FirstPage

The inflation technique for Causal Inference with Latent Variables

Elie Wolfe,[1,*] Robert W. Spekkens,[1,†] and Tobias Fritz[1,2,‡]

[1] *Perimeter Institute for Theoretical Physics, Waterloo, Ontario, Canada, N2L 2Y5*
[2] *Max Planck Institute for Mathematics in the Sciences, Leipzig, Germany*

(Dated: May 23, 2016)

The fundamental problem of causal inference is to infer if an observed probability distribution is compatible with some causal structure which may incorporate latent variables. Given a particular causal structure, it is therefore valuable to derive incompatibility inequalities, i.e. criteria whose violation witnesses the incompatibility of the violating distribution with the given causal structure. The problem of causal inference via incompatibility witnesses comes up in many fields. Special causal incompatibility inequalities are Bell inequalities (which distinguish non-classical from classical distributions) and Tsirelson inequalities (which distinguish quantum from post-quantum distributions), and Pearl's instrumental inequality. All of these are limited to very specific causal structures. Analogues of such inequalities for more-general causal structures, i.e., necessary criteria for either classical or quantum distributions to be realizable from the structure, are highly sought after.

We here introduce a technique for deriving such causal incompatibility inequalities, applicable to any causal structure. It consists of first *inflating* the causal structure and then translating weak constraints on the inflated structure into stronger constraints on the original structure. Moreover, we show how our technique can be tuned to yield either classical witnesses (i.e., that may have quantum violations), or post-classical witnesses (i.e., that hold even in the context of general probability theories), depending on whether or not the inflation implicitly broadcasts the value of a hidden variable. Concretely, we derive polynomial inequalities for the so-called Triangle scenario, and we show how all Bell inequalities also follow from our method. Furthermore, given both a causal structure and a specific probability distribution, our technique can be used to efficiently witness their incompatibility, without requiring explicit inequalities. The inflation technique is therefore both relevant and practical for general causal inference tasks with hidden variables.

* ewolfe@perimeterinstitute.ca
† rspekkens@perimeterinstitute.ca
‡ tobias.fritz@mis.mpg.de

I. INTRODUCTION

Given a probability distribution over some random variables, the problem of **causal inference** is to determine what causal relations among these variables and possibly also some unobserved variables could have generated this distribution. This type of problem arises in a wide variety of scientific disciplines, from sussing out biological pathways to enabling machine learning pearl2009causality,spirtes2011causation,studeny2005probabilistic,koller2009probabilistic [1–4]. A related problem is to determine, for a given set of causal relations, the set of all probability distributions that can be generated from them. A special case of both is the following decision problem: given a probability distribution and a causal hypothesis, determine whether the two are compatible, in the sense that the causal relations permitted by the hypothesis could in principle have generated the given distribution. In this article, we focus on techniques for solving the decision problem and for finding necessary conditions on a probability distribution for compatibility with a given causal hypothesis.

In the simplest setting, the causal hypothesis consists of a directed acyclic graph (DAG) whose nodes all correspond to *observed* variables. In this case, obtaining a verdict on the compatibility of a given distribution with the causal hypothesis is simple: the compatibility holds if and only if the distribution is Markov with respect to the DAG, which is to say that all of the conditional independence relations in the distribution are explained by the structure of the DAG. The compatible DAGs can be determined algorithmically solely from the distribution. ~~i.e. without having an *a priori* hypothesis~~ pearl2009causality [1].

A significantly more difficult case is when one considers a causal hypothesis which consists of a DAG whose nodes include **latent** variables, so that the set of observable variables is only a subset of the nodes of the DAG. This case occurs, e.g., in situations where one needs to deal with the possible presence of unobserved confounders, and is particularly relevant for experimental design in statistics.

It is useful to distinguish two varieties of this problem: (i) the causal hypothesis specifies the nature of the latent variables, for instance, that they are discrete and of a particular cardinality (the cardinality of a variable is the number of possible values it can take), and (ii) the nature of the latent variables is arbitrary.

Consider the first variety of causal inference problem. If the latent variables are all discrete then the mathematical problem which one must solve to infer the distributions that are compatible with the hypothesis is a quantifier elimination problem for some finite number of quantifiers. Say something here about quantifier elimination —RWS The parameters specifying the probability distribution over the observed variables can all be expressed as functions of the parameters specifying the conditional probabilities of each node given its parents. Many of the latter parameters are associated to the latent variables. However, if one can eliminate the parameters associated to the latent variables, one obtains constraints that refer exclusively to the probability distribution over the observed variables. Because this is a *nonlinear* quantifier elimination problem in the general case, it is infeasible to provide an exact solution except in particularly simple scenarios LeeSpekkens [5]. Nonetheless, because the mathematical problem to be solved is known in this case, any techniques developed for finding approximate solutions to problems of nonlinear quantifier elimination can be leveraged.

The second variety of causal inference problem, where the latent variables are arbitrary, is more difficult, but also the case that has been the focus of most research and that motivates the present work. It is possible that inference problems of this variety might also be reducible to quantifier elimination problems. This would be the case, for instance, if one could show that discrete latent variables of a certain finite cardinality (rather than arbitrary latent variables) are sufficient to generate all the distributions compatible with that DAG [1]. At present, therefore, the problem of providing a mathematical algorithm for deciding compatibility in this second case—let alone an efficient algorithm—remains open. Moreover, even if it *is* possible to achieve a reduction to the case of latent variables with finite cardinality, one would still be faced with a difficult nonlinear quantifier elimination problem. As such, heuristic techniques for obtaining nontrivial constraints, such as the one presented in this work, are still valuable in practice.

If one allows for latent variables, the condition that all of the conditional independence relations among the observed variables should be explained by the structure of the DAG is still a necessary condition for compatibility of a DAG with a given distribution, but in general it is no longer a sufficient condition for compatibility.

Historically, the insufficiency of the conditional independence relations for causal inference in the presence of latent variables was first noted by Bell in the context of the hidden variable problem in quantum physics bell1964einstein [6]. Bell considered an experiment for which considerations from relativity theory implied a very particular causal structure, and he derived an inequality that any distribution compatible with this structure (and with the quantum predictions) must satisfy. Bell also showed that this inequality was violated by distributions generated from entangled quantum states with particular choices of incompatible measurements. Later work, by Clauser, Horne, Shimony and Holte (CHSH) CHSHOriginal [7] showed how to derive inequalities directly from the causal structure. The CHSH inequality was the first example

[1] Denis Rosset has an unpublished proof purporting to upper bound the cardinality of sufficiently general latent variables. We do not pursue the question here.

of a compatibility condition that appealed to the strength of the correlations rather than simply the conditional independence relations inherent therein. Since then, many generalizations of the CHSH inequality have been derived for the same sort of causal structure [8].

The idea that such work is best understood as a contribution to the field of causal inference has only recently been appreciated [9–12], as has the idea that techniques developed by researchers in the foundations of quantum theory may be usefully adapted to causal inference [2].

Later on, Pearl derived another inequality, called the **instrumental inequality** [21], which provides a necessary condition for the compatibility of a distribution with a causal structure known as the *instrumental scenario* that applies, for instance, to certain kinds of noncompliance in drug trials.

Steudel and Ay [22] subsequently derived an inequality which must hold whenever a distribution on n variables is compatible with a causal structure where no set of more than c variables has a common ancestor (here $n, c \in \mathbb{N}$ are unrestricted). Subsequent work has focused on the case of $n = 3$ and $c = 2$, a causal structure that has been called the Triangle scenario [10, 23].

Recently, Henson, Lal and Pusey [11] have found a sufficient condition for a DAG to be interesting in the sense that conditional independence relations do not exhaust the set of constraints on the joint distributions that are compatible with the DAG. They have also explicitly presented a catalogue of all the interesting DAGs having seven or fewer nodes in Appendix ?? of Ref. [11]. The Bell scenario, the Instrumental scenario, and the Triangle scenario appear in the catalogue, but even for six or fewer nodes, there are many more cases to consider. Furthermore, the fraction of DAGs that are interesting increases as the total number of nodes increases. This highlights the need for moving beyond a case-by-case consideration of individual DAGs and developing techniques for deriving constraints beyond conditional independence relations that can be applied to any interesting DAG.

The challenge was taken up recently by... Summarize the Shannon inequalities stuff [14, 23, 24] and follow-up work on non-Shannon inequalities [15, 16, 25]. Also summarize Chaves' work on polynomial Bell inequalities. Summarize why these techniques are still wanting.

We here introduce a new technique for deriving necessary conditions on a distribution for compatibility with a given causal structure. This technique allows for, but is not limited to, the derivation of polynomial inequalities. As far as we know, our method is the first systematic tool for doing causal inference with latent variables that goes beyond observable conditional independence relations and does not assume any bounds on the number of values of each latent variable. While our method can be used to systematically generate necessary conditions for compatibility with a given causal structure, we do not know whether the set of inequalities thus generated are also sufficient. The fact that we have not yet been able to obtain Pearl's instrumental inequality from our method suggests that it may not be sufficient.

While we present our technique primarily as a tool for standard causal inference, we also comment on the extent to which the inequalities we derive are also necessary conditions on the compatibility of a distribution with nonclassical generalizations of the notion of a causal model [10–12, 14]. Some of the inequalities we derive require us to imagine that the value of a hidden variable can be distributed or *broadcast* to many different observed variables. The no-broadcasting theorem from quantum theory shows that this is not valid in the non-classical case, and from our perspective this is the reason for the existence of quantum violations of Bell inequalities. Moreover, our technique can also be applied in order to derive criteria that must be satisfied by all distributions that can be generated with latent nodes that are states in quantum theory or any other general probabilistic theory, simply by not assuming the possibility of broadcasting. Say something about how we anticipate deriving new inequalities that might be violated by quantum theory—RWS.

II. CAUSAL MODELS AND COMPATIBILITY

A **causal model** consists of a pair of objects: a **causal structure** and a set of **causal parameters**. We define each in turn.

We begin by recalling the definition of a directed acyclic graph (DAG), A DAG G consists of a set of nodes and directed edges (i.e., ordered pairs of nodes), which we denote by $\mathsf{Nodes}[G]$ and $\mathsf{Edges}[G]$ respectively. Each node corresponds to a random variable and a directed edge between two nodes corresponds to there being a direct causal influence from one variable to the other.

Our terminology for the causal relations between the nodes in a DAG is the standard one. The parents of a node X in a given graph G are defined as those nodes which have directed edges originating at them and terminating at X, i.e. $\mathsf{Pa}_G(X) = \{\, Y \mid Y \to X \,\}$. Similarly the children of a node X in a given graph G are defined as those nodes which have have directed edges originating at X and terminating at them, i.e. $\mathsf{Ch}_G(X) = \{\, Y \mid X \to Y \,\}$. If $\boldsymbol{U}$ is a set of nodes, then we put $\mathsf{Pa}_G(\boldsymbol{U}) := \bigcup_{X \in \boldsymbol{U}} \mathsf{Pa}_G(X)$ and $\mathsf{Ch}_G(\boldsymbol{U}) := \bigcup_{X \in \boldsymbol{U}} \mathsf{Ch}_G(X)$. The **ancestors** of a set

[2] The current article being another example of the phenomenon [13–20].

of nodes $\boldsymbol{U}$, denoted $\mathsf{An}_G(\boldsymbol{U})$, are defined as those nodes which have a directed *path* to some node in $\boldsymbol{U}$, *including* the nodes in $\boldsymbol{U}$ themselves. R: Does Pearl include U among the ancestors? I wonder if "ancestry" might be better terminology. Equivalently (dropping the G subscript), $\mathsf{An}(\boldsymbol{U}) := \bigcup_{n\in\mathbb{N}} \mathsf{Pa}^n(\boldsymbol{U})$, where $\mathsf{Pa}^n(\boldsymbol{U})$ is inductively defined via $\mathsf{Pa}^0(\boldsymbol{U}) := \boldsymbol{U}$ and $\mathsf{Pa}^{n+1}(\boldsymbol{U}) := \mathsf{Pa}(\mathsf{Pa}^n(\boldsymbol{U}))$.

A causal structure is a DAG that incorporates a distinction between two types of nodes: those that are observed, denoted $\mathsf{ObservedNodes}[G]$ and those that are latent, denoted $\mathsf{LatentNodes}[G]$. Following Ref. [HensonLalPusey], we will denote the observed nodes by triangles and the latent nodes by circles. Finally, we suppose that a specification of the causal structure also includes a specification of the nature of the random variable associated to each node [12, Appendix A], for instance, that it is continuous or that it is discrete and has a particular cardinality (the number of possible values that the variable can take). Henceforth, we will use the terms "DAG" and "causal structure" interchangeably, so that the specification of which variables are observed as well as their cardinalities is considered to be part of the DAG (unless we explicitly state otherwise). BeyondBellII

The set of causal parameters specifies, for each node, the conditional probability distribution over the values of the random variable associated to that node, given the values of the variables associated to the node's parents. (In the case of root nodes, the parents are the null set and the conditional probability distribution is simply a probability distribution.) We will denote a conditional probability distribution over a variable Y given a variable X by $P_{Y|X}$, while the particular conditional probability of the variable X taking the value x given that the variable Y takes the values y is denoted $P_{Y|X}(y|x)$. Therefore, a given set of causal parameters has the form

$$\{P_{A|\mathsf{Pa}_G(A)} : A \in \mathsf{Nodes}[G]\}. \tag{1}$$

A causal model, denoted M, constitutes a causal structure together with a set of causal parameters, $M := (G, \{P_{A|\mathsf{Pa}_G(A)} : A \in \mathsf{Nodes}[G]\})$.

A causal model specifies a joint distribution over all variables in the DAG via

$$P_{\mathsf{Nodes}[G]} = \bigotimes_{A\in\mathsf{Nodes}[G]} P_{A|\mathsf{Pa}_G(A)}, \tag{2}$$

{Markov}

where $\otimes$ denotes the standard tensor product of functions, so that $P_X \otimes P_Y(xy) := P_X(x)P_Y(y)$. This is typically called the Markov condition. Similarly, the joint distribution over the observed variables is obtained from the joint distribution over all variables by marginalization over the latent variables

$$P_{\mathsf{ObservedNodes}[G]} = \sum_{\{X: X\in\mathsf{LatentNodes}[G]\}} P_{\mathsf{Nodes}[G]}, \tag{3}$$

{MarkovOb

where $\sum_X$ denotes marginalization over the variable X, so that $(\sum_X P_{XY})(y) := \sum_x P_{XY}(xy)$.

A given distribution over observed variables is said to be **compatible** with a given causal structure if there is some choice of the causal parameters that yields the given distribution via Eqs. (3) and (2). Note that a given set of marginal distributions over sets of observed variables is said to be compatible with a given causal structure if and only if the joint distribution over observed variables that yields these marginals is compatible with the causal structure.

III. WITNESSING INCOMPATIBILITY USING THE INFLATION TECHNIQUE

We now introduce the notion of **an inflation of a causal model**. If the original causal model is associated to a DAG G, then a nontrivial inflation of this model is associated to a different DAG, G'. We refer to G' as an inflation of G. There are many possible choices of G' for a given G (specified below), hence many possible inflations of a given DAG. We denote the set of these by $\mathsf{Inflations}[G]$. The choice of an element $G' \in \mathsf{Inflations}[G]$ is the only freedom in the inflation of a causal model. Once a choice is made, the set of parameters of the inflated model M' is fixed uniquely by the set of parameters of the original model M by a function $\mathsf{Inflation}_{G\to G'}$ (specified below), such that $M' = \mathsf{Inflation}_{G\to G'}[M]$.

We begin by defining the condition under which a DAG G' is an inflation of a DAG G. This requires some preliminary definitions.

The **subgraph** of G induced by restricting attention to the set of nodes $\boldsymbol{V} \subseteq \mathsf{Nodes}[G]$ will be denoted $\mathsf{SubDAG}_G(\boldsymbol{V})$. It consists of the nodes $\boldsymbol{V}$ and the edges between pairs of nodes in $\boldsymbol{V}$ per the original DAG. Of special importance to us is the **ancestral subgraph** of $\boldsymbol{V}$, denoted $\mathsf{AnSubDAG}_G(\boldsymbol{V})$, which is the minimal subgraph containing the full ancestry of $\boldsymbol{V}$, $\mathsf{AnSubDAG}_G(\boldsymbol{V}) := \mathsf{SubDAG}_G(\mathsf{An}_G(\boldsymbol{V}))$.

Inflation involves a sort of copying operation on nodes of the DAG. Specifically, every node of G' can be understood as a copy of a node of G. If A denotes a node in G that has copies in G', then we denote these copies by $A_1, \ldots, A_k$, and the variable that indexes the copies is termed the **copy-index**. When two objects (e.g. nodes, sets of nodes, DAGs, etc...) are the same up to copy-indices, then we use $\sim$ to indicate this. For instance, we have $A_i \sim A_j \sim A$. This copying operation must also preserve the causal structure of the DAG, in a manner that is formalized by the following definition.

Definition 1. *The DAG G' is said to be an* ***inflation*** *of the DAG G, that is, $G' \in \mathsf{Inflations}[G]$, if and only if for every node A_i in G', the ancestral subgraph of A_i in G' is equivalent, under removal of the copy-index, to the ancestral subgraph of A in G,*

$$G' \in \mathsf{Inflations}[G] \quad \textit{iff} \quad \forall A_i \in \mathsf{Nodes}[G'] : \ \mathsf{AnSubDAG}_{G'}(A_i) \sim \mathsf{AnSubDAG}_{G}(A). \tag{4}$$ {eq:defin

To illustrate the notion of inflation, we consider the DAG of Fig. 1, which is called the *Triangle scenario* (for obvious reasons) and which has been studied by many authors [11 (Fig. E#8), 9 (Fig. 18b), 10 (Fig. 3), 23 (Fig. 6a), 26 (Fig. 1a), 27 (Fig. 8), 22 (Fig. 1b), 14 (Fig. 4b)] Different inflations of the Triangle scenario are depicted in Figs. 2 to 6.

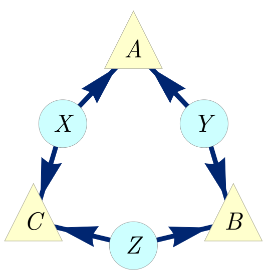

FIG. 1. The causal structure of the Triangle scenario.

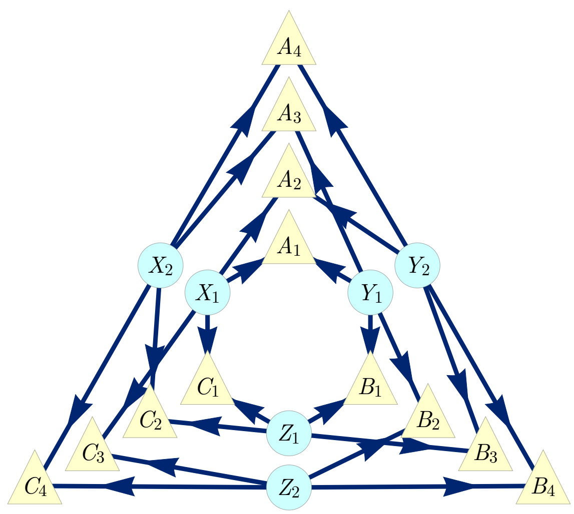

FIG. 2. An inflated DAG of the Triangle scenario where each latent node has been duplicated and each observable nodes node has been quadrupled. Note that no further duplication of observable nodes is needed, given that each has two latent nodes as parents in the original DAG and consequently there are only four possible choices of parentage of each observable node's counterpart in the inflated DAG.

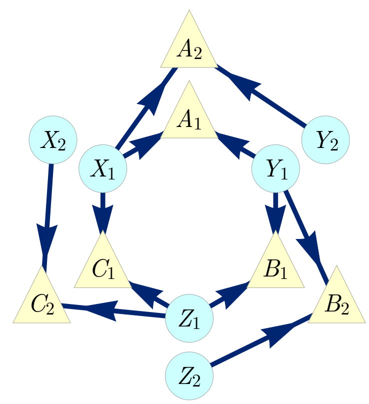

FIG. 3. Another inflation of the Triangle scenario consisting, also notably $\mathsf{AnSubDAG}_{(\text{Fig. 2})}(A_1 A_2 B_1 B_2 C_1 C_2)$.

We now turn to specifying the function $\mathsf{Inflation}_{G \to G'}$, that is, to specifying how a causal model transforms under inflation.

Definition 2. *Consider causal models M and M' where $\mathsf{DAG}[M] = G$ and $\mathsf{DAG}[M'] = G'$ and such that G' is an inflation of G. The causal model M' is said to be the* ***$G \to G'$ inflation of M****, that is, $M' = \mathsf{Inflation}_{G \to G'}[M]$, if and only if for every node A_i in G', the manner in which A_i depends causally on its parents within G' must be the same as the manner in which A depends causally on its parents within G. Noting that $A_i \sim A$ and that $\mathsf{Pa}_{G'}(A_i) \sim \mathsf{Pa}_G(A)$ (given Eq. (4)), one can formalize this condition as:*

$$\forall A_i \in \mathsf{Nodes}[G'] : \ P_{A_i | \mathsf{Pa}_{G'}(A_i)} = P_{A | \mathsf{Pa}_G(A)}, \tag{5}$$ {eq:funcd

To sum up then, the inflation of a causal model is a new causal model where (i) each given variable in the original DAG may have counterpart variables in the inflated DAG with ancestral subgraphs mirroring those of the originals, and (ii) where the manner in which variables depend causally on their parents in the inflated DAG is given by the manner in which their counterparts depend causally on their parents in the original DAG. Note that the operation of modifying a DAG and equipping the modified version with conditional probability distributions that mirror those of the original also appears in the *do calculus* and *twin networks* of Pearl [1].

