

The Inflation DAG Technique for Causal Inference with Hidden Variables

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~~The fundamental problem of causal inference is to infer from a given probability distribution over observed variables, what causal structures, possibly incorporating hidden variables, could have given rise to that distribution.~~

The fundamental problem of causal inference is to infer if an observed probability distribution is compatible with some causal structure hypothesis, possibly incorporating hidden variables. Given a particular causal structure, it is therefore valuable to derive incompatibility witnesses, i.e. criteria whose violation certifies 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 incompatibility witnesses 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 incompatibility witnesses, 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 criteria (i.e., that may have quantum violations), or post-classical criteria (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.

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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 [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~~ [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 [cite:LeeSpekkens]. 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 it is also reducible to a quantifier elimination problem. 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 (see, e.g. [?] [cite unpublished Rosset result]). However, it is not clear at present whether this is likely to be the case, and we do not pursue the question here. 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 [5]. 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) [7] showed how to derive inequalities directly from the causal structure. The CHSH inequality was the first example 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 [6]. The idea that such work is best understood as a contribution to the field of

causal inference, and therefore that The idea that such work is best understood as a contribution to the field of causal inference has only recently been appreciated [7, 10–12], as has the idea that techniques developed by researchers in the foundations of quantum theory may be usefully adapted to causal inference¹.

Move the following to the introduction of the quantum section: 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 [7]. 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.

Later on, Pearl derived another inequality, called the **instrumental inequality** [8], 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 [9] 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. [cite Fritz]

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 and follow-up work on nonShannn inequalities. 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. [provide citations] 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 CAUSAL INFERENCE

Definitions

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 $\text{Nodes}[G]$ and $\text{Edges}[G]$ 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.

¹ The current article being another example of the phenomenon [provide references].

$\text{Pa}_G(X) = \{Y \mid Y \rightarrow X\}$. Similarly the children of a node X in a given graph G are defined as those nodes which have directed edges originating at X and terminating at them, i.e. $\text{Ch}_G(X) = \{Y \mid X \rightarrow Y\}$. If \mathbf{U} is a set of nodes, then we put $\text{Pa}_G(\mathbf{U}) := \bigcup_{X \in \mathbf{U}} \text{Pa}_G(X)$ and $\text{Ch}_G(\mathbf{U}) := \bigcup_{X \in \mathbf{U}} \text{Ch}_G(X)$. The **ancestors** of a set of nodes \mathbf{U} , denoted $\text{An}_G(\mathbf{U})$, are defined as those nodes which have a directed *path* to some node in \mathbf{U} , including the nodes in \mathbf{U} themselves. **R: Does Pearl include \mathbf{U} among the ancestors? I wonder if “ancestry” might be better terminology.** Equivalently (dropping the G subscript), $\text{An}(\mathbf{U}) := \bigcup_{n \in \mathbb{N}} \text{Pa}^n(\mathbf{U})$, where $\text{Pa}^n(\mathbf{U})$ is inductively defined via $\text{Pa}^0(\mathbf{U}) := \mathbf{U}$ and $\text{Pa}^{n+1}(\mathbf{U}) := \text{Pa}(\text{Pa}^n(\mathbf{U}))$. A causal structure is a DAG that incorporates a distinction between two types of nodes: those that are observed, denoted $\text{ObservedNodes}[G]$ and those that are latent, denoted $\text{LatentNodes}[G]$. Following Ref. [HensonLalPusey], we will denote the observed nodes by triangles and the latent nodes by circles.² 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 (beyondBell111 [12, Appendix A], for instance, whether it is continuous or discrete, and, if the latter, the cardinality of the set of possible values that the variable can take.

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, denoted F_G , has the form

$$F_G \equiv \{P_{A|\text{Pa}_G(A)} : A \in \text{Nodes}[G]\}. \quad (1)$$

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

$$P(\text{Nodes}[G]) = \prod_{A \in \text{Nodes}[G]} P_{A|\text{Pa}_G(A)}, \quad (2) \quad \boxed{\{\text{Markov}\}}$$

(typically called the Markov condition), and the joint distribution over the observed variables is obtained from the joint distribution over all variables by marginalization over the latent variables

$$P(\text{ObservedNodes}[G]) = \sum_{\{X : X \in \text{LatentNodes}[G]\}} P(\text{Nodes}[G]). \quad (3) \quad \boxed{\{\text{MarkovObserved}\}}$$

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). ~~MarkovObserved~~

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 $\text{Inflations}[G]$. The choice of an element $G' \in \text{Inflations}[G]$ is the only freedom in the inflation of a causal model. Once a choice is made, the set of parameters of the inflation model M' is fixed uniquely by the set of parameters of the original model M by a function $\text{Inflation}[G \rightarrow G']$ (specified below), such that $M' = \text{Inflation}[G \rightarrow G']M$.

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

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, \dots, 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 $A_i \sim A_j \sim A$.

² Unlike Ref. [HensonLalPusey], who term these *generalized DAGs*, we will continue to refer to them as simply DAGs.

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 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 ,

$$G' \in \text{Inflations}[G] \quad \text{iff} \quad \forall A_i \in \text{Nodes}[G'] : \text{AnSubDAG}_{G'}[A_i] \sim \text{AnSubDAG}_G[A]. \quad (4) \quad \boxed{\text{fig:defin1}}$$

To illustrate the notion of the inflation of a DAG, 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), 7 (Fig. 18b), 10 (Fig. 3), 13 (Fig. 6a), 14 (Fig. 1a), 15 (Fig. 8), 9 (Fig. 1b), 16 (Fig. 4b)] Different inflations of the Triangle scenario are depicted in Figs. 2 to 6.

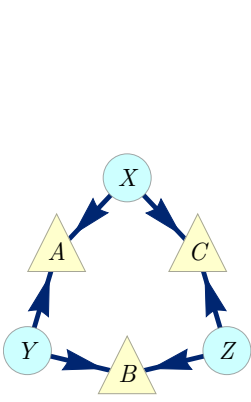


FIG. 1. The causal structure of the Triangle scenario.

fig:TriMainDAG

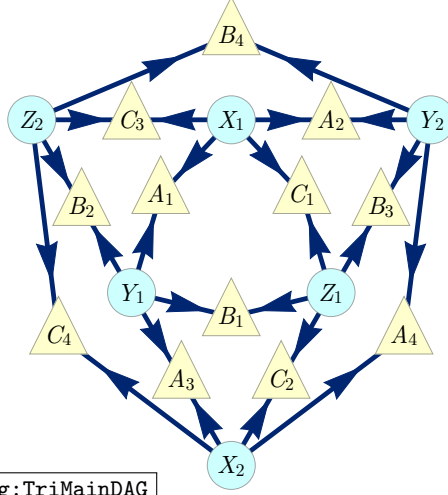


FIG. 2. An inflation DAG of the Triangle scenario where each latent node has been duplicated and each observable nodes node has been quadrupled. Note that no further duplication of observable nodes is needed, given that each has two latent nodes as parents in the original DAG and consequently there are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

fig:TriFullDouble

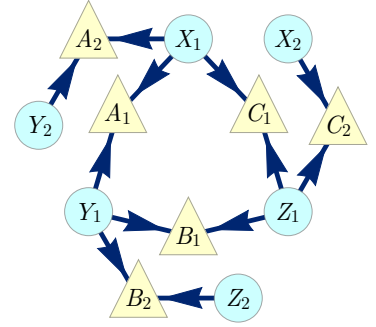


FIG. 3. Another inflation of the Triangle scenario consisting, also notably $\text{AnSubDAG}_{(\text{Fig. 2})}[A_1 A_2 B_1 B_2 C_1 C_2]$.

fig:Tri22

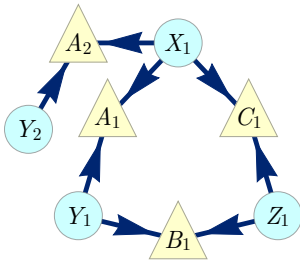


FIG. 4. A simple inflation of the Triangle scenario, also notably $\text{AnSubDAG}_{(\text{Fig. 3})}[A_1 A_2 B_1 C_1]$.

fig:AnSubDAG_inflation

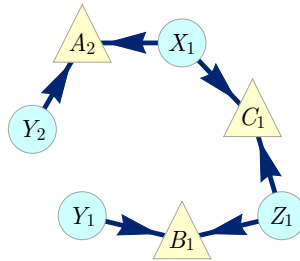


FIG. 5. An even simpler inflation of the Triangle scenario, also notably $\text{AnSubDAG}_{(\text{Fig. 4})}[A_2 B_1 C_1]$.

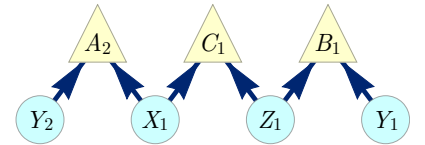


FIG. 6. Another representation of Fig. 5. Despite not containing the original scenario, this is a valid inflation per Eq. (4).

fig:TriDa

We now turn to specifying the function $\text{Inflation}[\]_{G \rightarrow G'}$, that is, to specifying how a causal model transforms under inflation. **PHYSICS needed here. Why mathematical abstraction? Explain that due to physical construct-ability, therefore we expect that models on the original DAG can be used to build a model on the inflation DAG...**

Definition 2. Consider causal models M and M' where $\text{DAG}[M] = G$ and $\text{DAG}[M'] = G'$ and such that G' is an inflation of G . The causal model M' is said to be the $G \rightarrow G'$ **inflation of M** , that is, $M' = \text{Inflation}[M]$, 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 $\text{Pa}_{G'}(A_i) \sim \text{Pa}_G(A)$ (given Eq. (4)), one can formalize this condition as:

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

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 inflation DAG with ancestral subgraphs mirroring those of the originals, and (ii) where the manner in which variables depend causally on their parents in the inflation 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].

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

$$\text{if } \text{AnSubDAG}_{G'}[U'] \sim \text{AnSubDAG}_G[U] \text{ then } P_{U'} = P_U. \quad (6) \quad \{\text{eq:coinc}\}$$

This follows from the fact that the probability distributions over U' and U depend only on their ancestral subgraphs and the parameters defined thereon, which by the definition of inflation are the same for U' and for U . It is useful to have a name for those sets of observed nodes in the inflation 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 $\text{InjectableSets}_{G' \rightarrow G}$.

$$U' \in \text{InjectableSets}_{G' \rightarrow G} \subseteq \text{ObservedNodes}[G'] \quad \text{iff} \quad \exists U \subseteq \text{ObservedNodes}[G] : \text{AnSubDAG}_{G'}[U'] \sim \text{AnSubDAG}_G[U]. \quad (7) \quad \{\text{eq:define}\}$$

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 inflation 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 $\text{ImagesInjectableSets}_{G' \rightarrow G}$.

$$U \in \text{ImagesInjectableSets}_{G' \rightarrow G} \quad \text{iff} \quad \exists U' \subseteq \text{ObservedNodes}[G'] : \text{AnSubDAG}_{G'}[U'] \sim \text{AnSubDAG}_G[U]. \quad (8) \quad \{\text{eq:define}\}$$

Clearly, $U \in \text{ImagesInjectableSets}_{G' \rightarrow G}$ iff $\exists U' \subseteq \text{InjectableSets}_{G' \rightarrow G}$ such that $U \sim U'$.

