Entropic Inequality Constraints from e-separation Relations in Directed Acyclic Graphs with Hidden Variables

Noam Finkelstein\textsuperscript{1} Beata Zjawin\textsuperscript{2, 3} Elie Wolfe\textsuperscript{2} Ilya Shpitser\textsuperscript{1} Robert W. Spekkens\textsuperscript{2}

\textsuperscript{1} Johns Hopkins University, Department of Computer Science, 3400 N Charles St, Baltimore, MD USA, 21218
\textsuperscript{2} Perimeter Institute for Theoretical Physics, 31 Caroline St. N, Waterloo, Ontario, Canada, N2L 2Y5
\textsuperscript{3} International Centre for Theory of Quantum Technologies, University of, Gdańsk, 80-308 Gdańsk, Poland

Abstract

Directed acyclic graphs (DAGs) with hidden variables are often used to characterize causal relations between variables in a system. When some variables are unobserved, DAGs imply a notoriously complicated set of constraints on the distribution of observed variables. In this work, we present entropic inequality constraints that are implied by e-separation relations in hidden variable DAGs with discrete observed variables. The constraints can intuitively be understood to follow from the fact that the capacity of variables along a causal pathway to convey information is restricted by their entropy; e.g. at the extreme case, a variable with entropy 0 can convey no information. We show how these constraints can be used to learn about the true causal model from an observed data distribution. In addition, we propose a measure of causal influence called the minimal mediary entropy, and demonstrate that it can augment traditional measures such as the average causal effect.

1 INTRODUCTION

A causal model of a system of random variables can be represented as a directed acyclic graph (DAG), where an edge from a node $X$ to a node $Y$ can be taken to mean that the random variable $X$ is a direct cause of the random variable $Y$. Such causal models can be used to algorithmically deduce highly non-obvious properties of the system. For example, it is possible to deduce that the probability distribution of observed variables in the system, called the observed data distribution, must satisfy certain constraints.

When some variables in the system are unobserved, the constraints implied by the causal model are not well understood, and, for computational reasons, cannot be feasibly enumerated in full for arbitrary graphs. As a result, a number of methods have been developed for quickly providing a subset of these constraints [1–3]. In this work, we contribute to this literature by describing entropic inequality constraints that hold whenever an e-separation relationship [4, 5] is present in the graph.

The idea underlying these inequality constraints is that mutual information between two variables in a graphical model must be explained by variability of variables (termed bottleneck variables) that are between them along some path. Such paths need not be directed; a bottleneck variable may constitute the base of a fork structure or the mediary variable in a chain structure along the path. Each such path has a limited capacity for carrying information, which can be quantified in terms of the entropies of the bottleneck variables on that path. At the extreme case, if there is a bottleneck variable along a path with zero entropy, then subsequent variables on that path cannot learn about prior variables through the path, because the bottleneck variable will hold a fixed value regardless of the values taken other any other variables, observed or unobserved. We will quantitatively relate the amount of information that can flow through a path to the entropies of its bottleneck variables below.

Constraints on the observed data distribution implied by a causal model have primarily been used to determine whether the observed data is compatible with a causal model, and to learn the true causal model directly from the observed data. Existing algorithms for learning causal models rely primarily on equality constraints. We suggest that incorporating our proposed inequality constraints, which can easily be read off a graphical model, can meaningfully improve these methods. In addition, we show how the entropy of latent variables can be linked to properties of the observed data distribution, yielding bounds on latent variable entropies or constraints on the observed data distribution.

We also demonstrate that our constraints can be used to bound an intuitive measure of the strength of a causal relationship between two variables, called the Minimum Mediary Entropy (MME). We show that the standard measure, called the Aver-
age Causal Effect (ACE), is not well suited to capturing the causal influence strength of a non-binary treatment on outcome, and can be misleading in some settings. For example, the ACE can be 0 even when treatment changes outcome for every subject in the population. The MME overcomes both of these issues, and can serve as an informative complement to the ACE.

The remainder of the paper is organized as follows. In Section 2, we discuss relevant material in causal inference and information theory. We present our constraints in Section 3, and several applications of the constraints in Section 4. Finally, a discussion of related work and directions for future study can be found in Section 5 and Section 6 respectively.

2 PRELIMINARIES

2.1 CAUSAL INFERENC BACKGROUND

We begin by introducing key ideas from the literature on graphical causal models. Suppose we are interested in a system of related phenomena, each of which can be represented by a random variable. We denote observed variables in the system as $Y$, unobserved variables as $U$, and the full set of variables as $V = Y \cup U$.

We let $G$ denote a DAG representing the system of interest. Each node in $G$ corresponds to a variable in $V$. The direct causes of each random variable $V$ are defined to be its parents in $G$, denoted $pa_G(V)$. We adopt a nonparametric structural equations view of the DAG [6, 7], under which the value of each variable $V$ is a function of its direct causes and exogenous noise, denoted $\epsilon_V$. The set of these structural equations is denoted $F = \{ f_V(pa_G(V), \epsilon_V) \mid V \in V \}$. In most causal analyses, the exact form of these functions is unknown. Nevertheless, if the structure of causal dependencies in a system is known to be summarized by a graph $G$, or, equivalently, to be described by some set of functions $F$, then the distribution $P(V)$ is known to factorize as

$$P(V) = \prod_{V \in V} P(V \mid pa_G(V)). \quad (1)$$

Equation (1) is the fundamental constraint that $G$ places on the distribution $P(V)$ — if the equality holds, then the distribution is in the model; otherwise it is not. When all variables are observed, each term in the factorization is identifiable from observed data, and the constraint may easily be checked. When not all variables are observed, there is no known polynomial-time algorithm for expressing the constraints that the factorization of the full joint distribution places on the observed data distribution. In theory, necessary and sufficient conditions for the observed data distribution to be in the model can be obtained through the use of quantifier elimination algorithms [8], but these have doubly exponential runtime and are prohibitively slow in practice.

