Exclusivity graph approach to Instrumental inequalities

Abstract

Instrumental tests have been widely used to derive causal relations between variables even in presence of unobserved latent factors, thus providing a powerful tool for different sciences ranging from xxx to xxx. Recently, much interest have been dedicated to the instrumental scenario since admits quantum violations with fewer resources respect to the Bell analogue, this property can be exploited to (drastically?) improve our current capacities to process information. Dire qualcosa della contextuality. Here, we present the instrumental inequality under a contextual approach, showing that the geometry of correlations within this framework allow us to find optimal xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx

Introduction

Inferring whether a variable A is the cause of another variable B is at the core of causal inference. However, unless interventions are available [1], one can cannot exclude that observed correlations between A and B are due to a latent common factor, thus hindering any causal conclusions. To cope with that, instrumental variables (IV) have been introduced [2, 3]. Under the assumption that they are independent of any latent common factors, IV can be used to put non-trivial bounds on the causal effect between A and B. To this aim, first, one has to guarantee that an appropriate instrument (fulling a set of causal constraints) has been employed, precisely the goal of the so-called instrumental tests [2, 3]. Their violation, at least in classical physics, is an unambiguous proof that some of the causal assumptions underlying the instrumental causal structure are not fulfilled, that is, one should identify and use another instrumental variable.

The first instrumental tests have been introduced by Pearl [2], in the form of inequalities providing a necessary condition for a given observed probability distribution to be compatible with the instrumental causal structure. Following that, Bonet [3] introduced a general framework, showing that the instrumental correlations define a polytope, a convex set from which the non-trivial boundaries are precisely the instrumental inequalities. Bonet's framework allows for a the derivation of new inequalities as well as proving general results, for instance, the fact that if variable A is continuous, no instrumental test exists. However, two main drawbacks are presented. First, the systematic derivation of new inequalities quickly becomes unfeasible as the variables' cardinality increases. Second, as recently shown, in quantum physics, violations of the instrumental tests are possible even though the whole process is indeed subjected to an instrumental causal structure [4, 5]. In the quantum case, instrumentality violations witness the presence of quantum entanglement as the latent factor and prove a stronger form of quantum non-locality as compared to the famous Bell's theorem [4]. As a consequence, typical bounds on the causal influence of A into B have to be reevaluated and reinterpreted in the presence of quantum effects [].

Our aim in this paper is to provide a novel and complementary framework to the analysis of instrumental tests and that addresses the two drawbacks mentioned above. The proposed method is based on a graph theoretical approach introduced in the foundations of quantum physics to analyze the possible correlations obtained in quantum experiments []. This method allow us to reproduce the classical results by Bonet and to straightforwardly generalize them in the quantum scenario. It also offer an easy way to check for the presence of gap between the quantum and classical case, for any causal scenario involving a single latent variable.

The paper is organized as follows: firstly we provide an introduction about the instrumental scenario, both from a classical perspective, as well as its quantum violation, and about the exclusivity approach. Then, we show a possible application of the exclusivity approach to the field of causal inference. Indeed, it is possible to exploit these graphs in order to obtain inequality constraints, as we show in particular for the instrumental scenario, in the case where the two parties can respectively choose among four and three three-outcome measurements.

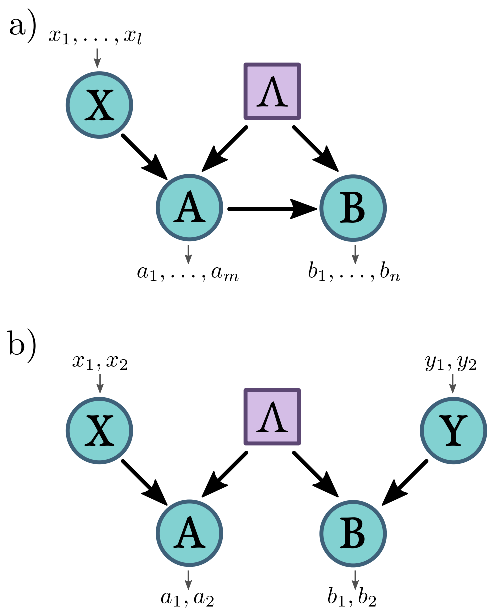

Figure 1: **a)** The directed acyclic graph (DAG) representing a general Instrumental scenario, with l possible values for the random variable X and m, n possible outcomes for A and B respectively **b)** The directed acyclic graph (DAG) of the CHSH scenario where all the variables X, Y, A and B can only take two possible values.