In the inflation of the triangle scenario depicted in Fig. 3, for example, the set of observed nodes $\{A_1 B_1 C_1\}$ 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 $\{A_2 C_1\}$ 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 inflation 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, $\{A_1 A_2 C_1\}$ is not injectable because it contains two copies of A , and $\{A_2 B_1 C_1\}$ is not injectable because its ancestral subgraph contains two copies of Y .

The fact that the sets $\{A_1 B_1 C_1\}$ and $\{A_2 C_1\}$ 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, $P'_{A_1 B_1 C_1} = P_{ABC}$ and $P'_{A_2 C_1} = P_{AC}$.

It is useful to express Eq. (7) in the language of injectable sets, namely, as

$$\text{if } U' \in \text{InjectableSets}_{G' \rightarrow G} \text{ and } U \sim U' \text{ then } P'_{U'} = P_U. \quad (9) \quad \{\text{keyinfer}\}$$

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 $\{P_U : U \in \text{ImagesInjectableSets}_{G' \rightarrow G}\}$ 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 $\{P'_{U'} : U' \in \text{InjectableSets}_{G' \rightarrow G}\}$ 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 $\mathbf{U} \in \text{ImagesInjectableSets}[\downarrow_{G' \rightarrow G}]$, 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 $\mathbf{U}' \in \text{InjectableSets}[\downarrow_{G' \rightarrow G}]$. But for a given pair \mathbf{U} and \mathbf{U}' such that $\mathbf{U} \sim \mathbf{U}'$, the parameters in the model M that determine the distribution on \mathbf{U} are, by the definition of inflation, precisely equal to the parameters in the model $M' = \text{Inflation}[M]_{G' \rightarrow G}$ that determine the distribution on \mathbf{U}' . Consequently, if there is a causal model M on G yielding the family $\{P_{\mathbf{U}} : \mathbf{U} \in \text{ImagesInjectableSets}[\downarrow_{G' \rightarrow G}]\}$ then there is a model M' on G' yielding the family $\{P'_{\mathbf{U}'} : \mathbf{U}' \in \text{InjectableSets}[\downarrow_{G' \rightarrow G}]\}$ with $P'_{\mathbf{U}'} = P_{\mathbf{U}}$.

We formalize the result as a lemma.

mainlemma

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

[Move the relevant figure here. Put the triangle and its inflation side by side. I think it's okay to repeat the triangle DAG in our figures.]

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,

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

and one would like to determine whether it is compatible with the Triangle scenario, that is, the DAG depicted in Fig. 3. 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. 6. The injectable sets in this case include $\{A_2C_1\}$ and $\{B_1C_1\}$. We therefore consider the marginals on these sets. fig:TriDagSubA2B1C1

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

$$P_{AC} = \frac{[00] + [11]}{2} \quad (11) \quad \boxed{\{j1\}}$$

$$P_{BC} = \frac{[00] + [11]}{2} \quad (12) \quad \boxed{\{j2\}}$$

But by lemma 3, this compatibility holds only if the following pair of marginals is compatible with the inflation DAG depicted in Fig. 6: mainlemma

$$P_{A_2C_1} = \frac{[00] + [11]}{2} \quad (13) \quad \boxed{\{k1\}}$$

$$P_{B_1C_1} = \frac{[00] + [11]}{2} \quad (14) \quad \boxed{\{k2\}}$$

It is not difficult to see that the latter pair of marginals is *not* compatible with our inflation 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 inflation DAG.

We have therefore certified that the joint distribution P_{ABC} of Eq. (10) is not compatible with the Triangle causal structure, recovering the seminal result of Steudel and Ay [9]. eq:ghzdistribution1

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

[Move the relevant figure here. Put the triangle and its inflation side by side. I think it's okay to repeat the triangle DAG in our figures.]

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

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

We call this the W-type distribution³.

To settle the compatibility question, we consider the inflation DAG of Fig. 3. The injectable sets in this case include $\{A_1 B_1 C_1\}$, $\{A_2 C_1\}$, $\{B_2 A_1\}$, $\{A_2 B_1\}$, $\{A_2\}$, $\{B_2\}$ and $\{C_2\}$.

Therefore, we turn our attention to determining whether the marginals of the W-type distribution on the images of these injectable sets are compatible with the triangle hypothesis. These marginals are:

$$P_{ABC} = \frac{[100] + [010] + [001]}{3} \quad (16) \quad \{\text{v4}\}$$

$$P_{AC} = \frac{[10] + [01] + [00]}{3} \quad (17) \quad \{\text{v1}\}$$

$$P_{BA} = \frac{[10] + [01] + [00]}{3} \quad (18) \quad \{\text{v2}\}$$

$$P_{CB} = \frac{[10] + [01] + [00]}{3} \quad (19) \quad \{\text{v3}\}$$

$$P_A = \frac{2}{3}[0] + \frac{1}{3}[1] \quad (20) \quad \{\text{v5}\}$$

$$P_B = \frac{2}{3}[0] + \frac{1}{3}[1] \quad (21) \quad \{\text{v6}\}$$

$$P_C = \frac{2}{3}[0] + \frac{1}{3}[1] \quad (22) \quad \{\text{v7}\}$$

But by lemma 3, this compatibility holds only if the following set of marginals is compatible with the inflation DAG depicted in Fig. 6:

$$P_{A_1 B_1 C_1} = \frac{[100] + [010] + [001]}{3} \quad (23) \quad \{\text{w4}\}$$

$$P_{A_2 C_1} = \frac{[10] + [01] + [00]}{3} \quad (24) \quad \{\text{w1}\}$$

$$P_{B_2 A_1} = \frac{[10] + [01] + [00]}{3} \quad (25) \quad \{\text{w2}\}$$

$$P_{C_2 B_1} = \frac{[10] + [01] + [00]}{3} \quad (26) \quad \{\text{w3}\}$$

$$P_{A_2} = \frac{2}{3}[0] + \frac{1}{3}[1] \quad (27) \quad \{\text{w5}\}$$

$$P_{B_2} = \frac{2}{3}[0] + \frac{1}{3}[1] \quad (28) \quad \{\text{w6}\}$$

$$P_{C_2} = \frac{2}{3}[0] + \frac{1}{3}[1] \quad (29) \quad \{\text{w7}\}$$

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 $C_2=1$,

$$A_2=1 \implies C_1=0 \quad (30) \quad \{\text{ws1}\}$$

$$B_2=1 \implies A_1=0 \quad (31) \quad \{\text{ws2}\}$$

$$C_2=1 \implies B_1=0 \quad (32) \quad \{\text{ws3}\}$$

³ Because its correlations are reminiscent of those one obtains for the quantum state appearing in Ref. [17], and which is called the W state.

Our inflation 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 inflation DAG. This fact, together with Eqs. (27)-(29), implies that A_2, B_2 , and C_2 sometimes all take the value 1,

$$\text{Sometimes } A_2=1, B_2=1, C_2=1. \quad (33) \quad \{\text{WW2}\}$$

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

$$\text{sometimes } A_1=0, B_1=0, C_1=0. \quad (34) \quad \{\text{WW3}\}$$

This, however, contradicts Eq. (23). Consequently, the set of marginals described in Eqs. (23)-(29) are *not* compatible with the DAG of Fig. 6. 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 [18, 19], see Sec. VIII 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 [13, 16, 20].
3. Moreover, *no* entropic inequality can witness the W-type distribution as unrealizable. Weilenmann and Colbeck [21] 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.* [22], 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 [5, 6, 23, 24] is compatible with a causal structure of the form of Fig. 7, as has been noted in several recent articles [5, 6, 23, 24] scenario [11 (Fig. E#2), 7 (Fig. 19), 13 (Fig. 1), 12 (Fig. 1), 25 (Fig. 2b), 26 (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*.

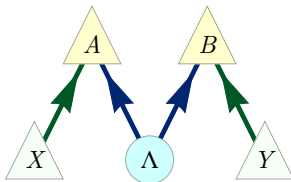


FIG. 7. The causal structure of the a bipartite Bell scenario. The local outcomes of Alice’s and Bob’s experimental probing is assumed to be a function of some latent common cause, in addition to their independent local experimental settings.

fig:NewBellDAG1

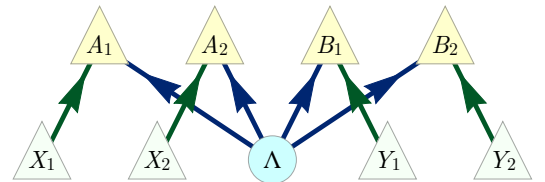


FIG. 8. An inflation DAG of the bipartite Bell scenario, where both local settings variables have been duplicated.

fig:BellDAG2

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 distribu-

tions⁴ over the binary variables X and Y , and

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

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 [cite: WoodSpekkens], 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 [cite] and later independently by Popescu and Rohrlich [27, 28]. 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. 8.