We now review $d$-separation and $e$-separation, which are properties of the graph $G$ that imply certain properties of distribution $P(V)$. We first introduce the notion of open and closed paths in conditional distributions. Triples in the graph of the form $A \rightarrow C \rightarrow B$ and $A \leftarrow C \rightarrow B$ are said to be open if we do not condition on $C$, and closed if we do condition on $C$. Triples of the form $A \rightarrow C \leftarrow B$, in which $C$ is called a collider, are closed if we do not condition on $C$ or any of its descendants, and open if we do. A path is said to be open under a conditioning set $C$ if all contiguous triples along that path are open under that conditioning set.

**Definition 1** ($d$-separation). Let $A$, $B$ and $C$ be sets of variables in a DAG. $A$ and $B$ are said to be $d$-separated by $C$ if all paths between $A$ and $B$ are closed after conditioning on $C$. This is denoted $(A \perp_d B \mid C)$.

It is a well-known consequence of Equation (1) that any $d$-separation relation $(A \perp_d B \mid C)$ in $G$ implies the corresponding conditional independence relation $A \perp B \mid C$ in the distribution $P(V)$. Conditional independence constraints of this form are about sub-populations in which the variables in $C$ take the same value for all subjects. We can only evaluate whether these constraints hold when all variables in $C$ are observed; otherwise there is no way to identify the relevant sub-populations. For that reason, it is impossible to determine whether conditional independences implied by $G$ hold if they have hidden variables in their conditioning sets, leading to the need for other mechanisms to test implications of these independencies.

To describe $e$-separation, we first introduce the idea that a node can be deleted from a graph by removing the node and all of its incoming and outgoing edges. $e$-separation can then be defined as follows.

**Definition 2** ($e$-separation). Let $A$, $B$, and $C$ be sets of variables in a DAG. $A$ and $B$ are said to be $e$-separated by $C$ after deletion of $D$ if $(A \perp_B C \mid D)$ after deletion of every variable in $D$. This is denoted $(A \perp_e B \mid C \text{ upon } \sim D)$.

Conditioning on $C$ may close some paths between $A$ and $B$, and open others. In the context of $e$-separation, the set $D$, which we refer to as a bottleneck for $A$ and $B$ conditional on $C$, is any set that includes at least one variable from each path between $A$ and $B$ that is open after conditioning on $C$. If no subset of $D$ is a bottleneck, then $D$ is called a minimal bottleneck. This terminology reflects the fact that, conditional on $C$, all information shared between $A$ and $B$ — that is, transferred from one to the other or transferred to each from a common source — must flow through $D$.

It has been shown that every $e$-separation relationship among observed variables in a graph $G$ corresponds to a constraint on the observed data distribution $P(Y)$ [4]. However, this result is not constructive, in the sense that it does not provide a strategy for deriving such constraints for a given $e$-
We will see that vide in Section 3 partially fulfill this role; they provide explicit constraints that hold everywhere in the model whenever an \( e \)-separation relationship obtains in a graph.

### 2.1.1 Node Splitting

We will see that \( e \)-separation is related to the idea of splitting nodes in a graph. We define a node-splitting operation as follows. Given a graph \( G \) and a vertex \( D \) in the graph, the node splitting operation returns a new graph \( G^\# \) in which \( D \) is split into two vertices. One of the vertices is still called \( D \), and it maintains all edges directed into \( D \) in the original graph \( G \), but none of its outgoing edges. This vertex keeps the name \( D \) because it will have the same distribution as \( D \) in the original graph, as all of its causal parents remain the same. The second random variable is labeled \( D^\# \), and it inherits all of the edges outgoing from \( D \) in the original graph, but none of its incoming edges. Examples of the node splitting operation are illustrated in Fig. 1.

By a result of Evans [4], \( (A \perp_{e} B | C \text{ upon } \neg D) \) in \( G \) if and only if \( (A \perp_{d} B | C, D^\#) \) in \( G^\# \). Note that the node splitting operation described here is closely related to the operation of node splitting in Single World Intervention Graphs in causal inference [7].

### 2.2 ENTROPIES

In this section, we review standard concepts in information theory, which we will use to express our inequality constraints. We begin with the definitions of entropy and mutual information.

**Definition 3.** The **entropy** of a random variable \( X \) is defined as 
\[
H(X) = -\sum_{x \in X} P(x) \log_2 P(x),
\]
with the joint entropy of \( X \) and \( Y \) defined analogously. The **mutual information** between \( X \) and \( Y \) is defined as 
\[
I(X : Y) = H(X) + H(Y) - H(X,Y).
\]

The entropy of a random variable can be thought of as the level of uncertainty one has about its value. Entropy is maximized by a uniform distribution over the domain of a random variable, as there is no reason to think any one value is more probable than another, and minimized by a point distribution, in which there is no uncertainty.