FiXme Note: non-Shannon

We are now in a position to describe the key property of the inflation of a causal model, the one that makes it useful for causal inference.

Let G and G' be DAGs with $G' \in \mathsf{Inflations}[G]$, let M and M' be causal models with $M' = \mathsf{Inflation}_{G\to G'}[M]$, and let P and P' be the joint distributions over observed variables arising in models M and M' respectively. Finally, let $P_{\boldsymbol{U}}$ and $P'_{\boldsymbol{U}'}$ denote the marginal distribution of P on $\boldsymbol{U}$ and of P' on $\boldsymbol{U}'$ respectively. For any sets of nodes $\boldsymbol{U}' \subseteq \mathsf{Nodes}[G']$ and $\boldsymbol{U} \subseteq \mathsf{Nodes}[G]$,

$$P_{\boldsymbol{U}'} = P_{\boldsymbol{U}} \quad \text{if} \quad \mathsf{AnSubDAG}_{G'}\big(\boldsymbol{U}'\big) \sim \mathsf{AnSubDAG}_{G}\big(\boldsymbol{U}\big). \tag{6}$$

This follows from the fact that the probability distributions over $\boldsymbol{U}'$ and $\boldsymbol{U}$ depend only on their ancestral subgraphs and the parameters defined thereon, which by the definition of inflation are the same for $\boldsymbol{U}'$ and for $\boldsymbol{U}$. It is useful to have a name for those sets of observed nodes in the inflated DAG G' which satisfy the antecedent of Eq. (6), that is, for which one can find a corresponding set in the original DAG G with a copy-index-equivalent ancestral subgraph. We say that such subsets of the observed nodes of G' are *injectable* into G and we call them the **injectable sets**. The set of all such subsets is denoted $\mathsf{InjectableSets}[G']$,

$$\begin{aligned}&\boldsymbol{U}' \in \mathsf{InjectableSets}[G'] \subseteq \mathsf{ObservedNodes}[G'] \\ &\quad \text{iff} \quad \exists \boldsymbol{U} \subseteq \mathsf{ObservedNodes}[G] : \mathsf{AnSubDAG}_{G'}\big(\boldsymbol{U}'\big) \sim \mathsf{AnSubDAG}_{G}\big(\boldsymbol{U}\big).\end{aligned} \tag{7}$$

Similarly, those sets of observed nodes in the original DAG G which satisfy the antecedent of Eq. (6), that is, for which one can find a corresponding set in the inflated DAG G' with a copy-index-equivalent ancestral subgraph, we describe as *images of the injectable sets*, and we denote the set of these by $\mathsf{ImagesInjectableSets}[G]$.

$$\boldsymbol{U} \in \mathsf{ImagesInjectableSets}[G] \quad \text{iff} \quad \exists \boldsymbol{U}' \subseteq \mathsf{ObservedNodes}[G'] : \mathsf{AnSubDAG}_{G'}\big(\boldsymbol{U}'\big) \sim \mathsf{AnSubDAG}_{G}\big(\boldsymbol{U}\big). \tag{8}$$

Clearly, $\boldsymbol{U} \in \mathsf{ImagesInjectableSets}[G]$ iff $\exists \boldsymbol{U}' \subseteq \mathsf{InjectableSets}[G']$ such that $\boldsymbol{U} \sim \boldsymbol{U}'$.

In the inflation of the triangle scenario depicted in Fig. 3, for example, the set of observed nodes $\{A_1B_1C_1\}$ is injectable because its ancestral subgraph is equivalent up to copy-indices to the ancestral subgraph of $\{ABC\}$ in the original DAG, and the set $\{A_2C_1\}$ is injectable because its ancestral subgraph is equivalent to that of $\{AC\}$ in the original DAG. Note that it is clear that a set of nodes in the inflated DAG can only be injectable if it contains at most one copy of any node from the original DAG. Similarly, it can only be injectable if its ancestral subgraph also contains at most one copy of any node from the original DAG. Thus, in Fig. 3, $\{A_1A_2C_1\}$ is not injectable because it contains two copies of A, and $\{A_2B_1C_1\}$ is not injectable because its ancestral subgraph contains two copies of Y.

The fact that the sets $\{A_1B_1C_1\}$ and $\{A_2C_1\}$ are injectable implies, via Eq. (6), that the marginals on each of these in the inflated causal model are precisely equal to the marginals on their counterparts, $\{ABC\}$ and $\{AC\}$, in the original causal model, that is, $P'_{A_1B_1C_1} = P_{ABC}$ and $P'_{A_2C_1} = P_{AC}$.

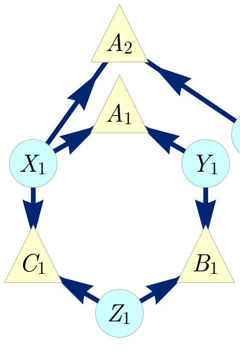

FIG. 4. A rather simple inflation of the Triangle scenario, also notably $\mathsf{AnSubDAG}_{(Fig.\ 3)}(A_1A_2B_1C_1)$.

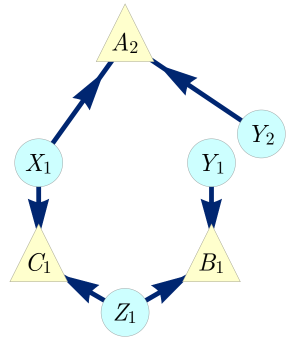

FIG. 5. An even simpler inflation of the Triangle scenario, also notably $\mathsf{AnSubDAG}_{(Fig.\ 4)}(A_2B_1C_1)$.

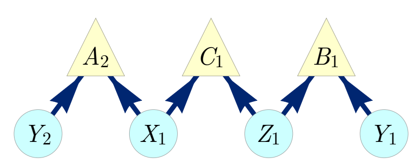

FIG. 6. Another representation of Fig. 5. Despite not containing the original scenario, this is a valid inflation per Eq. (4).

It is useful to express Eq. (6) in the language of injectable sets, namely, as

$$P'_{\boldsymbol{U}'} = P_{\boldsymbol{U}} \quad \text{if } \boldsymbol{U} \sim \boldsymbol{U}' \quad \text{and} \quad \boldsymbol{U}' \in \mathsf{InjectableSets}[G']. \tag{9}$$

{keyinfer

Finally, we can explain why inflation is relevant for deciding whether a distribution is compatible with a causal structure. For a family of marginal distributions $\{P_{\boldsymbol{U}} : \boldsymbol{U} \in \mathsf{ImagesInjectableSets}[G]$ to be compatible with G, there must be a causal model M that yields a joint distribution with this family as its marginals. Similarly, for a family of marginal distributions $\{P'_{\boldsymbol{U}'} : \boldsymbol{U}' \in \mathsf{InjectableSets}[G']$ to be compatible with G', there must be a causal model M' that yields a joint distribution with this family as its marginals. Now note that in the first problem, the only parameters of the model M that are relevant are those pertaining to nodes in the ancestral subgraph of some $\boldsymbol{U} \in \mathsf{ImagesInjectableSets}[G]$, and in the second problem, the only parameters of the model M' that are relevant are those pertaining to nodes in the ancestral subgraph of some $\boldsymbol{U}' \in \mathsf{InjectableSets}[G']$. But for a given pair $\boldsymbol{U}$ and $\boldsymbol{U}'$ such that $\boldsymbol{U} \sim \boldsymbol{U}'$, the parameters in the model M that determine the distribution on $\boldsymbol{U}$ are, by the definition of inflation, precisely equal to the parameters in the model $M' = \mathsf{Inflation}_{G \to G'}[M]$ that determine the distribution on $\boldsymbol{U}'$. Consequently, if there is a causal model M on G yielding the family $\{P_{\boldsymbol{U}} : \boldsymbol{U} \in \mathsf{ImagesInjectableSets}[G]$ then there is a model M' on G' yielding the family $\{P'_{\boldsymbol{U}'} : \boldsymbol{U}' \in \mathsf{InjectableSets}[G']$ with $P'_{\boldsymbol{U}'} = P_{\boldsymbol{U}}$.

We formalize the result as a lemma.

mainlemma **Lemma 3.** *Let G and G' be DAGs, with G' an inflation of G. Let $S' \subseteq \mathsf{InjectableSets}[G']$ be a collection of injectable sets on $\mathsf{ObservedNodes}[G']$, and let $S \subseteq \mathsf{ImagesInjectableSets}[G]$ be the images on $\mathsf{ObservedNodes}[G]$ of this collection. If the family of marginal distributions $\{P_{\boldsymbol{U}} : \boldsymbol{U} \in S\}$ is compatible with G, then the family of marginal distributions $\{P'_{\boldsymbol{U}'} : \boldsymbol{U}' \in S'\}$ satisfying $P'_{\boldsymbol{U}'} = P_{\boldsymbol{U}}$ where $U \sim U'$ is compatible with G'.*

We have thereby converted a question about compatibility with the original causal structure to one about compatibility with the inflated causal structure. If one can show that the new compatibility question is answered in the negative, one can infer that the original question is answered in the negative as well. Some simple examples serve to illustrate the idea.

[Define notational convention of $[x]$]

Example 1: **Witnessing the incompatibility of perfect three-way correlation with the Triangle scenario.**

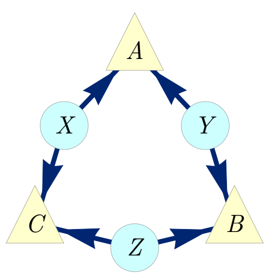

FIG. 7. The causal structure of the Triangle scenario. (Repeat of Fig. 1.) fig:TriMainDAGv2

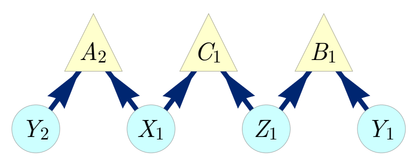

FIG. 8. A relevant inflation of the Triangle scenario. (Repeat of Fig. 6.) fig:TriDa

Consider the following causal inference problem. One is given a joint distribution over three binary variables, P_{ABC}, where the marginal on each variable is uniform and the three are perfectly correlated,

$$P_{ABC} = \frac{[000] + [111]}{2}, \quad \text{i.e.} \quad P_{ABC}(abc) = \begin{cases} \frac{1}{2} & \text{if } a{=}b{=}c, \\ 0 & \text{otherwise,} \end{cases} \tag{10}$$

{eq:ghzdi

and one would like to determine whether it is compatible with the Triangle scenario, that is, the DAG depicted in Fig. 7. Note that there are no conditional independence relations among the observed variables in this DAG, so there is no opportunity for ruling out the distribution on the grounds that it fails to reproduce the correct conditional independences.

To solve this problem, we consider the inflation of the Triangle scenario to the DAG depicted in Fig. 8. fig:TriDagSubA2B1C1v2 The injectable sets in this case include $\{A_2 C_1\}$ and $\{B_1 C_1\}$. We therefore consider the marginals on these sets.

Clearly, the given distribution is only compatible with the triangle hypothesis if the following pair of marginals of the given distribution are compatible with the triangle hypothesis:

$$P_{AC} = \frac{[00]+[11]}{2} \tag{11}$$

$$P_{BC} = \frac{[00]+[11]}{2} \tag{12}$$

But by lemma 3, this compatibility holds only if the following pair of marginals is compatible with the inflated DAG depicted in Fig. 8:

$$P_{A_2C_1} = \frac{[00]+[11]}{2} \tag{13}$$

$$P_{B_1C_1} = \frac{[00]+[11]}{2} \tag{14}$$

It is not difficult to see that the latter pair of marginals is *not* compatible with our inflated DAG. It suffices to note that the only joint distribution that exhibits perfect correlation between A_2 and C_1 and between B_1 and C_1 also exhibits perfect correlation between A_2 and B_1. But A_2 and B_1 have no common ancestors and hence must be marginally independent in the inflated DAG.

We have therefore certified that the joint distribution P_{ABC} of Eq. (10) is not compatible with the Triangle causal structure, recovering a result originally proven by Steudel and Ay [22].

Example 2: **Witnessing the incompatibility of the W-type distribution with the Triangle scenario**

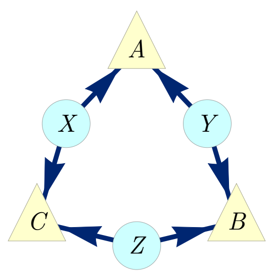

FIG. 9. The causal structure of the Triangle scenario. (Repeat of Fig. 1.)

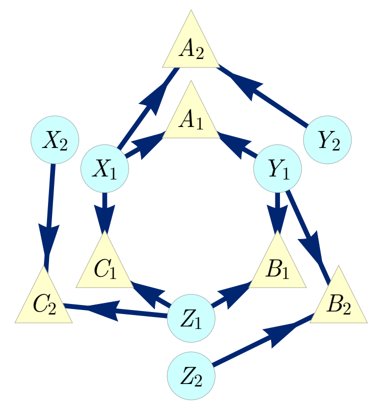

FIG. 10. A relevant inflation of the Triangle scenario. (Repeat of Fig. 3.)

Consider another causal inference problem concerning the triangle scenario, namely, that of determining whether the hypothesis of the triangle DAG is compatible with a joint distribution P_{ABC} of the form

$$P_{ABC} = \frac{[100]+[010]+[001]}{3}, \quad \text{i.e.,} \quad P_{ABC}(abc) = \begin{cases} \frac{1}{3} & \text{if } a{+}b{+}c{=}1, \\ 0 & \text{otherwise.} \end{cases} \tag{15}$$

We call this the W-type distribution[3].

To settle the compatibility question, we consider the inflated DAG of Fig. 10. The injectable sets in this case include $\{A_1B_1C_1\}$, $\{A_2C_1\}$, $\{B_2A_1\}$, $\{C_2B_1\}$, $\{A_2\}$, $\{B_2\}$ and $\{C_2\}$.

Therefore, we turn our attention to determining whether the marginals of the W-type distribution on the images of

[3] Because its correlations are reminiscent of those one obtains for the quantum state appearing in Ref. [28], and which is called the W state.

these injectable sets are compatible with the triangle hypothesis. These marginals are:

$$P_{ABC} = \frac{[100]+[010]+[001]}{3} \tag{16}$$
$$P_{AC} = \frac{[10]+[01]+[00]}{3} \tag{17}$$
$$P_{BA} = \frac{[10]+[01]+[00]}{3} \tag{18}$$
$$P_{CB} = \frac{[10]+[01]+[00]}{3} \tag{19}$$
$$P_{A} = \frac{2}{3}[0]+\frac{1}{3}[1] \tag{20}$$
$$P_{B} = \frac{2}{3}[0]+\frac{1}{3}[1] \tag{21}$$
$$P_{C} = \frac{2}{3}[0]+\frac{1}{3}[1] \tag{22}$$

But by lemma 3, this compatibility holds only if the following set of marginals is compatible with the inflated DAG depicted in Fig. 10:

$$P_{A_1B_1C_1} = \frac{[100]+[010]+[001]}{3} \tag{23}$$
$$P_{A_2C_1} = \frac{[10]+[01]+[00]}{3} \tag{24}$$
$$P_{B_2A_1} = \frac{[10]+[01]+[00]}{3} \tag{25}$$
$$P_{C_2B_1} = \frac{[10]+[01]+[00]}{3} \tag{26}$$
$$P_{A_2} = \frac{2}{3}[0]+\frac{1}{3}[1] \tag{27}$$
$$P_{B_2} = \frac{2}{3}[0]+\frac{1}{3}[1] \tag{28}$$
$$P_{C_2} = \frac{2}{3}[0]+\frac{1}{3}[1] \tag{29}$$

Eq. (24) implies that $C_1{=}0$ whenever $A_2{=}1$. Similarly, Eq. (25) implies that $A_1{=}0$ whenever $B_2{=}1$ and Eq. (26) implies that $B_1{=}0$ whenever $C_2{=}1$,

$$A_2{=}1 \implies C_1{=}0 \tag{30}$$
$$B_2{=}1 \implies A_1{=}0 \tag{31}$$
$$C_2{=}1 \implies B_1{=}0 \tag{32}$$

Our inflated DAG is such that A_2,B_2, and C_2 have no common ancestor and consequently, they are all marginally independent in any distribution consistent with this inflated DAG. This fact, together with Eqs. (27)-(29), implies that

$$\text{Sometimes}\quad A_2{=}1 \text{ and } B_2{=}1 \text{ and } C_2{=}1. \tag{33}$$

Finally, Eqs. (30)-(32) together with Eq. (33) imply

$$\text{Sometimes}\quad A_1{=}0 \text{ and } B_1{=}0 \text{ and } C_1{=}0. \tag{34}$$

This, however, contradicts Eq. (23). Consequently, the set of marginals described in Eqs. (23)-(29) are *not* compatible with the DAG of Fig. 10. By lemma 3, this implies that the set of marginals described in Eqs. (16)-(22)—and therefore the W-type distribution of which they are marginals—is not compatible with the DAG of the triangle scenario.

We have secured our verdict of incompatibility using logic reminiscent of Hardy's version of Bell's theorem [29, 30], see Sec. VI for further discussion of Hardy-type paradoxes and their applications.

To our knowledge, the fact that the W-type distribution of Eq. (15) is incompatible with the triangle DAG has not been demonstrated previously.

The incompatibility of the triangle DAG with the W-type distribution is difficult to infer from conventional causal inference techniques.

1. There are no conditional independence relations between the observable nodes of the Triangle scenario.
2. Shannon-type entropic inequalities cannot detect this distribution as not allowed by the Triangle scenario [14, 23, 24].
3. Moreover, *no* entropic inequality can witness the W-type distribution as unrealizable. Weilenmann and Colbeck [15] have constructed an inner approximation to the entropic cone of the Triangle causal structure, and the W-distribution lies inside this. In other words, a distribution with the same entropic profile as the W-type distribution *can* arise from the Triangle scenario.
4. The newly-developed method of covariance matrix causal inference due to Åberg *et al.* [16], which gives tighter constraints than entropic inequalities for the Triangle scenario, also cannot detect incompatibility with the W-type distribution.

Therefore, for this problem at least, the inflation technique appears to be more powerful.

Example 3: **Witnessing the incompatibility of PR-box correlations with the Bell scenario**

Bell's theorem concerns whether the distribution obtained in an experiment involving a pair of systems that are measured at space-like separation [6–8, 31] is compatible with a causal structure of the form of Fig. 11, as has been noted in several recent articles [6–8, 31] scenario [11 (Fig. E#2), 9 (Fig. 19), 23 (Fig. 1), 12 (Fig. 1), 32 (Fig. 2b), 33 (Fig. 2)]. Here, the observed variables are $\{A, B, X, Y\}$, and Λ is a latent variable acting as a common cause of A and B. We shall term this causal structure the *Bell scenario*.

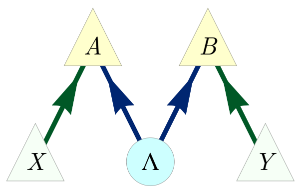

FIG. 11. The causal structure of the a bipartite Bell scenario. The local outcomes of Alice's and Bob's experimental probing is assumed to be a function of some latent common cause, in addition to their independent local experimental settings.

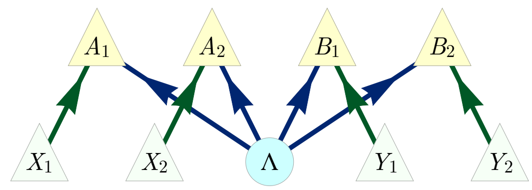

FIG. 12. An inflated DAG of the bipartite Bell scenario, where both local settings variables have been duplicated.

We consider the distribution $P_{ABXY} = P_{AB|XY} \otimes P_X \otimes P_Y$, where P_X and P_Y are arbitrary full-support distributions[4] over the binary variables X and Y, and

$$P_{AB|XY}(ab|xy) = \begin{cases} \frac{1}{2} & \text{if } \mathsf{mod}_2[a{+}b]{=}x{\cdot}y, \\ 0 & \text{otherwise.} \end{cases} \tag{35}$$

Note that the Bell scenario implies nontrivial conditional independences among the observed variables, namely, $X \perp Y$, $A \perp Y|X$, and $B \perp X|Y$ Problem: this notation has not been previously defined! and those that can be generated from these by the semi-graphoid axioms [9], and that these are all respected by this distribution. (In the context of a Bell experiment, where $\{X, A\}$ are space-like separated from $\{Y, B\}$, the conditional independences $A \perp Y|X$, and $B \perp X|Y$ encode the impossibility of sending signals faster than the speed of light.)

It is well known that this distribution is nonetheless incompatible with the Bell scenario, a fact that was first proven by Tsirelson [34] and later independently by Popescu and Rohrlich [35, 36]. The correlations described by this distribution are known to researchers in the field of quantum foundations as PR-box correlations (after Popescu and Rohrlich)[5]. Here we prove their incompatibility with the Bell scenario using the inflation technique.

We use the inflation of the Bell DAG shown in Fig. 12.

We begin by noting that $\{A_1B_1X_1Y_1\}$, $\{A_2B_1X_2Y_1\}$, $\{A_1B_2X_1Y_2\}$, $\{A_2B_2X_2Y_2\}$, $\{X_1\}$, $\{X_2\}$, $\{Y_1\}$, and $\{Y_2\}$ are

[4] In the literature on the Bell scenario, these variables are known as "settings". Generally, we may think of endogenous observable variables as settings, coloring them light green in the DAG figures. Settings variables are natural candidates for conditioning on.