We begin by noting that $\{A_1 B_1 X_1 Y_1\}$, $\{A_2 B_1 X_2 Y_1\}$, $\{A_1 B_2 X_1 Y_2\}$, $\{A_2 B_2 X_2 Y_2\}$, $\{X_1\}$, $\{X_2\}$, $\{Y_1\}$, and $\{Y_2\}$ are all injectable sets. By lemma 3, it follows that

$$P_{A_1 B_1 X_1 Y_1} = P_{ABXY} \quad (36) \quad \boxed{\text{PR1}}$$

$$P_{A_2 B_1 X_2 Y_1} = P_{ABXY} \quad (37) \quad \boxed{\text{PR2}}$$

$$P_{A_1 B_2 X_1 Y_2} = P_{ABXY} \quad (38) \quad \boxed{\text{PR3}}$$

$$P_{A_2 B_2 X_2 Y_2} = P_{ABXY} \quad (39) \quad \boxed{\text{PR4}}$$

$$P_{X_1} = P_X \quad (40) \quad \boxed{\text{PR5}}$$

$$P_{X_2} = P_X \quad (41) \quad \boxed{\text{PR6}}$$

$$P_{Y_1} = P_Y \quad (42) \quad \boxed{\text{PR7}}$$

$$P_{Y_2} = P_Y. \quad (43) \quad \boxed{\text{PR8}}$$

Using the definition of conditional probability, we infer that

$$P_{A_1 B_1 | X_1 Y_1} = P_{AB|XY} \quad (44) \quad \boxed{\text{PR1b}}$$

$$P_{A_2 B_1 | X_2 Y_1} = P_{AB|XY} \quad (45) \quad \boxed{\text{PR2b}}$$

$$P_{A_1 B_2 | X_1 Y_2} = P_{AB|XY} \quad (46) \quad \boxed{\text{PR3b}}$$

$$P_{A_2 B_2 | X_2 Y_2} = P_{AB|XY}. \quad (47) \quad \boxed{\text{PR4b}}$$

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 inflation DAG, that is, we have $P_{X_1 X_2 Y_1 Y_2} = P_{X_1} P_{X_2} P_{Y_1} P_{Y_2}$ 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

$$\text{Sometimes } X_1=0, X_2=1, Y_1=0, Y_2=1. \quad (48) \quad \boxed{\text{PRs}}$$

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

$$X_1=0, Y_1=0 \implies A_1=B_1, \quad (49) \quad \boxed{\text{PRs1}}$$

$$X_1=0, Y_2=1 \implies A_1=B_2, \quad (50) \quad \boxed{\text{PRs2}}$$

$$X_2=1, Y_1=0 \implies A_2=B_1, \quad (51) \quad \boxed{\text{PRs3}}$$

$$X_2=1, Y_2=1 \implies A_2 \neq B_2. \quad (52) \quad \boxed{\text{PRs4}}$$

Combining Eq. (53) with Eqs. (49)-(52), we obtain

$$\text{Sometimes } A_1=B_1, A_1=B_2, A_2=B_1, A_2 \neq B_2. \quad (53) \quad \boxed{\text{PRs}}$$

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.

No values of A_1, A_2, B_1, B_2 can jointly satisfy these conditions—the first three properties entail perfect correlation between A_2 and B_2 —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_0 is the value of A when $X = 0$, and similarly for the others. They note that if the Bell DAG describes the experiment, then by taking the product of the conditional of A_0 given λ with the conditional of A_1 given λ , etcetera, one obtains 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 the 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. [Is there a citation we can provide for this argument? —RWS](#)

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 DAG G and a subset of the observed nodes thereon, $S \subseteq \text{ObservedNodes}[G]$. Let I_S denote an inequality that is evaluated on a family of marginal distributions $\{P_U : U \in S\}$. The inequality I_S is termed a causal compatibility inequality for the DAG G just in case it is satisfied by every family of distributions $\{P_U : U \in S\}$ that is compatible with G .

Note that violation of a causal compatibility inequality witnesses the incompatibility of a distribution with the associated DAG, but the inequality being satisfied does not guarantee that the distribution is compatible with the DAG. 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](#): [mainlemma](#)

corollary

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

The proof is as follows. Suppose that the family $\{P_U : U \in S\}$ is compatible with G . By lemma [3](#), [mainlemma](#) it follows that the family $\{P_{U'} : U' \in S'\}$ where $P_{U'} := P_U$ 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 $\{P_{U'} : U' \in S'\}$ satisfies $I_{S'}$. But I_S evaluated on $\{P_U : U \in S\}$ is equal to $I'(S')$ evaluated on $\{P_{U'} : U' \in S'\}$, by the definition of I_S , and therefore because $\{P_{U'} : U' \in S'\}$ satisfies $I_{S'}$ it follows that $\{P_U : U \in S\}$ satisfies I_S . This implication holds for every $\{P_U : U \in S\}$ 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 $X \not\sim_{\emptyset} Y$. Generalizing to sets, $U \not\sim_{\emptyset} V$ indicates that no node in U shares a common ancestor with any node in V ,

$$U \not\sim_{\emptyset} V \quad \text{iff} \quad \text{An}(U) \cap \text{An}(V) = \emptyset. \quad (54)$$

Furthermore, the notation $U \not\sim_{\emptyset} V \not\sim_{\emptyset} W$ should be understood as indicating that $U \not\sim_{\emptyset} V$ and $V \not\sim_{\emptyset} W$ and $U \not\sim_{\emptyset} W$. Ancestral independence is equivalent to d -separation by the empty set [\[1–4\]](#). [pearl2009causality,spirtes2011causation,studeny2011causality](#)

Example 1: 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. [6](#). [fig:TriDagSub](#)
The injectable sets we make use of here are $\{A_2C_1\}$, $\{B_1C_1\}$ and $\{B_1\}$.

From corollary [4.1](#), [maincorollary](#) any causal compatibility inequality for the inflation DAG that can be evaluated on the marginal distributions for $\{A_2C_1\}$, $\{B_1C_1\}$ and $\{B_1\}$ will yield a causal compatibility inequality for the original DAG that

can be evaluated on the marginal distributions for $\{AC\}$, $\{BC\}$ and $\{B\}$. We begin, therefore, by identifying a simple example of a causal compatibility inequality for the inflation DAG that is of this sort.

The example we use assumes that 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 [\[30–34\]](#), [Pitowsky_1994](#), [Pitowsky1989](#), [Kellerer_marginal_1964](#), [Leggett_garg_1985](#), [araujo_cycle_2013](#)

$$\langle A_2C_1 \rangle + \langle B_2C_1 \rangle - \langle A_2B_1 \rangle \leq 1. \quad (55) \quad \{\text{eq:polym}\}$$

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* [Do we need an earlier description of the marginals problem?—RWS](#)).

But the DAG of Fig. [6](#) 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

$$A_2 \not\sim B_1 \implies \langle A_2B_1 \rangle = \langle A_2 \rangle \langle B_1 \rangle. \quad (56) \quad \{\text{corrfact}\}$$

Substituting the latter equality into Eq. [\(55\)](#), we have [eq:polymonogamyraw](#)

$$\langle A_2C_1 \rangle + \langle B_2C_1 \rangle \leq 1 + \langle A_2 \rangle \langle B_1 \rangle. \quad (57)$$

This is an example of a nontrivial causal compatibility inequality on the inflation DAG.

Finally, by corollary [4.1](#), we infer that [maincorollary](#)

$$\langle AC \rangle + \langle BC \rangle \leq 1 + \langle A \rangle \langle B \rangle, \quad (58) \quad \{\text{eq:polym}\}$$

is a causal compatibility inequality on the original DAG, that is, on the Triangle scenario. This inequality expresses a trade-off in the strength of the correlations that can be observed between any pair of observed nodes in the Triangle scenario: at most two such pairs can be perfectly correlated. [Is this an accurate description of the constraint? I don't see how to justify calling it "monogamy". —RWS](#)

Example 2: 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 this, consider again the inflation of the triangle scenario to the DAG depicted in Fig. [6](#). [fig:TriDagSubA2B1C1](#)

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

$$I(A_2 : C_1) + I(C_1 : B_1) - I(A_2 : B_1) \leq H(B_1), \quad (59) \quad \{\text{eq:MIraw}\}$$

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. [\[20\]](#). [Fritz2013marginal](#)

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

$$A_2 \not\sim B_1 \implies I(A_2 : B_1) = 0. \quad (60) \quad \{\text{entropic}\}$$

Substituting the latter equality into Eq. [\(59\)](#), we have [eq:MIraw](#)

$$I(A_2 : C_1) + I(C_1 : B_1) \leq H(B_1). \quad (61)$$

This is another example of a nontrivial causal compatibility inequality for the DAG of Fig. [6](#). [fig:TriDagSubA2B1C1](#)

By corollary [4.1](#), it follows that [maincorollary](#)

$$I(A : C) + I(C : B) \leq H(B), \quad (62) \quad \{\text{eq:monog}\}$$

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 3: A causal compatibility inequality expressed in terms of probabilities of certain joint valuations

Consider the inflation of the triangle scenario depicted in Fig. 3, 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,

$$P_{A_2B_2C_2}(111) \leq P_{A_1B_1C_1}(000) + P_{A_1B_2C_2}(111) + P_{B_1C_2A_2}(111) + P_{A_2C_1B_2}(111). \quad (\text{eq:Fritz2012bell})$$

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.

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

$$\begin{aligned} A_1B_2 \perp\!\!\!\perp C_2 &\implies P_{A_1B_2C_2} = P_{A_1B_2} \otimes P_{C_2}, \\ B_1C_2 \perp\!\!\!\perp A_2 &\implies P_{B_1C_2A_2} = P_{B_1C_2} \otimes P_{A_2}, \\ A_2C_1 \perp\!\!\!\perp B_2 &\implies P_{A_2C_1B_2} = P_{A_2C_1} \otimes P_{B_2}, \\ A_2 \perp\!\!\!\perp B_2 \perp\!\!\!\perp C_2 &\implies P_{A_2B_2C_2} = P_{A_2} \otimes P_{B_2} \otimes P_{C_2}. \end{aligned} \quad (\text{eq:tri22})$$

Substituting these equalities into Eq. [\(63\)](#), we obtain the polynomial inequality

$$P_{A_2}(1)P_{B_2}(1)P_{C_2}(1) \leq P_{A_1B_1C_1}(000) + P_{A_1B_2}(11)P_{C_2}(1) + P_{B_1C_2}(11)P_{A_2}(1) + P_{A_2C_1}(11)P_{B_2}(1). \quad (\text{eq:Fritz3raw})$$

This, therefore, is a causal compatibility inequality for the DAG of Fig. 3.

Finally, by [corollary 4.1](#), we infer that

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

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 inflation 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 inflation DAG.

In the rest of this article, we shall continue to rely only on the ancestral independences among observed variables within the inflation 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

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 inflation DAG. 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 \mathbf{U}' in the inflation DAG G' will be called **pre-injectable** whenever it is a union of injectable sets with disjoint ancestries.

$$\mathbf{U}' \in \text{PreInjectableSets}[G'] \quad \text{iff} \quad \exists \{\mathbf{U}_i \in \text{InjectableSets}[G']\} \quad \text{s.t.} \quad \mathbf{U}' = \bigcup_i \mathbf{U}_i \quad \text{and} \quad \forall i \neq j : \mathbf{U}_i \not\uparrow \mathbf{U}_j. \quad (67) \quad \boxed{\text{eq:definepreinjectable}}$$

Note that every injectable set is a trivial example of a pre-injectable set.

