

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, as in experiment design. **What is “experiment design”? Is this a technical term in statistics? –RWS**

It is useful to distinguish two varieties of this problem. In the first case, 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). In the second case, the nature of the latent variables is arbitrary.

Consider the first case. 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. The probability distribution over the observed variables are defined as a function of the conditional probabilities incorporating the latent variables, where this function is dictated by the DAG. If one can eliminate the parameters describing these conditional probabilities, while taking into account the constraint that probabilities are constrained to the unit interval, one is left with constraints that refer exclusively to the probability distribution over the observed variables. Because this is a nonlinear quantifier elimination problem, it is infeasible to provide an exact solution except in very simple cases [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 case, 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 for quantifiers that refer to the latent variables. 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.

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 it is no longer, in general, 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 which considerations of relativity theory suggested must have a particular causal structure, and 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 suitably entangled quantum states.¹

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

¹ This incompatibility has subsequently become known as *quantum nonlocality* [6]. 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 did not go beyond conditional independence relations.

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.

concerns noncompliance in drug trials. More recently, ^{Steudel2010ancestors} Steudel and Ay [9] have derived inequalities which witness the impossibility to model a given distribution on n variables in terms of a causal structure without a common (hidden) ancestor for any subset of at least c nodes, for any $n, c \in \mathbb{N}$. **Can the Steudel and Aye result be expressed more clearly?—RWS** The community of researchers who work on the foundations of quantum theory have also, over the years, derived many generalizations of the CHSH inequality ^{Brunner2013Bell} [6], but the idea that such work is usefully understood as a special case of the causal inference problem has only recently been appreciated ^{Woodspekkens, Fritzsche2012bell, Pusey2014gdag, BeyondB} [7, 10–12].

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 derive 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. $\text{Pa}_G(X) = \{Y \mid Y \rightarrow X\}$. 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 U is a set of nodes, then we put $\text{Pa}_G(U) := \bigcup_{X \in U} \text{Pa}_G(X)$ and $\text{Ch}_G(U) := \bigcup_{X \in U} \text{Ch}_G(X)$. The **ancestors** of a set of nodes U , denoted $\text{An}_G(U)$, are defined as those nodes which have a directed *path* to some node in U , including the nodes in U themselves. Equivalently (dropping the G subscript), $\text{An}(U) := \bigcup_{n \in \mathbb{N}} \text{Pa}^n(U)$, where $\text{Pa}^n(U)$ is inductively defined via $\text{Pa}^0(U) := U$ and $\text{Pa}^{n+1}(U) := \text{Pa}(\text{Pa}^n(U))$. 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

The set of causal parameters specifies, first of all, the nature of the random variable associated to each node, 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. It also 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

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

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

Should we worry about the fact that the conditional probability refers to variables whereas, strictly speaking, A refers to a node. Should we have a function $\text{Vars}[G]$ that specifies the variables? Note that a category-theoretic treatment of a causal model is cleaner in this respect insofar as the nodes are replaced with objects and these can be defined to encode dimensionality.

A DAG G and a set of causal parameters F_G defines a causal model, which we denote by

$$M = (G, F_G). \quad (2)$$

In this case, $\text{DAG}[M]$ and $\text{Params}[M]$ specify G and F_G respectively.

As is standard, a causal model M specifies a joint distribution over all variables in the DAG, namely,

$$P(\text{Nodes}[G]) = \prod_{A \in \text{Nodes}[G]} P_{A|\text{Pa}_G(A)}, \quad (3) \quad \boxed{\{\text{Markov}\}}$$

(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

$$P(\text{ObservedNodes}[G]) = \sum_{\{X: X \in \text{LatentNodes}[G]\}} P(\text{Nodes}[G]). \quad (4) \quad \boxed{\{\text{MarkovObs}\}}$$

In addition to the notion of a causal model, it is useful to have a notion of a **causal hypothesis**, which we define to be a set of causal models. We shall consider only causal hypotheses for which the models in the set share the same DAG. The most simple sort of causal hypothesis is one that includes the full set of causal models associated to a DAG G , which we denote by H_G^{full} . This is simply the hypothesis of a particular DAG, with no restriction on the set of parameters that supplement it. Examples of more refined hypotheses are provided below.

Causal hypotheses are judged on the basis of **observational constraints**. These are a restriction on the joint distribution over the observed variables, specified as a subset of the set of all possible joint distributions over the observed variables, which we denote by D^{obs} ³.

Causal inference is about judging the plausibility of different causal hypotheses given certain observational constraints. In this article, we will be concerned with a particular sort of causal inference problem, namely, a decision problem which takes as its input (i) a specification of observational constraints and (ii) a specification of a causal hypothesis, and which outputs whether or not the two are compatible with one another.

A causal hypothesis is deemed **compatible** with observational constraints if there is some causal model in the set defined by the causal hypothesis which yields a joint distribution in the set defined by the observational constraints,

$$H_G \text{ is compatible with } D^{\text{obs}} \text{ iff } \exists M \in H_G : P(\text{ObservedNodes}[G]) \in D^{\text{obs}}, \quad (5)$$

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

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

³ Note that despite the terminology, such constraints might derive from experiments that include interventions.

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][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.⁴

III. INFLATION: A TOOL FOR CAUSAL INFERENCE

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

⁴ 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. .

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

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 $A_i \sim A_j \sim A$. 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 ,

$$G' \in \text{Inflations}[G] \quad \text{iff} \quad \forall A_i \in \text{Nodes}[G'] : \text{AnSubDAG}_{G'}[A_i] \sim \text{AnSubDAG}_G[A]. \quad (6) \quad \text{\texttt{fig:defin}}$$

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.

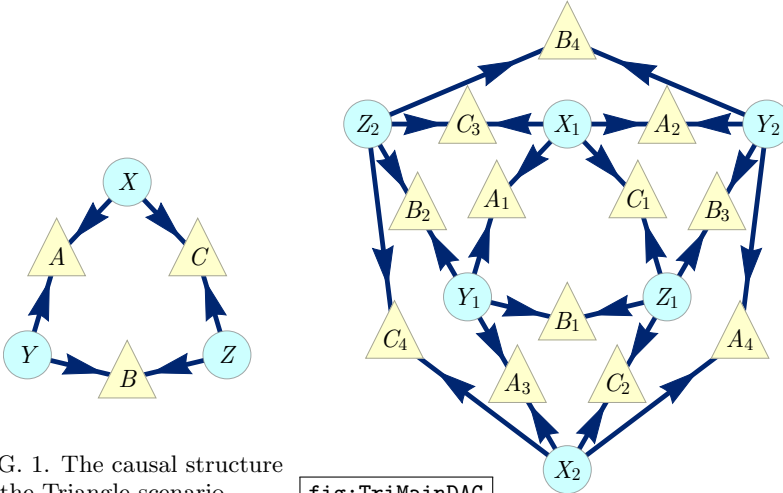


FIG. 1. The causal structure of the Triangle scenario.