Instrumental variables, estimation of causal influences and a new form of quantum non-locality

It has become standard to represent causal relations via directed acyclic graphs (DAG), where the nodes represent random variables interconnected by directed edges (arrows) accounting for their cause and effect relations [1]. A set of variables $(X_1, \ldots, X_n)$ form a Bayesian network with respect to the graph if every variable X_i can be expressed as a function of its parents PA_i and potentially an unobserved noise term U_i, such that U_i are jointly independent. This implies that the probability distribution of such variables should have a Markov decomposition [1]

$$p(x_1, \ldots, x_n) = \prod_{i=1}^{n} p(x_i | pa_i). \tag{1}$$

Importantly, a DAG typically implies non-trivial constraints over the probability distributions that are compatible with it. That is, simply from observational data and without the need of interventions, one can test whether some observed correlations are incompatible with some causal hypothesis.

Within this context, an important DAG is that corresponding to the instrumental scenario (see Fig.1-a). Following the Markov decomposition, any empirical data encoded in the probability distribution $p(a, b|x)$ and compatible with the instrumental causal structure can be decomposed as

$$p(a, b|x) = \sum_{\lambda} p(a|x, \lambda) p(b|a, \lambda) p(\lambda). \tag{2}$$

Two causal assumptions are employed to arrive at the decomposition above. First, the assumption that $p(x, \lambda) = p(x)p(\lambda)$ implying the independence of the instrument and the common ancestor. Second, the assumption that even though X and B can be correlated, all these correlations are mediated by A. In other terms, there is no direct causal influence between X and B and $p(b|x, a, \lambda) = p(b|a, \lambda)$.

The instrumental variable has been originally introduced to estimate parameters in econometric models of supply and demand [] and since then have found a wide range of applications in various other fields []. To illustrate its power, consider that variables A and B are related by a simple structural equation $B = \gamma A + \Lambda$, where Λ may represent a latent common factor. By assumption, the instrumental variable X should be independent of Λ, thus implying that the causal strength can be estimated as $\gamma = \mathrm{Cov}(X, B)/\mathrm{Cov}(X, A)$ where $\mathrm{Cov}(X, A) = \langle X, A \rangle - \langle X \rangle \langle A \rangle$ is the covariance between X and A. Strikingly, one can estimate the causal strength even without any information about the latent factor Λ. More generally and without assumptions about the functional dependence among the variables, the empirical data encoded in the probability distribution $p(a, b|x)$ can also be used to bound different quantifiers of causality between A and B [].

Clearly, however, to draw any causal conclusions, first it is necessary to certify that one has a valid instrument. This is achieved via instrumental inequalities, first introduced by Pearl []. If we allow the variables X, A, B to

[1]Uppercase letters label variables and lowercase label the values taken by them, for instance, $p(X_i = x_i, X_j = x_j) \equiv p(x_i, x_j)$.

take the values in the range $x = 1, \ldots, l$, $a = 1, \ldots, m$ and $b = 1, \ldots, n$ Pearl showed that the instrumental causal structure implies that

$$\sum_{j=0}^{n} P(a_i b_j | x_{k(i,j)}) \leq 1, \tag{3}$$

for all $i \in 1, \ldots, m$ and for all the possible functions $k(i,j)$ where $p(a = i, b = j | x = k) = p(a_i, b_j | x_k)$.