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

$$P(\mathbf{U}') = P(\mathbf{U}_1)P(\mathbf{U}_2) \cdots P(\mathbf{U}_n). \quad (68) \quad \boxed{\text{eq:preindependence}}$$

The situation, therefore, is this: for any constraints 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 derive from these constraints that *do* refer to the causal structure by substituting the equalities 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 inflation DAG.

The latter inequality can then be converted into a causal compatibility inequality for the original DAG using corollary 4.1. [THE END OF ROB'S EDITS. What follows from this point on is text from an old version of the paper. However, even the new version of what follows will need to edited to harmonize it with the new narrative in what has come before.]

We have defined causal inference as a decision problem, namely testing the compatibility of some observational data with some causal hypothesis. We've shown that this decision can be negatively answered by proxy, namely by demonstrating incompatibility of *inflated* data with an *inflated* hypothesis. The inflation technique can also be used to derive incompatibility witnesses, however, by **deriving constraints on the pre-injectable sets**. Any such constraint is also an implicit consequence of the original hypothesis, and hence a relevant criterion for compatibility.

The “big” problem, therefore, is rather straightforward: We seek to derive compatibility witnesses from the inflation hypothesis on the injectable sets. This task, however, is just a special instance of generic causal inference: Given some causal hypothesis, what can we say about how it constrains possible observable marginal distribution? Any technique for deriving incompatibility witnesses is therefore relevant when using the inflation technique. Interestingly, weak constraints from the inflation hypothesis translate into strong constraints pursuant to the original hypothesis.

In the discussion that follows we continue to assume that the original hypothesis is nothing more than supposing the causal structure to be given by the original DAG. Furthermore we presume that the joint distribution over all original observable variables is accessible. Moreover, we limit our attention to deriving polynomial inequalities in terms of probabilities. The potential of using inflation as tool for deriving entropic inequalities is considered separately in Appendix C.

In what follows we consider three different strategies for constraining possible marginal distributions from the inflation hypothesis.

- The full nonlinear strategy attempts to leverage many different kinds of constraints which are implicit in the inflation hypothesis. This strategy yields the strongest incompatibility witnesses, but relies on computationally-difficult nonlinear quantifier elimination.
- An intermediate strategy asks only if the various marginal distributions are compatible with *any* joint distribution, without regard to the specific causal structure of the inflation DAG whatsoever. Solving the marginal problem amounts to a special linear quantifier elimination computation, one which can be computed efficiently using convex hull algorithms. The resulting incompatibility witnesses are nevertheless still polynomial inequalities.
- Another strategy is based on probabilistic 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.

In the narrative below the marginal problem is discussed first; the nonlinear strategy is presented as supplementing the marginal problem with additional constraints. The most computationally efficient strategy is presented as a relaxation of the marginal problem, and is discussed separate from the other two strategies, namely in Sec. VIII.

Preliminary to every strategy, however, is the identification of the pre-injectable sets.

Identifying the Pre-Injectable Sets

injectable

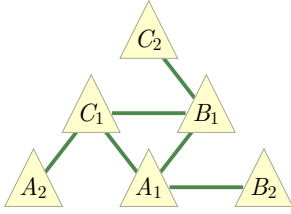


FIG. 9. The auxiliary injection graph corresponding to the inflation DAG in Fig. 3, wherein a pair of nodes are adjacent iff they are pairwise injectable.

fig:injection

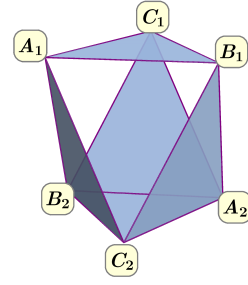


FIG. 10. The simplicial complex... Tobias - you please caption this? The 5 faces in this figure correspond to the 5 maximal pre-injectable sets per Fig. 3, namely $\{A_1B_1C_1\}$, $\{A_1B_2C_2\}$, $\{A_1B_2C_1\}$, $\{A_2B_2C_1\}$ and $\{A_2B_2C_2\}$.

fig:simpl

To identify the pre-injectable sets, we first identify the injectable sets. To this end, it is useful to construct an auxiliary graph from the inflation DAG. Let the nodes of these auxiliary graphs be the observable nodes in the inflation DAG. The **injection graph**, then, is the undirected graph in which a pair of nodes A_i and B_j are adjacent if $An(A_iB_j)$ is irredundant. The injectable sets are then precisely the cliques⁶ in this graph, per Eq. (7).

Determining the pre-injectable sets from there can be done via constructing another graph that we call the **independence graph**. Its nodes are the injectable sets, and we connect two of these by an edge if their ancestral subgraphs are disjoint. Then by definition, the pre-injectable sets can be obtained as the cliques in this graph. Taking the union of all the injectable sets in such a clique results in a pre-injectable set. Since it is sufficient to only consider the maximal pre-injectable sets, one can eliminate all those pre-injectable sets that are contained in other ones, as a final step.

Applying these prescriptions to the inflation DAG in Fig. 3 identifies ancestral independencies and (pre-)injectable sets as follows:

$$\begin{array}{ccccc}
 \begin{array}{l} A_2 \not\perp\!\!\!\perp B_1 \\ A_2 \not\perp\!\!\!\perp C_2 \\ B_2 \not\perp\!\!\!\perp A_2 \\ B_2 \not\perp\!\!\!\perp C_1 \\ C_2 \not\perp\!\!\!\perp A_1 \\ C_2 \not\perp\!\!\!\perp B_2 \end{array} & \begin{array}{l} \{A_2\} \not\perp\!\!\!\perp \{B_1B_2C_2\} \\ \{B_2\} \not\perp\!\!\!\perp \{A_2C_1C_2\} \\ \{C_2\} \not\perp\!\!\!\perp \{A_1A_2B_2\} \\ \{A_2\} \not\perp\!\!\!\perp \{B_2\} \not\perp\!\!\!\perp \{C_2\} \end{array} & \begin{array}{l} \{A_1B_1\} \\ \{B_1C_1\} \\ \{A_1C_1\} \\ \{A_2C_1\} \\ \{B_2A_1\} \\ \{C_2B_1\} \end{array} & \begin{array}{l} \{A_1B_2\} \\ \{B_1C_2\} \\ \{A_2C_1\} \\ \{A_1B_1C_1\} \end{array} & \begin{array}{l} \{A_1B_1C_1\} \\ \{A_1B_2C_2\} \\ \{A_2B_1C_2\} \\ \{A_2B_2C_1\} \\ \{A_2B_2C_2\} \end{array} \\
 \underbrace{\hspace{1.5cm}}_{\text{pairwise ancestral independencies}} & \underbrace{\hspace{1.5cm}}_{\text{maximal ancestral independencies}} & \underbrace{\hspace{1.5cm}}_{\text{pairwise injectable sets}} & \underbrace{\hspace{1.5cm}}_{\text{maximal injectable sets}} & \underbrace{\hspace{1.5cm}}_{\text{maximal pre-injectable sets}}
 \end{array} \tag{69}$$

eq:basic

such that the distributions on the pre-injectable sets relate to the original DAG distribution via

$$\forall_{abc} : \begin{cases} P_{A_1B_1C_1}(abc) = P_{ABC}(abc) \\ P_{A_1B_2C_2}(abc) = P_C(c)P_{AB}(ab) \\ P_{A_2B_1C_2}(abc) = P_A(a)P_{BC}(bc) \\ P_{A_2B_2C_1}(abc) = P_B(b)P_{AC}(ac) \\ P_{A_2B_2C_2}(abc) = P_A(a)P_B(b)P_C(c) \end{cases} \tag{70}$$

eq:prein

Eq. (70) is an equivalent restatement of Eq. (64). Having identified the pre-injectable sets (and how to use them), we next consider various ways to invoke constraints on the distributions over the pre-injectable sets.

Constraining Possible Distributions over Pre-Injectable Sets via the Marginal Problem

The most trivial constraint on possible marginal probabilities, regardless of causal structure, is simply the *existence of some joint probability distribution* from which the marginal distributions can be recovered through marginalization, i.e. the possible marginal distributions must be **marginally compatible**. This isn't really causal inference – as no hypothesis is considered – but rather more of a preliminary sanity check. If the marginal distributions are not marginally compatible, then the answer to “Can these marginal distributions be explained by this particular causal hypothesis?” is automatically “No”.

⁶ A clique is a subset of nodes such that every node in the subset is connected to every other node in the subset.

The necessary and sufficient conditions for marginal compatibility are easy enough to state. There must exist some joint distribution (a collection of nonnegative joint probabilities) such that the marginal distributions can be recovered (each marginal distribution is a sum over various joint probabilities). **Solving the marginal problem** means resolving these "exists" statements into quantifier-free inequalities such that satisfaction of all such inequalities is necessary and sufficient for marginal compatibility. An efficient algorithm to solve the marginal problem is given in Appendix A. The marginal problem comes up in a variety of applications, and has been studied extensively; see [20] for further references.

As an example, here's how the marginal problem would be phrased as a partial-existential-closure problem with respect to the five three-variable marginal distributions corresponding to the pre-injectable sets in Eq. (70). For simplicity, we assume that all observable variables are binary⁷.

In order for the five pre-injectable sets in Eq. (70) to be marginally compatible there must exist 64 nonnegative joint probabilities, i.e. satisfying

$$\forall_{a_1 a_2 b_1 b_2 c_1 c_2} : 0 \leq P_{A_1 A_2 B_1 B_2 C_1 C_2}(a_1 a_2 b_1 b_2 c_1 c_2), \quad (71) \quad \{\text{eq:nonne}$$

constrained further by marginal distributions given by

$$\begin{aligned} \forall_{a_1 b_1 c_1} : P_{A_1 B_1 C_1}(a_1 b_1 c_1) &= \sum_{a_2 b_2 c_2} P_{A_1 A_2 B_1 B_2 C_1 C_2}(a_1 a_2 b_1 b_2 c_1 c_2), \\ \forall_{a_1 b_2 c_2} : P_{A_2 B_2 C_2}(a_1 b_2 c_2) &= \sum_{a_2 b_1 c_1} P_{A_1 A_2 B_1 B_2 C_1 C_2}(a_1 a_2 b_1 b_2 c_1 c_2), \\ \forall_{a_2 b_1 c_2} : P_{A_2 B_1 C_2}(a_2 b_1 c_2) &= \sum_{a_1 b_2 c_1} P_{A_1 A_2 B_1 B_2 C_1 C_2}(a_1 a_2 b_1 b_2 c_1 c_2), \\ \forall_{a_2 b_2 c_1} : P_{A_2 B_2 C_1}(a_2 b_2 c_1) &= \sum_{a_1 b_1 c_2} P_{A_1 A_2 B_1 B_2 C_1 C_2}(a_1 a_2 b_1 b_2 c_1 c_2), \\ \forall_{a_2 b_2 c_2} : P_{A_2 B_2 C_2}(a_2 b_2 c_2) &= \sum_{a_1 b_1 c_1} P_{A_1 A_2 B_1 B_2 C_1 C_2}(a_1 a_2 b_1 b_2 c_1 c_2). \end{aligned} \quad (72) \quad \{\text{eqs}\}\{\text{eq:}$$

The marginal compatibility constraints in this case are, therefore, 64 inequalities and 40 equalities. Solving the marginal problem means eliminating 64 terms from those inequalities and equalities, namely any $p_{A_1 A_2 B_1 B_2 C_1 C_2}$.