fig:TriMainDAG

FIG. 2. An inflation DAG of the Triangle scenario where each latent node has been duplicated, resulting in four copies of each observable node.

fig:TriFullDouble

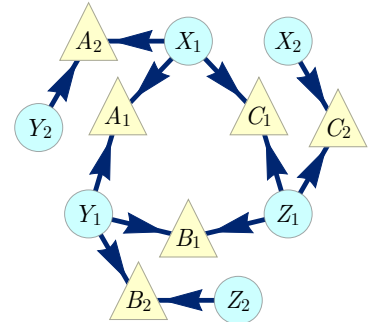


FIG. 3. Another inflation of the Triangle scenario consisting, also notably $\text{AnSubDAG}_{(\text{Fig. 2})}[A_1 A_2 B_1 B_2 C_1 C_2]$.

fig:Tri22

We now turn to specifying the function $\text{Inflation}[]_{G \rightarrow G'}$, that is, to specifying how a causal model transforms under inflation. One we've said how DAG inflated, then we need TWO things: How models (and hypothesis) inflate, and also how observational data inflates. Best to word intro to subject in a way that suggests we'll be getting around to both topics sequentially? 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. (6)), one can formalize this condition as:

$$\forall A_i \in \text{Nodes}[G'] : P_{A_i|\text{Pa}_{G'}(A_i)} = P_{A|\text{Pa}_G(A)}, \quad (7) \quad \{\text{eq:funcnd}\}$$

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* of Pearl [1].

Because causal hypotheses are sets of causal models, and the inflation map acts on causal models, it has an induced action on causal hypotheses. Let H_G^{full} denote the causal hypothesis that the DAG is G (the hypothesis consisting of the set of *all* causal models compatible with the DAG G). The induced action of the inflation map has the notable feature that $\text{Inflation}[H_G^{\text{full}}] \neq H_{G'}^{\text{full}}$ because even if there is no restriction on the set of parameters supplementing G , inflation imposes a restriction on the set of parameter supplementing G' . Specifically, if nodes A_i and A_j on G' are copies of a single node A on G , then the set of parameters on G' are constrained to satisfy $P_{A_i|\text{Pa}_{G'}(A_i)} = P_{A_j|\text{Pa}_{G'}(A_j)}$. This explains our earlier claim that the inflation map takes a causal hypothesis of type H1 and maps it to a causal hypothesis of type H4.

It remains to explain how a $G \rightarrow G'$ inflation acts on the observational data and to prove that compatibility in the original causal decision problem implies compatibility in the image of this problem under inflation. Both purposes are served by contemplating what inflation means for the joint distribution over observed variables induced by a causal model. Because inflation is a map on causal models, it has an induced action on the joint distribution over observed variables defined by a causal model. We begin by describing this action. In what follows, we assume that G and G' are DAGs with $G' \in \text{Inflations}[G]$ and that M and M' are causal models with $M' = \text{Inflation}[M]_{G \rightarrow G'}$. Finally, distributions that arise from M are denoted by P , and those arising from M' are denoted by P' .

Note, first of all, that for any sets of nodes $\mathbf{U} \subseteq \text{Nodes}[G']$ and $\tilde{\mathbf{U}} \subseteq \text{Nodes}[G]$,

$$\text{if } \text{AnSubDAG}_{G'}[\mathbf{U}] \sim \text{AnSubDAG}_G[\tilde{\mathbf{U}}] \text{ then } P'(\mathbf{U}) = P(\tilde{\mathbf{U}}). \quad (8) \quad \{\text{eq:coinc}\}$$

This follows from the fact that the probability distributions over \mathbf{U} and $\tilde{\mathbf{U}}$ depend only on their ancestral subgraphs and the parameters defined thereon, which by the definition of inflation are the same for \mathbf{U} and for $\tilde{\mathbf{U}}$.

It is useful to have a name for a set of observed nodes in the inflation DAG, $\mathbf{U} \subseteq \text{ObservedNodes}[G']$ satisfying the antecedent of Eq. (8), that is, such that one can find a corresponding set in the original DAG, $\tilde{\mathbf{U}} \subseteq \text{ObservedNodes}[G]$, which has an 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**,

$$\mathbf{U} \in \text{InjectableSets}[G' \rightarrow G] \text{ iff } \exists \tilde{\mathbf{U}} \subseteq \text{ObservedNodes}[G] : \text{AnSubDAG}_{G'}[\mathbf{U}] \sim \text{AnSubDAG}_G[\tilde{\mathbf{U}}]. \quad (9) \quad \{\text{eq:defin}\}$$

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

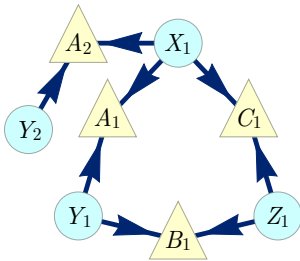


FIG. 4. A simple inflation of the Triangle scenario, also notably $\text{AnSubDAG}_{(\text{Fig. 3})}[A_1 A_2 B_1 C_1]$.

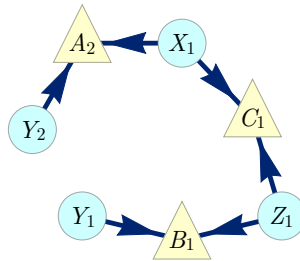


FIG. 5. An even simpler inflation of the Triangle scenario, also notably $\text{AnSubDAG}_{(\text{Fig. 3})}[A_1 A_2 B_1 C_1]$.

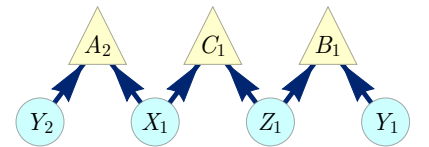


FIG. 6. Another representation of Fig. 5. Despite not containing the original scenario, it is a valid inflation per Eq. (6). fig:TriDa

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 sets of nodes of G' that will be of primary interest to us are not the injectable sets per se, but sets satisfying a slightly weaker constraint. To define the latter sorts of sets, which we term *pre-injectable*, we must first introduce some additional terminology.

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 ,

$$U \not\sim_{\emptyset} V \quad \text{iff} \quad \text{An}(U) \cap \text{An}(V) = \emptyset. \quad (10)$$

Ancestral independence is equivalent to d -separation by the empty set [pearl2009causality,spirtes2011causation,studeny2005probabil1-4].