Extending these results, Bonet [3] provided a general geometric framework for the derivation of instrumental inequalities. Instrumental correlations define a convex set, a polytope described by finitely many extremal points, or alternatively by a finite number of facets, the non-trivial of which are precisely instrumental inequalities. In particular, considering the case $(l, m, n) = (3, 2, 2)$ it was proven that there are two inequivalent classes of instrumental inequalities (those not obtained from each other by permuting the labels of a_i, b_j and x_k). One class corresponding to Pearl's inequality (3) and the other given by

$$\begin{aligned} P(a_1 b_1 | x_1) + P(a_2 b_2 | x_1) + P(a_1 b_1 | x_2) + \\ + P(a_2 b_1 | x_2) + P(a_1 b_2 | x_3) \leq 2. \end{aligned} \tag{4}$$

All these conclusions and results, however, rely on a classical description of causal and effect relations, that since Bell's theorem [] we know do not apply to the world governed by quantum mechanics. This has motivated the question of whether many of the cornerstones in causal inference have to reevaluated or reinterpreted in the presence of quantum effects []. Indeed, as recently shown [4], violations of the instrumental tests are possible even though the causal constraints underlying the instrumental scenario are fulfilled. As shown in the experimental implementation of the instrumental test [], this is possible due to the presence of quantum entanglement acting as latent common ancestor. Considering an entangled sources of photons, an alternative version of Bonet's inequality (written in terms of expectation values, upper bounded by 3, in the classical realm) has been tested, implying a violation of the inequality (4) with a value of 3.258 ± 0.020.

Altogether, this shows the necessity of a new unifying framework, not only considering what are the classical instrumental correlations but as well the ones achievable if the underlying latent factor might have a quantum origin. In the following we will achieve that by proposing a graph-theoretical approach to the analysis of instrumental inequalities.

The exclusivity graph approach

The graph-theoretical approach we propose here, was initially developed to the study of non-contextual inequalities [6] as well as Bell non-locality scenarios [**?**] and obtain their quantum violation. In this formalism, every possible event, i.e. every possible set of measurement outcomes $a_1 \ldots, a_n$ corresponding to given measurement settings $x_1, \ldots, x_n$ (each of which can be understood as an instrument), 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/instrument that can distinguish between them. Any linear constraint (like the instrumental inequalities) can be expressed defining a linear function

$$I_w(p) = \sum_{\substack{a_1, \ldots, a_n \\ x_1, \ldots, x_n}} w_{\substack{a_1, \ldots, a_n \\ x_1, \ldots, x_n}} p(a_1, \ldots, a_n | x_1, \ldots, x_n) \tag{5}$$

on the probabilities of possible events. This linear function can be represented by the weighted exclusivity graph G. Nicely, as it will be discussed below, bounds for the maximum values for $I_w(p)$ achievable in classical and quantum physical theories can be related to well-known graph invariants [], the independence number $\alpha(G, w)$ and the Lovász theta $\theta(G, w)$, respectively. In the following, we will briefly introduce these concepts and their interconnections, a more extensive and detailed account can be found in [6, 7, **?**]

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 customary to define the set $\mathrm{STAB}(G)$ as the convex hull of all the characteristic labellings of stable sets:

$$\mathrm{STAB}(G) = \{x : x \quad \text{is a stable labelling of} \quad G\}. \tag{6}$$

Using this definition the independence number becomes:

$$\alpha(G, w) = \max\{w \cdot x : x \in \mathrm{STAB}(G)\} \tag{7}$$

From these definitions we can see that $\alpha(G, w)$ corresponds to the classical bound of the inequality, since it is exactly 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:

$$\mathrm{TH}(G) = \{x : x_v = a_v^1 \text{ where } a_v \text{ is an orthonormal labelling of } G\} \quad (8)$$

It can be proved that this set includes all correlations permitted by quantum theory [2], but in general is larger as it contains correlations beyond those achieved by quantum mechanics [?]. Maximizing over $\mathrm{TH}(G)$ gives the Lovász theta:

$$\theta(G, w) = \{w \cdot x : x \in \mathrm{TH}(G)\} \quad (9)$$

which upper-bounds the maximum quantum value. This approach provides a useful condition to check if a given graph G admits a quantum violation. Indeed it can be proven 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" [?].

