Supplemental Materials

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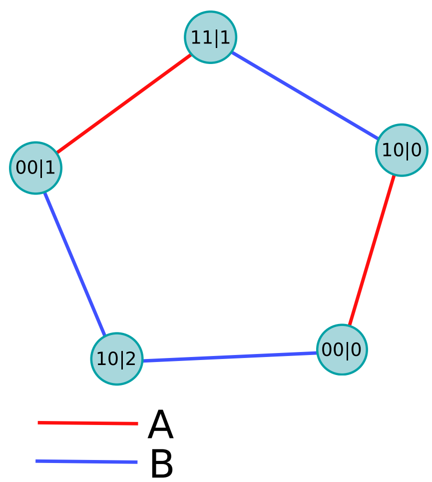

Figure 1: Edge colored exclusivity graph representation of the Bonet inequality. Exclusivity constraints for the party A and B are represented by red lines and blue lines respectively.

Building the exclusivity graph from DAG

In the following we describe in more details how to get from the DAG (Directed Acyclic Graph) representation of a causal model to the one for exclusivity graph. Starting from a generic causal model described by a DAG D, with N random variables $O_D = \{A_1, \ldots, A_N\}$ and M instruments $I_D = \{X_1, \ldots, X_M\}$, the exclusivity graph $G = (V, E)$ can be constructed, for example, using a simple breadth-first graph exploring algorithm. The procedure, described in algorithm 1, requires the DAG D and the list V of vertices to be explored, since we can be interested in building the graph only for a subset of events.

Edge colored multigraph technique for approximating the quantum bound

The Lovász theta of a graph, despite being efficiently computable, only gives an upper bound to the maximal quantum bound, since it ignores the additional constraints arising from the presence of different random variables A_i. Indeed the quantum bound is influenced not only by the exclusivity relations between the possible events in our scenario, but also on how those relations are derived from the variables $A_1, \ldots, A_N$.

To obtain a better approximation for the quantum bound we can follow the technique presented in [1]. This method consists in introducing an edge coloring in the exclusivity graph. This edge coloring encodes the information of which of the A_is is involved in the exclusivity constraints under consideration. In practice this corresponds to constructing an exclusivity graph G_i for each A_i. The resulting object is called a *multigraph*. Having defined a multigraph $G = G_1, \ldots, G_N$ for a given scenario the quantum bound is defined by the quantity:

$$\vartheta(G) = \max_v \sum_{i \in V} |v \cdot a_i^1 \otimes \cdots \otimes a_i^n|^2 \tag{1}$$

where $\{a_i^j\}$ is an orthonormal labelling for G_j and V is the set of vertices of G. This quantity, which can be seen as a generalization of the Lovász theta, is in general not efficiently computable, but, as described in [1], can be arbitrarily approximated by a hierarchy of semi-definite programs[2].

For example, in the case of the pentagon in the instrumental scenario we have two colors, and thus two graph G_A and G_B, corresponding to variables A and B respectively, as shown in Fig. 1. Applying the technique described above to this scenario yields a quantum bound of 2.2071, reproducing the known value for the quantum bound of the Bonet inequality given by $(3 + \sqrt{2})/2$.

Algorithm 1 Breadth-first graph exploration

```
function BUILD GRAPH(V, D)
    E ← ∅
    while V ≠ ∅ do
        INSERT(Q, V_1)                          ▷ Initialize the queue with the first element of V
        DELETE(V, V_1)
        while Q ≠ ∅ do
            v ← Q_1
            DELETE(Q, Q_1)
            for u ∈ V do
                if EXCLUSIVE(u, v) then
                    INSERT(E, (v, u))
                    INSERT(Q, u)
                    DELETE(V, u)                ▷ Visited nodes are removed from V
                end if
            end for
        end while
    end while
    return E
end function
```

As in the main text, here a, a' stand for the value of the outcome of the variable A in the events v, v', while $p_a, p_{a'}$ stand for the values of the parent nodes of A in D, $\mathrm{PA}(A)$.

```
function EXCLUSIVE(v, v', D)
    n ← true
    for A ∈ O_D do
        n ← n ∧ (p_a ≠ p_a' ∨ (p_a = p_a' ∧ a = a'))
    end for
    return ¬n
end function
```

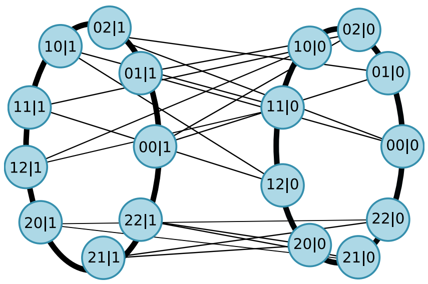

Figure 2: Exclusivity graph for the instrumental scenario 233, showing the impossibility of having cycles with more than 5 vertices. To simplify the figure cliques are represented by bold lines between vertices.

There are no quantum violation for instrumental scenarios with $l = 2$ settings.

It is easy to see that no quantum violation is possible for instrumental scenario with $l = 2$ possible settings for the instrumental variable X. This reduces to proving that there are no odd n-cycles nor n-anticycles as induced subgraphs in the corresponding exclusivity graph, with $n \geq 5$. To see this we can notice that any such graph is composed by two cliques (see for example Fig. 2), corresponding to the events with $x = 0$ and $x = 1$. Any n-cycle with at least 5 vertices must then have at least 3 mutually connected vertices belonging to the same x, so they can never form a cycle-graph. Similarly we can show that there cannot be any induced odd anticycle with 5 or more vertices.

There are no cycles C_n with $n \geq 7$ in the $l22$ 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 $l22$.

Two different events $ab|x$ and $a'b'|x'$, are exclusive 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. 3, 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

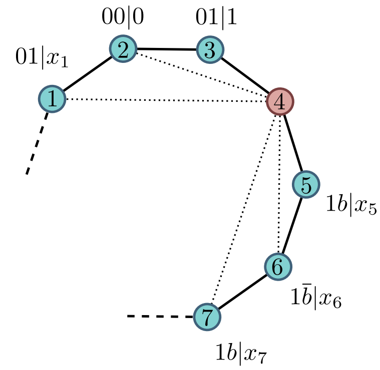

Figure 3: Proof of the impossibility of having cycles with 7 nodes or more in the $d22$ scenario.

$a = 1$. 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

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