A set of nodes U in the inflation DAG G' will be called **pre-injectable** whenever it is a union of injectable sets with disjoint ancestries.

$$U \in \text{PreInjectableSets}[G'] \quad \text{iff} \quad \exists \{U_i \in \text{InjectableSets}[G']\} \quad \text{s.t.} \quad U = \bigcup_i U_i \quad \text{and} \quad \forall i \neq j : U_i \not\sim_{\emptyset} U_j. \quad (11) \quad \boxed{\text{eq:defineprein}}$$

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 U is a pre-injectable set and U_1, U_2, \dots, U_n are the ancestrally independent components of U , then

$$P'(U) = P'(U_1)P'(U_2) \cdots P'(U_n). \quad (12)$$

Furthermore, because each injectable set of variables U_i satisfies Eq. (8), it follows that joint distributions on pre-injectable sets in the inflation model can be expressed in terms of distributions defined on the original causal model, eq:coincidingdistrodef

$$P'(U) = P(\tilde{U}_1)P(\tilde{U}_2) \cdots P(\tilde{U}_n). \quad (13) \quad \boxed{\text{eq:prein}}$$

This relation specifies precisely how the marginal distribution over any pre-injectable set in the inflated causal model is defined in terms of the distribution over the corresponding set of variables in the original causal model.

Because this relation involves only *observed variables* of the original and inflated causal models, one can use it to determine observational constraints for the inflated causal inference problem from observational constraints for the original problem.

In the original causal inference problem, whatever form the observational constraint takes, one can deduce its consequences for the marginals on subsets of variables that correspond to injectable sets with copy-indices dropped, that is, the marginals on subsets $\tilde{U} \subseteq \text{ObservedNodes}[G]$ satisfying $\tilde{U} \sim U$ where $U \in \text{InjectableSets}[G']$. Marginalization onto \tilde{U} is a map on probability distributions, but given that the observational constraint D^{obs} is a set of probability distributions, such marginalization has an induced action on D^{obs} . We denote the marginalization onto \tilde{U} of D^{obs} by $D_{\tilde{U}}^{\text{obs}}$. The set $D_{\tilde{U}}^{\text{obs}}$ captures the consequences of the observational constraints for the marginal distribution on \tilde{U} .

In the inflated causal inference problem, suppose the observational constraint D'^{obs} specifies a set of possibilities for the joint distribution on $\text{ObservedNodes}[G']$. For every pre-injectable set $U \in \text{PreInjectableSets}[G']$, let the image of D'^{obs} under marginalization on \tilde{U} be denoted by $D_{\tilde{U}}'^{\text{obs}}$. It is then clear from Eq. (13) that if U_1, U_2, \dots, U_n are the ancestrally independent components of U , as in Eq. (11), then eq:defineprein

$$\forall U \in \text{PreInjectableSets}[G'] : D_{\tilde{U}}'^{\text{obs}} \equiv \{P'(U) = \prod_i P(\tilde{U}_i) : P(\tilde{U}_i) \in D_{\tilde{U}_i}^{\text{obs}} \quad \forall i\}. \quad (14)$$

The key is this: if a given specification of marginals on deflated injectables is compatible with the original causal hypothesis, then the corresponding products of marginals on the pre-injectable sets is compatible with the inflated causal hypothesis. If a joint distribution is compatible with the original causal hypothesis, then its marginals on deflated injectables are as well, and we get the corresponding inference on the inflated problem. An observational constraint provides a bunch of joint distribution candidates for compatibility with the causal hypothesis and inflation turns these into a bunch of marginals candidates for compatibility with the inflated causal hypothesis.

If the observational constraint D^{obs} and the causal hypothesis H_G are compatible, then the observational constraint $\{D_U^{\text{obs}} : U \in \text{PreInjectableSets}[G']\}$ and the causal hypothesis $H_{G'} = \text{Inflation}[H_G]$ are compatible.

We need to define the notion of observational constraints on a set of marginal distributions. Let $\text{Subsets}[G]$ be the subsets of the nodes of G on which we impose our observational constraints. Let $(P(U) : U \in \text{Subsets}[G])$ be a collection of marginals associated to these subsets. Then the observational constraint on marginals is a set of such collections, denoted $D_{\text{marg}}^{\text{obs}}$.

Let the function $\text{JointDistObserved}[M]$ return the joint distribution over the observed nodes implied by causal model M , via Eqs. ???.

Compatibility in the original causal inference problem implies that

$$\exists M \in H_G : \text{JointDistObserved}[M] \in D^{\text{obs}} \quad (15)$$

We can now describe the image of the observational constraint D^{obs} under the $G \rightarrow G'$ inflation map, $D'^{\text{obs}} = \text{Inflation}[D^{\text{obs}}]_{G \rightarrow G'}$, as follows:

$$D'^{\text{obs}} \equiv \{P(\text{all}) : \text{marginals } P(\tilde{U}) : \tilde{U} \sim U \in \text{InjectableSets}[G'] \text{ are built from } D_0^{\text{obs}} \text{ via Eq. (I3)}\}. \quad (16)$$

??? If some distribution were compatible with the causal hypothesis in the original causal inference problem, then the counterpart of this distribution on the pre-injectable sets would be compatible with the inflated causal hypothesis. If some observational constraint were compatible with the causal hypothesis in the original causal inference problem, then the counterpart of this constraint on the pre-injectable sets would be compatible with the inflated causal hypothesis. This holds if and only if

$$\exists C \in H_{G,S} : P_C(\text{ObservedNodes}[G]) = P(O). \quad (17)$$

Every inflation $G \rightarrow G'$ defines a new causal inference problem for which the decision regarding compatibility is the same as for the original problem.

The causal hypothesis of the new causal inference problem is simply the image under a $G \rightarrow G'$ inflation of the causal hypothesis of the original causal inference problem, and one seeks to evaluate its compatibility with observational data that is determined by the observational data of the original in the following way.

Let O denote the image of \tilde{O} under the $G \rightarrow G'$ inflation, and consider the subsets of O that are pre-injectable relative to the $G \rightarrow G'$ inflation, denoted $\text{PreInjectableSets}[O]$. Recall that for every set of nodes $U \in \text{PreInjectableSets}[O]$ there is a partition $U = \bigcup_i U_i$ where the U_i are subsets of O that are injectable relative to the $G \rightarrow G'$ inflation and that are ancestrally independent. Recall also that, by the definition of a $G \rightarrow G'$ inflation, for any set of nodes $U_i \subseteq O$ that is injectable, one can find a set of nodes $\tilde{U}_i \subseteq \tilde{O}$ such that $\forall i : U_i \sim \tilde{U}_i$. The observational data of the new causal inference problem is that $\forall U \in \text{PreInjectableSets}[O] : P(U) = P(\tilde{U}_1)P(\tilde{U}_2) \dots P(\tilde{U}_n)$, where $P(\tilde{U}_i)$ is the marginal of $P(\tilde{O})$ on \tilde{U}_i .

Therefore the observational input to the new causal inference problem is not the distribution on O , but rather a specification of the marginals of this distribution on each of the pre-injectable sets of O under the $G \rightarrow G'$ inflation.