1 Exclusivity graph method applied to causal models

Next we show how the techniques presented in the previous section can be employed to analyze a broad class of causal models. Consider a DAG as in fig 2, with k observable variables A_k with potential causal arrows among them, l instruments X_l with no incoming edges, and a single unobservable latent variable Λ acting as a potential common factor for all A_k (but not to X_l).

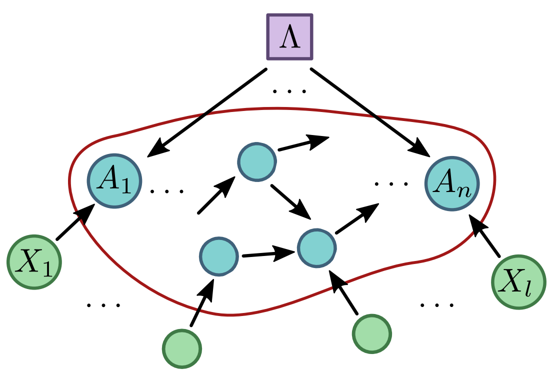

Figure 2: A represetantion of the class of causal structures to which our method can be applied. Those arewith k observable variables, l instruments and a single latent variable.

A *non-exclusivity* graph can be associated with such a DAG as follows:

[2] As proved in [?] this set corresponds to the level $1 + AB$ of the NPA (Navascués-Pironio-Acín) hierarchy [10].

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

As we will show next, considering the particular case of the instrumental scenario [], one can apply the graph-theoretical methods delineated before to the complement of this graph, $G = \bar{H}$, and its subgraphs. This allows to obtain instrumental inequalities and their respective quantum and classical bounds.

1.1 The Instrumental exclusivity graph

Without loss of generality we will restrict our attention to the case of dichotomic observables ($n = m = 2$), considering $p(ab|x)$ 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 the instrument assuming the value x. As detailed above, the non-exclusivity graph for the instrumental scenario is obtained by linking two events $ab|x$ and $a'b'|x'$ if there exists two functions $f : \mathcal{X} \rightarrow \mathcal{A}$ and $g : \mathcal{A} \rightarrow \mathcal{B}$ such that:

$$\begin{aligned} a = f(x) \quad &\text{and} \quad a' = f(x') \\ b = g(a) \quad &\text{and} \quad b' = g(a') \end{aligned} \quad (10)$$

As shown in figure 3, we construct the exclusivity graphs for various l and use the graph-theory methods described earlier to obtain the classical and quantum bounds for several inequalities in the instrumental scenario.

First, consider the case $l = 2$, for which Pearl's inequality (???) defines the only instrumental inequality. It has been shown that this inequality does not have a quantum violation []. For that, general probabilistic Bayesian networks, including classical and quantum causal models as particular cases, had to be introduced. In contrast, in our method it is straightforward not only to derive the classical bound to Pearl's inequality but also show that there is no quantum violation of the inequality. This follows immediately from the fact that the corresponding exclusivity graph (and its complement) does not contain any odd cyclic graph with more than 5 vertices, a necessary condition for any quantum violation.

For $l \geq 3$ we see that there might be a quantum violation, since the associated graph has as a subset a C_5 cyclic graph, i.e. the pentagon depicted in fig. 4 that is exactly

