Causal Bounds via Subgraph Inequalities

Lee M. Gunderson
Department of Statistical Science
University College London
l.gunderson@ucl.ac.uk

Davide Poderini
Department of Physics
University of Pavia
davide@poder.in

Gecia Bravo-Hermsdorff
School of Informatics
University of Edinburgh
gecia.bravo@gmail.com

We introduce a graphical algebraic notation that streamlines the derivation of causal inequalities, alleviating (some of) the combinatorial explosion inherent in generalizing the method of inflation. The proposed graph algebra is an application of the celebrated theory of *flag algebras* introduced by Razborov in 2007, which continues to serve as an instrumental tool in the derivation of many new results in extremal combinatorics in an impressive variety of settings. We demonstrate the utility of this algebra of rooted subgraphs by providing succinct proofs of bounds on the joint distribution of variables in a variety of correlation scenarios relevant to quantum networks.

Bell's theorem [5] stands as a cornerstone of quantum theory, with profound implications for both its foundational aspects and its applications in quantum information processing [27]. The violation of a Bell inequality can be seen as a demonstration of the incompatibility between classical and quantum predictions, based solely on the causal assumptions underlying an experiment. Notably, the discrepancy between classical and quantum causal predictions extends beyond the paradigmatic Bell scenario, generalizing to more complex causal structures. Driven by advances in quantum networks, a growing body of research has demonstrated that correlations among distant parties in causal networks composed of independent sources can also exhibit non-classical behavior [27].

Strikingly, such nonclassicality exhibits many peculiar aspects distinct from those observed in the standard Bell scenario, such as nonconvex boundaries, elucidating subtler aspects of nonclassicality and showing that the Bell inequality is but one facet of the feasibility iceberg. This raises a fundamental question of being able to characterize the constraints of causal structures that can give rise to nonclassical correlations. Despite its importance, this question remains exceptionally challenging to answer. Although numerous complementary approaches have been developed in recent years [8, 17, 20, 21, 16], their practical applicability remains limited to specific cases of interest and becomes computationally intractable as the scale of the system grows.

Causal assumptions can be encoded in a *d*irected *a*cyclic *g*raph (*DAG*), where the nodes represent random variables, each generated by a random mechanism that depends on the outcome of its parents (i.e., nodes in the DAG that have edges point to it). Additionally, node variables can be either observable variables or latent variables (also called sources). The causal compatibility problem asks whether a given probability distribution over the observable variables is compatible with a particular causal structure. This question can be asked in the classical setting (where all variables are classical) and in the quantum case, where the latent variables represent quantum systems.

The central message of this work is that the questions of causal compatibility can be translated to questions of extremal combinatorics. Using this connection we present a technique for deriving inequality constraints for the compatibility of a distribution in large-scale correlation scenarios. In particular, we show how methods employing flag algebras can streamline the derivation of causal inequalities, while the diversity of causal scenarios can offer new settings for problems in extremal combinatorics.

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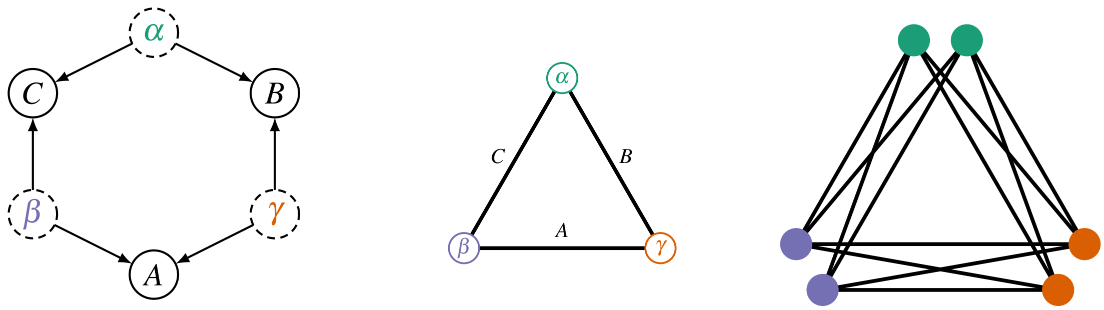

Figure 1: **The triangle scenario example.** The *triangle scenario* refers to a causal scenario with three observable variables, *A*lice, *B*ob, and *C*harlie, and three independent sources/latent variables: α (parent of B and C), β (parent of A and C), and γ (parent of A and B). On the *left* this scenario is represented as a DAG, with arrows indicating direct causal influence. The graph algebra represents such scenarios compactly using subgraphs with (colored) nodes referring to (type of) latent variables and edges referring to (the outcome of the) observed variables. Converting the picture on the *left* to a simpler representation as the *middle* triangle, allows one to succinctly represent equivalence classes of combinations of variables in the inflated structure on the *right*.

A Motivating Correspondence. The Finner bound for the triangle scenario (Fig. 1, *left*) [12, 26] corresponds to a well-known graph theory inequality—the density of triangles squared is upper-bounded by the edge density cubed [19]:

$$\underbrace{p(ABC) \leq \sqrt{p(A)p(B)p(C)}}_{\text{Finner bound}} \qquad \Longleftrightarrow \qquad \underbrace{\triangle\triangle \leq ///}_{\text{Kruskal-Katona theorem}} \tag{1}$$

The corresponding lower bound resisted proof until around 2007, when it was proven using flag algebras [23], a powerful tool in extremal combinatorics that has been fundamental to the derivation of many new results for: graphs [10, 3, 25, 15], hypergraphs [11, 2], graphons [19, 14], permutations [4], Ramsey numbers [18], phylogenic trees [1], binary trees [7], and tournament graphs [9].