[5] They are of interest because they represent a manner in which experimental correlations could deviate from the predictions of quantum theory while still being consistent with relativity.

all injectable sets. By lemma 3, it follows that

$$P_{A_1B_1X_1Y_1} = P_{ABXY} \tag{36}$$
$$P_{A_2B_1X_2Y_1} = P_{ABXY} \tag{37}$$
$$P_{A_1B_2X_1Y_2} = P_{ABXY} \tag{38}$$
$$P_{A_2B_2X_2Y_2} = P_{ABXY} \tag{39}$$
$$P_{X_1} = P_X \tag{40}$$
$$P_{X_2} = P_X \tag{41}$$
$$P_{Y_1} = P_Y \tag{42}$$
$$P_{Y_2} = P_Y. \tag{43}$$

Using the definition of conditional probability, we infer that

$$P_{A_1B_1|X_1Y_1} = P_{AB|XY} \tag{44}$$
$$P_{A_2B_1|X_2Y_1} = P_{AB|XY} \tag{45}$$
$$P_{A_1B_2|X_1Y_2} = P_{AB|XY} \tag{46}$$
$$P_{A_2B_2|X_2Y_2} = P_{AB|XY}. \tag{47}$$

Because $\{X_1\}$, $\{X_2\}$, $\{Y_1\}$, and $\{Y_2\}$ have no common ancestor, these variables must be marginally independent in any distribution compatible with the inflated DAG, that is, we have $P_{X_1X_2Y_1Y_2} = P_{X_1}P_{X_2}P_{Y_1}P_{Y_2}$ in any such distribution. Given the assumption that the distributions P_X and P_Y are full support, it follows from Eqs. (40)-(43) that

$$\text{Sometimes} \quad X_1{=}0, X_2{=}1, Y_1{=}0, Y_2{=}1. \tag{48}$$

Next, from Eqs. (44)-(47) together with the definition of PR box correlations, Eq. (35), we conclude that

$$X_1{=}0, Y_1{=}0 \implies A_1{=}B_1, \tag{49}$$
$$X_1{=}0, Y_2{=}1 \implies A_1{=}B_2, \tag{50}$$
$$X_2{=}1, Y_1{=}0 \implies A_2{=}B_1, \tag{51}$$
$$X_2{=}1, Y_2{=}1 \implies A_2 \neq B_2. \tag{52}$$

Combining Eq. (48) with Eqs, (49)-(52), we obtain

$$\text{Sometimes} \quad A_1{=}B_1, A_1{=}B_2, A_2{=}B_1, A_2 \neq B_2. \tag{53}$$

No values of A_1, A_2, B_1, B_2 can jointly satisfy these conditions—the first three entail perfect correlation between A_2 and B_2, while the fourth entails perfect anit-correlation—so we have reached a contradiction.

The mathematical structure of this proof parallels that of standard proofs of the incompatibility of PR-box correlations with the Bell DAG. Standard proofs focus on a set of variables $\{A_0, A_1, B_0, B_1\}$ where A_x is the value of A when $X = x$ and B_y is the value of B when $Y = y$, and note that the distribution $\sum_\lambda P(A_0|\lambda)P(A_1|\lambda)P(B_0|\lambda)P(B_1|\lambda)P(\lambda)$ is a joint distribution over $\{A_0, A_1, B_0, B_1\}$ for which the marginals on pairs $\{A_0, B_0\}$, $\{A_0, B_1\}$, $\{A_1, B_0\}$ and $\{A_1, B_1\}$ are those predicted by the Bell DAG. Finally, the existence of such a joint distribution rules out the possibility of having $A_1{=}B_1$, $A_1{=}B_2$, $A_2{=}B_1$ but $A_2 \neq B_2$ and therefore shows that the PR Box correlations are incompatible with the Bell DAG [37, 38].

IV. DERIVING CAUSAL COMPATIBILITY INEQUALITIES USING THE INFLATION TECHNIQUE

As noted in the introduction, the inflation technique can be used not only to witness the incompatibility of a given distribution with a given causal structure, but it can also be used to derive necessary conditions that a distribution must satisfy to be compatible with the given causal structure. When these necessary conditions are expressed as inequalities, we will refer to them as *causal compatibility inequalities*. Formally, we have:

Definition 4. *Consider a causal structure G and a set of the observed nodes thereon, $S \subseteq \mathsf{ObservedNodes}[G]$. Let I_S denote an inequality that is evaluated on a family of marginal distributions $\{P_{\boldsymbol{U}} : \boldsymbol{U} \in S\}$. The inequality I_S is* *termed a* **causal compatibility inequality for the causal structure G** *whenever it is satisfied by every family of distributions $\{P_{\boldsymbol{U}} : \boldsymbol{U} \in S\}$ that is compatible with the causal structure G.*

Note that violation of a causal compatibility inequality witnesses the incompatibility of a distribution with the associated causal structure, but the inequality being satisfied does not guarantee that the distribution is compatible with the causal structure. This is the sense in which it merely provides a *necessary* condition on compatibility.

The inflation technique is useful for deriving causal compatibility inequalities because of the following consequence of lemma 3:

Corollary 4.1. *Let G and G' be DAGs, with G' an inflation of G. Let $S' \subseteq \mathsf{InjectableSets}[G']$ be a family of injectable sets on $\mathsf{ObservedNodes}[G']$, and let $S \subseteq \mathsf{ImagesInjectableSets}[G]$ be the images on $\mathsf{ObservedNodes}[G]$ of this family. Let $I_{S'}$ (respectively I_S) be an inequality that is evaluated on the marginal distributions over the elements of S' (respectively S), that is, $\{P'_{\boldsymbol{U}'} : \boldsymbol{U}' \in S'\}$ (respectively $\{P_{\boldsymbol{U}} : \boldsymbol{U} \in S\}$). Suppose that I_S is obtained from $I_{S'}$ as follows: In the functional form of $I_{S'}$, replace $P'_{\boldsymbol{U}'}$ with $P_{\boldsymbol{U}}$ for the U such that $U \sim U'$. In this case, if $I_{S'}$ is a causal compatibility inequality for the causal structure G' then I_S is a causal compatibility inequality for the causal structure G*

The proof is as follows. Suppose that the family $\{P_{\boldsymbol{U}} : \boldsymbol{U} \in S\}$ is compatible with G. By lemma 3, it follows that the family $\{P'_{\boldsymbol{U}'} : \boldsymbol{U}' \in S'\}$ where $P'_{\boldsymbol{U}'} := P_{\boldsymbol{U}}$ for $U \sim U'$ is compatible with G'. Given that $I_{S'}$ is assumed to be a causal compatibility inequality for G', it follows that $\{P'_{\boldsymbol{U}'} : \boldsymbol{U}' \in S'\}$ satisfies $I_{S'}$. But I_S evaluated on $\{P_{\boldsymbol{U}} : \boldsymbol{U} \in S\}$ is equal to $I'(S')$ evaluated on $\{P'_{\boldsymbol{U}'} : \boldsymbol{U}' \in S'\}$, by the definition of I_S, and therefore because $\{P'_{\boldsymbol{U}'} : \boldsymbol{U}' \in S'\}$ satisfies $I_{S'}$ it follows that $\{P_{\boldsymbol{U}} : \boldsymbol{U} \in S\}$ satisfies I_S. This implication holds for *every* $\{P_{\boldsymbol{U}} : \boldsymbol{U} \in S\}$ that is compatible with G. Consequently, I_S is a causal compatibility inequality for G.

We now present some simple examples of causal compatibility inequalities for the Triangle scenario that one can derive from the inflation technique.

Some terminology and notation will facilitate the description of these examples. We refer to a pair of nodes which do not share any common ancestor as being **ancestrally independent**, for which we invent the notation $X \Lsh\emptyset\Rsh Y$. Generalizing to sets, $\boldsymbol{U} \Lsh\emptyset\Rsh \boldsymbol{V}$ indicates that no node in $\boldsymbol{U}$ shares a common ancestor with any node in $\boldsymbol{V}$,

$$\boldsymbol{U} \Lsh\emptyset\Rsh \boldsymbol{V} \quad \text{iff} \quad \mathsf{An}(\boldsymbol{U}) \cap \mathsf{An}(\boldsymbol{V}) = \emptyset. \tag{54}$$

Furthermore, the notation $\boldsymbol{U} \Lsh\emptyset\Rsh \boldsymbol{V} \Lsh\emptyset\Rsh \boldsymbol{W}$ should be understood as indicating that $\boldsymbol{U} \Lsh\emptyset\Rsh \boldsymbol{V}$ and $\boldsymbol{V} \Lsh\emptyset\Rsh \boldsymbol{W}$ and $\boldsymbol{U} \Lsh\emptyset\Rsh \boldsymbol{W}$. Ancestral independence is equivalent to d-separation by the empty set [1–4].

Example of a causal compatibility inequality expressed in terms of *correlators*

As in example 1 of the previous section, consider the inflation of the triangle scenario to the DAG depicted in Fig. 8. The injectable sets we make use of here are $\{A_2C_1\}$, $\{B_1C_1\}$, $\{A_2\}$, and $\{B_1\}$.

From corollary 4.1, any causal compatibility inequality for the inflated DAG that can evaluated on the marginal distributions for $\{A_2C_1\}$, $\{B_1C_1\}$, $\{A_2\}$, and $\{B_1\}$ will yield a causal compatibility inequality for the original DAG that can evaluated on the marginal distributions for $\{AC\}$, $\{BC\}$, $\{A\}$, and $\{B\}$. We begin, therefore by identifying a simple example of a causal compatibility inequality for the inflated DAG that is of this sort.

In our example, all of the observed variables are binary. For technical convenience, we assume that these take values in the set $\{-1, +1\}$, rather than taking values in the set $\{0, 1\}$ as was presumed in the last section.

We begin by noting that for *any* distribution on three binary variables $\{A_2B_1C_1\}$, that is, *regardless* of the causal structure in which they are embedded, the marginals on $\{A_2C_1\}$, $\{B_1C_1\}$ and $\{A_2B_1\}$ satisfy the following inequality [39–43],

$$\langle A_2C_1\rangle + \langle B_2C_1\rangle - \langle A_2B_1\rangle \leq 1. \tag{55}$$

This is an example of a constraint on pairwise correlators that arises from the presumption that they are consistent with a joint distribution. (The problem of deriving such constraints is the so-called *marginals problem*, dicussed in detail in Sec. V.)

But the DAG of Fig. 8 shows that A_2 and B_1 have no common ancestor and consequently any distribution compatible with the DAG must make A_2 and B_1 marginally independent. In terms of correlators, this can be expressed as

$$A_2 \Lsh\emptyset\Rsh B_1 \implies \langle A_2B_1\rangle = \langle A_2\rangle\langle B_1\rangle. \tag{56}$$

Substituting the latter equality into Eq. (55), we have

$$\langle A_2C_1\rangle + \langle B_2C_1\rangle \leq 1 + \langle A_2\rangle\langle B_1\rangle. \tag{57}$$

This is an example of a nontrivial causal compatibility inequality for the DAG of Fig. 8.

Finally, by corollary 4.1 and the fact that the DAG of Fig. 8 is an inflation of the Triangle scenario, we infer that

$$\langle AC\rangle + \langle BC\rangle \leq 1 + \langle A\rangle\langle B\rangle, \tag{58}$$

is a causal compatibility inequality for the Triangle scenario. This inequality expresses the fact that as long as A and B are not completely biased, there is a nontrivial tradeoff between the strength of AC correlations and the strength of BC correlations.

Given the symmetry of the triangle scenario under permutations of A, B and C, it is clear that the image of inequality (58) under any such permutation is also a valid causal compatibility inequality for the triangle scenario. Together, these inequalities imply monogamy[6] of correlations in the triangle scenario: if any two observed variables are perfectly correlated with unbiased marginals then they are both uncorrelated with the third.

Example of a causal compatibility inequality expressed in terms of *entropic quantities*

One way to derive constraints that are independent of the cardinality of the observed variables is to express these in terms of the mutual information between observed variables rather than in terms of correlators. The inflation technique can also be applied in such cases. To see how this works in the case of the triangle scenario, consider again the inflated DAG of Fig. 8.

One can follow the same logic as in the preceding example, but starting from a different constraint on marginals. For any distribution on three variables $\{A_2B_1C_1\}$ of arbitrary cardinality (again, regardless of the causal structure in which they are embedded), the marginals on $\{A_2C_1\}$, $\{B_1C_1\}$ and $\{A_2B_1\}$ satisfy the following inequality

$$I(A_2 : C_1) + I(C_1 : B_1) - I(A_2 : B_1) \leq H(B_1), \tag{59}$$

where $H(X)$ denotes the Shannon entropy of the distribution over X, and $I(X : Y)$ denotes the mutual information between X and Y for the marginal on X and Y. This was shown in Ref. [24].

The fact that A_2 and B_1 have no common ancestor in the inflated DAG implies that in any distribution that is compatible with the inflated DAG, A_2 and B_1 are marginally independent. This is expressed entropically as the vanishing of their mutual information,

$$A_2 \Lsh\emptyset\Rsh B_1 \implies I(A_2 : B_1) = 0. \tag{60}$$

Substituting the latter equality into Eq. (59), we have

$$I(A_2 : C_1) + I(C_1 : B_1) \leq H(B_1). \tag{61}$$

This is another example of a nontrivial causal compatibility inequality for the DAG of Fig. 8.

By corollary 4.1, it follows that

$$I(A : C) + I(C : B) \leq H(B), \tag{62}$$

is also a causal compatibility inequality for the Triangle scenario. This inequality was originally derived in Ref. [10]. Our rederivation in terms of inflation coincides with the proof technique found in Henson *et al.* [11].

Example of a causal compatibility inequality expressed in terms of *probabilities* of certain joint valuations

Consider the inflation of the triangle scenario depicted in Fig. 10, and consider the injectable sets$\{A_1B_1C_1\}$, $\{A_1B_2\}$, $\{B_1C_2\}$, $\{A_1, C_2\}$, $\{A_2\}$, $\{B_2\}$, and $\{C_2\}$. We here derive a causal compatibility inequality under the assumption that the observed variables are all binary, and we adopt the convention that they take values in the set $\{0, 1\}$.

We begin by noting that the following is a constraint that holds for any joint distribution over $\{A_1B_1C_1A_2B_2C_2\}$, regardless of the causal structure,

$$P_{A_2B_2C_2}(111) \leq P_{A_1B_1C_1}(000) + P_{A_1B_2C_2}(111) + P_{B_1C_2A_2}(111) + P_{A_2C_1B_2}(111). \tag{63}$$

To prove this claim, it suffices to check that the inequality holds for each of the 2^6 deterministic assignments of values to $\{A_1B_1C_1A_2B_2C_2\}$, from which the general case follows by linearity. A more intuitive proof will be provided in Sec. VI.

---

[6] We are here using the term "monogamy" in the same sort of manner in which it is used in the context of entanglement theory [provide references]

Next, we note that certain sets of variables have no common ancestors with other sets of variables in the inflated DAG, and we infer the marginal independence of the two sets, expressed now as a factorization of a joint probability distribution,

$$
\begin{aligned}
A_1B_2 \Lsh\emptyset\Rsh C_2 &\implies P_{A_1B_2C_2} = P_{A_1B_2} \otimes P_{C_2},\\
B_1C_2 \Lsh\emptyset\Rsh A_2 &\implies P_{B_1C_2A_2} = P_{B_1C_2} \otimes P_{A_2},\\
A_2C_1 \Lsh\emptyset\Rsh B_2 &\implies P_{A_2C_1B_2} = P_{A_2C_1} \otimes P_{B_2},\\
A_2 \Lsh\emptyset\Rsh B_2 \Lsh\emptyset\Rsh C_2 &\implies P_{A_2B_2C_2} = P_{A_2} \otimes P_{B_2} \otimes P_{C_2}.
\end{aligned}
\tag{64}
$$
{eq:tri22

eq:FritzF3raw
Substituting these equalities into Eq. (63), we obtain the polynomial inequality

$$
P_{A_2}(1)P_{B_2}(1)P_{C_2}(1) \leq P_{A_1B_1C_1}(000) + P_{A_1B_2}(11)P_{C_2}(1) + P_{B_1C_2}(11)P_{A_2}(1) + P_{A_2C_1}(11)P_{B_2}(1). \tag{65}
$$

This, therefore, is a causal compatibility inequality for the DAG of Fig. 10.

maincorollary
Finally, by corollary 4.1, we infer that

$$
P_A(1)P_B(1)P_C(1) \leq P_{ABC}(000) + P_{AB}(11)P_C(1) + P_{BC}(11)P_A(1) + P_{AC}(11)P_B(1) \tag{66}
$$
{eq:Fritz

is a causal compatibility inequality for the Triangle scenario.

What is distinctive about this inequality is that—through the presence of the term $P_{ABC}(000)$—it takes into account genuine three-way correlations. This inequality is strong enough to demonstrate the incompatibility of the W-type distribution of Eq. (15) with the Triangle scenario: it suffices to note that for this distribution, the right-hand side of the inequality vanishes while the left-hand side does not.

Of the known techniques for witnessing the incompatibility of a distribution with a DAG or deriving necessary conditions for compatibility, the most straightforward is to consider the constraints implied by ancestral independences among the observed variables of the DAG. The constraints derived in the last two sections have all made use of this basic technique, but at the level of the inflated DAG rather than the original DAG. The constraints that one thereby infers for the original DAG reflect facts about its causal structure that cannot be expressed in terms of ancestral independences among its observed variables. The inflation technique manages to expose these facts in the ancestral independences among observed variables of the inflated DAG.

In the rest of this article, we shall continue to rely only on the ancestral independences among observed variables within the inflated DAG to infer compatibility constraints on the original DAG. Nonetheless, it is possible that the inflation technique can also amplify the power of *other* techniques for deriving compatibility constraints, in particular, techniques that do not merely consider ancestral independences among the observed variables. This question, however, is left for future research.

V. DERIVING POLYNOMIAL INEQUALITIES SYSTEMATICALLY

sec:ineqs

In all of the examples from the previous section, the inequality with which one starts—a constraint upon marginals that is independent of the causal structure—involves sets of observed variables that are not all injectable. Each of these sets can, however, be partitioned into disjoint subsets each of which *is* injectable where the partitioning represents ancestral independence in the inflated DAG. For instance, in the first example from the previous section, the set $\{A_2B_1\}$ can be partitioned into the singleton sets $\{A_2\}$ and $\{B_1\}$ which are ancestrally independent and each of which is injectable. It is useful to have a name for such sets of observed variables: we will call them **pre-injectable**. We begin by defining this notion carefully before describing our general inflation technique.

A set of nodes $\boldsymbol{U}'$ in the inflated DAG G' will be called **pre-injectable** whenever it is a union of injectable sets with disjoint ancestries,

$$
\boldsymbol{U}' \in \mathsf{PreInjectableSets}[G'/_G] \quad \text{iff} \quad \exists\{\boldsymbol{U}_i \in \mathsf{InjectableSets}[G']\} \quad \text{s.t.} \quad \boldsymbol{U}' = \bigcup_i \boldsymbol{U}_i \quad \text{and} \quad \forall i \neq j : \boldsymbol{U}_i \Lsh\emptyset\Rsh \boldsymbol{U}_j. \tag{67}
$$
{eq:defpr

Note that every injectable set is a trivial example of a pre-injectable set. A pre-injectable set is said to be maximal if it is not a subset of a larger pre-injectable set.

Because ancestral independence in the DAG implies statistical independence for any probability distribution compatible with the DAG, it follows that if $\boldsymbol{U}'$ is a pre-injectable set and $\boldsymbol{U}_1, \boldsymbol{U}_2, \ldots, \boldsymbol{U}_n$ are the ancestrally independent components of $\boldsymbol{U}'$, then

$$P'(\boldsymbol{U}') = P'(\boldsymbol{U}_1)P'(\boldsymbol{U}_2)\cdots P'(\boldsymbol{U}_n). \tag{68}$$

The situation, therefore, is this: for any constraints that one can derive for the marginals on the pre-injectable sets based on the existence of a joint distribution (and hence without reference to the causal structure), one can infer constraints that *do* refer to the causal structure by substituting within these constraints equalities of the form of Eq. (68). Thus, an inequality derived from the marginal problem, after applying the equalities of Eq. (68), becomes a causal compatibility inequality for the inflated DAG.

The latter inequality can then be converted into a causal compatibility inequality for the original DAG using corollary 4.1.

T: A lot of the things in this section *also* need to be done when checking for satisfiability only, such as identifying the pre-injectable sets and writing down all the constraints.

This section considers the problem of how to derive these sorts of causal compatibility inequalities for a generic causal structure.

We limit our attention to deriving causal compatibility inequalities expressed in terms of probabilities. Note, however, that the inflation technique can also be used to derive inequalities expressed in terms of entropies, as our second example from the previous section demonstrated. Indeed, we show in Appendix D that the inflation technique implies the core lemma for deriving non-Shannon-type inequalities.

To obtain a complete solution of the marginal problem, one must determine all the facets of the **marginal polytope**, for which we discuss algorithms in Appendix A. The causal compatibility inequalities one thereby obtains are polynomial in the probabilities. The rest of this section describes the steps for deriving all such inequalities.

Computing all the facets of the marginal polytope is computationally costly. It is therefore useful to also consider relaxations of the marginal problem that are less computationally burdensome. One such relaxation is to merely derive a collection of linear inequalities which bound the marginal polytope. We describe one such approach based on possibilistic Hardy-type paradoxes, which we connect to the hypergraph transversal problem. This strategy requires the least computational effort, but is limited in that it only yields polynomial inequalities of a very particular form. We describe this approach in Sec. VI.

Preliminary to every strategy, however, is the identification of the pre-injectable sets, so we begin with this problem.