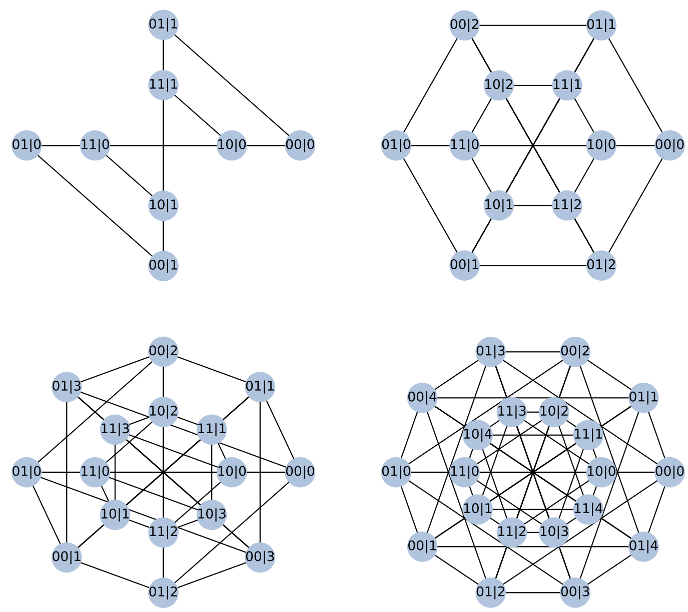

Figure 3: The exclusivity graph for the instrumental scenario $l22$ with $l = 2, 3, 4, 5$ respectively from top left to bottom right. To simplify the representation cliques are represented with the bold lines in the figure.

the Bonet's inequality (4). For cyclic graphs it is known that $\alpha(C_n) = \lfloor n/2 \rfloor$ and $\theta(C_n) = n\cos(\pi/n)/(1 + \cos(\pi/n))$. For $n = 5$ it follows directly the gap between the classical and quantum theories, since the classical limit is given by $\alpha(C_5) = 2$ and the quantum one given by $\theta(C_5) = \sqrt{5}$.

In this framework (4) seems analogous to the KCBS contextual inequality[8]. 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 [7], using which we find a value of $(3 + \sqrt{2})/2$.

As it will be shown below, no other odd anticycle besides C_5 is present for any l, that is, if we increase the cardinality of the instrumental variable.

This does not mean that different inequalities cannot be devised by clever choices of vertices and weights. For example for the 422 scenario we can find the inequality.

$$\begin{aligned}&p(00|10) + p(11|11) + p(01|20) + p(10|21) +\\&+ p(00|00) + p(10|01) + p(01|30) + p(11|31) +\\&- p(01|10) - p(10|11) - p(00|20) - p(11|21) +\\&- p(01|00) - p(11|01) - p(00|30) - p(10|31) \leq 2\end{aligned} \tag{11}$$

correponds to the two sets of events whose exclusivity graphs are depicted in fig. 5. 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.6), and, as pointed out above, both arise from the non-classicality of the C_5 graph.

Discussion

[Can we add an example with more outcomes?]

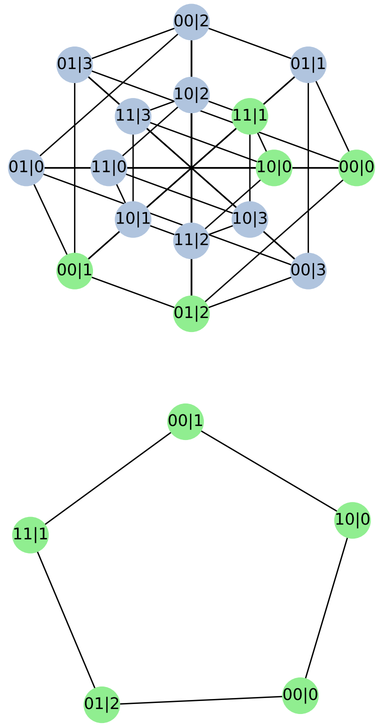

Figure 4: The exclusivity graph of the bonet inequality, as an induced subgraph of complete one of the 322 instrumental scenario.

Acknowledgements

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Methods

There are no cycles C_n with $n \geq 7$ in the $d22$ instrumental scenario.

In the following we prove that there cannot be a odd anticycle with more than 5 vertices in the exclusivity graph associated to an instrumental scenario of the type $d22$.

From the exclusivity conditions (11), given two events $ab|x$ and $a'b'|x'$, they are connected by edge if one of these two conditions is true:

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

Suppose we have a cycle C_n with $n \geq 7$, as in fig. 7, and consider that node 2 in this graph corresponds to an event which we can arbitrarily identify as $00|0$. Among its neighbors 1 and 3, one will necessarily need to satisfy rule 2 (they cannot both satisfy rule 1 or the three nodes would be a clique So without loss of generality we can assign the event $01|1$ to 3. Since nodes $5, 6, 7$ must not satisfy rule 2 with both 2 and 3, then they must have $a = 1$. Moreover 7 and 5 must have the same b, different from 6. In the same way 1 must not satisfy rule 2 with $6, 5$ and 3, so it needs to have $a = 0$ and $b = 1$. At this point, since we only have values $\{0, 1\}$ for a, we cannot avoid node 4 to be linked to one of the nodes $1, 2, 6, 7$. Thus, the corresponding graph cannot be a cycle.