The mutual information between \( X \) and \( Y \) can be thought of as the amount of certainty we gain about the value of one, on average, if we learn the value of the other. It is maximized when one of \( X \) and \( Y \) is a deterministic function of the other, and is minimized when they are independent.

The entropy \( H(X \mid Y=y) \) of \( X \) conditional on a specific value of \( Y=y \) is obtained by replacing the distribution \( P(X) \) in Definition 3 with \( P(X \mid Y=y) \). The **conditional entropy** of \( X \) given \( Y \), denoted \( H(X \mid Y) \), is defined as the expected value of \( H(X \mid Y=y) \). Conditional mutual information is analogously defined.

### 3 E-SEPARATION CONSTRAINTS

We have already described the intuition behind our constraints, which can be roughly summarized by the observation that the statistical dependence between random variables must be limited by the total amount of information that can flow through any bottleneck between them. We now describe how the tools introduced in Section 2 help us formalize this intuition.

First, we describe why \( e \)-separation helps formalize the idea of blocking “all paths” between two sets of variables. Consider the instrumental variable graph, depicted in Fig. 1(c). \( A \) and \( B \) are only \( d \)-separated by the set \( \{D, U\} \), where \( U \) is unobserved. Consequently, they are not \( d \)-separated by any set consisting entirely of observed variables. They are, however, \( e \)-separated after deletion of the observed variable \( D \). This tells us that all paths between \( A \) and \( B \) are through \( D \), and we can take advantage of observed properties of \( D \) to bound the dependence between them even when nothing is known about the unobserved variable \( U \). A similar story can be told about the Unrelated Confounders scenario depicted in Fig. 1(a).

When all variables are observed, \( e \)-separation does not imply any constraints that are not implied by \( d \)-separation, which follows from the fact that \( d \)-separation implies all constraints in such cases [9]. However, as illustrated by the examples in Figs. 1(a) and 1(c), \( e \)-separation allows us to identify bottlenecks consisting entirely of observed variables between \( A \) and \( B \) even when paths between \( A \) and \( B \) cannot be closed by any manner of conditioning on observed variables. To show how \( e \)-separation lead to entropic constraints, we will make use of Theorem 4.2 in [4], reframed as follows.
Theorem 4. (Evans [4, Theorem 4.2])
Suppose \((A \perp^B C \mid \bar{D})\) in \(\mathcal{G}\), and that no variable in \(C\) is a descendant of any in \(D\). Then there exists a distribution \(P^*\) over \(A, B, C, D, D^\#\) such that
\[
P(A=a,B=b,D=d \mid C=c) = P^*(A=a,B=b,D=d \mid C=c,D^\# = d)
\]
with \(A \perp B \mid C,D^\#\) in \(P^*\). If furthermore no variable in \(A\) is a descendant of any in \(D\), then there exists a distribution \(P^*\) such that \(P(B=b,D=d \mid A=a,C=c) = P^*(B=b,D=d \mid A=a,C=c,D^\# = d)\) with \(A \perp B \mid C,D^\#\) in \(P^*\).  

We provide the following intuition for this theorem. Our graph \(\mathcal{G}\) represents the causal relationships within a system of random variables in the real world. The graph \(\mathcal{G}^\#\) represents an alternative world in which the causal effects of \(D\) are “spoofed” by some random variable \(D^\#\). That is, children of \(D\) in \(\mathcal{G}\), which should be functions of \(D\), are instead fooled into being functions of \(D^\#\).

In the alternative world represented by \(\mathcal{G}^\#\), we suppose that the functional form \(f_V\) of a variable \(V\) in terms of its parents stays the same for all variables that are shared between graphs. This means that all non-descendants of \(D\) have the same joint distribution in our world and in the alternative world, as neither their parents nor the functions defining them in terms of their parents have changed. By contrast, descendants of \(D\) in \(\mathcal{G}\) will have a different distribution in the alternative world, as their distributions are now functions of the distribution of \(D^\#\), which may be different from that of \(D\), and is unknown.

Now, suppose we condition on a particular value of \(D^\# = d\) in \(\mathcal{G}^\#\). Then, because the functional form of the causal mechanisms is shared across worlds, the descendants of \(D\) in \(\mathcal{G}\) have the same distribution as they have when \(D=d\) in the observed world. In addition, all of the non-descendants of \(D^\#\) are marginally independent from \(D^\#\), because it has no ancestors so all connecting paths must be collider paths. Therefore, both its non-descendants and its descendants have the same joint distribution they would have had when \(D=d\) in the original graph. The results in the theorem then follow when we note that \(C\), and optionally \(A\), are non-descendants of \(D\), and that the relevant independence properties hold in the world of \(\mathcal{G}^\#\).