Identifying the Pre-Injectable Sets

To identify the pre-injectable sets of an inflated DAG, we must first identify the *injectable* sets. This problem can be reduced to identifying the injectable pairs, because it is the case that if all of the pairs in a set of nodes are injectable, then so too is the set itself. The latter claim is proven as follows. Let $\varphi : G' \to G$ be the projection map from the inflated DAG G' to the original DAG G, corresponding to removing the copy-indices. Then φ has the characteristic feature that it takes edges to edges: if $A \to B$ in G', then also $\varphi(A) \to \varphi(B)$ in G. Conversely, if $\varphi(A) \to \varphi(B)$ in G then also $A \to B$ in G'; this follows from the assumption that G' is an inflation of G. Note that a set of observed variables $\boldsymbol{U} \subset G'$ is injectable if and only if the restriction of φ to the ancestors of $\boldsymbol{U}$ is an injective map. But now injectivity of a map means precisely that no two different elements of the domain get mapped to the same element of the codomain. So if $\boldsymbol{U}$ is injectable, then so is each of its two-element subsets; conversely, if $\boldsymbol{U}$ is not injectable, then φ maps two nodes among the ancestors of $\boldsymbol{U}$ to the same node, which means that there are two nodes in the ancestry that differ only by copy index. Each of these two nodes must be an ancestor of at least some node in $\boldsymbol{U}$; if one chooses two such descendants, then one gets a two-element subset of $\boldsymbol{U}$ such that φ is not injective on the ancestry of that subset, and therefore this two-element set of observed nodes is not injectable.

To enumerate the injectable sets, it is useful to encode certain features of the inflated DAG in an undirected graph which we call the **injection graph**. The nodes of the injection graph are the observed nodes of the inflated DAG, and a pair of nodes A_i and B_j are connected by an edge in the injection graph if the pair $\{A_iB_j\}$ is injectable. Recalling that a "clique" is a subset of nodes such that every node in the subset is connected by an edge to every other node in the subset, it follows from the property noted above that the injectable sets are precisely the cliques of the injection graph. The inflation technique requires one to enumerate all of the injectable sets, not just the maximal ones. Consequently, all of the nonempty cliques, not just the maximal cliques, are of interest. For example, applying these prescriptions to the inflated DAG in Fig. 3 results in the injection graph of Fig. 13.

Given a characerization of the injectable sets, the pre-injectable sets can be described in terms of another graphical construction that we call the **ancestral independence graph**. The nodes of the independence graph are the injectable sets of the inflated DAG, and two nodes are connected by an edge if the associated injectable sets are ancestrally independent in the inflated DAG. It follows, therefore, that the pre-injectable sets correspond to the cliques of the ancestral independence graph, specifically, the union of all the injectable sets associated to the nodes of the clique. For the inflation technique, it is sufficient to consider the maximal pre-injectable sets. For the inflated DAG in Fig. 3, the ancestral independence graph is depicted in Fig. ??.

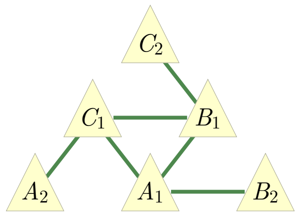

FIG. 13. The auxiliary injection graph corresponding to the inflated DAG in Fig. 3, wherein a pair of nodes are adjacent iff they are pairwise injectable.

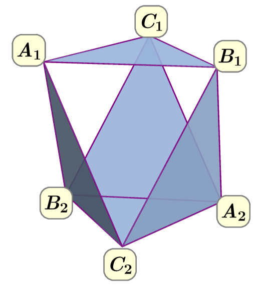

FIG. 14. The simplicial complex of pre-injectable sets for the inflation of Fig. 3. The 5 faces correspond to the maximal pre-injectable sets, namely $\{A_1B_1C_1\}$, $\{A_1B_2C_2\}$, $\{A_2B_1C_2\}$, $\{A_2B_2C_1\}$ and $\{A_2B_2C_2\}$.

From Figs. 13 and ??, we easily infer the injectable sets and the maximal pre-injectable sets, as well as the partition of the maximal pre-injectable sets into ancestrally independent subsets, for the inflated DAG in Fig. 3 to be:

$$\underbrace{\begin{matrix}\{A_1\},\ \{B_1\},\ \{C_1\},\\ \{A_2\},\ \{B_2\},\ \{C_2\},\\ \{A_1B_1\},\ \{A_1C_1\},\ \{B_1C_1\},\\ \{A_1B_2\}.\ \{A_2C_1\},\ \{B_1C_2\},\\ \{A_1B_1C_1\}\end{matrix}}_{\text{injectable sets}} \qquad \underbrace{\begin{matrix}\{A_1B_1C_1\}\\ \{A_1B_2C_2\}\\ \{B_1C_2A_2\}\\ \{C_1A_2B_2\}\\ \{A_2B_2C_2\}\end{matrix}}_{\substack{\text{maximal}\\ \text{pre-injectable sets}}} \qquad \underbrace{\begin{matrix}\{A_1B_2\} \perp \{C_2\}\\ \{B_1C_2\} \perp \{A_2\}\\ \{C_1A_2\} \perp \{B_2\}\\ \{A_2\} \perp \{B_2\} \perp \{C_2\}\end{matrix}}_{\substack{\text{relevant}\\ \text{ancestral independences}}} \tag{69}$$

Using the ancestral independence relations, the marginal distributions for the maximal pre-injectable sets factorize in the manner described by the right-hand side of Eq. (64). Having described how to identify the pre-injectable sets and what factorization relations are implied by ancestral independences in the causal structure, we now turn to a discussion of how to obtain constraints on the marginal distributions over the pre-injectable sets,

Constraining Distributions over Pre-Injectable Sets via the Marginals Problem

For a given family of probability distributions, each defined on a subset of the variables, determining whether there exists a joint probabiity distribution over the full set of variables from which all of these can be obtained as marginal distributions is known as the *marginals problem*. For some of its history and for further references, see [24]; for a more recent account using the language of presheaves, see [44].

To specify such a problem, one must specify the full set of variables to be considered, denoted $\boldsymbol{X}$, together with a family of subsets of $\boldsymbol{X}$, denoted $(\boldsymbol{U}_1, \ldots, \boldsymbol{U}_n)$ and called **contexts**. A family of contexts can be visualized through the simplicial complex that they generate, as the example in Fig. 14 illustrates. Every joint distribution $P_{\boldsymbol{X}}$ defines a family of marginal distributions, $(P_{\boldsymbol{U}_1}, \ldots, P_{\boldsymbol{U}_n})$ through marginalization, $P_{\boldsymbol{U}_i} := \sum_{\boldsymbol{X}\setminus\boldsymbol{U}_i} P_{\boldsymbol{X}}$. A *marginals problem* concerns the converse inference. What is given is a family of distributions $(P_{\boldsymbol{U}_1}, \ldots, P_{\boldsymbol{U}_n})$, and what is sought are the conditions under which one can find a joint distribution $\hat{P}_{\boldsymbol{X}}$ which has all the given distributions as marginals, that is, which has $\hat{P}_{\boldsymbol{U}_i} = P_{\boldsymbol{U}_i}$ for all i, where $\hat{P}_{\boldsymbol{U}_i} := \sum_{\boldsymbol{X}\setminus\boldsymbol{U}_i} \hat{P}_{\boldsymbol{X}}$.

There is a simple necessary condition: in order for $\hat{P}_{\boldsymbol{X}}$ to exist, the marginals clearly must be consistent, in the sense that marginalizing $P_{\boldsymbol{U}_i}$ and $P_{\boldsymbol{U}_j}$ to the variables in $\boldsymbol{U}_i \cap \boldsymbol{U}_j$ results in the same distribution. As we have already seen in the previous section, in many cases this is not sufficient[7]. So what are the necessary and sufficient conditions? To answer this question, it helps to realize two things:

- Every joint distribution $P_{\boldsymbol{X}}$ is a convex combination of deterministic assignments of values to all variables (delta distributions), and conversely.
- The map $P_{\boldsymbol{X}} \to (P_{\boldsymbol{U}_1}, \ldots, P_{\boldsymbol{U}_n})$ is linear.

Hence the image of the map $P_{\boldsymbol{X}} \to (P_{\boldsymbol{U}_1}, \ldots, P_{\boldsymbol{U}_n})$ is exactly the convex hull of the deterministic assignments of values at the level of marginals. Since there are only finitely many such deterministic assignments, this convex hull is a

[7] Depending on how the contexts intersect with one another, this *may* be sufficient. A criterion for when this occurs has been found by Vorob'ev [45].

polytope called the **marginal polytope** [46]. Together with the above set of equations, the facet inequalities of the marginal polytopes form necessary and sufficient conditions for the marginal problem to have a solution.

Thus solving the marginal problem is an instance of a facet enumeration problem, or equivalently a linear quantifier elimination problem; Appendix A gives an overview of how to solve this in practice. Given a facet of the marginal polytope—or any other linear inequality that bounds it—we can construct a polynomial inequality for our original causal inference problem by plugging in the factorization relations of Lemma 3. Doing the same with the equations of coinciding submarginals shows that these are trivially satisfied, and thus it is only the inequalities that are of interest to us.

As an example, here's how the marginal problem can be phrased as a linear quantifier elimination problem in the case of the five three-variable marginal distributions corresponding to the pre-injectable sets in **??**. The putative joint distribution is nonnegative,

$$\forall a_1a_2b_1b_2c_1c_2 : \ P_{A_1A_2B_1B_2C_1C_2}(a_1a_2b_1b_2c_1c_2) \geq 0, \tag{70}$$

and is required to reproduce the given marginal distributions via

$$\begin{aligned}
\forall a_1b_1c_1 &: \ P_{A_1B_1C_1}(a_1b_1c_1) = \sum\nolimits_{a_2b_2b_2} P_{A_1A_2B_1B_2C_1C_2}(a_1a_2b_1b_2c_1c_2),\\
\forall a_1b_2c_2 &: \ P_{A_2B_2C_2}(a_1b_2c_2) = \sum\nolimits_{a_2b_1c_1} P_{A_1A_2B_1B_2C_1C_2}(a_1a_2b_1b_2c_1c_2),\\
\forall a_2b_1c_2 &: \ P_{A_2B_1C_2}(a_2b_1c_2) = \sum\nolimits_{a_1b_2c_1} P_{A_1A_2B_1B_2C_1C_2}(a_1a_2b_1b_2c_1c_2),\\
\forall a_2b_2c_1 &: \ P_{A_2B_2C_1}(a_2b_2c_1) = \sum\nolimits_{a_1b_1c_2} P_{A_1A_2B_1B_2C_1C_2}(a_1a_2b_1b_2c_1c_2),\\
\forall a_2b_2c_2 &: \ P_{A_2B_2C_2}(a_2b_2c_2) = \sum\nolimits_{a_1b_1c_1} P_{A_1A_2B_1B_2C_1C_2}(a_1a_2b_1b_2c_1c_2).
\end{aligned} \tag{71}$$

For example in the case of binary variables, we therefore have 64 inequalities and 40 equalities, although the latter are not all independent. Doing the facet enumeration means eliminating 64 unknowns from those inequalities and equalities, namely any $P_{A_1A_2B_1B_2C_1C_2}(\_\_\_\_\_\_)$, and to thereby compute the inequalities that constrain the marginal probabilities.

Linear quantifier elimination is already widely used in causal inference to derive entropic inequalities [14, 23, 24]. In that task, however, the quantifiers being eliminated are those entropies which refer to hidden variables. By contrast, the probabilities we consider here are exclusively in terms of observable variables right from the very start (although not in terms of the original observables). The unknowns we eliminate are the not-pre-injectable joint probabilities, which are, at least on first look, quite different from probabilities involving hidden variables; Sec. VII will partly elucidate the relation.

Note that the marginal problem can be solved by computing *either* a convex hull *or* by eliminating quantifiers from linear inequalities. The derivation of entropic inequalities, by contrast, is strictly a linear quantifier elimination task, and cannot be recast as a convex hull problem. As such, while convex hull enumerations tools *are* useful to derive polynomial inequalities via the inflation technique, they are *not* available for the derivation of entropic inequalities; see Appendix A for further details.

VI. DERIVING HARDY-TYPE CONSTRAINTS FOR THE MARGINAL PROBLEM

In the literature on Bell inequalities, it has been noticed that incompatibility with the Bell scenario DAG can sometimes be witnessed by only looking at which probabilities are zero and which ones are nonzero. In other words, instead of considering the *probability* of a composite outcome, the inconsistency of some marginal distributions can be evident from considering only the *possibility* or *impossibility* of each composite outcome. This is due to Hardy [29], and hence such **possibilistic constraints** are also known as **Hardy-type paradoxes**, in the sense that the "paradox" is said to occur whenever the constraint is violated. For more background on Hardy's paradoxes, see Refs. [37, 50–53]; a partial classification of Hardy-type paradoxes in Bell scenarios can be found in Ref. [30]

The usual presentation of a Hardy-type paradox takes the following form: Even though events $E_1, \ldots, E_n$ never occur (are not possible), some other event E_0 *does* occur sometimes (is possible). However, the logical relations between these events are such that whenever E_0 occurs, then also at least one of $E_1, \ldots, E_n$ occurs, and this is in contradiction with the previous statement.

The following example illustrates a Hardy-type paradox. Suppose a plague has suddenly wiped out a population of rats. Three kinds of autopsies are performed on different samples of the dead rats. Autopsies checking specifically for heart and brain disease find that every rat suffered from at least one of those conditions i.e. the event [Brain=☺, Heart=☺]

is found to be *not possible*. In a slightly different vein, suppose further that autopsies specifically checking for brain and lung diseases find that every dead rat afflicted by brain disease also suffered from lungs disease, i.e. the event [Brain=☹, Lungs=☺] is not possible. Logic (and the absence of sampling bias) then dictates that an autopsy for heart and lung disease will never find both heart and lungs simultaneously healthy. If some medical examiner checking rats heart and lung conditions then finds that *it is possible* for a rat to have [Heart=☺, Lungs=☺], this would be considered an occurrence of a Hardy-type paradox.

The possibilistic constraint which is equivalent to a Hardy-type paradox is as follows,

$$\mathsf{Never}[E_1] \wedge \ldots \wedge \mathsf{Never}[E_n] \implies \mathsf{Never}[E_0], \tag{72}$$

although it can be expressed more fundamentally in conjuctive form, i.e.

$$[E_0] \implies [E_1] \vee \ldots \vee [E_n]. \tag{73}$$

Any possibilistic constraint can be immediately translated into a stronger probabilistic one, as noted by Mansfield2012 Mansfield and Fritz [30]. The probabilistic variant states than *whenever* the event E_0 occurs than at least one of the events $E_1..E_N$ should also occur. Applying the union bound to the probability of the right-hand side we obtain

$$P(E_0) \le \sum_{j=1}^{n} P(E_j). \tag{74}$$

In order to derive causal incompatibility witnesses via consistency of the marginal distributions, therefore, we may consider the task of **enumerating** Hardy-type paradoxes, each of which we can then express as an inequality in terms of probabilities. In the following, we explain how to determine *all* such constraints for *any* marginal problem.

To start with a simple example, suppose that we are in a marginal scenario where the pairwise joint distributions of three variables A, B and C are given. One Hardy-type possibilistic constraint which we would want to enumerate is

$$[\mathbf{A{=}1}, \mathbf{C{=}1}] \implies [\mathbf{A{=}1}, B{=}1] \vee [B{=}0, \mathbf{C{=}1}], \tag{75}$$

resulting in the probabilistic constraint

$$P_{AC}(\mathbf{11}) \le P_{AB}(\mathbf{1}1) + P_{BC}(0\mathbf{1}). \tag{76}$$ {eq:trivm

Eq. (76) is a necessary condition for the existence of a joint distribution of P_{AB}, P_{AC}, and P_{BC}; it is equivalent to Eq. (55) and therefore also implies the polynomial inequality Eq. (58).

We outline the general procedure using a slightly more sophisticated example. Consider the marginal scenario of Fig. 14, where the contexts are $\{A_1B_1C_1\}$, $\{A_1B_2C_2\}$, $\{A_2B_1C_2\}$, $\{A_2B_2C_1\}$ and $\{A_2B_2C_2\}$, pursuant to Eq. (69). Now a possibilistic constraint on this marginal problem consists of a logical implication with one joint outcome as the **antecedent** and a disjunction of joint outcomes as the **consequent**. In the following, we explain how to generate *all* such implications which are tight in the sense that their right-hand sides are minimal.

First we fix the antecedant by choosing some context and a composite outcome for it. In order to generate all possibilistic constraints, one will have to perform this procedure for *every* context as the antecedent and every choice of joint outcome thereupon. For the sake of concreteness we take $[\mathbf{A_2{=}1}, \mathbf{B_2{=}1}, \mathbf{C_2{=}1}]$ to be the fixed antecedent.

The consequent will be a conjunction of composite outcomes in marginal contexts, with the additional property that all outcomes of variables that also occur in the antecedent carry the same outcome. For the implication to be valid, the consequent must further be such that **for any *joint* composite outcome which extends the antecedent's marginal composite outcome, also at least one of the marginal composite outcomes in the consequent must occur.**

To formally determine all valid consequents, we first consider two hypergraphs. The nodes in the first hypegraph correspond to every possible composite outcome for every possible context. The hyperedges correspond to every possible joint outcome of all variables. A hyperedge (joint composite outcome) contains a node (marginal composite outcome) iff the hyperedge is an extension of the node; for example the hyperedge $[A_1{=}0, \mathbf{A_2{=}1}, B_1{=}0, \mathbf{B_2{=}1}, C_1{=}1, \mathbf{C_2{=}1}]$ is an extension of the node $[A_1{=}0, \mathbf{B_2{=}1}, \mathbf{C_2{=}1}]$. In our example following Fig. 14, this initial hypergraph has $5 \cdot 2^3 = 40$ nodes and $2^6 = 64$ hyperedges.

The second hypergraph is a sub-hypergraph of the first one. We delete from the first graph all nodes and hyperedges which contradict the outcomes supposed by the antecedent. For example, the node $[\mathbf{A_2{=}1}, \mathbf{B_2{=}0}, C_1{=}1]$ contradicts the antecedent $[\mathbf{A_2{=}1}, \mathbf{B_2{=}1}, \mathbf{C_2{=}1}]$. We also delete the node corresponding to the antecedent itself. In our example, this final resulting hypergraph has $2^3 + 3 \cdot 2^1 = 14$ nodes and $2^3 = 8$ hyperedges.

All valid (minimal) consequents are (minimal) **transversals** of this latter hypergraph. A transversal is a set of nodes which has the property that it intersects every hyperedge in at least one node. In order to get implications which are as tight as possible, it is sufficient to enumerate only the minimal transversals. Doing so is a well-studied problem in computer science with various natural reformulations and for which manifold algorithms have been developed [54].

In our example, it is not hard to check that the right-hand side of

$$\begin{aligned}[\mathbf{A_2{=}1}, \mathbf{B_2{=}1}, \mathbf{C_2{=}1}] \quad \implies \quad & [A_1{=}0, B_1{=}0, C_1{=}0] \vee [A_1{=}1, \mathbf{B_2{=}1}, \mathbf{C_2{=}1}] \\ & \vee [\mathbf{A_2{=}1}, B_1{=}1, \mathbf{C_2{=}1}] \vee [\mathbf{A_2{=}1}, \mathbf{B_2{=}1}, C_1{=}1]\end{aligned} \tag{77}$$

is such a minimal transversal: every assignment of values to all variables which extends the assignment on the left-hand side satisfies at least one of the terms on the right, but this ceases to hold as soon as one removes any one term on the right.

We convert these implications into inequalities in the usual way, by replacing "⇒" by "≤" at the level of probabilities and the disjunctions by sums. For example the possibilistic constraint Eq. (77) translates to the probabilistic constraint

$$P_{A_2B_2C_2}(\mathbf{111}) \leq P_{A_1B_1C_1}(000) + P_{A_1B_2C_2}(\mathbf{111}) + P_{A_2B_1C_2}(\mathbf{111}) + P_{A_2B_2C_1}(\mathbf{111}) \tag{78}$$

i.e. Eq. (63). Therefore Eq. (77) recovers Eq. (63), and hence Eq. (77) can be thoughts of as the fundamental progenitor of Eq. (66).

Inequalities resulting from hypergraph transversals are generally weaker than those that result from completely solving the marginal problem. Nevertheless, many Bell inequalities are of this form—such as the CHSH inequality which follows in this way from Hardy's original implication. So it seems that this method is still sufficiently powerful to generate plenty of interesting inequalities. At the same time, it should be significantly easier to perform in practice than the full-fledged linear (let alone nonlinear) quantifier elimination, even if one does it for every possible antecedent.

In conclusion, linear quantifier elimination is the preferable tool for deriving inequalities whenever it is computationally tractable; but whenever it is not, then enumerating hypergraph transversals presents a good alternative.

VII. BELL SCENARIOS AND INFLATION

To further illustrate the power of our inflated DAG approach, we now demonstrate how to recover all Bell inequalities [7, 8, 31] via our method. To keep things simple we only discuss the case of a bipartite Bell scenario with two values for both "settings" and "outcome" variables here, but the case of more parties and/or more values per variable is totally analogous.

The causal structure associated to the Bell [6–8, 31] experiment [11 (Fig. E#2), 9 (Fig. 19), 23 (Fig. 1), 12 (Fig. 1), 32 (Fig. 2b), 33 (Fig. 2)] is depicted here in Fig. 11. The observable variables are A, B, X, Y, and Λ is the latent common cause of A and B. In a Bell scenario, one traditionally works with the conditional distribution $P_{AB|XY}$, to be understood as an array of distributions indexed by the possible values of X and Y, instead of with the original distribution P_{ABXY}, which is what we do.