The Flag Philosophy. The theme of flag algebras is to fix the limiting object once and for all.[1] While the method of inflation [28, 20] reasons about counterfactual distributions resulting from n independent copies of the latent sources, flag algebras takes this to the limit ($n \to \infty$). As the size of the larger network tends to infinity, its statistics converge to those of the true distribution. Any such larger network with the desired statistics may be used as a protocol certifying the possibility of such a distribution. Likewise, the impossibility of such an object results in a bound on the possible statistics.

A particularly important class of causal structures is that of correlation scenarios [13], which is the class of bipartite DAGs connecting source nodes to observable nodes. For the classical setting, a causal compatibility problem in a general causal structure can be mapped to a causal compatibility problem in a correlation scenario [20]. Correlation scenarios are often illustrated with arrows pointing from the latent variables/sources to the observed variables, such as the triangle scenario shown at the left of Fig. 1. To make the connection between causal inequalities and (extremal) graph theory, the latent variables become nodes in a graph, while the observed variables become (outcome-valued) edges between the nodes.

Intuitively, one can think of rooted subgraphs as representing tensors, with each latent variable/node in the subgraph representing an index that ranges over the n options for that latent variable in a large

[1]We refer the reader to [22, 24, 19] for a formal presentation.

inflated network. The entries of the tensor are given by the product of the variables corresponding to the edges of the rooted subgraph. Subgraphs with no edges correspond to tensors with 1 for every entry. For example, the rooted subgraph is an all-ones tensor with size $n \times n \times n$.

While the different types of latent nodes must be kept track of, they can often be implied by the relative positions of the nodes. For example, given the triangular arrangement in Figure 1, the rooted subgraph, can be seen to have an edge representing Alice's outcomes as a function of the β and γ indices (with the isolated α node essentially adding a "dummy" index[2]). Likewise, represents Bob's outcomes, and represents Charlie's. The gluing algebra of subgraphs is simply the entrywise product of these objects, which corresponds to combining subgraphs by "gluing" together their corresponding nodes. For example, the product of Alice and Bob's outcomes is represented as $()() = $. In this presentation, we take the outcomes to be $\{+1,-1\}$.[3] This has the interesting feature (for classical variables) of canceling pairs of identical edges, as $(\pm 1)^2 = 1$. For example: $()() = $.

A quick cut inflation and a GHZ-type upper bound. Now, let's see how to use this notation to derive a quick bound on the probability that $A = B = C$ in the triangle scenario with uniform marginals. We represent a cut inflation using two copies of the α latent variable/node, and use the gluing algebra to multiply the following two linear combinations of flags: $0 \leq (\; - \;)(\; - \;) = \; - \; - \; + \;$. As the entries of these linear combinations (in parentheses) are nonnegative, so too is their product.

Averaging over all entries of the tensors (represented by filling in the nodes) gives observable statistics: $0 \leq \; - \; - \; + \; = 1 - \langle AB \rangle - \langle AC \rangle + \langle B \rangle \langle C \rangle$. Notice that the disconnected subgraphs become a product of expectations, as the outcomes of their components are independent. For the case of uniform marginals, $\langle A \rangle = \langle B \rangle = \langle C \rangle = 0$, and we obtain: $\; + \; = \langle AB \rangle + \langle AC \rangle \leq 1$ (and cyclic permutations). To obtain a bound on GHZ-type distributions, consider the following linear combination:

$$Q(\;) \equiv \tfrac{1}{4}(\; + \; + \; + \;) = \begin{cases} 1 & \text{if } A = B = C \\ 0 & \text{otherwise} \end{cases} \tag{2}$$

Combining these results, we obtain an upper bound on the probability that all three outcomes agree:

$$p(A = B = C) = \Big\langle Q(\;) \Big\rangle = \tfrac{1}{4}(1 + \; + \; + \;) \leq \tfrac{5}{8} \tag{3}$$

Summary and future directions. Our example illustrates that this can be a promising approach for the study of correlation scenarios, and potentially a broader class of causal structures, suggesting a profound connection between these frameworks. Leveraging the well-established technique of flag algebras, we are able to derive powerful results that already capture key features of the problem, such as its inherent nonconvexity. These findings not only provide a powerful tool for the characterization of the classical causal constraints, but also lay the groundwork for exploring more complex scenarios. Notably, while we have focused on the dichotomic case for simplicity, the framework can be generalized to observable outcomes of arbitrary cardinality. Looking ahead, it would be highly interesting to extend this approach to the quantum case, i.e., promoting classical latent sources to quantum states. Such an extension could provide new insights into the boundaries of quantum correlations and their implications for quantum information processing and foundational studies.

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[2] One can think of the isolated nodes as being placeholders, akin to the function NEWAXIS() in Python.

[3] For homomorphism densities in graph theory, the outcomes are typically taken to be $\{0,1\}$. Our approach here is equivalent, amounting to a sort of "change of basis" (see Chapter 6 of [6]).

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