In general, we cannot know what this \(P^*\) distribution is, because we never get to observe this alternate world. But when we condition on \(D^\#\), we are removing precisely the randomness we do not know about, yielding a distribution that we do know about. The fact that \(P^*\) agrees with \(P\) on a subset of their domains, and that it contains known independences, is sufficient to derive informative constraints,

\[\text{as seen below.}\]

3.1 ENTROPIC CONSTRAINTS FROM \(E\)-SEPARATION
We now show how the notion of \(e\)-separation permits the formulation of entropic inequality constraints. In these constraints, we use mutual information to represent dependence between sets of variables, and entropy to measure the information-carrying capacity of paths connecting them.

Theorem 5. (Proof in Appendix C.)
Suppose the variables in \(D\) are discrete. Whenever \((A \perp^B C \mid \bar{D})\), then \(I(A : B \mid C,D) \leq H(D)\). If in addition no element of \(C\) is a descendant of any in \(D\), then for any value \(c\) in the domain of \(C\), the following stronger constraints hold:
\[
I(A : B \mid C=c,D) \leq H(D) \quad \text{and} \quad I(A : B \mid C,D) \leq H(D) \quad \text{if and only if} \quad I(A : B,D \mid C) \leq H(D) \quad \text{if and only if} \quad I(A : C,D) \leq H(D) \quad \text{if and only if} \quad I(A : B,D \mid C) \leq H(D) \quad \text{if and only if} \quad I(A : C,D) \leq H(D)
\]

This theorem potentially allows us to efficiently discover many entropic inequalities implied by any given graph, such as those implied by Fig. 2. In some cases, as in Fig. 2(a), the theorem recovers all Shannon-type entropic inequality constraints implied by the graph [10–12]. In other cases, as in Fig. 2(b), the graph implies a Shannon-type entropic inequality constraint beyond what Theorem 5 can recover, per a result in [13]. Indeed, entropic inequality constraints can be implied by graphs not exhibiting \(e\)-separation relations whatsoever, such as the triangle scenario [11, 14].

The linear quantifier elimination of [10–12] will always discover all the entropic inequalities which can be inferred from Theorem 5. However, the quantifier elimination method is computationally expensive, and is essentially intractable for graphs involving more than six or seven variables (observed and latent combined). Theorem 5, by contrast, provides an approach that is computationally tractable, but is capable of discovering fewer entropic constraints.

Finally, it would be possible to prove the converse of Theorem 5 holds. In particular, if \((A \notin^\# B \mid C \mid \bar{D})\) in \(\mathcal{G}\) and the variables in \(D\) are discrete, then there necessarily exists some distribution \(P\) over \(A, B, C, D\), in the marginal model of \(\mathcal{G}\) such that \(\text{mutual info} \geq H(D)\) when evaluated on \(P\).

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1In causal inference problems, a distribution \(P^*\) that satisfies the relevant conditions for this result may be constructed from counterfactual random variables \(A(d), B(d), D(d)\) and \(C(d)\).
We have seen that \( A \) is \( d \)-separated from \( B \) by \( \{C, D\} \), then \( A \) is also \( e \)-separated from \( B \) by \( C \) upon deleting \( D \).

This demonstrates that for any \( d \)-separation relation in the graph, it is possible to obtain an entropic constraint corresponding to any minimal bottleneck \( D \) through an \( e \)-separation relation. More precisely, when \( A \) is \( d \)-separated from \( B \) by \( \{C, D\} \), then by Proposition 6, it is also the case that \( A \) is \( e \)-separated from \( B \) given \( C \) upon deleting \( D \), and therefore Theorem 5 can be applied to obtain entropic constraints. Note, however, that these are necessarily weaker than the entropic constraint \( I(A : B | C, D) = 0 \), which follows from the \( d \)-separation relation itself.

In summary, every \( d \)-separation relation in the graph is an instance of \( e \)-separation, but not vice-versa. When an instance of \( e \)-separation is also an instance of \( d \)-separation, then all the inequality constraints implied by \( e \)-separation are rendered defunct by the stronger equality constraints implied by \( d \)-separation.

We now show that a similar pattern of deprecating inequalities by equalities occurs in the presence of Verma inequalities when certain counterfactual interventions are identifiable.

**Proposition 7.** Consider a graph \( G \) which exhibits the \( e \)-separation relation \( (A \perp_B B \mid C \text{ upon } \neg D) \) and where no element of \( C \) is a descendant of any in \( D \). If the counterfactual distribution \( P(A(D=d),B(D=d),D(D=d) \mid C) \) is identifiable, then the inequalities of Theorem 5 are logically implied whenever the stronger equality constraints

\[
I(A(D=d):B(D=d) \mid C) = 0
\]

are satisfied for all values of \( d \). Note that Equation (5) is satisfied if and only if the margin of the identified counterfactual distribution factorizes, i.e., when

\[
P(A(D=d),B(D=d) \mid C) = \sum_d p(A(D=d),B(D=d),D(D=d)=d' \mid C)
\]

exhibits \( A(D=d) \perp B(D=d) \mid C \).

The proof directly follows from that of Theorem 5. In proving Theorem 5, we derive entropic inequalities by relating the entropies pertaining to \( P(A,B,D \mid C) \) to entropies pertaining to the \( P^* \) distribution posited by Theorem 4. That is, Theorem 5 is an entropic consequence of Theorem 4. If the conditions of Proposition 7 are satisfied, then the conditions of Theorem 4 are also automatically satisfied since one can then explicitly reconstruct

\[
P^*(A,B,D=d \mid C,D# = d#) = P(A(D=d#),B(D=d#),D(D=d#) = d \mid C).
\]

There is no opportunity to violate the entropic inequalities of Theorem 5 once the observational data has been confirmed as consistent with Theorem 4. In other words, in order to violate the inequalities of Theorem 5 it must be the case that no \( P^* \) consistent with Theorem 4 can be constructed, but this contradicts the explicit recipe of Equation (7).