Summarizing, we have:

Lemma 3. *If a causal hypothesis H_G is compatible with the observational data D^{obs} then the image of this causal hypothesis under a $G \rightarrow G'$ inflation is compatible with the image of this observational data under a $G \rightarrow G'$ inflation.*

For the specific sorts of causal inference problems we consider in this article, the observational data is a specification of a joint distribution over the set O of observed variables, $P(\tilde{O})$, and its image under inflation is a specification of certain marginals of the joint distribution over the inflation of O , namely, $\forall U \in \text{PreInjectableSets}[O] : P(U) = P(\tilde{U}_1)P(\tilde{U}_2) \dots P(\tilde{U}_n)$.

It follows that any incompatibility witnesses that one can derive for the new causal inference problem immediately yield incompatibility witnesses for the original causal inference problem. Indeed, any manner of incompatibility witnesses from the standard toolkit of causal inference can be applied to the new problem to yield generally novel incompatibility witnesses for the original problem. Any causal inference tool, therefore, can potentially have its power augmented by combining it with the inflation technique.

New narrative.

A given joint distribution being compatible with the original causal hypothesis does not imply that it is compatible with the inflated causal hypothesis. Indeed, the observed variables are not even the same in the two cases. However, certain tuples of marginals being compatible with the original causal hypothesis do imply that an inflation of the tuple of marginals (where each marginal now applies to the copy-index-equivalent variables in the inflated DAG) is compatible with the inflated causal hypothesis.

Thus any tricks that can be used to infer incompatibility or provide a necessary condition for compatibility of the inflated tuple of marginals with the inflated causal hypothesis can be used to infer incompatibility or provide a necessary condition for compatibility of the original causal inference problem.

Example 1: Perfect correlation cannot arise from the Triangle scenario.

Consider the following causal inference problem. The observational data is a joint distribution over three binary-outcome variables, P_{ABC}^{obs} , where the marginal on each variable is uniform and the three are perfectly correlated,

$$P_{ABC}^{\text{obs}} = \frac{[000] + [111]}{2}, \quad \text{i.e.} \quad P_{ABC}^{\text{obs}}(abc) = \begin{cases} \frac{1}{2} & \text{if } a=b=c, \\ 0 & \text{otherwise.} \end{cases} \quad (18) \quad \boxed{\text{eq:ghzdi}}$$

The causal hypothesis is that the DAG corresponds to the triangle scenario, depicted in Fig. 3. The problem is to decide whether the observational data is compatible with this causal hypothesis.

To solve this problem, we consider its image under the inflation of the triangle scenario to the DAG depicted in Fig. 6. The sets $\{A_2C_1\}$ and $\{B_1C_1\}$ are injectable (hence trivially pre-injectable). The set $\{A_2B_1\}$ is also pre-injectable because the singleton sets $\{A_2\}$ and $\{B_1\}$ are each injectable and $A_2 \not\rightarrow B_1$. Therefore, the inflated observational data for our new causal inference problem includes

$$\begin{aligned} P_{A_2C_1}^{\text{obs-inf}} &= P_{AC}^{\text{obs}} = \frac{[00] + [11]}{2} \\ P_{B_1C_1}^{\text{obs-inf}} &= P_{BC}^{\text{obs}} = \frac{[00] + [11]}{2} \\ P_{A_2B_1}^{\text{obs-inf}} &= P_A^{\text{obs}} \otimes P_B^{\text{obs}} = \frac{[0] + [1]}{2} \otimes \frac{[0] + [1]}{2}. \end{aligned} \quad (19) \quad \boxed{\text{eqs}\{\text{eq:ghzdist}, \text{eq:triangle}\}}$$

The question is whether such constraints are compatible with the causal hypothesis that the DAG is that of Fig. 6, where the parameters supplementing the DAG are unrestricted but for the constraint that the latent variables Y_1 and Y_2 are identically distributed.

It is not difficult to see that the answer to the question is negative, and that this verdict can be rendered without even appealing to the form of the inflation DAG. It suffices to make use of results concerning the marginals problem, namely, that there is no joint distribution $P_{A_2B_1C_1}$ having marginals of the form given in Eqs. (19). To see this, 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 .

We have therefore certified that the joint distribution P_{ABC}^{obs} of Eq. (18) is not compatible with the Triangle causal structure, recovering the seminal result of Steudel and Ay [9]. eq:ghzdistribution1

Example 2: The W-type distribution cannot arise from the Triangle scenario

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}^{W} of the form

$$P_{ABC}^{\text{W}} = \frac{[100] + [010] + [001]}{3}, \quad \text{i.e.} \quad P_{ABC}^{\text{obs}}(abc) = \begin{cases} \frac{1}{3} & \text{if } a+b+c=1, \\ 0 & \text{otherwise.} \end{cases} \quad (20) \quad \boxed{\text{eq:wdist}}$$

We call this the W-type distribution⁵.

To prove the incompatibility of P^{W} with the Triangle causal structure, we consider the inflation DAG of Fig. 3. The sets $\{A_2C_1\}$, $\{B_2A_1\}$, $\{A_2B_1\}$ and $\{A_1B_1C_1\}$ are injectable. The set $\{A_2B_2C_2\}$ is pre-injectable because the singleton sets $\{A_2\}$, $\{B_2\}$ and $\{C_2\}$ are injectable and *all* ancestrally independent. It follows that we must consider

⁵ Because its correlations are reminiscent of those one obtains for the quantum state appearing in Ref. [17], and which is called the W state. 3Qubits2Ways

the inflated observational data

$$P_{A_2 C_1}^{W\text{-inf}} = P_{AC}^W = \frac{[10] + [01] + [00]}{3} \quad (21) \quad \{\text{W1}\}$$

$$P_{B_2 A_1}^{W\text{-inf}} = P_{BA}^W = \frac{[10] + [01] + [00]}{3} \quad (22) \quad \{\text{W2}\}$$

$$P_{C_2 B_1}^{W\text{-inf}} = P_{CB}^W = \frac{[10] + [01] + [00]}{3} \quad (23) \quad \{\text{W3}\}$$

$$P_{A_1 B_1 C_1}^{W\text{-inf}} = P_{ABC}^W = \frac{[100] + [010] + [001]}{3} \quad (24) \quad \{\text{W4}\}$$

$$P_{A_2 B_2 C_2}^{W\text{-inf}} = P_A^W \otimes P_B^W \otimes P_C^W = \frac{[1] + 2 \cdot [0]}{3} \otimes \frac{[1] + 2 \cdot [0]}{3} \otimes \frac{[1] + 2 \cdot [0]}{3} \quad (25) \quad \{\text{W5}\}$$

Eq. (21) implies that $C_1=0$ whenever $A_2=1$. Similarly, $A_1=0$ whenever $B_2=1$ and $B_1=0$ whenever $C_2=1$. Eq. (25) implies that A_2, B_2 , and C_2 are uncorrelated and uniformly distributed, which means that sometimes they all take the value 1. Summarizing, we have

$$A_2=1 \implies C_1=0$$

$$B_2=1 \implies A_1=0$$

$$C_2=1 \implies B_1=0$$

and sometimes $A_2=1, B_2=1, C_2=1$.