In the Bell scenario DAG, the maximal pre-injectable sets are

$$\begin{aligned}&\{A_1B_1X_1X_2Y_1Y_2\}\\&\{A_1B_2X_1X_2Y_2Y_2\}\\&\{A_2B_1X_1X_2Y_2Y_2\}\\&\{A_2B_2X_1X_2Y_2Y_2\},\end{aligned} \tag{79}$$

where notably every maximal pre-injectable set contains all "settings" variables X_1 to Y_2. The marginal distributions on these pre-injectable sets are then specified by the original observable distribution via

$$\forall abx_1x_2y_1y_2: \begin{cases} P_{A_1B_1X_1X_2Y_1Y_2}(abx_1x_2y_1y_2) = P_{ABXY}(abx_1y_1)P_X(x_2)P_Y(y_2), \\ P_{A_1B_2X_1X_2Y_1Y_2}(abx_1x_2y_1y_2) = P_{ABXY}(abx_1y_2)P_X(x_2)P_Y(y_1), \\ P_{A_2B_1X_1X_2Y_1Y_2}(abx_1x_2y_1y_2) = P_{ABXY}(abx_2y_1)P_X(x_1)P_Y(y_2), \\ P_{A_2B_2X_1X_2Y_1Y_2}(abx_1x_2y_1y_2) = P_{ABXY}(abx_2y_2)P_X(x_1)P_Y(y_1), \\ \qquad P_{X_1X_2Y_1Y_2}(x_1x_2y_1y_2) = P_X(x_1)P_X(x_2)P_Y(y_1)P_Y(y_2). \end{cases} \tag{80}$$

By dividing each of the first four equations by the fifth, we obtain

$$\forall abx_1x_2y_1y_2: \begin{cases} P_{A_1B_1|X_1X_2Y_1Y_2}(ab|x_1x_2y_1y_2) = P_{AB|XY}(ab|x_1y_1), \\ P_{A_1B_2|X_1X_2Y_1Y_2}(ab|x_1x_2y_1y_2) = P_{AB|XY}(ab|x_1y_2), \\ P_{A_2B_1|X_1X_2Y_1Y_2}(ab|x_1x_2y_1y_2) = P_{AB|XY}(ab|x_2y_1), \\ P_{A_2B_2|X_1X_2Y_1Y_2}(ab|x_1x_2y_1y_2) = P_{AB|XY}(ab|x_2y_2). \end{cases} \tag{81}$$

{eq:bellf

The existence of a joint distribution over all six variables—i.e. the existence of a solution to the marginal problem—implies in particular

$$\forall abx_1x_2y_1y_2: \quad P_{A_1B_1|X_1X_2Y_1Y_2}(ab|x_1x_2y_1y_2) = \sum\nolimits_{a',b'} P_{A_1A_2B_1B_2X_1X_2Y_1Y_2}(aa'bb'|x_1x_2y_1y_2), \tag{82}$$

and similarly for the other three conditional distributions under consideration. For consistency with the causal hypothesis, therefore, the original distribution must satisfy in particular

$$\forall ab: \begin{cases} P_{AB|XY}(ab|00) = \sum_{a',b'} P_{A_1A_2B_1B_2X_1X_2Y_1Y_2}(aa'bb'|0101) \\ P_{AB|XY}(ab|10) = \sum_{a',b'} P_{A_1A_2B_1B_2X_1X_2Y_1Y_2}(a'abb'|0101) \\ P_{AB|XY}(ab|01) = \sum_{a',b'} P_{A_1A_2B_1B_2X_1X_2Y_1Y_2}(aa'b'b|0101) \\ P_{AB|XY}(ab|11) = \sum_{a',b'} P_{A_1A_2B_1B_2X_1X_2Y_1Y_2}(a'ab'b|0101) \end{cases} \tag{83}$$

{eq:final

The possibility to write the conditional probabilities in the Bell scenario in this form is equivalent to the existence of a latent variable model, as noted in Fine's Theorem FineTheorem [55]. Thus, if an inflated model exists with the required marginals, then a latent variable model of the original distribution exists as well (and conversely, trivially). Hence the inflated DAG of Fig. 12 provides necessary and sufficient conditions for the consistency of the original observed distribution with the Bell scenario causal structure.

Moreover, it is possible to describe the marginal polytope over the pre-injectable sets of Eq. (79), due to the fact that the "settings" variables X_1 to Y_4 occur in all four contexts. This description is easier to state for the marginal *cone*, by which we mean the convex cone spanned by the marginal polytope, i.e. the convex cone consisting of all nonnegative linear combinations of deterministic assignments of values, or equivalently the convex cone of all measures on the set of joint outcomes. This cone lives in $\oplus_{i=1}^4 \mathbb{R}^{2^6} = \oplus_{i=1}^4 (\mathbb{R}^2)^{\otimes 6}$, where each tensor factor has basis vectors corresponding to the two possible outcomes of each variable, and the direct summands enumerate the four contexts. Now the marginal cone is precisely the set of all nonnegative linear combinations of the points

$$\begin{aligned} &(e_{A_1} \otimes e_{B_1} \otimes e_{X_1} \otimes e_{X_2} \otimes e_{Y_1} \otimes e_{Y_2}) \\ \oplus\, &(e_{A_1} \otimes e_{B_2} \otimes e_{X_1} \otimes e_{X_2} \otimes e_{Y_1} \otimes e_{Y_2}) \\ \oplus\, &(e_{A_2} \otimes e_{B_1} \otimes e_{X_1} \otimes e_{X_2} \otimes e_{Y_1} \otimes e_{Y_2}) \\ \oplus\, &(e_{A_2} \otimes e_{B_2} \otimes e_{X_1} \otimes e_{X_2} \otimes e_{Y_1} \otimes e_{Y_2}), \end{aligned}$$

where all six variables range over their deterministic outcomes. Since the last four tensor factors occur in every direct summand in exactly the same way, the resulting marginal cone is linearly isomorphic to the cone generated by all vectors of the form

$$[(e_{A_1} \otimes e_{B_1}) \oplus (e_{A_1} \otimes e_{B_2}) \oplus (e_{A_2} \otimes e_{B_1}) \oplus (e_{A_2} \otimes e_{B_2})] \otimes [e_{X_1} \otimes e_{X_2} \otimes e_{Y_1} \otimes e_{Y_2}]$$

in $\mathbb{R}^{2^2} \otimes \mathbb{R}^{2^4}$. Now since the first four variables in the first tensor factor vary completely independently of the latter four variables in the second tensor factor, the resulting cone will be precisely the tensor product namioka_tensor_1969 [56] of two cones: first, the cone generated by all vectors of the form

$$(e_{A_1} \otimes e_{B_1}) \oplus (e_{A_1} \otimes e_{B_2}) \oplus (e_{A_2} \otimes e_{B_1}) \oplus (e_{A_2} \otimes e_{B_2}),$$

and second the one spanned by all $e_{X_1} \otimes e_{X_2} \otimes e_{Y_1} \otimes e_{Y_2}$. While the latter cone is simply the standard positive cone of $\mathbb{R}^8$, the former cone is the cone generated by the "local polytope" or "Bell polytope" that is traditionally used in the context of Bell scenarios Brunner2013Bell [8, Sec. II.B]. Standard results on tensor products of cones and polytopes bogart_hom_2013 [57] therefore imply that our marginal polytope is the tensor product of the Bell polytope, corresponding to the A_1 to B_2 part, with a simplex corresponding to the X_1 to Y_2 "settings" part. This implies that the facets of our marginal polytope are precisely the pairs consisting of a facet of the Bell polytope and a facet of the simplex. For example, in this way we obtain one version of the CHSH inequality as a facet of the marginal polytope,

$$\sum_{a,b,x,y} (-1)^{a+b+xy} P_{A_x B_y X_1 X_2 Y_1 Y_2}(ab0101) \leq 2 P_{X_1 X_2 Y_1 Y_2}(0101).$$

Upon using Eq. (81), this becomes

$$\sum_{a,b} (-1)^{a+b} \big(P_{ABXY}(ab00) P_X(1) P_Y(1) + P_{ABXY}(ab01) P_X(1) P_Y(0) \\ + P_{ABXY}(ab10) P_X(0) P_Y(1) - P_{ABXY}(ab11) P_X(0) P_Y(0) \big) \leq P_X(0) P_X(1) P_Y(0) P_Y(1),$$

so that dividing by the right-hand side results in essentially the conventional form of the CHSH inequality,

$$\sum_{a,b} (-1)^{a+b} \left(P_{AB|XY}(ab|00) + P_{AB|XY}(ab|01) + P_{AB|XY}(ab|10) - P_{AB|XY}(ab|11) \right) \leq 2.$$

In conclusion, the inflation technique is powerful enough to get a precise characterization of all distributions consistent with the Bell causal structure, and our technique for generating polynomial inequalities while solving the marginal problem recovers all Bell inequalities.

VIII. QUANTUM CAUSAL INFERENCE AND THE NO-BROADCASTING THEOREM

sicallity

Mention that the distinction between whether the nodes of the DAG represent variables or quantum algebras or post-quantum things is something that is part of the causal parameters, not the causal structure. We must therefore revise our description of a causal model to accommodate quantum and post-quantum causal models. Specifically, we drop the claim that the nodes are variables. Fortunately, the notion of observed versus latent and of the cardinality of an object can be made theory-independent. —RWS

In the causal inference problems with latent nodes that we have considered so far, the latent nodes correspond to unobserved random variables. This describes things that come up in *classical* physics (and things outside of physics). In *quantum* physics, however, the latent nodes may instead carry *quantum systems*. Whenever this is allowed, we say that the DAG represents a **quantum causal structure**. Some quantum causal structures are famously capable of generating distributions over the observable variables that would not be possible classically[8].

The set of quantumly realizable distributions is superficially quite similar to the classical subset [10, 11]. For example, classical and quantum distributions alike respect all conditional independence relations implied by the common underlying causal structure [11]. It is an interesting problem to find quantum distributions that are not realizable classically, or to show that there are no such distributions on a given DAG.

However, this is by no means an easy task. For example, recent work has found that quantum causal structure also implies many of the entropic inequalities that hold classically [11, 13, 26]. To date, no quantum distribution has been found to violate a Shannon-type entropic inequality on observable variables derived from the Markov conditions on all nodes [10, 58]. Fine-graining the scenario by conditioning on root variables ("settings") leads to a different kind of entropic inequality, and these have proven somewhat quantum-sensitive [23, 59, 60]. Such inequalities are still limited, however, in that they only apply in the presence of observable root nodes[9], and they still fail to witness certain distributions as classically impossible [10, 23].

We hope that polynomial inequalities derived from broadcasting inflated DAGs will provide an additional tool for witnessing certain quantum distributions as non-classical. For example due to the results of Sec. VII, it seems conceivable that these inequalities will be much stronger and provide much tighter constraints than entropic inequalities.

It is worth pondering how it is possible that some of the inequalities that can be derived via inflation—such as Bell inequalities—have quantum violations, i.e. why one cannot expect them to be valid for all quantum distributions as well. The reason for this is that duplicating an outgoing edge in a DAG during inflation amounts to **broadcasting** the value of the random variable. For example while the information about X in Fig. 1 was "sent" to A and C, the information about X_1 is sent to A_1 *and* A_2 and C in the inflation Fig. 4. Since quantum theory satisfies a

[8] The incompatibility of quantum correlations with practical causal structure which generates them is known as Bell's theorem [31]. The particular distributions which violate Bell inequalities are known as nonlocal correlations [8]. Although the term suggests the existence of nonlocal interactions, in the sense that the actual causal structure may be different from the hypothesized one, this interpretation is at odds with the fact that no nonlocal interactions have been observed in nature, implying that their presence would require fine-tuning [9]. A less problematic alternative conclusion from Bell's theorem is the impossibility to model quantum physics in terms of the usual notions of "classical" probability theory.

[9] Rafael Chaves and E.W. are exploring the potential of entropic analysis based on conditioning on non-root observable nodes. This generalizes the method of entropic inequalities, and might be capable of providing much stronger entropic witnesses.

no-broadcasting theorem [61, 62], one cannot expect such broadcasting to be possible quantumly. More generally, there is an analogous no-broadcasting theorem in the regime of epistemically restricted general probabilistic theories (GPTs) [62–65], so that the same statement applies in many theories other than quantum theory. As a consequence, a quantum or general probabilistic causal model on the original DAG does generally not inflate to a "quantum inflated model" or "general probabilistic inflated model" on the inflated DAG.

Some inflations, such as the one of Fig. 5, do not require such broadcasting. By remove A_1 from the broadcasting inflation of Fig. 4 we obtain the non-broadcasting inflation of Fig. 5. In Fig. 5 the channel from X to A is merely *redirected* from it original configuration in Fig. 1; there is no broadcasting of information required.

Definition 5. *$G' \in \mathsf{Inflations}[G]$ is* ***non-broadcasting*** *if every latent node in G' has at most one copy of each $A \in \mathsf{Nodes}[G]$ among its children.*

It follows that every quantum causal model can be inflated to a non-broadcasting DAG, so that one obtains a quantum and general probabilistic analogue of Lemma 3 in the non-broadcasting case. Constraints derived from non-broadcasting inflations are therefore valid also for quantum and even general probabilistic distributions. In the specific case of the entropic monogamy inequality for the Triangle scenario, i.e. Eq. (62) here, this was originally noticed in Ref. [11]. Another example is Eq. (58), which was derived from the non-broadcasting inflation of Fig. 6. Eq. (58) too, therefore, is a necessary criterion for compatibility with the Triangle scenario even when the latent nodes are allowed to carry quantum or general probabilistic systems. Since the perfect-correlation distribution considered in Eq. (10) violates both of these inequalities, it evidently cannot be generated within the Triangle scenario even with quantum or general probabilistic states on the hidden nodes. This was also pointed out in Ref. [11].

On the other hand, by intentionally using broadcasting in an inflated DAG, we can specifically try to witness certain quantum or general probabilistic distributions as non-classical. This is exactly what happens in Bell's theorem.

Even when using broadcasting inflated DAGs, it may still be possible to derive inequalities valid for quantum distributions if one appropriately the nonnegativity inequalities in the marginal problem, e.g. such as Eq. (70). The modification would replace demanding nonnegativity of the full joint distribution with instead demanding the nonnegativity of only quantum-physically-meaningful marginal probability distributions.

Even when using broadcasting inflated DAGs, it may still be possible to derive inequalities valid for quantum distributions if one appropriately modifies Sec. V to generate a different initial set of nonnegativity inequalities. This new set should capture the nonnegativity of only quantum-physically-meaningful marginal probability distributions. Indeed, a quantum causal model on the original DAG can potentially be inflated to a quantum inflated model on the inflated DAG in terms of the logical broadcasting maps of Coecke and Spekkens [66]. From this perspective, a broadcasting inflated DAG is an abstract logical concept, as opposed to a feasible physical construct. However, this would result in a joint distribution over all observable variables that may have some negative probabilities, and one cannot expect Eq. (70) to hold in general. But one can still try to reformulate the marginal problem so as to refer only to the existence of joint distributions on non-broadcastings sets rather than the existence of a full joint distribution from which the marginal distributions might be recovered. Here, a set $\boldsymbol{U}$ of observable nodes is non-broadcasting if $\mathsf{An}(\boldsymbol{U})$ does not contain two distinct copies of a node both sharing a common latent parent.

An analysis along these lines has already been carried out successfully by Chaves *et al.* [26] in the derivation of entropic inequalities that are valid for all quantum distributions. Although Chaves *et al.* [26] do not invoke inflated DAGs, they do seem to employ a similar type of structure to model the conditioning of a variable on a "setting" variable, and this also gives rise to non-broadcasting sets. Chaves *et al.* [26] take pains to avoid including full joint probability distributions in any of their initial entropic inequalities, precisely as we would want to do in constructing our initial probability inequalities, and they successfully derive quantumly valid entropic inequalities. But so far, no inequalities polynomial in the probabilities have been derived using this method.

A tight set of inequalities characterizing quantum distributions would provide the ultimate constraints on what quantum theory allows. Deriving additional inequalities that hold for quantum distributions is therefore a priority for future research.

IX. PROSPECTS FOR THE INFLATION TECHNIQUE

Corollary ?? implies that *any* causal compatibility inequality on the inflated DAG can be translated into a causal compatibility inequality on the original DAG. Consequently *any* technique for deriving causal compatibility inequalities can potentially be leveraged by the inflation technique. And, as we noted in Sec. ??, even weak constraints at the level of the inflated DAG can translate into strong constraints at the level of the original DAG.

We here consider two possibilities for constraints that might be leveraged by the inflation technique.

Constraining Possible Distributions over Pre-Injectable Sets via Conditional Independence Relations

The marginal problem asks about the existence of *any* joint distribution which recovers the given marginal distributions. In causal inference, however, there are plenty of other constraints on the sorts of joint distributions which are consistent with some causal hypothesis. The minimal constraint embedded in any causal hypothesis is the idea of causal structure. Thus it is natural to supplement the marginal problem with additional constraints, motivated by causal structure, constraining the hypothetical distribution over observable variables of the inflated DAG.

The most familiar causally-motivated constraints on a joint distribution are **conditional independence relations**, say among observable variables. Conditional independence relations are inferred by d-separation; if $\boldsymbol{X}$ and $\boldsymbol{Y}$ are d-separated in the (inflation) DAG by $\boldsymbol{Z}$, then we infer the conditional independence $\boldsymbol{X}\perp\boldsymbol{Y}|\boldsymbol{Z}$. The d-separation criterion is explained at length in [1, 3, 9, 11], so we elect not to review it here.

Every conditional independence relation can be translated into a nonlinear constraint on probabilities, as $\boldsymbol{X}\perp\boldsymbol{Y}|\boldsymbol{Z}$ implies $P(\boldsymbol{xy}|\boldsymbol{z}) = P(\boldsymbol{x}|\boldsymbol{z})P(\boldsymbol{y}|\boldsymbol{z})$ for all $\boldsymbol{x}$, $\boldsymbol{y}$, and $\boldsymbol{z}$. As we generally prefer to work with unconditional probabilities, we rewrite this as follows: If $\boldsymbol{X}$ and $\boldsymbol{Y}$ are d-separated by $\boldsymbol{Z}$, then $P_{\boldsymbol{XYZ}}(\boldsymbol{xyz})P_{\boldsymbol{Z}}(\boldsymbol{z}) = P_{\boldsymbol{XZ}}(\boldsymbol{xz})P_{\boldsymbol{YZ}}(\boldsymbol{yz})$ for all $\boldsymbol{x}$, $\boldsymbol{y}$, and $\boldsymbol{z}$. Such nonlinear constraints can be incorporated as further restrictions on the sorts of joint distributions consistent with the inflated DAG, supplementing the basic nonnegativity of probability constraints of the marginal problem discussed above.

For example, in Fig. 3 we find that A_1 and C_2 are d-separated by $\{A_2B_2\}$, and so one might incorporate the family of nonlinear equalities $P_{A_1A_2B_2C_2}(a_1a_2b_2c_2)P_{A_2B_2}(a_2b_2) = P_{A_1A_2B_2}(a_1a_2b_2)P_{A_2B_2C_2}(a_2b_2c_2)$ for all a_1, a_2, b_2 and c_2. Every probability that appears in an equation like this must occur as a marginal as well, i.e. it can be written as a sum of various joint probabilities, as in

$$\forall a_2b_2:\ P_{A_2B_2}(a_2b_2) = \sum\nolimits_{a_1b_1c_1c_2} P_{A_1A_2B_1B_2C_1C_2}(a_1a_2b_1b_2c_1c_2). \tag{84}$$

In particular, the number of unknown quantities to be eliminated is still the same, but now the system of equations and inequalities is nonlinear.

Many modern computer algebra systems have functions capable of tackling nonlinear quantifier elimination symbolically[10]. Currently, however, it is generally not practical to perform nonlinear quantifier elimination on large polynomial systems with many quantifiers. It may help to exploit results on the particular algebraic-geometric structure of these particular systems [47]. But also without using quantifier elimination, the nonlinear constraints can be easily accounted for numerically. Upon substituting numerical values for all the injectable probabilities, the former quantifier elimination problem is converted to simpler existence problem: Do there exist joint probabilities that satisfy the full set of linear and nonlinear constraints numerically? Most computer algebra systems can resolve such *satisfiability* questions quite easily[11].

It is also possible to use a mixed strategy of linear and nonlinear quantifier elimination, such as Chaves [17] advocates. The explicit results of [17] are therefore consequences of any inflated DAG, achieved by applying a mixed quantifier elimination strategy. T: I don't see where the "therefore" comes from. Are Rafael's results a special case of inflation? If so, we should explain this in one or two sentences, but maybe not here.

Constraining Possible Distributions over Pre-Injectable Sets via Coinciding Marginals

Even if the original hypothesis does not constrain possible causal models beyond d-separation, The inflation hypothesis is (in all nontrivial cases) more than just that: every inflated model also satisfies $P(A_i|\mathsf{Pa}(A_i)) = P(A_j|\mathsf{Pa}(A_j))$, per Eq. (5). This implies cases that distributions over certain sets of nodes must coincide in any inflated model. For example, $P_{\boldsymbol{X}} = P_{\boldsymbol{Y}}$ certainly holds whenever $\boldsymbol{X}$ and $\boldsymbol{Y}$ are injectable and $\tilde{\boldsymbol{X}} = \tilde{\boldsymbol{Y}}$, but adding this constraint to the quantifier elimination problem does not help as both sides of this equations are already determined by the original distribution. However, this type of equation also follows in some cases when $\boldsymbol{X}$ and $\boldsymbol{Y}$ are not injectable. For example, $P_{A_1A_2B_1} = P_{A_1A_2B_2}$ follows from Fig. 3 and the inflation hypothesis, even though $\{A_1A_2B_1\}$ and $\{A_1A_2B_2\}$ are not injectable sets.