See Refs. [15, 16, 18] for details on how to derive the form of the equality constraints summarized by Equation (6). We note here that \( P(A(D=d),B(D=d),D(D=d)=d \mid C) \) is certainly identifiable if \( D \) is not a member of the same district \((16)\) as any element in \( \{A,B\} \) within the subgraph of \( G \) over \( \{A,B,C,D\} \) and their ancestors. We also note that the identifiability of merely \( P(A(D=d),B(D=d) \mid C) \) but not of \( P(A(D=d),B(D=d),D(D=d)=d \mid C) \) negates the implication from Equation (6) to Theorem 5. In Ap-
3.3 CONSTRAINTS AND BOUNDS INVOLVING LATENT VARIABLES

In this section, we consider $d$-separation relations with hidden variables in the conditioning set. Because we cannot condition on hidden variables, there is no way to check whether the corresponding independence constraints hold in the full data distribution. However, if we have access to auxiliary information about these hidden variables – such as information about their entropy or their cardinality – it is possible to obtain inequality constraints on the observed data distribution.

**Proposition 8.** (Proof in Appendix C.)

If $(A \perp_{d} B \mid C, U)$ and $H(U \mid A, B, C = c) \geq 0$, for any value $c$ in the domain of $C$:

$$H(U \mid C = c) \geq I(A : B \mid C = c)$$

(8)

Note that Proposition 8 holds even if $A$, $B$, and $C$ are continuously valued variables.

In many scenarios, we may have more (or be more interested in) information pertaining to the cardinality of a hidden variable than its entropy. We take the cardinality of a set of variables to be the product of the cardinalities of the variables in the set. An upper bound on the cardinality of $U$ entails an upper bound on its entropy. As observed above, the entropy of a random variable is maximized when it takes a uniform distribution. If we let $|U|$ denote the cardinality of $U$, and recall that the entropy of a uniformly distributed variable with cardinality $m$ is simply $\log_2(m)$, then $\log_2|U| \succ H(U)$. The next corollary then follows immediately from Proposition 8, since $H(U \mid \cdot) \geq 0$ whenever $U$ has finite cardinality:

**Corollary 8.1.** If $(A \perp_{d} B \mid C, U)$, then for any value $c$ in the domain of $C$, the cardinality of $U$ may be lower-bounded:

$$|U| \geq \max_c 2^{I(A : B \mid C = c)} \geq 2^{I(A : B \mid C)}.$$  

(9)

Finally, we note that both of these inequalities can also be used if we do not know anything about the properties of $U$, but would like to infer lower bounds for its entropy and cardinality from the observed data. In Section 4.2, we will explore a scenario in genetics in which these bounds and constraints may be of use.

**Remark 9.** Constraints given in Proposition 8 and Corollary 8.1 are stronger than can be obtained from the $e$-separation relation $(A \perp_e B \mid C \upon U)$ on its own.

Figure 3: Two hidden variable DAGs that share equality constraints over observed variables, but (a) contains $e$-separation relations that are not in (b).

To demonstrate Remark 9, we consider a set of structural equations consistent with Fig. 1(a). Suppose that $D$ takes the value 0 when $U_1 \neq U_2$, and the value 1 otherwise, and that $A$ and $B$ take the value 0 if $D$ is 0, and values equal to $U_1$ and $U_2$ respectively if $D$ is 1. It follows that $A$ and $B$ are always equal, and therefore $I(A : B) = H(A)$. Now, suppose that $U_1$ and $U_2$ only take values not equal to 0, and that there are at least two values that each takes with nonzero probability. It immediately follows that $H(D) < H(A)$, and therefore that $H(D) < I(A : B)$, as $D$ and $A$ by construction take the value 0 with the same probability, but there is strictly more entropy in the remainder of $A$’s distribution because $D$ is binary and $A$ takes at least two other values with nonzero probability.

4 APPLICATIONS

In this section, we explore several applications of the constraints developed above. In Sections 4.1 and 4.2, we show how our results can be used to learn about causal models from observational data. In Section 4.3, we further leverage the importance of the entropy of variables along a causal pathway to posit a new measure of causal strength, and observe that this measure can be bounded by an application of Theorem 5.

4.1 CAUSAL DISCOVERY

In this section, we present an example in which two hidden variable DAGs with the same equality constraints present different entropic inequality constraints. The ability to distinguish between models that share equality constraints has the potential to advance the field of causal discovery, in which causal DAGs are learned directly from the observed data. Causal discovery algorithms for learning hidden variable DAGs currently do so using only equality constraints. Our approach may be useful as a post-processing addition to such methods, whereby any graph found to satisfy the equality constraints in the observed data is tested against the entropic inequality constraints implied by $e$-separation relations in the model.

The hidden variable DAGs in Fig. 3, adapted from Ap-
pendix B in Ref. [19], share the same conditional independence constraints: $Y_1 \perp Y_3 \mid Y_2 Y_5$ and $Y_1 \perp Y_5$, but exhibit different $\varepsilon$-separation relations.