Linear quantifier elimination is already widely used in causal inference to derive entropic inequalities [13, 16, 20]. 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. The quantifiers we eliminate are the not-pre-injectable joint probabilities, which are quite different from probabilities involving hidden variables.

When solving the marginal problem is too difficult, one may consider solving a relaxation of it, instead. One extremely computationally amenable relaxation of the marginal problem is to enumerate probabilistic Hardy-type paradoxes. This is discussed later on in Sec. VIII.

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 marginal distributions. In causal inference, however, there are plenty of other constraints on the sorts of joint distributions which are compatible 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, on the hypothetical inflation-DAG observable joint distribution.

The most familiar causally-motivated constraints on a joint distribution are **conditional independence relations**, in particular, observable conditional independence relations. Conditional independence relations are inferred by d -separation; if \mathbf{X} and \mathbf{Y} are d -separated in the (inflation) DAG by \mathbf{Z} , then we infer the conditional independence $\mathbf{X} \perp \mathbf{Y} | \mathbf{Z}$. The d -separation criterion is explained at length in [1, 3, 7, 11], so we elect not to review it here.

Every conditional independence relation can be translated into a nonlinear constraint on probabilities, as $\mathbf{X} \perp \mathbf{Y} | \mathbf{Z}$ implies $p(\mathbf{x}\mathbf{y}|\mathbf{z}) = p(\mathbf{x}|\mathbf{z})p(\mathbf{y}|\mathbf{z})$ for all \mathbf{x} , \mathbf{y} , and \mathbf{z} . As we generally prefer to work with unconditional probabilities, we rewrite this as follows: If \mathbf{X} and \mathbf{Y} are d -separated by \mathbf{Z} , then $p_{\mathbf{X}\mathbf{Y}\mathbf{Z}}(\mathbf{x}\mathbf{y}\mathbf{z})p_{\mathbf{Z}}(\mathbf{z}) = p_{\mathbf{X}\mathbf{Z}}(\mathbf{x}\mathbf{z})p_{\mathbf{Y}\mathbf{Z}}(\mathbf{y}\mathbf{z})$ for all \mathbf{x} , \mathbf{y} , and \mathbf{z} . Such nonlinear constraints can be incorporated as further restrictions on the sorts of joint distributions compatible with the inflation DAG, supplementing the basic nonnegativity of probability constraints of the marginal problem.

For example, in Fig. 3 we find that A_1 and C_2 are d -separated by $\{A_2 B_2\}$, and so one might incorporate the family of nonlinear equalities $p_{A_1 A_2 B_2 C_2}(a_1 a_2 b_2 c_2)p_{A_2 B_2}(a_2 b_2) = p_{A_1 A_2 B_2}(a_1 a_2 b_2)p_{A_2 B_2 C_2}(a_2 b_2 c_2)$ for all a_1 , a_2 , b_2 and c_2 .

⁷ If the observables are not binary, then the resulting binary-outcome inequalities are necessary for marginal compatibility, in that they should hold for any course-graining of the observational data into two classes, but the binary-outcome inequalities are no longer sufficient.

Note that every semi-marginal probability introduced in some nonlinear condition independence equation should also be *defined* by marginalization, i.e. as a sum of various joint probabilities, so that one need not eliminate further quantifiers. The relevant substitutions of this example would be

$$\begin{aligned} \forall_{a_2 b_2} : & P_{A_2 B_2}(a_2 b_2) \rightarrow \sum_{a_1 b_1 c_1 c_2} P_{A_1 A_2 B_1 B_2 C_1 C_2}(a_1 a_2 b_1 b_2 c_1 c_2), \\ \forall_{a_1 a_2 b_2 c_2} : & P_{A_1 A_2 B_2 C_2}(a_1 a_2 b_2 c_2) \rightarrow \sum_{b_1 c_1} P_{A_1 A_2 B_1 B_2 C_1 C_2}(a_1 a_2 b_1 b_2 c_1 c_2), \\ \forall_{a_1 a_2 b_2} : & P_{A_1 A_2 B_2}(a_1 a_2 b_2) \rightarrow \sum_{b_1 c_1 c_2} P_{A_1 A_2 B_1 B_2 C_1 C_2}(a_1 a_2 b_1 b_2 c_1 c_2) \end{aligned} \quad (73)$$

etc.

Many modern computer algebra systems have functions capable of tackling nonlinear quantifier elimination symbolically⁸. Currently, however, it is not practical to perform nonlinear quantifier elimination on large polynomial systems with many quantifiers. It may be possible to exploit results on the particular algebraic-geometric structure of these particular systems [35]. 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 a universal quantifier existence problem: Do there exist quantifier that satisfy the full set of linear and nonlinear numeric (as opposed to symbolic) constraints? Most computer algebra systems can resolve such *satisfiability* questions quite rapidly⁹.

It is also possible to use a mixed strategy of linear and nonlinear quantifier elimination, such as Chaves [37] advocates. The explicit results of Ref. [37] are therefore consequences of any inflation DAG, achieved by applying a mixed quantifier elimination strategy.

Constraining Possible Distributions over Pre-Injectable Sets via Coinciding Marginals

The inflation hypothesis is more than just causal structure, however, even if the original hypothesis did not constrain possible causal models beyond the original DAG. By restricting to exclusively *inflation* models, however, we require $P(A_i | \text{Pa}_{G'}(A_i)) = P(A_j | \text{Pa}_{G'}(A_j))$, per Eq. (5). Consequently, the distributions over different injectable sets must occasionally coincide, i.e. $P(\mathbf{X}) = P(\mathbf{Y})$ whenever both \mathbf{X} and \mathbf{Y} are injectable, and $\tilde{\mathbf{X}} = \tilde{\mathbf{Y}}$. Sometimes sets of random variables which are *not* injectable, however, can also be shown to have necessarily coinciding distributions. For example, we can verify that $P(A_1 A_2 B_1) = P(A_1 A_2 B_2)$ follows from Fig. 3, even though $\{A_1 A_2 B_1\}$ and $\{A_1 A_2 B_2\}$ are not injectable sets.

Equations such as $\forall_{a_1 a_2 b} : p_{A_1 A_2 B_1}(a_1 a_2 b) = p_{A_1 A_2 B_2}(a_1 a_2 b)$ are also intrinsic parts 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 are discuss in Appendix B.

Move this paragraph up, Tobias? EW 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 [38–40], nor to the nonlinear inequalities which account for interventions to a given causal structure [26, 41].

VI. BELL SCENARIOS AND INFLATION

To further illustrate our inflation-DAG approach, we demonstrate how to recover all Bell inequalities [6, 23, 24] via our method. To keep things simple we only discuss the case of a bipartite Bell scenario with two possible “settings” here, but the cases of more settings and/or more parties are totally analogous.

Consider the causal structure associated to the Bell/CHSH [5, 6, 23, 24] experiment [11 (Fig. E#2), 7 (Fig. 19), 13 (Fig. 1), 12 (Fig. 1), 25 (Fig. 2b), 26 (Fig. 2)], depicted here in Fig. 7. The observable variables are A, B, X, Y , and Λ is the latent common cause of A and B .

In the Bell scenario DAG, one usually works with the conditional distribution $P(AB|XY)$ instead of with the original distribution $P(ABXY)$. The conditional distribution is an *array* of distributions over A and B , indexed by the possible values of X and Y . The maximal pre-injectable sets then are

$$\begin{aligned} & \{A_1 B_1, X_1 X_2 Y_1 Y_2\} \\ & \{A_1 B_2, X_1 X_2 Y_2 Y_2\} \\ & \{A_2 B_1, X_1 X_2 Y_1 Y_2\} \\ & \{A_2 B_2, X_1 X_2 Y_2 Y_2\}, \end{aligned} \quad (74)$$

⁸ For example *Mathematica*TM’s `Resolve` command, *Redlog*’s `rlposqe`, or *Maple*TM’s `RepresentingQuantifierFreeFormula`, etc.
⁹ For example *Mathematica*TM `Reduce`ExistsRealQ` function. Specialized satisfiability software such as SMT-LIB’s `check-sat` [36] are particularly apt for this purpose.

where we have put commas in order to clarify that every maximal pre-injectable set contains *all* “settings” variables. These pre-injectable sets are specified by the original observable distribution via

$$\forall_{abx_1x_2y_1y_2} : \begin{cases} P_{A_1B_1X_1X_2Y_1Y_2}(abx_1x_2y_1y_2) = P_{ABXY}(abx_1y_1)P_X(x_2)P_Y(y_2), \\ P_{A_1B_2X_1X_2Y_1Y_2}(abx_1x_2y_1y_2) = P_{ABXY}(abx_1y_2)P_X(x_2)P_Y(y_1), \\ P_{A_2B_1X_1X_2Y_1Y_2}(abx_1x_2y_1y_2) = P_{ABXY}(abx_2y_1)P_X(x_1)P_Y(y_2), \\ P_{A_2B_2X_1X_2Y_1Y_2}(abx_1x_2y_1y_2) = P_{ABXY}(abx_2y_2)P_X(x_1)P_Y(y_1), \\ P_{X_1X_2Y_1Y_2}(x_1x_2y_1y_2) = P_X(x_1)P_X(x_2)P_Y(y_1)P_Y(y_2). \end{cases} \quad (75)$$

By dividing the first four inequalities by the latter we obtain

$$\forall_{abx_1x_2y_1y_2} : \begin{cases} P_{A_1B_1|X_1X_2Y_1Y_2}(ab|x_1x_2y_1y_2) = P_{AB|XY}(ab|x_1y_1) \\ P_{A_1B_2|X_1X_2Y_1Y_2}(ab|x_1x_2y_1y_2) = P_{AB|XY}(ab|x_1y_2) \\ P_{A_2B_1|X_1X_2Y_1Y_2}(ab|x_1x_2y_1y_2) = P_{AB|XY}(ab|x_2y_1) \\ P_{A_2B_2|X_1X_2Y_1Y_2}(ab|x_1x_2y_1y_2) = P_{AB|XY}(ab|x_2y_2). \end{cases} \quad (76)$$