Hence equations such as $\forall a_1a_2b:\ P_{A_1A_2B_1}(a_1a_2b) = P_{A_1A_2B_2}(a_1a_2b)$ are also consequnces of the inflation hypothesis, and may be incorporated into either linear or nonlinear quantifier eliminations in order to derive stronger incompatibility witnesses. The details of how to recognize coinciding distributions beyond the obvious coincidences implied by injectable or pre-injectable sets and under what conditions they may yield tighter inequalities are discussed in Appendix B.

T: yes, this should be moved, to some place where also the second to last paragraph goes. Maybe end of introduction, a paragraph on related work? As far as we can tell, our inequalities are not related to the nonlinear incompatibility witnesses which have been derived specifically to constrain classical networks [18–20], nor to the nonlinear inequalities which account for interventions to a given causal structure [33, 49].

---

[10] For example *Mathematica*™'s `Resolve` command, *Redlog*'s `rlposqe`, or *Maple*™'s `RepresentingQuantifierFreeFormula`, etc.

[11] For example *Mathematica*™ `Reduce`ExistsRealQ` function. Specialized satisfiability software such as SMT-LIB's `check-sat` [48] are particularly apt for this purpose.

X. CONCLUSIONS

Our main contribution is a new way of deriving causal incompatibility witnesses, namely the inflated DAG approach. An inflated DAG naturally carries inflated models, and the existence of an inflated model implies inequalities which constrain the set of distributions on observable nodes compatible with the original causal structure. Polynomial inequalities can be obtained through *linear* inequalities which are necessary conditions for a collection of given marginal distributions to arise from a joint distribution (marginal problem). For deriving such inequalities in turn, we have considered the methods of computing all facets of the marginal polytope via facet enumeration, and deriving looser constraints more efficiently by enumerating hypergraph transversals.

The resulting polynomial inequalities are necessary conditions on a joint distribution to be explained by the causal structure. We currently do not know to what extent they can also be considered sufficient, and there is somewhat conflicting evidence: as we have seen, the inflated DAG approach reproduces all Bell inequalities; but on the other hand, we have not been able to use it to rederive Pearl's instrumental inequality, although the instrumental scenario also contains only one latent node. By excluding the W-type distribution on the Triangle scenario, we have seen that our polynomial inequalities are stronger than entropic inequalities in at least some cases.

A single causal structure has unlimited potential inflations. Selecting a good inflation from which strong polynomial inequalities can be derived is an interesting challenge. To this end, it would be desirable to understand how particular features of the original causal structure are exposed when different nodes in the DAG are duplicated. By isolating which features are exposed in each inflation, we could conceivably quantify the causal inference strength of each inflation. In so doing, we might find that inflated DAGs beyond a certain level of variable duplication need not be considered. The multiplicity beyond which further inflation is irrelevant may be related to the maximum degree of those polynomials which tightly characterize a causal scenario. Presently, however, it is not clear how to upper bound either number, or whether finite upper bounds can even be expected.

Concerning the relation to quantum theory, our method turns the quantum no-broadcasting theorem [61, 62] on its head by crucially relying on the fact that classical hidden variables *can* be cloned. The possibility of classical cloning motivates the inflated DAG method, and is often critical for deriving strong incompatibility witnesses. We have found that in the case of non-broadcasting inflations, our method also yields causal incompatibility witnesses that constitute necessary constraints even for *quantum* or *general probabilistic* causal scenarios, a common desideratum in recent works [10–13, 26].

It would be enlightening to understand the extent to which our (classical) polynomial inequalities are violated in quantum theory. A variety of techniques exist for estimating the amount by which a Bell inequality [67, 68] is violated in quantum theory, but even finding a quantum violation of one of our *polynomial* inequalities presents a new task for which we currently lack a systematic approach. Nevertheless, we know that there exists a difference between classical and quantum also beyond Bell scenarios [10, Theorem 2.16], and we hope that our polynomial inequalities will perform better in witnessing this difference than entropic inequalities do [11, 26].

ACKNOWLEDGMENTS

T.F. would like to thank Guido Montúfar for discussion and references. E.W. would like to thank Rafael Chaves and TC Fraser for suggestions which have improved this manuscript. Research at Perimeter Institute is supported by the Government of Canada through Industry Canada and by the Province of Ontario through the Ministry of Economic Development and Innovation.

Appendix A: Algorithms for Solving the Marginal Problem

By solving the marginal problem, what we mean is to determine all the facets of the marginal polytope for a given marginal scenario. Since the vertices of this polytope are precisely the deterministic assignments of values to all variables, which are easy to enumerate, solving the marginal problem is an instance of a **facet enumeration problem**: given the vertices of a convex polytope, determine its facets. This is a well-studied problem in combinatorial optimization for which a variety of algorithms are available [69].

A generic facet enumeration problem takes a matrix of vertices $V \in \mathbb{R}^{n\times d}$, where each row is a vertex, and asks what is the set of points $x \in \mathbb{R}^d$ that can be written as a convex combination of the vertices using weights $w \in \mathbb{R}^n$ that are nonnegative and normalized,

$$\left\{ x \in \mathbb{R}^d \;\middle|\; \exists w \in \mathbb{R}^n : \; x = wV, \;\; w \geq 0, \;\; \sum_i w_i = 1 \right\}. \tag{A.1}$$

The oldest-known method for facet enumeration relies on **linear quantifier elimination** in the form of Fourier-Motzkin (FM) elimination [70, 71]. This refers to the fact that one starts with the system $x = wV$, $w \geq 0$ and $\sum_i w_i = 1$, which is the half-space representation of a convex polytope (a simplex), and then one needs to project onto x-space by *eliminating* the variables w to which the existential *quantifier* $\exists w$ refers. The Fourier-Motzkin algorithm is a particular method for performing this quantifier elimination one variable at a time; when applied to Eq. (A.1), it is equivalent to the *double description method* [72, 73]. Linear quantifier elimination routines are available in many software tools[12]. The authors found it convenient to custom-code a linear elimination routine in *Mathematica*™.

Other algorithms for facet enumeration that are not based on linear quantifier elimination include the following. *Lexicographic reverse search* (LRS) [77], which explores the entire polytope by repeatedly pivoting from one facet to an adjacent one, and is implemented in `lrs`. Equality Set Projection (ESP) [78, 79] is also based on pivoting from facet to facet, though its implementation is less stable[13]. These algorithms could be interesting to use in practice, since each pivoting step churns out a new facet; by contrast, Fourier-Motzkin type algorithms only generate the entire list of facets at once, after all the quantifiers have been eliminated one by one.

It may also be possible to exploit special features of marginal polytopes in order to facilitate their facet enumeration, such as their high degree of symmetry: permuting the outcomes of each variable maps the polytope to itself, which already generates a sizeable symmetry group, and oftentimes there are additional symmetries given by permuting some of the variables. This simplifies the problem of facet enumeration [81, 82], and it may be interesting to apply the dedicated software[14] to the facet enumeration problem of marginal polytopes [83–85].

TABLE I. A comparison of different approaches for constraining the distributions on the pre-injectable sets. The primary divide is producing inequalities, as in the more difficult first three approaches, versus satisfiability which can witness the infeasibility of specific distributions. The approaches subdivide further into nonlinear, linear, and possibilistic variants.

Approach	General problem	Standard algorithm(s)	Difficulty
Nonlinear quantifier elimination	Real quantifier elimination	Cylindrical algebraic decomposition, see [17]	Very hard
Solve marginal problem	Facet enumeration	Fourier-Motzkin [70, 71, 75, 80, 86], lexicographic reverse search [77]	Hard
Enumerate Hardy-type paradoxes	Hypergraph transversals	See Eiter *et al.* [54]	Very easy
Nonlinear satisfiability	Nonlinear optimization	See [48], and semidefinite relaxations [87]	Easy
Linear satisfiability	Linear programming	Simplex method [88, 89]	Very easy

---

[12] For example *MATLAB*™'s `MPT2`/`MPT3`, *Maxima*'s `fourier_elim`, *lrs*'s `fourier`, or *Maple*™'s (v17+) `LinearSolve` and `Projection`. The efficiency of most of these software tools, however, drops off markedly when the dimension of the final projection is much smaller than the initial space of the inequalities. FM elimination aided by Chernikov rules [74, 75] is implemented in *qskeleton* [76].

[13] ESP [78–80] is supported by `MPT2` but not `MPT3`, and by the (undocumented) option of projection in the *polytope* (v0.1.1 2015-10-26) python module.

[14] Such as `PANDA`, `Polyhedral`, or `SymPol`.

Appendix B: On Identifying Coinciding Marginal Distributions

Whenever one considers some inflated DAG, the corresponding inflated causal hypothesis includes the constraint that every copy of a variable in the inflated DAG has the same functional dependence on its parents, i.e. Eq. (5). In particular, this implies that the single-variable marginal distribution of all copies are equal,

$$\forall i, j \in \mathbb{N}: \; P_{A_i} = P_{A_j}. \tag{B.1}$$

As we will see in the following, the inflation hypothesis also implies similar constraints on the marginal distributions of certain *sets* of variables.

Given sets of nodes $\boldsymbol{U}$ and $\boldsymbol{Y}$ in an inflated DAG G', let us say that a map $\varphi : \mathsf{SubDAG}(\boldsymbol{U}) \to \mathsf{SubDAG}(\boldsymbol{V})$ is a **copy isomorphism** if it is a graph isomorphism[15] such that $\varphi(X) \sim X$ for all $X \in \boldsymbol{U}$, meaning that φ maps every node $X \in \boldsymbol{U}$ to a node $\varphi(X) \in \boldsymbol{Y}$ that is equivalent to X under dropping the copy index.

Furthermore, we say that a copy isomorphism $\varphi : \mathsf{SubDAG}(\boldsymbol{U}) \to \mathsf{SubDAG}(\boldsymbol{V})$ is an **inflationary isomorphism** whenever it can be extended to a copy isomorphism $\Phi : \mathsf{AnSubDAG}(\boldsymbol{U}) \to \mathsf{AnSubDAG}(\boldsymbol{V})$. If one starts with such a Φ, then one can reconstruct φ by restricting the domain of Φ to $\boldsymbol{U}$. If the image of this restriction is $\boldsymbol{V}$, then one obtains an inflationary isomorphism; that this restriction is indeed a copy isomorphism follows automatically. So in practice, one can either start with $\varphi\mathsf{SubDAG}(\boldsymbol{U}) \to \mathsf{SubDAG}(\boldsymbol{V})$ and try to extend it to $\Phi : \mathsf{AnSubDAG}(\boldsymbol{U}) \to \mathsf{AnSubDAG}(\boldsymbol{V})$, or start with such a Φ and see whether it restricts to a $\varphi : \mathsf{SubDAG}(\boldsymbol{U}) \to \mathsf{SubDAG}(\boldsymbol{V})$.

By the very definition of inflated model, the inflation hypothesis implies an equation between marginal distributions:

Lemma 6. *If $\varphi : \mathsf{SubDAG}(\boldsymbol{U}) \to \mathsf{SubDAG}(\boldsymbol{V})$ is an inflationary isomorphism, then $P_{\boldsymbol{U}} = P_{\boldsymbol{V}}$ in any inflated model, where the variables in $\boldsymbol{U}$ and $\boldsymbol{V}$ are matched up according to φ.*

In order to equate the distribution $P_{\boldsymbol{U}}$ with the distribution $P_{\boldsymbol{V}}$, one needs to specify a correspondence between the variables that make up $\boldsymbol{U}$ and those that make up $\boldsymbol{V}$. This is exactly the data provided by φ. If φ is not the identity map, then the resulting equation $P_{\boldsymbol{U}} = P_{\boldsymbol{V}}$ is nontrivial equation even when $\boldsymbol{U} = \boldsymbol{V}$: in this case, the equation is effectively requiring $P_{\boldsymbol{U}}$ to be invariant under permuting the variables according to the automorphism φ.

We illustrate Lemma 6 with an example. For the inflation of Fig. 3, the map

$$\varphi \; : \; A_1 \mapsto A_1, \qquad A_2 \mapsto A_2, \qquad B_1 \mapsto B_2$$

is a copy isomorphism between the non-ancestral subgraphs of $\boldsymbol{U} = \{A_1 A_2 B_1\}$ and $\boldsymbol{V} = \{A_1 A_2 B_2\}$, since it maps each copy to a copy of the same type, and trivially implements a graph isomorphism between $\mathsf{SubDAG}(\boldsymbol{U})$ and $\mathsf{SubDAG}(\boldsymbol{V})$, since neither of these graphs has any edges. There is a unique choice to extend φ to a copy isomorphism $\mathsf{AnSubDAG}(\boldsymbol{U}) \to \mathsf{AnSubDAG}(\boldsymbol{V})$ given by each of Y_2, X_1, and Y_1 mapping to itself, as well as $Z_1 \mapsto Z_2$.

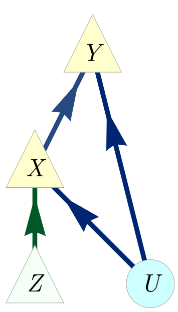

FIG. 15. The instrumental scenario of Pearl [21].

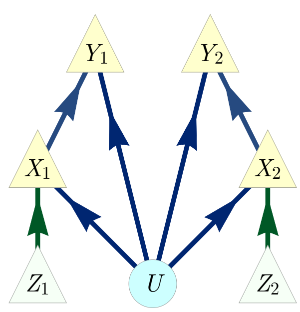

FIG. 16. An inflated DAG of the instrumental scenario which illustrates why coinciding ancestral subgraphs doesn't necessarily imply coinciding marginal distributions.

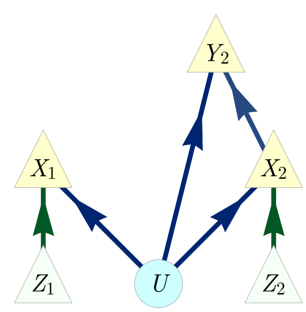

FIG. 17. The ancestral subgraph of Fig. 16 for either $\{X_1 Y_2 Z_1\}$ or $\{X_1 Y_2 Z_2\}$.

[15] A graph isomorphism is a bijective map between the nodes of one graph and the nodes of another, such that the action of the map transforms the complete *set of edges* defining the first graph into the complete set of edges comprising the second graph.

Therefore φ is indeed an inflationary isomorphism. From Lemma 6, we then conclude that any inflated model satisfies $P_{A_1A_2B_1} = P_{A_1A_2B_2}$.

To be clear, the existence of a copy isomorphism between ancestral subgraphs is *not*, by itself, a sufficient criterion to justify coinciding distributions. Nor is the existence of a copy isomorphism between non-ancestral subgraphs. Rather, the ancestral subgraph isomorphism must reduce to the non-ancestral subgraph isomorphism. The following example illustrates why the existence of a copy isomorphism between ancestral subgraphs is not, by itself, a sufficient criterion to justify coinciding distributions.

Consider the inflated DAG in Fig. 16. The identity map implements the only possible copy isomorphism $\mathsf{AnSubDAG}\big(X_1Y_2Z_1\big) \to \mathsf{AnSubDAG}\big(X_1Y_2Z_2\big)$, since both of these ancestral subgraphs are the DAG of Fig. 17. Nevertheless there is no inflationary isomorphism between $X_1Y_2Z_1$ and $X_1Y_2Z_2$, since the non-ancestral subgraphs of these two sets of nodes are not even copy isomorphic, i.e. $\mathsf{SubDAG}\big(X_1Y_2Z_1\big) \not\sim \mathsf{SubDAG}\big(X_1Y_2Z_2\big)$!

One can try to make use of Lemma 6 when deriving polynomial inequalities with inflation via solving the marginal problem, by imposing $P_{\boldsymbol{U}} = P_{\boldsymbol{V}}$ as an additional constraint for every inflationary isomorphism $\varphi : \mathsf{SubDAG}\big(\boldsymbol{U}\big) \to \mathsf{SubDAG}\big(\boldsymbol{V}\big)$ between sets of observable nodes. This is advantageous to speed up to the linear quantifier elimination, since one can solve each of the resulting equations for one of the unknown joint probabilities and thereby eliminate that probability directly without Fourier-Motzkin elimination.

Moreover, one could also hope that these additional equations would result in tighter constraints on the marginal problem, which then results in better polynomial inequalities. However, our computations have so far not revealed any example of such a tightening. In some cases, this lack of impact can be explained as follows. Suppose that $\varphi : \mathsf{SubDAG}\big(\boldsymbol{U}\big) \to \mathsf{SubDAG}\big(\boldsymbol{V}\big)$ is an inflationary isomorphism which is not just the restriction of a copy isomorphism between the ancestral subgraphs, but even the restriction of a copy automorphism $\Phi' : G' \to G'$ of the entire inflated DAG onto itself; in particular, this assumption implies that Φ' also restricts to a copy isomorphism $\Phi : \mathsf{AnSubDAG}\big(\boldsymbol{U}\big) \to \mathsf{AnSubDAG}\big(\boldsymbol{V}\big)$ between the ancestral subgraphs. In this case, the irrelevance of the additional constraint $P_{\boldsymbol{U}} = P_{\boldsymbol{V}}$ to the marginal problem for inflated models can be explained by the following argument.

Suppose that some joint distribution P solves the unconstrained marginal problem, i.e. without requiring $P_{\boldsymbol{U}} = P_{\boldsymbol{V}}$. Now apply Φ' to the variables in P, switching the variables around, to generate a new distribution P'. Because the set of marginal distributions that arise from inflated models is invariant under this switching of variables, we conclude that P' is also a solution to the unconstrained marginal problem. Taking the uniform mixture of P and P' is therefore still a solution of the unconstrained marginal problem. But this uniform mixture also satisfies the supplementary constraint $P_{\boldsymbol{U}} = P_{\boldsymbol{V}}$. Hence the supplementary constrained is satisfiable automatically whenever the unconstrained marginal problem is solvable, which makes adding the constraint irrelevant.

Note that the argument does not apply if the inflationary isomorphism $\varphi : \boldsymbol{U} \to \boldsymbol{V}$ cannot be extended to a copy isomorphism of the entire inflated DAG. It also does not apply if one uses the conditional independence relations on the inflated DAG as well, since this destroys linearity. We do not know what happens in either of these cases.

Appendix C: Using Inflation to Certify a DAG as "Interesting"

By considering all possible d-separation triples implied by a given DAG one can infer that certain conditional independence (CI) relations must hold in an observable joint distribution compatible with the given DAG. In the presence of nontrivial latent nodes, the set of *observable* CI relations is a strict subset of the set of all possible CI relations. Part of Ref. [11] is concerned with identifying DAGs for which satisfying all observable CI relations is *not* a sufficient criterion for compatibility of any observable distribution with a given DAG. Henson *et al.* [11] use the term **interesting** to refer to any DAG which exhibits a discrepancy between the set of observable distributions genuinely compatible with it and the set of observable distributions compatible with merely its observable CI relations.

Henson *et al.* [11] derived novel necessary criteria on the structure of a DAG in order for it to be interesting, and they conjectured that their criteria may, in fact, be necessary and sufficient. As evidence in favour of this conjecture, they enumerated all possible DAGs with no more than six nodes satisfying their criteria for further testing. They found only 21 classes of potentially interesting DAGs after accounting for symmetry. Of those 21, Henson *et al.* [11] further proved that 18 were unambiguously interesting by writing down an explicit incompatible distribution which nevertheless satisfied the DAGs observable CI relations. Incompatibility of the constructed distribution was certified by means of entropic inequalities.

That left three classes of DAGs as *potentially* interesting. For each of these, Henson *et al.* [11] derived all Shannon-type entropic inequalities in two different ways, once by accounting for non-observable CI relations and once without. The existence of *novel* Shannon-type inequalities upon accounting for non-observable CI relations is evidence for the DAG being interesting. The only loophole is that perhaps those novel Shannon-type inequalities are actually non-novel non-Shannon-type inequalities implied by the observable CI relations alone.

One way to close this loophole would be to show that the novel Shannon-type inequalities imply constraints beyond some inner approximation to the genuine entropy cone absent non-observable CI relations, perhaps along the lines of Ref. [15]. Another is to use incompatibility witnesses beyond entropic inequalities to identify some CI-respecting incompatible observable distribution. Pienaar [25] accomplished precisely this, and should be credited with the original insight to explicitly consider the different values that an observable root variable might take. In the following, we demonstrate how the inflation technique can be used for this purpose. So far, we have only considered one of the three enigmatic causal structures, namely Fig. 18.

The following representative polynomial inequalities follow from Hardy-type derivations, per Sec. VI.

$$P_A(0)P_{ADE}(000) \leq P_{AE}(00)P_{AF}(00) + P_A(0)P_{ADF}(001) \tag{C.1}$$

$$P_A(0)P_{ADE}(100) \leq P_{AE}(10)P_{AF}(00) + P_A(1)P_{ADF}(001) \tag{C.2}$$

For example, the second inequality may be explicitly derived as follows. One Hardy-type probabilistic inequality required for consistency of marginal distributions is

$$P_{A_1A_2DE_2}(0100) \leq P_{A_1A_2F_1E_2}(0100) + P_{A_1A_2DF_1}(0101). \tag{C.3}$$

Applying factorization as per the independence relations of the inflated DAG, we obtain the precursor to Eq. (C.2), namely

$$P_{A_1}(0)P_{A_2DE_2}(100) \leq P_{A_1F_1}(01)P_{A_2E_2}(00) + P_{A_2}(1)P_{A_1DF_1}(001). \tag{C.4}$$

A distribution incompatible with Fig. 18 discovered by Pienaar [25] is given by

$$P^{\text{JP}}_{ADEF} = \frac{[0000]+[0101]+[1000]+[1110]}{4}, \quad \text{i.e.} \quad P^{\text{JP}}_{ADEF}(adef) = \begin{cases} \frac{1}{4} & \text{if } e{=}a{\cdot}d \text{ and } f{=}(a{\oplus}1){\cdot}d, \\ 0 & \text{otherwise.} \end{cases} \tag{C.5}$$

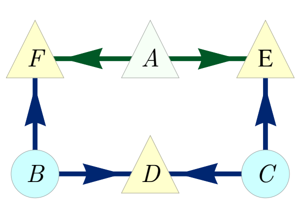

FIG. 18. DAG #15 in Ref. [11].