In Fig. 3(a), $(Y_1 \perp \varepsilon Y_3 Y_4 \mid Y_2 \perp \varepsilon Y_3)$, $(Y_1 Y_2 \perp \varepsilon Y_4 \mid Y_1 \perp \varepsilon Y_3)$, and $(Y_2 \perp \varepsilon Y_4 \mid Y_1 \perp \varepsilon Y_3)$. Applying Theorem 5 in each case, we obtain the three inequality constraints $I(Y_1 Y_2 Y_3 Y_5 \mid Y_2) \leq H(Y_5 \mid Y_2)$, $I(Y_2 Y_3 Y_4 Y_1) \leq H(Y_3 Y_1)$, and $I(Y_1 Y_2 Y_3 Y_4) \leq H(Y_3)$. 

In Fig. 3(b), we have added an edge, which removes some $\varepsilon$-separation relations. We are left with $(Y_1 \perp \varepsilon Y_3 Y_4 \mid Y_2 \perp \varepsilon Y_3)$, and $(Y_2 \perp \varepsilon Y_4 \mid Y_1 \perp \varepsilon Y_3)$. We can again apply Theorem 5 in each case, yielding the inequality constraints $I(Y_1 Y_3 Y_5 \mid Y_2) \leq H(Y_5 \mid Y_2)$ and $I(Y_2 Y_3 Y_4 Y_1) \leq H(Y_3 Y_1)$. The second of these constraints is shared by the graph in Fig. 3(a), and the first is strictly weaker than a constraint in Fig. 3(a).

Models similar to those shown in Fig. 3 sometimes arise in time-series data, where the variables in the chain represent observations taken at consecutive time steps. In such models, it is often assumed that treatments no longer have a direct effect on outcomes after a certain number of time steps. Here, that assumption is encoded in the lack of a direct edge from $Y_1$ to $Y_1$ in Fig. 3(a). We have shown above that this kind of assumption can be falsified even when it does not imply any additional equality constraints, as is often the case. In particular, if the stronger constraints implied by Fig. 3(a) are violated, but the weaker constraints of Fig. 3(b) are not, then the assumption is falsified.

### 4.2 CAUSAL DISCOVERY IN THE PRESENCE OF LATENT VARIABLES

![Diagram](attachment:image)

Figure 4: Identifying direct causal influence in the presence of a confounder with limited cardinality.

In this section, we consider a very simple possible application of the constraints and bounds relating to entropies of unobserved variables in genetics. Consider a causal hypothesis wherein the presence or absence of an unobserved gene influences two aspects of an organism’s phenotype. Suppose that due to genetic sequencing studies, the number of variants of the gene in the population — i.e. the cardinality of the corresponding random variable — is known. Two possible hypotheses regarding the causal structure are depicted in Fig. 4, where $U$ represents the gene and $X$ and $Y$ are the phenotype aspects. In Fig. 4(a), one presumes no causal influence of $X$ on $Y$, whereas in Fig. 4(b), direct causal influence is allowed. In the former case, knowledge of the number of variants of the gene constrains the mutual information between the phenotypes, while in the latter case it is not constrained.

Thus, for certain types of statistical dependencies between $X$ and $Y$, one can rule out the hypothesis of Fig. 4(a). For example, suppose we know the cardinality of $U$ to be 3. Corollary 8.1 then implies the constraint that the mutual information between $X$ and $Y$ cannot exceed $\log_2(3) \approx 1.584$. Suppose further that we observe the distribution depicted in Table 1. The mutual information between $X$ and $Y$ in this distribution is $\approx 1.594$. Because this mutual information violates the constraint implied by the model in Fig. 4(a), we know this model cannot be correct, and conclude that Fig. 4(b) is correct. More generally, strong statistical dependence between high cardinality variables cannot be explained by a low cardinality common cause and requires a direct influence between them.

|          | 0   | 1   | 2   | 3   |
|----------|-----|-----|-----|-----|
| $X$      |     |     |     |     |
| 0        | 0.002 | 0.001 | 0.400 | 0.001 |
| 1        | 0.003 | 0.005 | 0.005 | 0.066 |
| 2        | 0.224 | 0.003 | 0.003 | 0.001 |
| 3        | 0.002 | 0.281 | 0.001 | 0.002 |

Table 1: An example joint distribution over two variables $X$ and $Y$, each with cardinality 4.

Conversely, suppose Fig. 4(a) is known to be correct, and that there is no direct causal influence between the two aspects of phenotype. If the cardinality of $U$ is not known, it can be bounded from below directly from observed data, according to Corollary 8.1. In this case, the lower bound would be $2^{I(X;Y)} \approx 2^{1.594} \approx 3.018$. It follows that $U$ must have a cardinality of 4 or above in this setting. The ability to extract such information from observational data may be useful in making substantive scientific decisions, or in guiding future sequencing studies.

In many applied data analyses, different variables may be observed for different subjects, i.e., data on some variables is “missing” for some subjects. A recent line of work has focused on properties of missing data models that can be represented as DAGs [20]. Although the bounds and constraints above have been developed in the context of fully unobserved variables, they can also be used in missing data DAG models, for variables that are not observed for all subjects.