If we then impose marginal compatibility according to the marginal problem we find that the (minimal!) consequence of the inflation hypothesis is

$$P_{A_1B_1|X_1X_2Y_1Y_2}(ab|x_1x_2y_1y_2) = \sum_{a_2,b_2} P_{A_1A_2B_1B_2X_1X_2Y_1Y_2}(a_1a_2b_1b_2|x_1x_2y_1y_2) \quad (77)$$

etc. For the inflated observation data to be compatible with the inflation hypothesis, therefore, we would require

$$\forall_{ab} : \begin{cases} P_{AB|XY}(ab|00) = \sum_{a',b'} P_{A_1A_2B_1B_2X_1X_2Y_1Y_2}(aa'bb'|0101) \\ P_{AB|XY}(ab|10) = \sum_{a',b'} P_{A_1A_2B_1B_2X_1X_2Y_1Y_2}(a'abb'|0101) \\ P_{AB|XY}(ab|01) = \sum_{a',b'} P_{A_1A_2B_1B_2X_1X_2Y_1Y_2}(aa'b'b|0101) \\ P_{AB|XY}(ab|11) = \sum_{a',b'} P_{A_1A_2B_1B_2X_1X_2Y_1Y_2}(a'ab'b|0101) \end{cases} \quad (78) \quad \boxed{\text{eq:final}}$$

The existence of an *array* of distributions, i.e. Eq. (78), is equivalent to the existence of a **hidden variable model**, as noted in Fine’s Theorem ^{FineTheorem} [29]. Thus, an inflation model exists if and only if a hidden-variable model exists for the original observable variables.

In conclusion, we therefore find in the case of the inflation DAG Fig. 8, the inflation method yields *tight* incompatibility witnesses for the Bell causal structure, i.e. the Bell/CHSH inequalities, just by requiring marginal compatibility of the pre-injectable sets. More generally, we can use Fine’s theorem to show that applying the marginal problem to suitable inflation DAGs can reproduce *all* Bell inequalities, for any standard Bell scenario, no matter how many parties or settings or possible outcomes.

VII. QUANTUM CAUSAL INFERENCE AND THE NO-BROADCASTING THEOREM

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.

The set of quantumly realizable distributions is superficially quite similar to the classical subset ^{pusey2014gdag, fritz2012bel} [10, 11]. For example, classical and quantum distributions alike respect all conditional independence relations implied by the common underlying causal structure ^{pusey2014gdag} [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 ^{pusey2014gdag, chaves2015infoquantum, chavesNoSignalling} also implies many of the entropic inequalities that hold classically [11, 14, 42]. 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 ^{chaves2012entropic, fritz2012bell} [10, 43]. 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 ^{braunstein1988entropic, schumacherInequality, chaves2} [13, 44, 45]. Such inequalities are still

limited, however, in that they only apply in the presence of observable root nodes¹⁰, and they still fail to witness certain distributions as classically infeasible [10, 13].

We hope that polynomial inequalities derived from broadcasting inflation DAGs will provide an additional tool for witnessing certain quantum distributions as non-classical. For example due to the results of Sec. VI, 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 is sent to A_1 and A_2 and C in the inflation Fig. 4. Since quantum theory satisfies a no-broadcasting theorem [46, 47], 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) [47–50], 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 inflation model” or “general probabilistic inflation model” on the inflation DAG.

Some inflations, such as the one of Fig. 6, do not require such broadcasting.

Definition 5. $G' \in \text{Inflations}[G]$ is **non-broadcasting** if every latent node in G' has at most one copy of each $A \in \text{Nodes}[G]$ 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 inflation 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 inflation 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. (71). 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 inflation 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 inflation model on the inflation DAG in terms of the logical broadcasting maps of Coecke and Spekkens [51]. From this perspective, a broadcasting inflation 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. (71) 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 U of observable nodes is non-broadcasting if $\text{An}(U)$ does not two distinct copies of a node which have a parent in common.

An analysis along these lines has already been carried out successfully by Chaves *et al.* [14] in the derivation of entropic inequalities that are valid for all quantum distributions. Although Chaves *et al.* [14] do not invoke inflation 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.* [14] 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.

¹⁰ 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.

VIII. DERIVING HARDY-TYPE CONSTRAINTS FOR THE MARGINAL PROBLEM

In the literature on Bell inequalities, it has been noticed that the incompatibility with the Bell scenario DAG can sometimes be witnessed by only looking at which joint probabilities are zero and which ones are nonzero. In other words, instead of considering the probability of a joint outcome, some distributions can be witnesses as infeasible by only considering the *possibility* or *impossibility* of each joint outcome. This was originally noticed by Hardy [18], and hence such **possibilistic constraints** are also known as **Hardy-type paradoxes**. For a systematic account of Hardy-type paradoxes in Bell scenarios, see Ref. [19], although see also Refs. [52–56].

The usual presentation of a Hardy-type paradox takes the following form: Even though events $E_1..E_N$ never occur (are not possible), nevertheless some other event E_0 *does* occur sometimes (is possible). The impossibility of events $E_1..E_N$ *should* prohibit the possibility of E_0 , under the marginal distributions of all the variables in all the events are compatible.

The following observational data 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 for heart and brain disease find that rats always presented with one condition but never with *both* conditions, i.e. the events $[Brain_-, Heart_-]$ and $[Brain_+, Heart_+]$ are taken to be *not possible*. Suppose the autopsies checking for heart and lung diseases similarly find that all dead rats are afflicted by some disease but with no possibility of dual diagnoses, i.e. the events $[Heart_-, Lungs_-]$ and $[Heart_+, Lungs_+]$ are not possible. Logic should then dictate lung disease ought to be perfectly correlated with brain disease, because both those conditions are perfectly anticorrelated with heart disease. If some medical examiner checking rats for brain and lung disease then finds that *it is possible* for a rat to have brain disease without heart disease, this would be considered a violation of a Hardy-type paradox.

Hardy-type paradoxes are predicated on assuming the existence of a solution to the marginal problem. Thus, ensuring the observational data avoids any Hardy-type paradoxes is a necessary condition for solving the marginal problem. Liang *et al.* [56, Section III.C] discuss the use of possibilistic constraints to certify the incompatibility of marginal distributions in contexts of than Bell scenarios.

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

$$\text{Never}[E_1] \bigwedge \text{Never}[E_2] \bigwedge \dots \text{Never}[E_N] \implies \text{Never}[E_0] \quad (79)$$

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

$$[E_0] \implies [E_1] \bigvee [E_2] \bigvee \dots [E_N]. \quad (80)$$

Any possibilistic constraint can be immediately translated into a stronger probabilistic one, as noted by Mansfield and Fritz [19]. The probabilistic variant states that *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

$$p(E_0) \leq \sum_{n=1}^N p(E_n). \quad (81)$$

In order to derive causal incompatibility witnesses via marginal compatibility, therefore, we may consider the task of **enumerating** Hardy-type paradoxes, each of which we can then express as an inequalities 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

$$[A=1, C=1] \implies [A=1, B=1] \bigvee [B=0, C=1] \quad (82)$$

corresponding to the probabilistic constraint

$$P_{AC}(\mathbf{11}) \leq P_{AB}(\mathbf{11}) + P_{BC}(\mathbf{01}). \quad (83) \quad \{\text{eq:trivial}\}$$

Eq. (83) is a necessary condition for the marginal compatibility of $P(AB)$, $P(AC)$, and $P(BC)$; it is equivalent to Eq. (55).

We outline the general procedure using a slightly more sophisticated example. Consider the marginal scenario of Fig. 10, where the contexts are $\{A_1 B_1 C_1\}$, $\{A_1 B_2 C_2\}$, $\{A_2 B_1 C_2\}$, $\{A_2 B_2 C_1\}$ and $\{A_2 B_2 C_2\}$, 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 antecedent 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 $[A_2=1, B_2=1, C_2=1]$ to be the fixed antecedent.

The consequent will be a conjunction of composite outcomes restricted to marginal contexts, and further restricted so that all marginal composite outcomes in the consequent are compatible with that specified by the consequent. For the implication to be valid, however, 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 hypergraph correspond to every possible joint outcome for every possible marginal context. The hyperedges in the first hypergraph correspond to every possible joint outcome for the joint context over 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 $[A_1=0, A_2=1, B_1=0, B_2=1, C_1=1, C_2=1]$ is an extension of the node $[A_1=0, B_2=1, C_2=1]$. In our example following Fig. 10, 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 supposition of the composite event per our fixed antecedent. For example, the node $[A_2=1, B_2=0, C_1=1]$ contradicts the antecedent $[A_2=1, B_2=1, C_2=1]$. 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 the sets of nodes which have the property that they intersect 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 [57].

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

$$[A_2=1, B_2=1, C_2=1] \implies [A_1=0, B_1=0, C_1=0] \bigvee \text{And}[A_1=1, B_2=1, C_2=1] \bigvee [A_2=1, B_1=1, C_2=1] \bigvee [A_2=1, B_2=1, C_1=1] \quad (84) \quad \boxed{\text{eq:F3imp}}$$

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 the implications into inequalities in the usual way, by replacing “ \implies ” by “ \leq ” at the level of probabilities and the disjunctions by sums, so the possibilistic constraint Eq. (84) translates to the probabilistic constraint

$$P_{A_2 B_2 C_2}(\mathbf{111}) \leq P_{A_1 B_1 C_1}(\mathbf{111}) + P_{A_1 B_2 C_2}(a_1 \mathbf{11}) + P_{A_2 B_1 C_2}(\mathbf{111}) + P_{A_2 B_2 C_1}(\mathbf{111}) \quad (85) \quad \boxed{\text{eq:F3raw}}$$

Eq. (85) is equivalent to Eq. (63); therefore applying it the inflation depicted in Fig. 3 recovers Eq. (66).

Since also many Bell inequalities are of this form—such as the CHSH inequality which follows in this way from Hardy’s original implication—we conclude that this method is still sufficiently powerful to generate plenty of interesting inequalities, and at the same time significantly easier to perform in practice than the full-fledged linear (let alone nonlinear) quantifier elimination.

We note that the connection between classical propositional logic and linear inequalities has been used previously in the task of causal inference. Noteworthy examples of works deriving causal infeasibility criteria via classical logic are Pitowsky [31] and Ghirardi and Marinatto [58], see also Refs. [30, 32–34]. Novel this work, however, is the use of the hypergraph transversals problem to formally enumerate relevant logical implications.