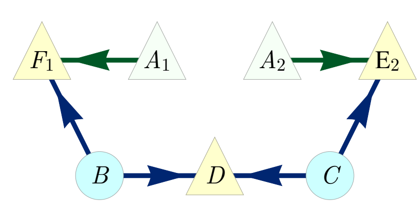

FIG. 19. A useful inflation of Fig. 18.

This distribution is indeed rejected by Eq. (C.2), although it satisfies the observable CI relations, which state that $A \perp D$ and $E \perp F|A$ [11]. Another way to see that this distribution is not compatible with Eq. (C.2) is by noting that the marginal distribution P^{JP}_{DEF} is not even compatible with the triangle scenario, since it violates inequality #8 of Appendix E. This is the same inequality which rejects the W-distribution of Eq. (15). Yet another interesting point is that P^{JP} not only satisfies all Shannon-type entropic inequalities pertinent to Fig. 18, but lies within an inner approximation to the genuine entropy cone for that scenario[16]. In other words, there exists a distribution with the same joint and marginal entropies as P^{JP} which *is* compatible with Fig. 18.

Finally, it may be worth noting that the inflation of Fig. 19 is precisely the "bilocality" scenario considered by Branciard *et al.* [27], so that inflation also permits us to translate every "bilocality" inequality into an inequality for the interesting DAG of Fig. 18.

[16] This is due to Weilenmann and Colbeck (private correspondence).

Appendix D: The Copy Lemma and Non-Shannon type Entropic Inequalities

onShannon

As it turns out, the inflation technique is also useful outside of the problem of causal inference. As we argue in the following, inflation is secretly what underlies the **Copy Lemma** in the derivation of non-Shannon type entropic inequalities [90, Chapter 15]. The following formulation of the Copy Lemma is the one of Kaced [91].

Lemma 7. *Let A, B and C be random variables with distribution P_{ABC}. Then there exists a fourth random variable A' and joint distribution $P_{AA'BC}$ such that:*

1. $P_{AB} = P_{A'B}$,
2. $A' \perp AC \mid B$.

copylemma

The proof via inflation is as follows.

Proof. We begin by noting that every possible joint distribution P_{ABC} is compatible with a DAG of the form of Fig. 20. This follows from the fact that one may take X to be any **sufficient statistic** for the joint variable (A, C) given B, such as $X := (A, B, C)$. Next, we consider the inflation of Fig. 20 depicted in Fig. 21. The maximal injectable sets are $\{A_1B_1C_1\}$ and $\{A_2B_1\}$. By lemma 3, because P_{ABC} is assumed to be compatible with Fig. 20, it follows that the marginals $\{P_{A_1B_1C_1}, P_{A_2B_1}\}$, where $P_{A_1B_1C_1} := P_{ABC}$ and $P_{A_2B_1} := P_{AB}$, are compatible with the inflated model with the DAG of Fig. 21. The fact that A_2 is d-separated from A_1C_1 by B_1 in Fig. 21 implies that the joint distribution can be expressed as $P_{A_1A_2B_1C_1} := P_{A_1B_1C_1}P_{A_2B_1}/P_{B_1}$. By construction, $P_{A_1A_2B_1C_1}$ has $P_{A_1B_1} = P_{A_2B_1} = P_{AB}$ and satisfies the conditional independence relation $A_2 \perp A_1C_1 \mid B_1$. □

While it is also not hard to write down a distribution with the desired properties explicitly [90, Lemma 15.8], the fact that one can rederive it using the inflation technique is significant.

All the non-Shannon type inequalities derived by Dougherty *et al.* [92] are obtained by applying some Shannon type inequality to the distribution that is implied to exist by the Copy Lemma. Our result shows, therefore, that one can understand these non-Shannon type inequalities for a DAG as arising from Shannon type inequalities applied to an inflation of the DAG. Indeed, it may be that the inflation technique may be a more general-purpose tool for deriving non-Shannon type entropic inequalities. A natural question is whether more sophisticated applications of the inflation technique might result in *new* examples of such inequalities.

Note that this inflation is non-broadcasting. The Copy Lemma is therefore valid even in the paradigm of quantum mechanics or any generalized probability theory, as we would expect. [R:Why do we expect this?]

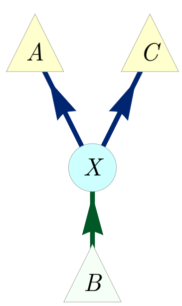

FIG. 20. A causal structure that is compatible with any distribution P_{ABC}.

fig:beforecopy

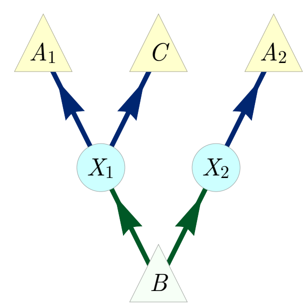

fig:aftercopy

FIG. 21. An inflation of Fig. 20. [Add subscripts to B and C in keeping with our notational convention. —RWS]

Appendix E: Classifying polynomial inequalities for the Triangle scenario

c:38ineqs

The following polynomial inequalities for the Triangle scenario have been derived via the linear quantifier elimination method of Sec. V using the inflated DAG of Fig. 3. Initially this has resulted in 64 symmetry classes of inequalities, where the symmetries are given by permuting the variables and inverting the outcomes. For the resulting 64 inequalities, numerical checks have found violations of only 38 of them: although they are all facets of the marginal polytope over the distributions on pre-injectable sets, there is no guarantee that they are also nontrivial inequalities at the level of the original DAG, and this has indeed turned out not to be the case for 26 of these symmetry classes of inequalities. Moreover, it is still likely to be the case that some of these inequalities are redundant; we have not yet checked whether for every inequality there is a distribution which violates the inequality but satisfies all others.

In the following table, the inequalities are listed in expectation-value form, where we assume the two possible outcomes of each variables to be $\{-1, +1\}$. Each row in the table gives the coefficients with one inequality, which is then ≥ 0.

TABLE II. List of inequalities as table of coefficients. This is a machine-readable version of the table on Page 32. tab:machi

	constant	$\langle A\rangle$	$\langle B\rangle$	$\langle C\rangle$	$\langle AB\rangle$	$\langle AC\rangle$	$\langle BC\rangle$	$\langle ABC\rangle$	$\langle A\rangle\langle B\rangle$	$\langle A\rangle\langle C\rangle$	$\langle B\rangle\langle C\rangle$	$\langle C\rangle\langle AB\rangle$	$\langle B\rangle\langle AC\rangle$	$\langle A\rangle\langle BC\rangle$	$\langle A\rangle\langle B\rangle\langle C\rangle$
(#1):	1	0	0	0	1	1	0	0	0	0	1	0	0	0	0
(#2):	2	0	0	0	0	-2	0	0	0	0	0	-1	0	0	1
(#3):	3	1	1	1	3	-1	0	0	0	0	-1	1	-1	0	1
(#4):	3	1	1	-1	3	1	0	0	0	0	1	-1	-1	0	1
(#5):	3	0	0	1	-2	0	-2	0	1	0	0	-1	-1	0	1
(#6):	3	0	1	0	1	0	-2	0	-1	1	0	1	-1	0	1
(#7):	3	0	1	0	1	0	-2	0	1	-1	0	1	1	0	-1
(#8):	3	1	1	1	2	2	2	-1	1	1	1	1	1	1	-1
(#9):	3	1	1	1	2	0	-2	1	1	-1	1	1	1	-1	-1
(#10):	4	0	0	2	-2	-2	0	-1	2	0	2	1	1	1	0
(#11):	4	0	-2	0	-2	0	-3	1	0	0	1	1	-1	0	1
(#12):	4	0	0	-2	-2	-2	-3	1	2	0	1	1	1	0	-1
(#13):	4	0	0	0	2	-2	1	1	2	2	-1	1	-1	0	-1
(#14):	4	0	0	0	2	-2	1	1	-2	2	-1	1	1	0	1
(#15):	4	0	0	0	-2	0	3	1	2	0	1	-1	-1	0	1
(#16):	4	0	0	-2	-2	-2	-2	1	2	0	0	1	1	-1	0
(#17):	4	0	0	0	-2	-2	-2	1	2	2	2	1	1	1	0
(#18):	5	1	1	1	3	1	-4	0	-2	0	1	1	-1	0	1
(#19):	5	1	1	1	3	-1	-4	0	2	-2	1	1	1	0	-1
(#20):	5	1	-1	1	1	2	-2	-2	-2	-1	1	1	-2	-2	0
(#21):	5	3	1	1	1	3	1	-1	2	0	0	-2	0	0	2
(#22):	5	1	1	1	1	2	-2	-1	0	-1	-1	2	1	1	-2
(#23):	5	-1	1	1	1	1	-1	1	-2	-2	2	-2	-2	-2	0
(#24):	5	1	1	1	2	1	-1	1	-1	0	2	-1	-2	-2	1
(#25):	5	1	1	1	-1	2	2	1	-2	-1	-1	2	1	-1	-2
(#26):	6	0	0	0	-3	-4	0	0	1	2	2	-1	-2	-2	1
(#27):	6	0	2	0	3	-4	0	0	1	2	0	1	-2	-2	1
(#28):	6	-2	2	0	-3	-5	0	0	1	1	0	1	-1	-2	2
(#29):	6	0	0	0	1	-3	2	0	1	1	-4	1	-1	-2	-2
(#30):	6	0	0	2	0	3	-5	0	-2	1	1	2	1	1	-2
(#31):	6	0	0	-2	2	-2	1	0	-4	2	-1	2	2	1	1
(#32):	6	0	0	0	-3	-2	-2	-2	1	0	4	-1	-2	0	1
(#33):	7	1	1	1	2	1	-3	3	1	-2	2	3	2	-2	-1
(#34):	8	0	0	0	-4	-2	-2	-3	4	2	-2	1	-1	-3	2
(#35):	8	2	-2	0	1	-6	0	1	-1	0	2	2	1	-3	3
(#36):	8	2	0	0	6	1	-2	1	0	1	2	-1	-2	-3	3
(#37):	8	0	-2	-2	0	-6	1	1	2	0	-1	3	1	-2	-3
(#38):	8	0	0	2	2	1	-6	1	-2	1	0	3	2	-1	-3

nontriv

(#1): $0 \le 1 + \langle B \rangle \langle C \rangle + \langle AB \rangle + \langle AC \rangle$

(#2): $0 \le 2 + \langle A \rangle \langle B \rangle \langle C \rangle - \langle C \rangle \langle AB \rangle - 2 \langle AC \rangle$

(#3): $0 \le 3 + \langle A \rangle + \langle B \rangle + \langle C \rangle - \langle B \rangle \langle C \rangle + \langle A \rangle \langle B \rangle \langle C \rangle + 3 \langle AB \rangle + \langle C \rangle \langle AB \rangle - \langle AC \rangle - \langle B \rangle \langle AC \rangle$

(#4): $0 \le 3 + \langle A \rangle + \langle B \rangle - \langle C \rangle + \langle B \rangle \langle C \rangle + \langle A \rangle \langle B \rangle \langle C \rangle + 3 \langle AB \rangle - \langle C \rangle \langle AB \rangle + \langle AC \rangle - \langle B \rangle \langle AC \rangle$

(#5): $0 \le 3 + \langle A \rangle \langle B \rangle + \langle C \rangle + \langle A \rangle \langle B \rangle \langle C \rangle - 2 \langle AB \rangle - \langle C \rangle \langle AB \rangle - \langle B \rangle \langle AC \rangle - 2 \langle BC \rangle$

(#6): $0 \le 3 + \langle B \rangle - \langle A \rangle \langle B \rangle + \langle A \rangle \langle C \rangle + \langle A \rangle \langle B \rangle \langle C \rangle + \langle AB \rangle + \langle C \rangle \langle AB \rangle - \langle B \rangle \langle AC \rangle - 2 \langle BC \rangle$

(#7): $0 \le 3 + \langle B \rangle + \langle A \rangle \langle B \rangle - \langle A \rangle \langle C \rangle - \langle A \rangle \langle B \rangle \langle C \rangle + \langle AB \rangle + \langle C \rangle \langle AB \rangle + \langle B \rangle \langle AC \rangle - 2 \langle BC \rangle$

(#8): $0 \le 3 + \langle A \rangle + \langle B \rangle + \langle A \rangle \langle B \rangle + \langle C \rangle + \langle A \rangle \langle C \rangle + \langle B \rangle \langle C \rangle - \langle A \rangle \langle B \rangle \langle C \rangle + 2 \langle AB \rangle + \langle C \rangle \langle AB \rangle + 2 \langle AC \rangle + \langle B \rangle \langle AC \rangle + 2 \langle BC \rangle + \langle A \rangle \langle BC \rangle - \langle ABC \rangle$

(#9): $0 \le 3 + \langle A \rangle + \langle B \rangle + \langle A \rangle \langle B \rangle + \langle C \rangle - \langle A \rangle \langle C \rangle + \langle B \rangle \langle C \rangle - \langle A \rangle \langle B \rangle \langle C \rangle + 2 \langle AB \rangle + \langle C \rangle \langle AB \rangle + \langle B \rangle \langle AC \rangle - 2 \langle BC \rangle - \langle A \rangle \langle BC \rangle + \langle ABC \rangle$

(#10): $0 \le 4 + 2 \langle A \rangle \langle B \rangle + 2 \langle C \rangle + 2 \langle B \rangle \langle C \rangle - 2 \langle AB \rangle + \langle C \rangle \langle AB \rangle - 2 \langle AC \rangle + \langle B \rangle \langle AC \rangle + \langle A \rangle \langle BC \rangle - \langle ABC \rangle$

(#11): $0 \le 4 - 2 \langle B \rangle + \langle B \rangle \langle C \rangle + \langle A \rangle \langle B \rangle \langle C \rangle - 2 \langle AB \rangle + \langle C \rangle \langle AB \rangle - \langle B \rangle \langle AC \rangle - 3 \langle BC \rangle + \langle ABC \rangle$

(#12): $0 \le 4 + 2 \langle A \rangle \langle B \rangle - 2 \langle C \rangle + \langle B \rangle \langle C \rangle - \langle A \rangle \langle B \rangle \langle C \rangle - 2 \langle AB \rangle + \langle C \rangle \langle AB \rangle - 2 \langle AC \rangle + \langle B \rangle \langle AC \rangle - 3 \langle BC \rangle + \langle ABC \rangle$

(#13): $0 \le 4 + 2 \langle A \rangle \langle B \rangle + 2 \langle A \rangle \langle C \rangle - \langle B \rangle \langle C \rangle - \langle A \rangle \langle B \rangle \langle C \rangle + 2 \langle AB \rangle + \langle C \rangle \langle AB \rangle - 2 \langle AC \rangle - \langle B \rangle \langle AC \rangle + \langle BC \rangle + \langle ABC \rangle$

(#14): $0 \le 4 - 2 \langle A \rangle \langle B \rangle + 2 \langle A \rangle \langle C \rangle - \langle B \rangle \langle C \rangle + \langle A \rangle \langle B \rangle \langle C \rangle + 2 \langle AB \rangle + \langle C \rangle \langle AB \rangle - 2 \langle AC \rangle + \langle B \rangle \langle AC \rangle + \langle BC \rangle + \langle ABC \rangle$

(#15): $0 \le 4 + 2 \langle A \rangle \langle B \rangle + \langle B \rangle \langle C \rangle + \langle A \rangle \langle B \rangle \langle C \rangle - 2 \langle AB \rangle - \langle C \rangle \langle AB \rangle - \langle B \rangle \langle AC \rangle + 3 \langle BC \rangle + \langle ABC \rangle$

(#16): $0 \le 4 + 2 \langle A \rangle \langle B \rangle - 2 \langle C \rangle - 2 \langle AB \rangle + \langle C \rangle \langle AB \rangle - 2 \langle AC \rangle + \langle B \rangle \langle AC \rangle - 2 \langle BC \rangle - \langle A \rangle \langle BC \rangle + \langle ABC \rangle$

(#17): $0 \le 4 + 2 \langle A \rangle \langle B \rangle + 2 \langle A \rangle \langle C \rangle + 2 \langle B \rangle \langle C \rangle - 2 \langle AB \rangle + \langle C \rangle \langle AB \rangle - 2 \langle AC \rangle + \langle B \rangle \langle AC \rangle - 2 \langle BC \rangle + \langle A \rangle \langle BC \rangle + \langle ABC \rangle$

(#18): $0 \le 5 + \langle A \rangle + \langle B \rangle - 2 \langle A \rangle \langle B \rangle + \langle C \rangle + \langle B \rangle \langle C \rangle + \langle A \rangle \langle B \rangle \langle C \rangle + 3 \langle AB \rangle + \langle C \rangle \langle AB \rangle + \langle AC \rangle - \langle B \rangle \langle AC \rangle - 4 \langle BC \rangle$

(#19): $0 \le 5 + \langle A \rangle + \langle B \rangle + 2 \langle A \rangle \langle B \rangle + \langle C \rangle - 2 \langle A \rangle \langle C \rangle + \langle B \rangle \langle C \rangle - \langle A \rangle \langle B \rangle \langle C \rangle + 3 \langle AB \rangle + \langle C \rangle \langle AB \rangle - \langle AC \rangle + \langle B \rangle \langle AC \rangle - 4 \langle BC \rangle$

(#20): $0 \le 5 + \langle A \rangle - \langle B \rangle - 2 \langle A \rangle \langle B \rangle + \langle C \rangle - \langle A \rangle \langle C \rangle + \langle B \rangle \langle C \rangle + \langle AB \rangle + \langle C \rangle \langle AB \rangle + 2 \langle AC \rangle - 2 \langle B \rangle \langle AC \rangle - 2 \langle BC \rangle - 2 \langle A \rangle \langle BC \rangle - 2 \langle ABC \rangle$

(#21): $0 \le 5 + 3 \langle A \rangle + \langle B \rangle + 2 \langle A \rangle \langle B \rangle + \langle C \rangle + 2 \langle A \rangle \langle B \rangle \langle C \rangle + \langle AB \rangle - 2 \langle C \rangle \langle AB \rangle + 3 \langle AC \rangle + \langle BC \rangle - \langle ABC \rangle$

(#22): $0 \le 5 + \langle A \rangle + \langle B \rangle + \langle C \rangle - \langle A \rangle \langle C \rangle - \langle B \rangle \langle C \rangle - 2 \langle A \rangle \langle B \rangle \langle C \rangle + \langle AB \rangle + 2 \langle C \rangle \langle AB \rangle + 2 \langle AC \rangle + \langle B \rangle \langle AC \rangle - 2 \langle BC \rangle + \langle A \rangle \langle BC \rangle - \langle ABC \rangle$

(#23): $0 \le 5 - \langle A \rangle + \langle B \rangle - 2 \langle A \rangle \langle B \rangle + \langle C \rangle - 2 \langle A \rangle \langle C \rangle + 2 \langle B \rangle \langle C \rangle + \langle AB \rangle - 2 \langle C \rangle \langle AB \rangle + \langle AC \rangle - 2 \langle B \rangle \langle AC \rangle - \langle BC \rangle - 2 \langle A \rangle \langle BC \rangle + \langle ABC \rangle$

(#24): $0 \le 5 + \langle A \rangle + \langle B \rangle - \langle A \rangle \langle B \rangle + \langle C \rangle + 2 \langle B \rangle \langle C \rangle + \langle A \rangle \langle B \rangle \langle C \rangle + 2 \langle AB \rangle - \langle C \rangle \langle AB \rangle + \langle AC \rangle - 2 \langle B \rangle \langle AC \rangle - \langle BC \rangle - 2 \langle A \rangle \langle BC \rangle + \langle ABC \rangle$

(#25): $0 \le 5 + \langle A \rangle + \langle B \rangle - 2 \langle A \rangle \langle B \rangle + \langle C \rangle - \langle A \rangle \langle C \rangle - \langle B \rangle \langle C \rangle - 2 \langle A \rangle \langle B \rangle \langle C \rangle - \langle AB \rangle + 2 \langle C \rangle \langle AB \rangle + 2 \langle AC \rangle + \langle B \rangle \langle AC \rangle + 2 \langle BC \rangle - \langle A \rangle \langle BC \rangle + \langle ABC \rangle$

(#26): $0 \le 6 + \langle A \rangle \langle B \rangle + 2 \langle A \rangle \langle C \rangle + 2 \langle B \rangle \langle C \rangle + \langle A \rangle \langle B \rangle \langle C \rangle - 3 \langle AB \rangle - \langle C \rangle \langle AB \rangle - 4 \langle AC \rangle - 2 \langle B \rangle \langle AC \rangle - 2 \langle A \rangle \langle BC \rangle$

(#27): $0 \le 6 + 2 \langle B \rangle + \langle A \rangle \langle B \rangle + 2 \langle A \rangle \langle C \rangle + \langle A \rangle \langle B \rangle \langle C \rangle + 3 \langle AB \rangle + \langle C \rangle \langle AB \rangle - 4 \langle AC \rangle - 2 \langle B \rangle \langle AC \rangle - 2 \langle A \rangle \langle BC \rangle$