### 4.3 QUANTIFYING CAUSAL INFLUENCE

The traditional approach to measuring the strength of a causal relationship is by contrasting how different an outcome would be, on average, under two different treatments. Formally, if $X$ is a cause of $Y$, the ACE is defined as $E[Y(X = x) - Y(X = x')]$. While the ACE is a very useful construct, we suggest that it has two important shortcomings, and present an alternative measure of causal strength called the Minimal
Mediary Entropy or MME. The MME is based on the idea – explored throughout this work – that the entropy of variables along a causal pathway provide insight into the amount of information that can travel along that pathway.

In a scenario where treatment can be discerned to always cause outcome, we might expect the ACE as a measure of causal influence, to be large. The example below shows that this is not necessarily the case.

Example 1. Consider a randomized binary treatment \( X \) and a ternary outcome \( Y \), with \( P(Y=0 | X=0) = P(Y=2 | X=0) = 0.5 \), and \( P(Y=1 | X=1) = 1 \). In this setting, \( \text{ACE} = 0 \), even though treatment affects outcome for every subject in the population.

In less extreme settings, the ACE may be very small even when treatment affects outcome for almost every subject in the population, or very large, even when very few subjects have an outcome that is affected by treatment.

The ACE is likewise not always well suited to measuring the strength of a causal relationship when the treatment variable is non-binary. In such situations, no causal contrast represents the causal influence, and the number of possible contrasts grows combinatorially in the cardinality of treatment. We now define the MME and discuss how it can overcome these issues.

\[
\begin{align*}
\text{(a)} & \quad X \rightarrow C \rightarrow Y \\
\text{(a')} & \quad X \rightarrow C \rightarrow Y \\
\text{(b)} & \quad X \rightarrow C \rightarrow Y \\
\text{(b')} & \quad X \rightarrow C \rightarrow Y 
\end{align*}
\]

Figure 5: Modifying DAGs (a) and (b) by inserting a latent mediary \( W \) between \( X \) and \( Y \) yields DAGs (a’) and (b’) respectively. Note that in (a), even though \( X \) and \( Y \) are latent confounded, corollary 10.1 gives \( \text{MME}_{X \rightarrow Y} \geq I(A:Y|C) \) by exploiting the fact that \( A \in an(X) \). Also note that in (b), even though \( X \) affects \( Y \) both directly and indirectly though \( D \), corollary 10.1 gives \( \text{MME}_{X \rightarrow Y} \geq I(X:Y|D) - H(D) \) for the direct effect.

**Definition 10 (Minimal Mediary Entropy (MME) for Direct Effect).** Given a DAG \( \mathcal{G} \) containing a directed edge \( X \rightarrow Y \), let \( \mathcal{G}'_{X \rightarrow W \rightarrow Y} \) denote the graph constructed by substituting the single edge \( X \rightarrow Y \) in \( \mathcal{G} \) with the set of four edges \( \{X \rightarrow W \rightarrow Y, \ W \leftarrow U_{WY} \rightarrow Y\} \), introducing auxiliary latent variables \( W \) and \( U_{WY} \).

We then define \( \text{MME}_{X \rightarrow Y} \) as the smallest entropy \( H(W) \) over all structural equations models reproducing the observed data distribution over \( \mathcal{G}'_{X \rightarrow W \rightarrow Y} \) in which \( W \) has finite cardinality.

Fig. 5 illustrates the process of edge substitution. Essentially, the edge \( X \rightarrow Y \) in \( \mathcal{G} \) is interrupted to pass through \( W \) in \( \mathcal{G}'_{X \rightarrow W \rightarrow Y} \), such that the auxiliary latent variable \( W \) fully mediates the direct effect of \( X \) on \( Y \). Note that caveat that MME is defined in terms of minimizing the entropy of \( W \) over finite cardinality \( W \) capable of reproducing the observed statistics. If \( W \) were allowed to be a continuously valued variable, then the observed data distribution would always be reproducible with arbitrarily small \( H(W) \), due to the total lack of restriction in the instrumental model with a continuous mediary [21].

With the presumption of finite cardinality \( W \) by fiat, however, we are in a position to exploit Theorem 5 in order to practically lower bound the MME.

**Corollary 10.1. (Proof in Appendix C.)**

Suppose that graphical construction \( \mathcal{G}'_{X \rightarrow W \rightarrow Y} \) exhibits the \( \epsilon \)-separation relation \( \{A \perp B | C \text{ upon } \bar{\{D,W\}}\} \) and furthermore no element of \( \{A,C\} \) is a descendant of any in \( \{D,W\} \), where \( A, B, C, \) and \( D \) are nonoverlapping subsets \( \{C,D\} \) possibly empty) of the observed variables in \( \mathcal{G} \), and all the variables within \( D \) are discrete. Then

\[
\text{MME}_{X \rightarrow Y} \geq I(A:B | C,D) - H(D|C). \tag{10}
\]

Suppose that \( P_0 \) is a distribution in the model of the extended graph \( \mathcal{G}'_{X \rightarrow W \rightarrow Y} \), such that \( P_0 \) marginalizes to the observed data distribution. Then the entropy \( H(W) \) in \( P_0 \) is necessarily an upper bound on \( \text{MME}_{X \rightarrow Y} \), i.e. we have found a \( W \) with entropy \( H(W) \) that fully mediates the causal influence of \( X \) on \( Y \). Since \( W \) could always reproduce the observed data by simply copying the values of \( X \), we have a trivial upper bound of \( \text{MME}_{X \rightarrow Y} \leq H(X) \).