We expect that this enumeration of minimal transversals will be computationally much more tractable than the linear quantifier elimination, even if one does it for every possible left-hand side of the implication. We reiterate that inequalities resulting from hypergraph transversals, however, are a subset of the inequalities that result from completely solving the marginal problem. Consequently, linear quantifier elimination is the preferable tool for deriving inequalities whenever the more general linear elimination strategy is computationally tractable.

To illustrate our method on a concrete example, in Appendix D we provide a list of polynomial inequalities that we have derived for the Triangle scenario.

IX. CONCLUSIONS

Our main contribution is a new way of deriving causal infeasibility criteria, namely the inflation DAG approach. An inflation DAG naturally carries inflation models, and the existence of an inflation model implies inequalities, containing gedankenprobabilities, which implicitly constrains the set of distribution compatible with the original causal structure. If desirable, one can further eliminate the gedankenprobabilities via quantifier elimination. Polynomial inequalities can be obtained through *linear* elimination techniques, or through further relaxation to purely *possibilistic* constraints.

These 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 inflation 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.

The most elementary of all causal infeasibility criteria are the conditional independence (CI) relations. Our method explicitly incorporates all marginal independence relations implied by a causal structure. We have found that some CI relations also appear to be implied by our polynomial inequalities. In future research we hope to clarify the process through which CI relations are manifested as properties of the inflation DAG.

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.

Our method turns the quantum no-broadcasting theorem [\[NoCloningQuantum1996, NoCloningGeneral2006\]](#) on its head by crucially relying on the fact that classical hidden variables *can* be cloned. The possibility of classical cloning motivates the inflation DAG method, and underpins the implied causal infeasibility criteria. We have speculated about generalizing our method to obtain causal infeasibility criteria that constitute necessary constraints even for *quantum* causal scenarios, a common desideratum in recent works [\[Fritz2012bell, Pusey2014dag, Chaves2015infoquantum, ChavesNoSignalling, BeyondBellII\]](#). 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 [\[NPA2008Long, 13822NPA1\]](#) 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.

The difference between classical ontic-state duplication and quantum no-broadcasting makes the inequalities that result from our consideration to be especially suited for distinguishing the set of quantum-realizable distributions from its subset of classically-realizable distributions. Causal infeasibility criteria that are sensitive to the classical-quantum distinction are precisely the sort of generalizations of the Bell inequalities which are sought after, in order to study the quantum features of generalized causal scenarios. Entropic inequalities have been lacking in this regard [\[Fritz2012bell, Pusey2014g\]](#), and the inflation DAG considerations proposed here constitute an alternative strategy that holds some promise.

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Appendix A: Algorithms for Solving the Marginal Problem

Algorithms

Geometrically, linear quantifier elimination is equivalent to projecting a high-dimensional polytope in halfspace representation (inequalities and equalities) into a lower-dimensional quotient space.

Polytope projection is a well-understood problem in computational optimization, and a surprising variety of algorithms are available for the task [61–63]. The oldest-known method for polytope projection, i.e. linear quantifier elimination, is an algorithm known as Fourier-Motzkin (FM) elimination [64, 65], although Fourier-Cernikov elimination variant [66, 67], as well as Block Elimination and Vertex Enumeration [68], are also fairly popular. More advanced polytope projection algorithms, such as Equality Set Projection (ESP) and Parametric Linear Programming, have also recently become available [61–63]. ESP could be an interesting algorithm to use in practice, because each internal iteration of ESP churns out a new facet; by contrast, FM algorithms only generate the entire list of facets after their final internal iteration, after all the quantifiers have been eliminated one by one.

Linear quantifier elimination routines are available in many software tools¹¹. We have found custom-coding an linear elimination routine in *Mathematica*TM to be most efficient, see Appendix A for further detail.

The generic task of polytope projection assumes that the initial polytope is given *only* in halfspace representation. If, however, a **dual description** of the initial polytope is available, i.e. we are also given its extremal vertices, then the projection problem can be significantly optimized [68, 70]. Such dual-description algorithms are used, for example, by modern convex hull solvers. The marginal problem can be explicitly recast as a special convex hull problem, which can be seen as follows.

A generic convex hull problem takes a matrix of vertices \hat{V} , where each row is a vertex, and asks what is the set of coordinates \vec{x} such that \vec{x} can be achieved as a convex combination of the vertices. Formally, it amounts to resolving a partial-existential-closure problem pertaining the existing of nonnegative weights, i.e.

$$\exists_{\vec{w}} : \text{And}[\vec{w} \cdot \hat{V} = \vec{x}, \sum_i w_i = 1, \forall_i w_i \geq 0]. \quad (\text{A-1})$$

It should be evident from Eqs. (71–72) that the marginal problem is precisely of this form. The individual probabilities of the joint outcome correspond to the weights in the convex hull problem. Recasting the marginal problem as a convex hull problem means that optimized convex hull algorithms can be used to directly solve the marginal problem. Fine’s Theorem [29] also follows along these lines. Fine’s theorem states that the existence of a joint distribution is equivalent to having the observables marginal distribution lie inside the convex hull of all deterministic joint distributions. Tobias, can you say the previous sentence better perhaps?

Indeed, the authors found that the software *lrs* [lrs] was capable of solving the marginal problem rather efficiently.

TABLE I. A comparison of different approaches for constraining the distributions on the pre-injectable sets. The primary divide is quantifier elimination, which is more difficult but produces inequalities, versus satisfiability which can witness the infeasibility of a specific distribution. The approaches subdivide further subdivided into nonlinear, linear, and possibilistic variants.

Approach	General problem	Standard algorithm(s)	Difficulty
Nonlinear quantifier elimination	Real quantifier elimination	Cylindrical algebraic decomposition, see [37]	Very hard
Nonlinear satisfiability	Nonlinear optimization	See [36], and semidefinite relaxations [71]	Easy
Linear quantifier elimination	Polytope projection	Fourier-Motzkin elimination, see [63–65, 67, 72]	Hard
Solve marginal problem	Convex Hull	Dual-description linear elimination, see [68, 70]	Moderate
Linear satisfiability	Linear programming	Simplex method, see [73, 74]	Very easy
Enumerate Hardy paradoxes	Hypergraph transversals	See Eiter <i>et al.</i> [57]	Very easy

¹¹ For example *MATLAB*TM’s **MPT2/MPT3**, *Mazima*’s **fourier.elim**, *lrs*’s **fourier**, or *Maple*TM’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 Cernikov rules [66, 67] is implemented in *qskeleton* [69]. ESP [61–63] 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.

Appendix B: On Identifying All Coinciding Marginal Distributions

ngdetails

A **bijection** between two sets of elements is a bijective map (\leftrightarrow) from one set of elements to another. Let us define a **copy bijection** (\leftrightarrow) to be a bijective map such that every pair of elements which are mapped to each other are equivalent under dropping the copy index. We've informally been using the notion of a copy bijection previously, in that sets of nodes $\mathbf{X} \sim \mathbf{Y}$ iff

We call two sets of observable nodes \mathbf{X} and \mathbf{Y} **inflationarily isomorphic** (relative to some inflation DAG G') if there exists an isomorphism $\text{AnSubDAG}_{G'}[\mathbf{X}] \leftrightarrow \text{AnSubDAG}_{G'}[\mathbf{Y}]$ which has the additional two properties that, when restricting to \mathbf{X} , the morphism bijectively maps $\mathbf{X} \leftrightarrow \mathbf{Y}$, and that furthermore the isomorphism maps *copies to copies*, i.e. the morphism is a permutation of indices when restricted to any original-scenario node-type. For example in Fig. 3, the sets $\mathbf{X} = \{A_1 A_2 B_1\}$ and $\mathbf{Y} = \{A_1 A_2 B_2\}$ are inflationarily isomorphic.

If two sets \mathbf{X} and \mathbf{Y} are inflationarily isomorphic then we can conclude that $P(\mathbf{X}) = P(\mathbf{Y})$ in any inflation model.

Coinciding ancestral subgraphs is not, by itself, a strong enough condition to justify coinciding distributions; rather the variables in question must play similar *roles* in their coinciding ancestral subgraphs, hence the precise definition of inflationary isomorphism. To illustrate this, consider the inflation DAG in Fig. 11. We have $\text{AnSubDAG}_{(\text{Fig. 11})}[X_2 Y_2 Z_1] \sim \text{AnSubDAG}_{(\text{Fig. 11})}[X_1 Y_2 Z_2]$, since both of these ancestral subgraphs are the entire DAG. Nevertheless $X_2 Y_2 Z_1$ is *not* inflationarily isomorphic to $X_1 Y_2 Z_2$, because any copy-to-copy isomorphism between $\text{AnSubDAG}_{(\text{Fig. 11})}[X_2 Y_2 Z_1]$ and $\text{AnSubDAG}_{(\text{Fig. 11})}[X_1 Y_2 Z_2]$ fails to map $X_2 Y_2 Z_1$ to $X_1 Y_2 Z_2$ when restricted to the domain $X_2 Y_2 Z_1$.

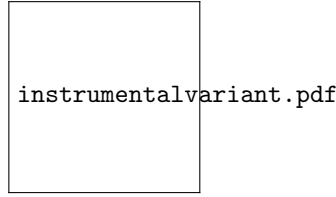


FIG. 11. An inflation DAG which illustrates why coinciding ancestral subgraphs don't necessarily imply coinciding distributions.

fig:ancestralsubgraphnotenough

Equality constraint expressing coinciding distributions can be used to supplement the marginal problem, and may be of practical use for reducing the dimensionality of the problem (number of quantifiers which need to be eliminated).

However, we are not aware of any case in which this would actually result in tighter exclusions for the distributions on the original DAG. In many cases, this can be explained by the following argument.

Suppose two sets \mathbf{X} and \mathbf{Y} are inflationarily isomorphic, such that a copy-to-copy isomorphism exists which takes $\text{AnSubDAG}_{G'}[\mathbf{X}] \leftrightarrow \text{AnSubDAG}_{G'}[\mathbf{Y}]$. If the copy-to-copy isomorphism can be extended to some copy-to-copy automorphism of the entire inflation DAG G' then the constraint $P_{\mathbf{X}} = P_{\mathbf{Y}}$ is not relevant for the distributions on the original DAG. The proof is as follows.

If \hat{P} solves the unsupplemented marginal problem, then switching the variables in \hat{P} according to the automorphism still solves the unsupplemented marginal problem, since the given marginal distributions are preserved by the automorphism. Now taking the uniform mixture of this new distribution with \hat{P} results in a distribution that still solves the marginal problem, and in addition satisfies the supplemented constraint $P_{\mathbf{X}} = P_{\mathbf{Y}}$.