References

[1] J. Pearl, *Causality: models, reasoning, and inference.* Cambridge University Press, (2000).

[2] J. Pearl, *On the testability of causal models with latent and instrumental variables*, Proceedings of the Eleventh conference on Uncertainty in artificial intelligence. Morgan Kaufmann Publishers Inc. (1995).

[3] B. Bonet, *Instrumentality tests revisited*, Proceedings of the Seventeenth conference on Uncertainty in artificial intelligence. Morgan Kaufmann Publishers Inc. (2001).

[4] R. Chaves, G. Carvacho, I. Agresti, V. Di Giulio, L. Aolita, S. Giacomini, F. Sciarrino, *Quantum violation of an instrumental test*, Nature Physics 14.3 291 (2018).

[5] T. Van Himbeeck, J. B. Brask, S. Pironio, R. Ramanathan, A. B. Sainz, E. Wolfe, *Quantum violations in the Instrumental scenario and their relations to the Bell scenario*, arXiv preprint arXiv:1804.04119 (2018).

[6] A. Cabello, S. Severini, A. Winter, *Graph-theoretic approach to quantum correlations*, Physical review letters, 112(4), 040401 (2014).

[7] R. Rabelo, C. Duarte, A. J. López-Tarrida, M. T. Cunha, A. Cabello, A. *Multigraph approach to quantum non-locality*, Journal of Physics A: Mathematical and Theoretical, 47(42), 424021 (2014).

[8] A. A. Klyachko, M. A. Can, S. Binicioğlu, A. S. Shumovsky. *Simple test for hidden variables in spin-1 systems.* Physical review letters, 101(2), 020403 (2008).

[9] M. Navascués, Y. Guryanova, M. J. Hoban, & A. Acín, *Almost quantum correlations.* Nature Communications 6, (2015).

[10] M. Navascués, S. Pironio, & A Acín, *A convergent hierarchy of semidefinite programs characterizing the set of quantum correlations.* New Journal of Physics 10, 073013 (2008).

[11] E. Tomita, A. Tanaka, & H. Takahashi, *The worst-case time complexity for generating all maximal cliques and computational experiments.* Theoretical Computer Science 363, 28–42 (2006).

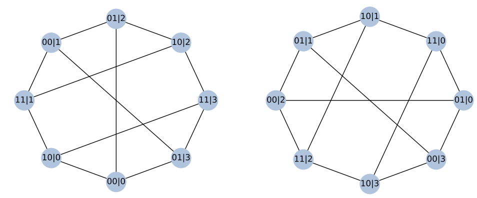

Figure 5: The exclusivity graph for the 422 Instrumental scenario.

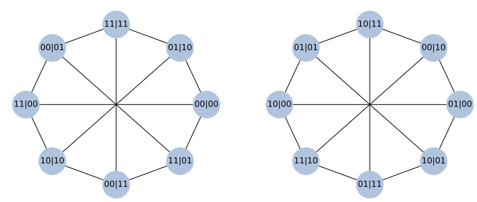

Figure 6: The exclusivity graphs for the the CHSH inequality in the Bell scenario.

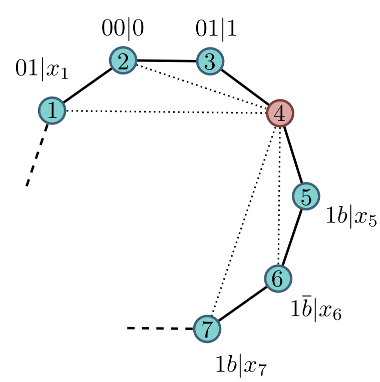

Figure 7: Proof of the impossibility of having cycles with 7 nodes or more in the $d22$ scenario.