(#28): $0 \le 6 - 2 \langle A \rangle + 2 \langle B \rangle + \langle A \rangle \langle B \rangle + \langle A \rangle \langle C \rangle + 2 \langle A \rangle \langle B \rangle \langle C \rangle - 3 \langle AB \rangle + \langle C \rangle \langle AB \rangle - 5 \langle AC \rangle - \langle B \rangle \langle AC \rangle - 2 \langle A \rangle \langle BC \rangle$

(#29): $0 \le 6 + \langle A \rangle \langle B \rangle + \langle A \rangle \langle C \rangle - 4 \langle B \rangle \langle C \rangle - 2 \langle A \rangle \langle B \rangle \langle C \rangle + \langle AB \rangle + \langle C \rangle \langle AB \rangle - 3 \langle AC \rangle - \langle B \rangle \langle AC \rangle + 2 \langle BC \rangle - 2 \langle A \rangle \langle BC \rangle$

(#30): $0 \le 6 - 2 \langle A \rangle \langle B \rangle + 2 \langle C \rangle + \langle A \rangle \langle C \rangle + \langle B \rangle \langle C \rangle - 2 \langle A \rangle \langle B \rangle \langle C \rangle + 2 \langle C \rangle \langle AB \rangle + 3 \langle AC \rangle + \langle B \rangle \langle AC \rangle - 5 \langle BC \rangle + \langle A \rangle \langle BC \rangle$

(#31): $0 \le 6 - 4 \langle A \rangle \langle B \rangle - 2 \langle C \rangle + 2 \langle A \rangle \langle C \rangle - \langle B \rangle \langle C \rangle + \langle A \rangle \langle B \rangle \langle C \rangle + 2 \langle AB \rangle + 2 \langle C \rangle \langle AB \rangle - 2 \langle AC \rangle + 2 \langle B \rangle \langle AC \rangle + \langle BC \rangle + \langle A \rangle \langle BC \rangle$

(#32): $0 \le 6 + \langle A \rangle \langle B \rangle + 4 \langle B \rangle \langle C \rangle + \langle A \rangle \langle B \rangle \langle C \rangle - 3 \langle AB \rangle - \langle C \rangle \langle AB \rangle - 2 \langle AC \rangle - 2 \langle B \rangle \langle AC \rangle - 2 \langle BC \rangle - 2 \langle ABC \rangle$

(#33): $0 \le 7 + \langle A \rangle + \langle B \rangle + \langle A \rangle \langle B \rangle + \langle C \rangle - 2 \langle A \rangle \langle C \rangle + 2 \langle B \rangle \langle C \rangle - \langle A \rangle \langle B \rangle \langle C \rangle + 2 \langle AB \rangle + 3 \langle C \rangle \langle AB \rangle + \langle AC \rangle + 2 \langle B \rangle \langle AC \rangle - 3 \langle BC \rangle - 2 \langle A \rangle \langle BC \rangle + 3 \langle ABC \rangle$

(#34): $0 \le 8 + 4 \langle A \rangle \langle B \rangle + 2 \langle A \rangle \langle C \rangle - 2 \langle B \rangle \langle C \rangle + 2 \langle A \rangle \langle B \rangle \langle C \rangle - 4 \langle AB \rangle + \langle C \rangle \langle AB \rangle - 2 \langle AC \rangle - \langle B \rangle \langle AC \rangle - 2 \langle BC \rangle - 3 \langle A \rangle \langle BC \rangle - 3 \langle ABC \rangle$

(#35): $0 \le 8 + 2 \langle A \rangle - 2 \langle B \rangle - \langle A \rangle \langle B \rangle + 2 \langle B \rangle \langle C \rangle + 3 \langle A \rangle \langle B \rangle \langle C \rangle + \langle AB \rangle + 2 \langle C \rangle \langle AB \rangle - 6 \langle AC \rangle + \langle B \rangle \langle AC \rangle - 3 \langle A \rangle \langle BC \rangle + \langle ABC \rangle$

(#36): $0 \le 8 + 2 \langle A \rangle + \langle A \rangle \langle C \rangle + 2 \langle B \rangle \langle C \rangle + 3 \langle A \rangle \langle B \rangle \langle C \rangle + 6 \langle AB \rangle - \langle C \rangle \langle AB \rangle + \langle AC \rangle - 2 \langle B \rangle \langle AC \rangle - 2 \langle BC \rangle - 3 \langle A \rangle \langle BC \rangle + \langle ABC \rangle$

(#37): $0 \le 8 - 2 \langle B \rangle + 2 \langle A \rangle \langle B \rangle - 2 \langle C \rangle - \langle B \rangle \langle C \rangle - 3 \langle A \rangle \langle B \rangle \langle C \rangle + 3 \langle C \rangle \langle AB \rangle - 6 \langle AC \rangle + \langle B \rangle \langle AC \rangle + \langle BC \rangle - 2 \langle A \rangle \langle BC \rangle + \langle ABC \rangle$

(#38): $0 \le 8 - 2 \langle A \rangle \langle B \rangle + 2 \langle C \rangle + \langle A \rangle \langle C \rangle - 3 \langle A \rangle \langle B \rangle \langle C \rangle + 2 \langle AB \rangle + 3 \langle C \rangle \langle AB \rangle + \langle AC \rangle + 2 \langle B \rangle \langle AC \rangle - 6 \langle BC \rangle - \langle A \rangle \langle BC \rangle + \langle ABC \rangle$

causality [1] J. Pearl, *Causality: Models, Reasoning, and Inference* (Cambridge University Press, 2009).

causation [2] P. Spirtes, C. Glymour, and R. Scheines, *Causation, Prediction, and Search*, Lecture Notes in Statistics (Springer New York, 2011).

abilistic [3] M. Studený, *Probabilistic Conditional Independence Structures*, Information Science and Statistics (Springer London, 2005).

abilistic [4] D. Koller, *Probabilistic Graphical Models: Principles and Techniques* (MIT Press, Cambridge, MA, 2009).

eSpekkens [5] C. M. Lee and R. W. Spekkens, "Causal inference via algebraic geometry: necessary and sufficient conditions for the feasibility of discrete causal models," arXiv:1506.03880 (2015).

4einstein [6] J. S. Bell, "On the Einstein-Podolsky-Rosen paradox," Physics **1**, 195 (1964).

HOriginal [7] J. F. Clauser, M. A. Horne, A. Shimony, and R. A. Holt, "Proposed experiment to test local hidden-variable theories," Phys. Rev. Lett. **23**, 880 (1969).

r2013Bell [8] N. Brunner, D. Cavalcanti, S. Pironio, V. Scarani, and S. Wehner, "Bell nonlocality," Rev. Mod. Phys. **86**, 419 (2014).

dSpekkens [9] C. J. Wood and R. W. Spekkens, "The lesson of causal discovery algorithms for quantum correlations: causal explanations of Bell-inequality violations require fine-tuning," New J. Phys. **17**, 033002 (2015).

z2012bell [10] T. Fritz, "Beyond Bell's theorem: correlation scenarios," New J. Phys. **14**, 103001 (2012).

y2014gdag [11] J. Henson, R. Lal, and M. F. Pusey, "Theory-independent limits on correlations from generalized Bayesian networks," New J. Phys. **16**, 113043 (2014).

ondBellII [12] T. Fritz, "Beyond Bell's theorem II: Scenarios with arbitrary causal structure," Comm. Math. Phys. **341**, 391 (2015).

ignalling [13] R. Chaves and C. Budroni, "Entropic nonsignalling correlations," arXiv:1601.07555 (2015).

inference [14] R. Chaves, L. Luft, T. O. Maciel, D. Gross, D. Janzing, and B. Schölkopf, "Inferring latent structures via information inequalities," in *Proc. of the 30th Conference on Uncertainty in Artificial Intelligence* (AUAI, 2014) pp. 112–121.

6entropic [15] M. Weilenmann and R. Colbeck, "Non-Shannon inequalities in the entropy vector approach to causal structures," personal communication (2016).

ovariance [16] J. Aberg, R. Chaves, D. Gross, A. Kela, and K. U. von Prillwitz, "Inferring causal structures with covariance information," poster session, Quantum Networks conference (2016).

olynomial [17] R. Chaves, "Polynomial Bell inequalities," Phys. Rev. Lett. **116**, 010402 (2016).

rNetworks [18] A. Tavakoli, P. Skrzypczyk, D. Cavalcanti, and A. Acín, "Nonlocal correlations in the star-network configuration," Phys. Rev. A **90**, 062109 (2014).

tNetworks [19] D. Rosset, C. Branciard, T. J. Barnea, G. Pütz, N. Brunner, and N. Gisin, "Nonlinear Bell inequalities tailored for quantum networks," Phys. Rev. Lett. **116**, 010403 (2016).

cNetworks [20] A. Tavakoli, "Bell-type inequalities for arbitrary noncyclic networks," Phys. Rev. A **93**, 030101 (2016).

trumental [21] J. Pearl, "On the testability of causal models with latent and instrumental variables," in *Proc. 11th Conference on Uncertainty in Artificial Intelligence*, AUAI (Morgan Kaufmann, San Francisco, CA, 1995) pp. 435–443.

ancestors [22] B. Steudel and N. Ay, "Information-theoretic inference of common ancestors," Entropy **17**, 2304 (2015).

2014novel [23] R. Chaves, L. Luft, and D. Gross, "Causal structures from entropic information: geometry and novel scenarios," New J. Phys. **16**, 043001 (2014).

3marginal [24] T. Fritz and R. Chaves, "Entropic inequalities and marginal problems," IEEE Trans. Info. Theo. **59**, 803 (2013).

teresting [25] J. Pienaar, "Towards a characterisation of interesting causal graphs," unpublished, Quantum Networks conference (2016).

foquantum [26] R. Chaves, C. Majenz, and D. Gross, "Information–theoretic implications of quantum causal structures," Nat. Comm. **6**, 5766 (2015).

relations [27] C. Branciard, D. Rosset, N. Gisin, and S. Pironio, "Bilocal versus nonbilocal correlations in entanglement-swapping experiments," Phys. Rev. A **85**, 032119 (2012).

bits2Ways [28] W. Dür, G. Vidal, and J. I. Cirac, "Three qubits can be entangled in two inequivalent ways," Phys. Rev. A **62**, 062314 (2000).

:PRL:1665 [29] L. Hardy, "Nonlocality for two particles without inequalities for almost all entangled states," Phys. Rev. Lett. **71**, 1665 (1993).

field2012 [30] S. Mansfield and T. Fritz, "Hardy's non-locality paradox and possibilistic conditions for non-locality," Foundations of Physics **42**, 709 (2012).

l1966lhvm [31] J. S. Bell, "On the problem of hidden variables in quantum mechanics," Rev. Mod. Phys. **38**, 447 (1966).

convexity [32] J. M. Donohue and E. Wolfe, "Identifying nonconvexity in the sets of limited-dimension quantum correlations," Phys. Rev. A **92**, 062120 (2015).

elaxation [33] G. V. Steeg and A. Galstyan, "A sequence of relaxations constraining hidden variable models," in *Proc. 27th Conference on Uncertainty in Artificial Intelligence* (AUAI, 2011) pp. 717–726.

[34] B. S. Cirel'son, "Quantum generalizations of Bell's inequality," Lett. Math. Phys. **4**, 93 (1980).

[35] S. Popescu and D. Rohrlich, "Quantum nonlocality as an axiom," Found. Phys. **24**, 379 (1994).

[36] J. Barrett and S. Pironio, "Popescu-rohrlich correlations as a unit of nonlocality," Phys. Rev. Lett. **95**, 140401 (2005).

[37] Y.-C. Liang, R. W. Spekkens, and H. M. Wiseman, "Specker's parable of the overprotective seer: A road to contextuality, nonlocality and complementarity," Phys. Rep. **506**, 1 (2011).

[38] D. Roberts, *Aspects of Quantum Non-Locality*, Ph.D. thesis, University of Bristol (2004).

[39] I. Pitowsky, "George Boole's 'conditions of possible experience' and the quantum puzzle," Br. J. Philos. Sci. **45**, 95 (1994).

[40] I. Pitowsky, *Quantum Probability - Quantum Logic*, Lecture Notes in Physics, Berlin Springer Verlag, Vol. 321 (Springer Berlin Heidelberg, 1989).

[41] H. G. Kellerer, "Verteilungsfunktionen mit gegebenen Marginalverteilungen," Z. Wahrscheinlichkeitstheorie **3**, 247 (1964).

[42] A. J. Leggett and A. Garg, "Quantum mechanics versus macroscopic realism: is the flux there when nobody looks?" Phys. Rev. Lett. **54**, 857 (1985).

[43] M. Araújo, M. Túlio Quintino, C. Budroni, M. Terra Cunha, and A. Cabello, "All noncontextuality inequalities for the n-cycle scenario," Phys. Rev. A **88**, 022118 (2013), arXiv:1206.3212.

[44] S. Abramsky and A. Brandenburger, "The sheaf-theoretic structure of non-locality and contextuality," New Journal of Physics **13**, 113036 (2011).

[45] N. N. Vorob'ev, "Consistent families of measures and their extensions," Theory Probab. Appl. **7**, 147 (1960).

[46] T. Kahle, "Neighborliness of marginal polytopes," Beiträge Algebra Geom. **51**, 45 (2010).

[47] L. D. Garcia, M. Stillman, and B. Sturmfels, "Algebraic geometry of Bayesian networks," J. Symbol. Comp. **39**, 331 (2003), arXiv:math/0301255.

[48] C. Barrett, P. Fontaine, and C. Tinelli, "The Satisfiability Modulo Theories Library (SMT-LIB)," `www.SMT-LIB.org` (2016).

[49] C. Kang and J. Tian, "Polynomial constraints in causal bayesian networks," in *Proc. of the 23rd Conference on Uncertainty in Artificial Intelligence* (AUAI, 2007) pp. 200–208.

[50] A. Garuccio, "Hardy's approach, Eberhard's inequality, and supplementary assumptions," Phys. Rev. A **52**, 2535 (1995).

[51] A. Cabello, "Bell's theorem with and without inequalities for the three-qubit greenberger-horne-zeilinger and W states," Phys. Rev. A **65**, 032108 (2002).

[52] D. Braun and M.-S. Choi, "Hardy's test versus the Clauser-Horne-Shimony-Holt test of quantum nonlocality: Fundamental and practical aspects," Phys. Rev. A **78**, 032114 (2008).

[53] L. Mancinska and S. Wehner, "A unified view on Hardy's paradox and the CHSH inequality," arXiv:1407.2320 (2014).

[54] T. Eiter, K. Makino, and G. Gottlob, "Computational aspects of monotone dualization: A brief survey," Discrete Appl. Math. **156**, 2035 (2008).

[55] A. Fine, "Hidden variables, joint probability, and the Bell inequalities," Phys. Rev. Lett. **48**, 291 (1982).

[56] I. Namioka and R. Phelps, "Tensor products of compact convex sets," Pacific J. Math. **31**, 469 (1969).

[57] T. Bogart, M. Contois, and J. Gubeladze, "Hom-polytopes," Math. Z. **273**, 1267 (2013), arXiv:1111.3880.

[58] R. Chaves and T. Fritz, "Entropic approach to local realism and noncontextuality," Phys. Rev. A **85**, 032113 (2012).

[59] S. L. Braunstein and C. M. Caves, "Information-theoretic Bell inequalities," Phys. Rev. Lett. **61**, 662 (1988).

[60] B. W. Schumacher, "Information and quantum nonseparability," Phys. Rev. A **44**, 7047 (1991).

[61] H. Barnum, C. M. Caves, C. A. Fuchs, R. Jozsa, and B. Schumacher, "Noncommuting mixed states cannot be broadcast," Phys. Rev. Lett. **76**, 2818 (1996).

[62] H. Barnum, J. Barrett, M. Leifer, and A. Wilce, "Cloning and broadcasting in generic probabilistic theories," quant-ph/0611295 (2006).

[63] R. W. Spekkens, "Evidence for the epistemic view of quantum states: A toy theory," Phys. Rev. A **75**, 032110 (2007).

[64] H. Barnum and A. Wilce, "Post-classical probability theory," arXiv:1205.3833 (2012).

[65] P. Janotta and H. Hinrichsen, "Generalized probability theories: what determines the structure of quantum theory?" J. Phys. A **47**, 323001 (2014).

[66] B. Coecke and R. W. Spekkens, "Picturing classical and quantum Bayesian inference," Synthese **186**, 651 (2011).

[67] M. Navascués, S. Pironio, and A. Acín, "A convergent hierarchy of semidefinite programs characterizing the set of quantum correlations," New J. Phys. **10**, 073013 (2008).

[68] K. F. Pál and T. Vértesi, "Quantum bounds on bell inequalities," Phys. Rev. A **79**, 022120 (2009).

[69] D. Avis, D. Bremner, and R. Seidel, "How good are convex hull algorithms?" Computational Geometry **7**, 265 (1997).

[70] A. Fordan, *Projection in Constraint Logic Programming* (Ios Press, 1999).

[71] G. B. Dantzig and B. C. Eaves, "Fourier-Motzkin elimination and its dual," J. Combin. Th. A **14**, 288 (1973).

[72] T. S. Motzkin, H. Raiffa, G. L. Thompson, and R. M. Thrall, "The double description method," in *Contributions to theory of games*, Annals of Mathematics Studies, Vol. 2 (Princeton University Press, 1953) pp. 51–73.

ukuda1996 [73] K. Fukuda and A. Prodon, "Double description method revisited," Combinatorics and Computer Science: 8th Franco-Japanese and 4th Franco-Chinese Conference , 91 (1996).

hapot2012 [74] D. V. Shapot and A. M. Lukatskii, "Solution building for arbitrary system of linear inequalities in an explicit form," Am. J. Comp. Math. **02**, 1 (2012).

rakov2015 [75] S. I. Bastrakov and N. Y. Zolotykh, "Fast method for verifying Chernikov rules in Fourier-Motzkin elimination," Comp. Mat. & Math. Phys. **55**, 160 (2015).

qskeleton [76] S. Bastrakov, "qskeleton," `sbastrakov.github.io/qskeleton` (2016), polyhedral computation software for Fourier-Motzkin elimination with Chernikov rules.

is2000lrs [77] D. Avis, "A revised implementation of the reverse search vertex enumeration algorithm," in *Polytopes — Combinatorics and Computation*, DMV Seminar, Vol. 29, edited by G. Kalai and G. M. Ziegler (Birkhäuser Basel, 2000) pp. 177–198.

4equality [78] C. Jones, E. C. Kerrigan, and J. Maciejowski, *Equality set projection: A new algorithm for the projection of polytopes in halfspace representation*, Tech. Rep. (Cambridge University Engineering Dept, 2004).

hesis2005 [79] C. Jones, *Polyhedral Tools for Control*, Ph.D. thesis, University of Cambridge (2005).

Jones2008 [80] C. N. Jones, E. C. Kerrigan, and J. M. Maciejowski, "On polyhedral projection and parametric programming," J. Optimiz. Theo. Applic. **138**, 207 (2008).

ries_2009 [81] D. Bremner, M. Dutour Sikiric, and A. Schürmann, "Polyhedral representation conversion up to symmetries," in *Polyhedral computation*, CRM Proc. Lecture Notes, Vol. 48 (Amer. Math. Soc., 2009) pp. 45–71, arXiv:math/0702239.

rmann2013 [82] A. Schürmann, "Disc. geom. optim." (Springer International Publishing, Heidelberg, 2013) Chap. Exploiting Symmetries in Polyhedral Computations, pp. 265–278.

aibel2010 [83] V. Kaibel, L. Liberti, A. Schürmann, and R. Sotirov, "Mini-workshop: Exploiting symmetry in optimization," Oberwolfach Rep. , 2245 (2010).

ools_2012 [84] T. Rehn and A. Schürmann, "C++ tools for exploiting polyhedral symmetries," in *Proceedings of the Third International Congress Conference on Mathematical Software*, ICMS'10 (Springer-Verlag, Berlin, Heidelberg, 2010) pp. 295–298.

anda_2015 [85] S. Lörwald and G. Reinelt, "Panda: a software for polyhedral transformations," EURO Journal on Computational Optimization , 1 (2015).

ctionCone [86] E. Balas, "Projection with a minimal system of inequalities," Comp. Optimiz. Applic. **10**, 189 (1998).

mial_2012 [87] M. Laurent and P. Rostalski, "The approach of moments for polynomial equations," in *Handbook on Semidefinite, Conic and Polynomial Optimization*, edited by M. F. Anjos and J. B. Lasserre (Springer, 2012) pp. 25–60.

entingCRA [88] K. Korovin, N. Tsiskaridze, and A. Voronkov, "Implementing conflict resolution," Perspectives of Systems Informatics , 362 (2012).

implexSAT [89] F. Bobot, S. Conchon, E. Contejean, M. Iguernelala, A. Mahboubi, A. Mebsout, and G. Melquiond, "A simplex-based extension of fourier-motzkin for solving linear integer arithmetic," Automated Reasoning , 67 (2012).

work_2008 [90] R. W. Yeung, *Information Theory and Network Coding* (Springer US, Boston, MA, 2008) Chap. Beyond Shannon-Type Inequalities, pp. 361–386.

ence_2013 [91] T. Kaced, "Equivalence of two proof techniques for non-Shannon-type inequalities," in *Information Theory Proceedings (ISIT)* (IEEE, 2013) pp. 236–240, arXiv:1302.2994.

onshannon [92] R. Dougherty, C. F. Freiling, and K. Zeger, ""non-shannon information inequalities in four random variables"," CoRR **abs/1104.3602** (2011).

stBibItem