But these constraints clearly imply that

$$\text{sometimes } A_1=0, B_1=0, C_1=0,$$

which contradicts Eq. (24).

Again, we have reached our verdict here simply by noting that the distributions defined in Eqs. (21)-(25) cannot arise as the marginals of a single distribution on $A_1, B_1, C_1, A_2, B_2, C_2$. Specifically, we have leveraged an approach to the marginal problem inspired by Hardy's version of Bell's theorem [18, 19], see Sec. VIII for further discussion of Hardy-type paradoxes and their applications.

We have thus established that the distribution P_{ABC}^W of Eq. (20) is incompatible with the triangle DAG. To our knowledge, this fact 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 Aberg *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: The PR-box cannot arise from the Bell scenario

Consider the causal structure associated to the Bell [5, 6, 23, 24] scenario [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 .

We consider the distribution $P_{ABXY}^{\text{obs}} = P_{AB|XY}^{\text{PR}} \otimes P_X^{\text{free}} \otimes P_Y^{\text{free}}$, where P_X^{free} and P_Y^{free} are arbitrary full-support

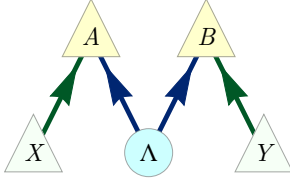


FIG. 7. The causal structure of the bipartite Bell scenario. The local outcomes of Alice's and Bob's experimental probing is assumed to be a function of some latent common cause, in addition to their independent local experimental settings.

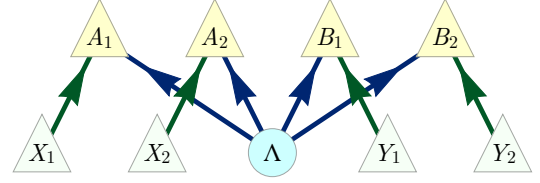


FIG. 8. An inflation DAG of the bipartite Bell scenario, where both local settings variables have been duplicated.

fig:BellD

fig:NewBellDAG1

distributions⁶ over the binary variables X and Y , and

$$P_{AB|XY}^{\text{PR}}(ab|xy) = \begin{cases} \frac{1}{2} & \text{if } \text{mod}_2[a+b]=x \cdot y, \\ 0 & \text{otherwise.} \end{cases} \quad (26)$$

{eq:PRbox}

The correlations described by this distribution are known as PR-box correlations after Popescu and Rohrlich, and they are well-known to be incompatible with the the Bell scenario [27, 28]. Here we prove this incompatibility using the inflation technique.

We use the inflation of the Bell DAG shown in Fig. 8.

We begin by recognizing that $\{A_1 B_1 X_1 Y_1\}$, $\{A_2 B_1 X_2 Y_1\}$, $\{A_1 B_2 X_1 Y_2\}$, and $\{A_2 B_2 X_2 Y_2\}$ are all injectable sets, and that $\{X_1 X_2 Y_1 Y_2\}$ is a pre-injectable set because the singleton sets $\{X_1\}$, $\{X_2\}$, $\{Y_1\}$, and $\{Y_2\}$ are all injectable and ancestrally independent of one another. It follows that the observable data inflates according to

$$\begin{aligned} P_{A_1 B_1 X_1 Y_1}^{\text{obs-inf}} &= P_{ABXY}^{\text{obs}} \\ P_{A_2 B_1 X_2 Y_1}^{\text{obs-inf}} &= P_{ABXY}^{\text{obs}} \\ P_{A_1 B_2 X_1 Y_2}^{\text{obs-inf}} &= P_{ABXY}^{\text{obs}} \\ P_{A_2 B_2 X_2 Y_2}^{\text{obs-inf}} &= P_{ABXY}^{\text{obs}} \\ P_{X_1 X_2 Y_1 Y_2}^{\text{obs-inf}} &= P_X^{\text{free}} \otimes P_X^{\text{free}} \otimes P_Y^{\text{free}} \otimes P_Y^{\text{free}} \end{aligned} \quad \text{and hence} \quad \begin{aligned} P_{A_1 B_1 X_1 Y_1}^{\text{obs-inf}} &= P_{AB|XY}^{\text{PR}} \\ P_{A_2 B_1 X_2 Y_1}^{\text{obs-inf}} &= P_{AB|XY}^{\text{PR}} \\ P_{A_1 B_2 X_1 Y_2}^{\text{obs-inf}} &= P_{AB|XY}^{\text{PR}} \\ P_{A_2 B_2 X_2 Y_2}^{\text{obs-inf}} &= P_{AB|XY}^{\text{PR}} \end{aligned} \quad (27)$$

{eqs}{eq:}

Given the assumption that the distributions P_X^{free} and P_Y^{free} are full support, it follows from Eqs. (27) that sometimes $\{X_1, X_2, Y_1, Y_2\} = \{0, 1, 0, 1\}$. For these values, Eqs. (27) specifies perfect correlation between A_1 and B_1 . Similarly, it the inflated observational data also specified perfect correlation between A_1 and B_2 , perfect correlation between A_2 and B_1 , and perfect *anticorrelation* between A_2 and B_2 . Those four requirements are not mutually compatible, however: since perfect correlation is transitive, the first three properties entail perfect correlation between A_2 and B_2 .

The mathematical structure of this proof parallels that of standard proofs of the incompatibility of PR-box correlations with the Bell structure. 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. The fact that there must be a joint distribution over these variables can be inferred from the structure of the Bell DAG and the fact that one can assume without loss of generality that the causal dependencies are deterministic (a result known as Fine's theorem [29]). It is then sufficient to note that the marginals given by the PR-box correlations do not arise from any joint distribution. Nonetheless, our proof is conceptually distinct insofar as the variables to which we apply the marginals problem are not conditioned on a setting value. And we do not require Fine's theorem.

Many causal inference techniques can be used to derive sufficient conditions for the incompatibility of the causal hypothesis $H_{G', S'}$ with the observational data $\forall U \in \text{PreinjectableSets}[O] : P(U) = P(\tilde{U}_1)P(\tilde{U}_2) \dots P(\tilde{U}_n)$. We will call sets of such conditions **incompatibility witnesses**.

⁶ 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.

IV. EXAMPLE APPLICATIONS OF THE INFLATION TECHNIQUE

Here are some examples of causal incompatibility witnesses for the Triangle scenario which we can derive by considering the inflation DAG of Fig. 6.

