lfloor n/2 \rfloor$ we immediately derive that the classical limit is 2. Analogously knowing that $\theta(C_n) = n\cos(\pi/n)/(1 + \cos(\pi/n))$ we get $\sqrt{5}$ as an upper bound for the quantum limit.

In this framework (2) seems analogous to the KCBS contextual inequality. The difference here is that the quantum limit is not $\sqrt{5}$, which we cannot obtain in a bipartite scenario. To find a tight bound we must apply other methods to our graph, like the ones in [6], using which we find a value of $(3 + \sqrt{2})/2$.

It can be easily proved (see Appendix) that no other odd anticycle beside C_5 is present for any l, so from this point of view, we can say that any quantum violation for a general $l22$ instrumental scenario has essentially the same origin: it stems from the non classicality of the C_5 graph.

This does not mean that different inequalities cannot be devised by clever choices of vertices and weights. For example the inequality for the 422 scenario presented in [**?**]

$$\langle AB \rangle_1 - \langle AB \rangle_2 + \langle B \rangle_0 - \langle B \rangle_3 \leq 2 \tag{11}$$

correponds to the two sets of events whose exclusivity graphs are depicted in fig. 6. The maximum classical value for both, given by the independence number of the graphs, is 3, while their minimum is 1, which gives the maximum value of 2 as in (11) when taken with opposite sign. This inequality has a structure very similar to the CHSH (showed in fig.7), and, as pointed out above, both arise from the non-classicality of the C_5 graph.

Finding optimal inequalities

The presence of an odd cycle graph guarantees only that $\mathrm{STAB}(G) \subset \mathrm{TH}(G)$, but does not say anything on the values of $\theta(G)$ and $\alpha(G)$. Nonetheless, if that condition is satisfied there must be some optimal choice of weights w for which we can obtain a maximum quantum violation. Formally if n is the number of nodes of G, we want to find the maximum:

$$\max_{w \in [0,1]^n} \{\theta(G, w) - \alpha(G, w)\} \tag{12}$$

Using the definition (8) and (6), and remembering that $\mathrm{STAB}(G)$ is a convex hull of a finite number of characteristic labellings we can rewirte the previous maximization as:

$$\Delta = \min\{I_y : y \, \text{is a maximal stable labelling}\} \quad \text{where} \tag{13}$$

$$I_y = \max_{\substack{w \in [0,1]^n \\ x \in \mathrm{TH}(G)}} \{w \cdot (x - y)\} \tag{14}$$

The maximization (14) for each y is efficient, being a semi-definite program, but unfortunately it has to be run for each maximal stable set in G which are $\sim 3^{n/3}$ in the worst case. Also to enumerate all the maximal independent sets we used the Tomita version of the Bron–Kerbosch algorithm which has the same worst case complexity.

Proof

Here we prove that there cannot be a odd antihole with more than 5 vertices in the exclusivity graph associated to an instrumental scenario of the type $l22$.

Remind that, from the exclusivity conditions **??**, given two events $ab|x$ and $a'b'|x'$, they are connected by edge if either

1. $x = x'$.

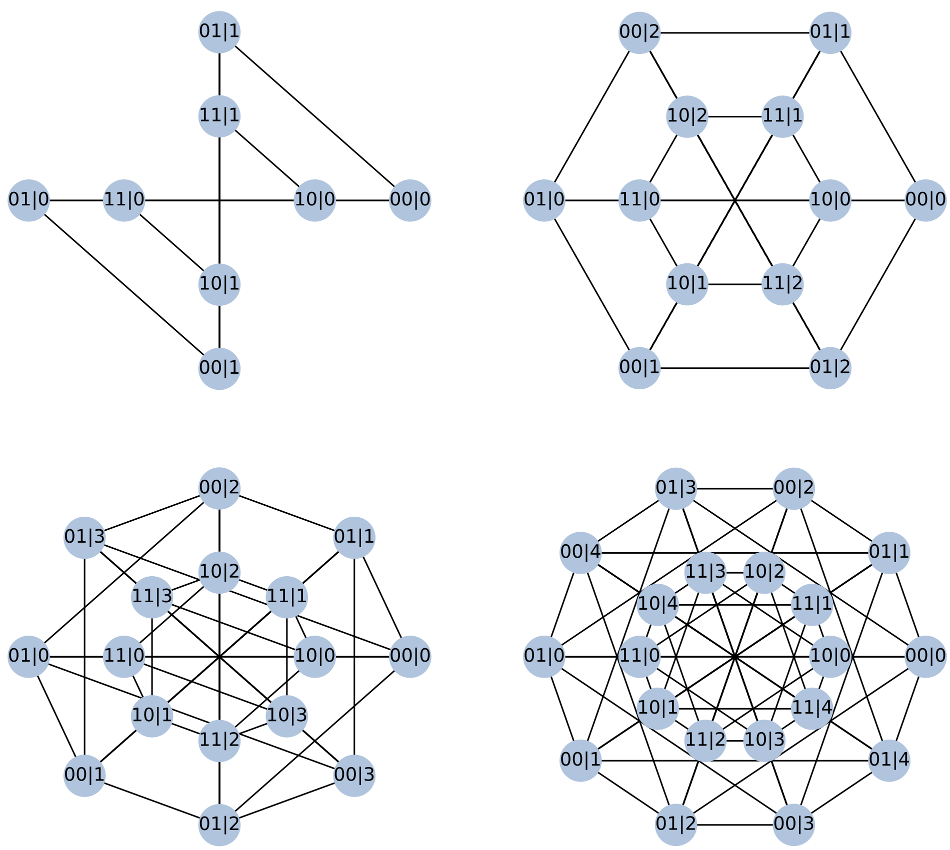

FIG. 4. The exclusivity graph for the instrumental scenario for $l = 2, 3, 4, 5$ from top left to bottom right. In the figure the bold lines represent cliques.

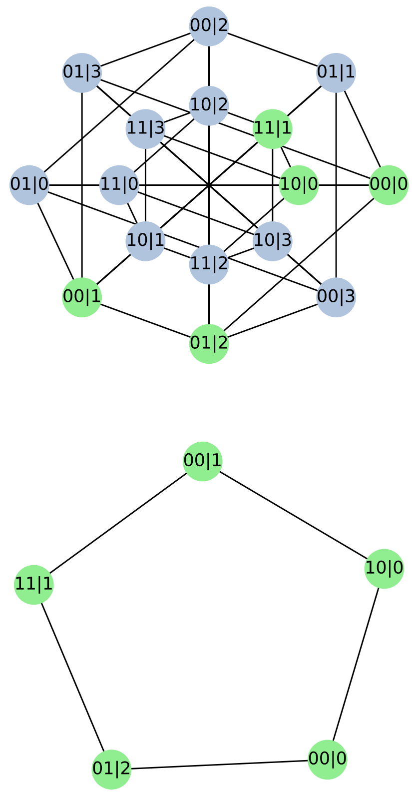

FIG. 5. The exclusivity graph of the bonet inequality.

2. $a = a'$ and $b \neq b'$.

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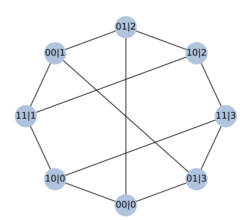

FIG. 6. The exclusivity graph for the 422 Instrumental scenario.

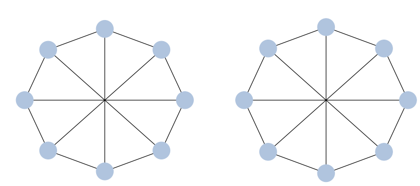

FIG. 7. The exclusivity graphs for the the CHSH scenario.