Note that the argument does not apply if there is no copy-to-copy automorphism which restricts to $\text{AnSubDAG}_{G'}[\mathbf{X}] \sim \text{AnSubDAG}_{G'}[\mathbf{Y}]$, and it also does not apply if one uses the conditional independence relations on the inflation DAG as well, since this destroys linearity. We do not know what happens in either of these cases.

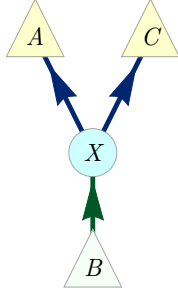


FIG. 12. A causal structure that is compatible with any distribution P_{ABC} .

fig:beforecopy

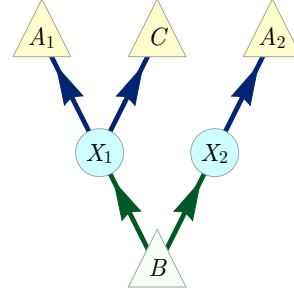


FIG. 13. An inflation.

fig:aftercopy

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

As it turns out, the inflation DAG 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 [\[75, Chapter 15\]](#). The following formulation of the copy lemma is the one of Kaced [\[76\]](#).

Lemma 6. *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. $P_{AB} = P_{AB'}$,
2. $A' \perp AC \mid B$.

Proof. Consider the original DAG of Fig. 12 and the associated inflation DAG of Fig. 13. If the original distribution P_{ABC} is compatible with Fig. 12, then the associated inflation model marginalizes to a distribution $P_{AA'BC}$ which has the required properties. Hence it remains to be shown that every P_{ABC} is compatible with Fig. 12. But this is easy: take λ to be any sufficient statistic for the joint variable (A, B) given C , such as $\lambda := (A, B, C)$. \square

While it is also not hard to write down a distribution with the desired properties explicitly [\[75, Lemma 15.8\]](#), our purpose of rederiving the lemma via inflation is our hope that more sophisticated applications of the inflation technique will result in *new* non-Shannon type entropic inequalities.

Appendix D: 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 inflation 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 $\{-1, +1\}$.

T: it may be better to list this as a table of coefficients, as e.g. in [arXiv:1101.2477](#), p.14/15?

TABLE II. List of coefficients

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	0	0	0	1	1	0	0	0	0	1	0	0	0	0
2	0	0	0	0	-2	0	0	0	0	0	-1	0	0	1
3	1	1	1	3	-1	0	0	0	0	-1	1	-1	0	1
3	1	1	-1	3	1	0	0	0	0	1	-1	-1	0	1
3	0	0	1	-2	0	-2	0	1	0	0	-1	-1	0	1
3	0	1	0	1	0	-2	0	-1	1	0	1	-1	0	1
3	0	1	0	1	0	-2	0	1	-1	0	1	1	0	-1
3	1	1	1	2	2	2	-1	1	1	1	1	1	1	-1
3	1	1	1	2	0	-2	1	1	-1	1	1	1	-1	-1
4	0	0	2	-2	-2	0	-1	2	0	2	1	1	1	0
4	0	-2	0	-2	0	-3	1	0	0	1	1	-1	0	1
4	0	0	-2	-2	-2	-3	1	2	0	1	1	1	0	-1
4	0	0	0	2	-2	1	1	2	2	-1	1	-1	0	-1
4	0	0	0	2	-2	1	1	-2	2	-1	1	1	0	1
4	0	0	0	-2	0	3	1	2	0	1	-1	-1	0	1
4	0	0	-2	-2	-2	-2	1	2	0	0	1	1	-1	0
4	0	0	0	-2	-2	-2	1	2	2	2	1	1	1	0
5	1	1	1	3	1	-4	0	-2	0	1	1	-1	0	1
5	1	1	1	3	-1	-4	0	2	-2	1	1	1	0	-1
5	1	-1	1	1	2	-2	-2	-2	-1	1	1	-2	-2	0
5	3	1	1	1	3	1	-1	2	0	0	-2	0	0	2
5	1	1	1	1	2	-2	-1	0	-1	-1	2	1	1	-2
5	-1	1	1	1	1	-1	1	-2	-2	2	-2	-2	-2	0
5	1	1	1	2	1	-1	1	-1	0	2	-1	-2	-2	1
5	1	1	1	-1	2	2	1	-2	-1	-1	2	1	-1	-2
6	0	0	0	-3	-4	0	0	1	2	2	-1	-2	-2	1
6	0	2	0	3	-4	0	0	1	2	0	1	-2	-2	1
6	-2	2	0	-3	-5	0	0	1	1	0	1	-1	-2	2
6	0	0	0	1	-3	2	0	1	1	-4	1	-1	-2	-2
6	0	0	2	0	3	-5	0	-2	1	1	2	1	1	-2
6	0	0	-2	2	-2	1	0	-4	2	-1	2	2	1	1
6	0	0	0	-3	-2	-2	-2	1	0	4	-1	-2	0	1
7	1	1	1	2	1	-3	3	1	-2	2	3	2	-2	-1
8	0	0	0	-4	-2	-2	-3	4	2	-2	1	-1	-3	2
8	2	-2	0	1	-6	0	1	-1	0	2	2	1	-3	3
8	2	0	0	6	1	-2	1	0	1	2	-1	-2	-3	3
8	0	-2	-2	0	-6	1	1	2	0	-1	3	1	-2	-3
8	0	0	2	2	1	-6	1	-2	1	0	3	2	-1	-3

Appendix E: Other possibilities for the form of the observational data and causal hypotheses

A causal hypothesis is deemed **compatible** with a given distribution over observed variables if there is some causal model in the set defined by the causal hypothesis which yields this distribution,

$$H_G \text{ is compatible with } D^{\text{obs}} \text{ iff } \exists M \in H_G : P(\text{ObservedNodes}[G]) \in D^{\text{obs}}, \quad (\text{A-1})$$

where $P(\text{ObservedNodes}[G])$ is fixed by the causal model M through Eqs. ^{Markov}(2) and ^{MarkovObserved}(3).

In broad strokes, the inflation DAG technique is a way of mapping a causal inference problem of this sort to a new such problem where the observational and causal inputs of the new problem are determined by the observational and causal inputs of the original problem and where compatibility between the observational and causal inputs of the original problem implies compatibility between the observational and causal inputs of the new problem. The technique is useful because, as we show, simple witnesses of incompatibility in the new problem yield nontrivial witnesses of incompatibility in the original problem.

The inflation DAG technique can accommodate many different forms for the observational constraints and for the causal hypothesis that appear in the original problem. It also imposes a restriction on the forms for the observational constraints and the causal hypothesis appearing in the new problem. It is therefore useful to pause and consider the range of possibilities for the two inputs of a causal decision problem.

Possibilities for the form of the observational constraints include a specification of:

- O1 a joint distribution over the observed variables.
- O2 a confidence interval around a joint distribution over the observed variables
- O3 conditional independence relations among the observed variables
- O3 marginals of the joint distribution for certain subsets of the observed variables

In addition to this sort of variety, one can imagine that the statistical dependences among a set of variables may be specified not by a joint distribution but by covariance matrices or the values of entropic quantities such as mutual information. Combinations of these possibilities are also possible.

The specification of the joint distribution, example O1, is the most restrictive form that the observational constraints can take. Specifying a region, example O2, provides a means of expressing uncertainty about the joint distribution. Specifying conditional independences, example O3, is the form of observational data that has been most thoroughly exploited in the development of tools for causal inference. If one specifies marginals, as in example O4, then the causal inference problem becomes a version of the marginals problem (described in the introduction), but where the space of joint distributions from which the marginals may arise is constrained by the causal hypothesis.

The inflation DAG technique can be applied for *any* of these types of observational constraints. Nonetheless, the particular concrete applications of the inflation DAG technique that we will describe in detail in this article will consider problems where the joint distribution is specified, i.e., constraints of the form of O1. The new causal inference problem to which this original problem is mapped by inflation, however, is one where the constraints concern marginals, i.e., they are of the form of O4.

It is also useful to exhibit some of the possibilities for the form that the causal hypothesis may take:

- H1 the full set of causal models for a particular DAG G
- H2 the full set of causal models for a particular DAG G excluding those that yield conditional independence relations beyond those implied by d-separation in G
- H3 the set of causal models for a particular DAG G wherein there are constraints on the manner in which particular nodes causally depend on their parents and/or constraints on the cardinality of the set of values for particular latent variables
- H4 the set of causal models for a particular DAG G wherein the manner in which a particular node causally depends on its parents is constrained to be equivalent, under some mapping between nodes, to the manner in which another node causally depends on its parents

In all cases, we have left implicit the trivial constraint that the causal hypothesis must include only those DAGs for which the set of observed nodes coincides with the set of variables described in the observational data.

The motivation for considering hypotheses of the form of H2 rather than H1 is the principle that a causal explanation should not be fine-tuned [reference] ^{WoodSpekkens}[7]. If, for some observational data, a causal hypothesis of type H1 is compatible but one of type H2 is not, then it means that the conditional independences in the observational data are not a

consequence of the causal structure, but rather are a consequence of the choice of parameters. Such an explanation can be criticized on the grounds that it is fine-tuned. Finding a causal hypothesis of type H2 that is compatible with the observational data implies that one has a non-fine-tuned explanation of that data. The fine-tuning issue will come up in Sec. VII where we discuss quantum causal models. *Note, not there yet...*

An example of a causal hypothesis of type H3 is that of an additive noise model: if an observed variable Y has an observed variable X and a latent variable U as parents, then the noise is deemed additive if $Y = \alpha X + \beta U$ for some scalars α and β [provide references]. Clearly, the conditional probability distributions $P_{Y|XU}$ that can be achieved in such an additive noise model are a subset of the valid conditional distributions. More general constraints on the conditional distributions have also been explored alongside constraints on the sizes of the latent variables [cite Lee-Spekkens].

A causal hypothesis of type H4 involves a novel and unusual sort of constraint, which has not, to our knowledge been studied previously. We include it on our list because it is the sort of causal hypothesis that appears in the new causal problem that is defined by our inflation DAG technique. Insofar as it is usually assumed that the manner in which one node in a DAG causally depends on its parents should be completely independent of the manner in which another depends on its parents—sometimes described as the assumption of *autonomy* of different causal mechanisms [Pearl]—it is quite conceivable that hypotheses of type H4 have *no* significance besides the role that they play in the inflation DAG technique.¹²

The inflation map takes a causal hypothesis of type H1 and maps it to a causal hypothesis of type H4.

¹² We could say something here about how this suggests that one does better to think of the inflation DAG in terms of counterfactuals and twin diagrams. .

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