For technical convenience, let us assume that all observed variables take values in $\{-1, +1\}$. By virtue of the existence of a joint distribution of A_2 , B_1 and C_1 , we can conclude [30–34], ^{pitowsky_boole_1994, Pitowsky1989, Kellereer_marginal_1964, leggett}

$$\langle A_2 C_1 \rangle + \langle B_2 C_1 \rangle - \langle A_2 B_1 \rangle \leq 1. \quad (28) \quad \{\text{eq:polym}\}$$

A consequence of the manner in which observational data is inflated per Fig. 6, i.e. the non-distribution-specific relations which appear as part of Eqs. (19), we can therefore conclude that if an observable distribution is compatible with the Triangle scenario DAG it must satisfy

$$\langle AC \rangle + \langle BC \rangle \leq 1 + \langle A \rangle \langle B \rangle, \quad (29) \quad \{\text{eq:polym}\}$$

which we think of as a sort of monogamy inequality: it is impossible for C to be strongly correlated with both A and B , unless A and B are both strongly biased.

Alternatively, we could also assume variables with any number of outcomes and start with the inequality [20] ^{fritz2013marginal}

$$I(A_2 : C_1) + I(C_1 : B_1) - I(A_2 : B_1) \leq H(B_1), \quad (30)$$

which also simply follows from the existence of a joint distribution of all variables. Again, implicit per Eqs. (19) is that that the third term vanishes regardless of what the observable distribution might be, purely as a consequence of *how* observable distributions are inflated pursuant to Fig. 6. We therefore derive

$$I(A : C) + I(C : B) \leq H(B), \quad (31) \quad \{\text{eq:monog}\}$$

which is the original entropic monogamy inequality derived for the Triangle scenario in [10]. ^{fritz2012bell} Our rederivation in terms of inflation is essentially the proof of Henson *et al.* [11]. ^{passey2014dag}

Slightly more involved but otherwise analogous considerations can be applied to the inflation DAG of Fig. 3, where in particular we have the pre-injectable sets $\{A_1 B_1 C_1\}$, $\{A_1 B_2 C_2\}$, $\{A_2 B_1 C_2\}$, $\{A_2 B_2 C_1\}$ and $\{A_2 B_2 C_2\}$, resulting in the factorization relations

$$\begin{aligned} P_{A_1 B_1 C_1} &= P_{ABC}, \\ P_{A_1 B_2 C_2} &= P_{AB} \otimes P_C, \\ P_{B_1 C_2 A_2} &= P_{BC} \otimes P_A, \\ P_{A_2 C_1 B_2} &= P_{AC} \otimes P_B, \\ P_{A_2 B_2 C_2} &= P_A \otimes P_B \otimes P_C. \end{aligned} \quad (32) \quad \{\text{eq:tri22}\}$$

In this case, let us assume binary variables with values in $\{0, 1\}$. Now we can again use the existence of a joint distribution over all six observable variables, which implies e.g. the inequality

$$P_{A_2 B_2 C_2}(111) \leq P_{A_1 B_1 C_1}(000) + P_{A_1 B_2 C_2}(111) + P_{B_1 C_2 A_2}(111) + P_{A_2 C_1 B_2}(111), \quad (33) \quad \{\text{eq:Fritz}\}$$

which one can show to be valid for every joint distribution of all six variables simply by checking that it holds on every deterministic assignments of values, from which the general case follows by linearity. Applying the above factorization relations turns this into the polynomial inequality

$$P_A(1)P_B(1)P_C(1) \leq P_{ABC}(000) + P_{AB}(11)P_C(1) + P_{BC}(11)P_A(1) + P_{AC}(11)P_B(1), \quad (34) \quad \{\text{eq:Fritz}\}$$

which is yet another necessary condition for compatibility with the Triangle scenario causal structure, and now takes genuine three-way correlations into account. A consequence of this inequality is again that the W-type distribution per Eq. (20) is found to be incompatible with the Triangle scenario, since the right-hand side vanishes but the left-hand side does not.

Appendix D provides a list of further polynomial inequalities that we have derived for the Triangle scenario using the method developed in the following section.

V. DERIVING POLYNOMIAL INEQUALITIES SYSTEMATICALLY

sec:ineqs

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.

injectable

Identifying the Pre-Injectable Sets

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 $\text{An}(A_i B_j)$ is irredundant. The injectable sets are then precisely the cliques⁷ in this graph, per Eq. (9).

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

⁷ A clique is a subset of nodes such that every node in the subset is connected to every other node in the subset.

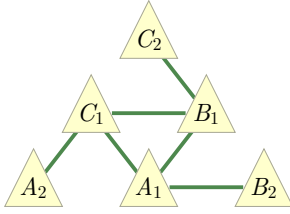


FIG. 9. The auxiliary injection graph corresponding to the inflation DAG in Fig. 3, wherein a pair of nodes are adjacent iff they are pairwise injectable.

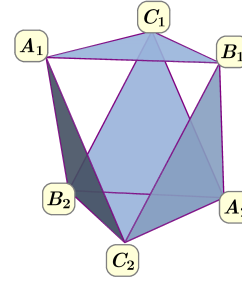


FIG. 10. The simplicial complex... The 5 faces in this figure correspond to the 5 maximal pre-injectable sets per Fig. 3, namely $\{A_1B_1C_1\}$, $\{A_1B_2C_2\}$, $\{A_1B_2C_1\}$, $\{A_2B_2C_1\}$ and $\{A_2B_2C_2\}$.

sets as follows:

$$\begin{array}{ccccc}
 \begin{array}{l} A_2 \not\sim B_1 \\ A_2 \not\sim C_2 \\ B_2 \not\sim A_2 \\ B_2 \not\sim C_1 \\ C_2 \not\sim A_1 \\ C_2 \not\sim B_2 \end{array} & \begin{array}{l} \{A_2\} \not\sim \{B_1B_2C_2\} \\ \{B_2\} \not\sim \{A_2C_1C_2\} \\ \{C_2\} \not\sim \{A_1A_2B_2\} \\ \{A_2\} \not\sim \{B_2\} \not\sim \{C_2\} \end{array} & \begin{array}{l} \{A_1B_1\} \\ \{B_1C_1\} \\ \{A_1C_1\} \\ \{A_2C_1\} \\ \{B_2A_1\} \\ \{C_2B_1\} \end{array} & \begin{array}{l} \{A_1B_2\} \\ \{B_1C_2\} \\ \{A_2C_1\} \\ \{A_1B_1C_1\} \end{array} & \begin{array}{l} \{A_1B_1C_1\} \\ \{A_1B_2C_2\} \\ \{A_2B_1C_2\} \\ \{A_2B_2C_1\} \\ \{A_2B_2C_2\} \end{array} \\
 \text{pairwise} & \text{maximal} & \text{pairwise} & \text{maximal} & \text{maximal} \\
 \text{ancestral} & \text{ancestral} & \text{injectable} & \text{injectable} & \text{pre-injectable} \\
 \text{independencies} & \text{independencies} & \text{sets} & \text{sets} & \text{sets}
 \end{array} \tag{35}$$

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

$$\forall_{abc} : \begin{cases} P_{A_1B_1C_1}(abc) = P_{ABC}(abc) \\ P_{A_1B_2C_2}(abc) = P_C(c)P_{AB}(ab) \\ P_{A_2B_1C_2}(abc) = P_A(a)P_{BC}(bc) \\ P_{A_2B_2C_1}(abc) = P_B(b)P_{AC}(ac) \\ P_{A_2B_2C_2}(abc) = P_A(a)P_B(b)P_C(c) \end{cases} \tag{36}$$

Eq. (36) is an equivalent restatement of Eq. (32). 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”.

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. (36). For simplicity, we assume that all observable variables are binary⁸.

⁸ 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.

In order for the five pre-injectable sets in Eq. (36) to be marginally compatible there must exist 64 nonnegative joint probabilities, i.e. satisfying

$$\forall_{a_1 a_2 b_1 b_2 c_1 c_2} : 0 \leq P_{A_1 A_2 B_1 B_2 C_1 C_2}(a_1 a_2 b_1 b_2 c_1 c_2), \quad (37) \quad \boxed{\text{[eq:nonne}}$$

constrained further by marginal distributions given by

$$\begin{aligned} \forall_{a_1 b_1 c_1} : P_{A_1 B_1 C_1}(a_1 b_1 c_1) &= \sum_{a_2 b_2 c_2} P_{A_1 A_2 B_1 B_2 C_1 C_2}(a_1 a_2 b_1 b_2 c_1 c_2), \\ \forall_{a_1 b_2 c_2} : P_{A_2 B_2 C_2}(a_1 b_2 c_2) &= \sum_{a_2 b_1 c_1} P_{A_1 A_2 B_1 B_2 C_1 C_2}(a_1 a_2 b_1 b_2 c_1 c_2), \\ \forall_{a_2 b_1 c_1} : P_{A_2 B_1 C_2}(a_2 b_1 c_2) &= \sum_{a_1 b_2 c_2} P_{A_1 A_2 B_1 B_2 C_1 C_2}(a_1 a_2 b_1 b_2 c_1 c_2), \\ \forall_{a_2 b_2 c_1} : P_{A_2 B_2 C_1}(a_2 b_2 c_1) &= \sum_{a_1 b_1 c_2} P_{A_1 A_2 B_1 B_2 C_1 C_2}(a_1 a_2 b_1 b_2 c_1 c_2), \\ \forall_{a_2 b_2 c_2} : P_{A_2 B_2 C_2}(a_2 b_2 c_2) &= \sum_{a_1 b_1 c_1} P_{A_1 A_2 B_1 B_2 C_1 C_2}(a_1 a_2 b_1 b_2 c_1 c_2). \end{aligned} \quad (38) \quad \boxed{\text{[eqs]{eq:}}$$

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 $p_{A_1 A_2 B_1 B_2 C_1 C_2}(a_1 a_2 b_1 b_2 c_1 c_2)$ Hyttinen2013marginal, chaves2019

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. pearl2009causality, studeny2005probabilistic, woodspekkens, pusey2014gd

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 . 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

$$\begin{aligned} \forall_{a_2 b_2} : P_{A_2 B_2}(a_2 b_2) &\rightarrow \sum_{a_1 b_1 c_1 c_2} P_{A_1 A_2 B_1 B_2 C_1 C_2}(a_1 a_2 b_1 b_2 c_1 c_2), \\ \forall_{a_1 a_2 b_2 c_2} : P_{A_1 A_2 B_2 C_2}(a_1 a_2 b_2 c_2) &\rightarrow \sum_{b_1 c_1} P_{A_1 A_2 B_1 B_2 C_1 C_2}(a_1 a_2 b_1 b_2 c_1 c_2), \\ \forall_{a_1 a_2 b_2} : P_{A_1 A_2 B_2}(a_1 a_2 b_2) &\rightarrow \sum_{b_1 c_1 c_2} P_{A_1 A_2 B_1 B_2 C_1 C_2}(a_1 a_2 b_1 b_2 c_1 c_2) \end{aligned} \quad (39)$$

etc.

Many modern computer algebra systems have functions capable of tackling nonlinear quantifier elimination symbolically⁹. Currently, however, it is not practical to perform nonlinear quantifier elimination on large polynomial

⁹ For example *Mathematica*TM's **Resolve** command, *Redlog*'s **rlposqe**, or *Maple*TM's **RepresentingQuantifierFreeFormula**, etc.

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 rapidly¹⁰.

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. (7). 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

$$\begin{aligned} &\{A_1 B_1, X_1 X_2 Y_1 Y_2\} \\ &\{A_1 B_2, X_1 X_2 Y_2 Y_2\} \\ &\{A_2 B_1, X_1 X_2 Y_2 Y_2\} \\ &\{A_2 B_2, X_1 X_2 Y_2 Y_2\}, \end{aligned} \tag{40}$$

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

$$\forall_{abx_1 x_2 y_1 y_2} : \begin{cases} P_{A_1 B_1 X_1 X_2 Y_1 Y_2}(abx_1 x_2 y_1 y_2) = P_{ABXY}(abx_1 y_1) P_X(x_2) P_Y(y_2), \\ P_{A_1 B_2 X_1 X_2 Y_1 Y_2}(abx_1 x_2 y_1 y_2) = P_{ABXY}(abx_1 y_2) P_X(x_2) P_Y(y_1), \\ P_{A_2 B_1 X_1 X_2 Y_1 Y_2}(abx_1 x_2 y_1 y_2) = P_{ABXY}(abx_2 y_1) P_X(x_1) P_Y(y_2), \\ P_{A_2 B_2 X_1 X_2 Y_1 Y_2}(abx_1 x_2 y_1 y_2) = P_{ABXY}(abx_2 y_2) P_X(x_1) P_Y(y_1), \\ P_{X_1 X_2 Y_1 Y_2}(x_1 x_2 y_1 y_2) = P_X(x_1) P_X(x_2) P_Y(y_1) P_Y(y_2). \end{cases} \tag{41}$$

¹⁰ For example *Mathematica*TM `Reduce`ExistsRealQ` function. Specialized satisfiability software such as SMT-LIB’s `check-sat` [36] are particularly apt for this purpose.

By dividing the first four inequalities by the latter we obtain

$$\forall_{abx_1x_2y_1y_2} : \begin{cases} P_{A_1B_1|X_1X_2Y_1Y_2}(ab|x_1x_2y_1y_2) = P_{AB|XY}(ab|x_1y_1) \\ P_{A_1B_2|X_1X_2Y_1Y_2}(ab|x_1x_2y_1y_2) = P_{AB|XY}(ab|x_1y_2) \\ P_{A_2B_1|X_1X_2Y_1Y_2}(ab|x_1x_2y_1y_2) = P_{AB|XY}(ab|x_2y_1) \\ P_{A_2B_2|X_1X_2Y_1Y_2}(ab|x_1x_2y_1y_2) = P_{AB|XY}(ab|x_2y_2). \end{cases} \quad (42)$$

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

$$P_{A_1B_1|X_1X_2Y_1Y_2}(ab|x_1x_2y_1y_2) = \sum_{a_2,b_2} P_{A_1A_2B_1B_2X_1X_2Y_1Y_2}(a_1a_2b_1b_2|x_1x_2y_1y_2) \quad (43)$$

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

$$\forall_{ab} : \begin{cases} P_{AB|XY}(ab|00) = \sum_{a',b'} P_{A_1A_2B_1B_2X_1X_2Y_1Y_2}(aa'bb'|0101) \\ P_{AB|XY}(ab|10) = \sum_{a',b'} P_{A_1A_2B_1B_2X_1X_2Y_1Y_2}(a'abb'|0101) \\ P_{AB|XY}(ab|01) = \sum_{a',b'} P_{A_1A_2B_1B_2X_1X_2Y_1Y_2}(aa'b'b|0101) \\ P_{AB|XY}(ab|11) = \sum_{a',b'} P_{A_1A_2B_1B_2X_1X_2Y_1Y_2}(a'ab'b|0101) \end{cases} \quad (44) \quad \boxed{\text{eq:final}}$$

The existence of an *array* of distributions, i.e. Eq. (44), is equivalent to the existence of a **hidden variable model**, as noted in Fine's Theorem [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 [10, 11]. For example, classical and quantum distributions alike respect all conditional independence relations implied by the common underlying causal structure [11]. It is an interesting problem to find quantum distributions that are not realizable classically, or to show that there are no such distributions on a given DAG.

However, this is by no means an easy task. For example, recent work has found that quantum causal structure also implies many of the entropic inequalities that hold classically [11, 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 [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 [13, 44, 45]. Such inequalities are still limited, however, in that they only apply in the presence of observable root nodes¹¹, 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**

¹¹ 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.

the value of the random variable. For example while the information about X in Fig. 1 was “sent” to A and C , the information about X_1 is sent to A_1 and A_2 and C in the inflation Fig. 4. Since quantum theory satisfies a 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 4. $G' \in \text{Inflations}[G]$ 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 5 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. (31) here, this was originally noticed in Ref. [11]. Another example is Eq. (29), which was derived from the non-broadcasting inflation of Fig. 6. Eq. (29) 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. (18) 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. (37). 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. (37) 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.

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 witnessed as impossible 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].

sec:TSEM

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. ^{LSW} 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,

$$\text{Never}[E_1] \bigwedge \text{Never}[E_2] \bigwedge \dots \text{Never}[E_N] \implies \text{Never}[E_0] \quad (45)$$

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

$$[E_0] \implies [E_1] \bigvee [E_2] \bigvee \dots [E_N]. \quad (46)$$

Any possibilistic constraint can be immediately translated into a stronger probabilistic one, as noted by ^{Mansfield2012} Mansfield and Fritz [19]. The probabilistic variant states than *whenever* the event E_0 occurs than at least one of the events $E_1..E_N$ should also occur. Applying the union bound to the probability of the right-hand side we obtain

$$p(E_0) \leq \sum_{n=1}^N p(E_n). \quad (47)$$

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

$$[A=1, C=1] \implies [A=1, B=1] \bigvee [B=0, C=1] \quad (48)$$

corresponding to the probabilistic constraint

$$P_{AC}(\mathbf{11}) \leq P_{AB}(\mathbf{11}) + P_{BC}(\mathbf{01}). \quad (49)$$

{eq:trivm

Eq. (49) is a necessary condition for the marginal compatibility of $P(AB)$, $P(AC)$, and $P(BC)$; it is equivalent to Eq. (28).

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. (35). 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 $[A_1=0, \mathbf{A_2=1}, B_1=0, \mathbf{B_2=1}, C_1=1, \mathbf{C_2=1}]$ is an extension of the node $[A_1=0, \mathbf{B_2=1}, \mathbf{C_2=1}]$. In our example following Fig. 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 $[\mathbf{A_2=1}, \mathbf{B_2=0}, C_1=1]$ contradicts the antecedent $[\mathbf{A_2=1}, \mathbf{B_2=1}, \mathbf{C_2=1}]$. We also delete the node corresponding to the antecedent itself. In our example, this final resulting hypergraph has $2^3 + 3 \cdot 2^1 = 14$ nodes and $2^3 = 8$ hyperedges.

All valid (minimal) consequents are (minimal) **transversals** of this latter hypergraph. A transversal is 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

$$[\mathbf{A_2=1}, \mathbf{B_2=1}, \mathbf{C_2=1}] \implies [A_1=0, B_1=0, C_1=0] \bigvee \text{And}[\mathbf{A_1=1}, \mathbf{B_2=1}, \mathbf{C_2=1}] \bigvee [\mathbf{A_2=1}, B_1=1, \mathbf{C_2=1}] \bigvee [\mathbf{A_2=1}, \mathbf{B_2=1}, C_1=1] \quad (50) \quad \{\text{eq:F3imp}\}$$

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. (50) translates to the probabilistic constraint

$$P_{A_2 B_2 C_2}(\mathbf{111}) \leq P_{A_1 B_1 C_1}(111) + P_{A_1 B_2 C_2}(a_1 \mathbf{11}) + P_{A_2 B_1 C_2}(\mathbf{111}) + P_{A_2 B_2 C_1}(\mathbf{111}) \quad (51) \quad \{\text{eq:F3raw}\}$$

Eq. (51) is equivalent to Eq. (33); therefore applying it the inflation depicted in Fig. 3 recovers Eq. (34).

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.

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] [46, 47] 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, Pusey2014gdag, Chaves2015introquantum, ChavesNoSignalling, BeyondBellII, Fritz2012bell, Pusey2014gdag, Chaves2015introquantum, 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 [59, 60] 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, Pusey2014gdag, Fritz2012bell, Pusey2014gdag], 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 tools¹². 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. (37–38) 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

¹² 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 $X_2 Y_2 Z_1$.

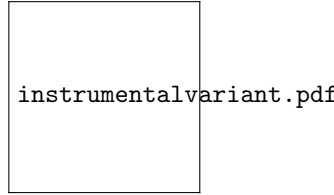


FIG. 11. An inflation DAG which illustrates why coinciding ancestral subgraphs don't necessarily imply coinciding distributions.

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.

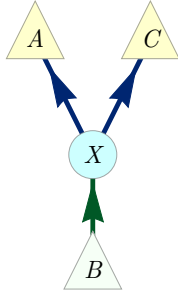


FIG. 12. A causal structure that is compatible with any distribution P_{ABC} .

fig:beforecopy

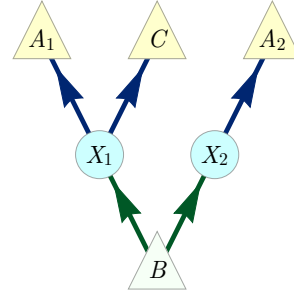


FIG. 13. An inflation.

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 5. *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

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- | | |
|------------|---|
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