This upper bound can typically be improved by even partially exploring the space of the distributions in \( \mathcal{G}'_{X \rightarrow W \rightarrow Y} \).

Consider the simple model \( X \rightarrow Y \) with \( |X| = 3 \) and \( |Y| = 3 \), and the observed data distribution \( P(X=x, Y=y) = \frac{27}{32} \) if \( x = y \) and \( \frac{5}{32} \) if \( x \neq y \). Our corollary gives us a lower bound on \( \text{MME}_{X \rightarrow Y} \geq I(X:Y) \approx 0.150 \), contrasted with the trivial upper bound \( \text{MME}_{X \rightarrow Y} \leq H(X) \approx 1.585 \). We can improve the trivial upper bounding by noting that this distribution

\[3\]If a latent confounder were added between \( X \) and \( W \), then although \( W \) would still mediate \( X \rightarrow Y \), \( X \) and \( Y \) would share a source of unobserved confounding, altering the causal model.

\[4\]Consider example 1 which has \( \text{ACE}_{X \rightarrow Y} = 0 \). That example has the feature that \( I(X:Y) = H(X) \). Accordingly the lower bound of \( \text{MME}_{X \rightarrow Y} \geq I(X:Y) \) is evidently tight, given the trivial upper bounder \( \text{MME}_{X \rightarrow Y} \leq H(X) \).
can be reproduced by the following functional relationships:

\[ \begin{align*}
W = 0 & \quad \text{and} \quad Y = U_{WY} \quad \text{when} \quad U_{WY} = X \\
W = 1 & \quad \text{and} \quad Y = \text{uniformly random} \quad \text{when} \quad U_{WY} \neq X
\end{align*} \]

and taking \( U_{WY} \) to be a uniform random distribution with cardinality three. In this model for \( G'_{X \rightarrow W \rightarrow Y} \) we obtain \( P(W=0) = \frac{1}{3} \), corresponding to \( \text{MME}_{X \rightarrow W} \leq H(W) \approx 0.918 \).

5 RELATED WORK

This work builds most directly on Ref. [4], in which \( e \)-separation was introduced and Theorem 4 was derived, both of which are essential to our results. It follows in the tradition of a line of literature that aims to derive symbolic expressions of restrictions on the observed data distribution implied by a causal model with latent variables, including Refs. [2, 18, 22]. Entropic constraints were previously considered in Refs. [10–12]. The entropic constraint for the instrumental scenario appears as Equation (5) in Ref. [11], see also Appendix E of Ref. [23]. Our work is also closely related to work in the literature on information theory on how much information can pass through channels of varying types [24]. Our proposed measure of causal strength, the \( \text{MME} \), is motivated by weaknesses in standard causal strength measures (e.g. ACE), which was previously discussed in Ref. [25].

Our results are also related to the causal discovery literature, which seeks to find the causal structures compatible with an observed data distribution [26]. The inequality constraints posed above can be used to check the outputs of existing causal discovery algorithms [26–28].

6 CONCLUSION

In this work, we present inequality constraints implied by \( e \)-separation relations in hidden variable DAGs. We have shown that these constraints can be used for a number of purposes, including adjudicating between causal models, bounding the cardinalities of latent variables, and measuring the strength of a causal relationship. \( e \)-separation relations can be read directly off a hidden variable DAG, leading to constraints that can be easily obtained.

This work opens up two avenues for future work. The first is that our constraints demonstrate a practical use of \( e \)-separation relations, and should motivate the study of fast algorithms for enumerating all such relations in hidden variable DAGs. The second is that the constraints suggest that equality-constraint-based causal discovery algorithms can be improved; understanding how the inequality constraints can best be used to this end will take careful study.

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References

[1] E. Wolfe, R. W. Spekkens, and T. Fritz, “The Inflation Technique for Causal Inference with Latent Variables,” *J. Caus. Inf.* 7, 70 (2019).

[2] C. Kang and J. Tian, “Inequality Constraints in Causal Models with Hidden Variables,” in *Proc. 22nd Conf. UAI* (AUAI, 2006) pp. 233–240.

[3] D. Poderini, R. Chaves, I. Agresti, G. Carvacho, and F. Sciarrino, “Exclusivity graph approach to Instrumental inequalities,” in *Proc. 35th Conf. UAI* (AUAI, 2019).

[4] R. J. Evans, “Graphical methods for inequality constraints in marginalized DAGs,” in *Proc. 2012 IEEE Intern. Work. MLSP* (IEEE, 2012) pp. 1–6.

[5] J. Pienaar, “Which causal structures might support a quantum–classical gap?” *New J. Phys.* 19, 043021 (2017).

[6] J. Pearl, “Causal inference in statistics: An overview,” *Statist. Surv.* 3, 96– (2009).

[7] T. S. Richardson and J. M. Robins, *Single World Intervention Graphs* (Now Publishers Inc, 2013).

[8] D. Geiger and C. Meek, “Quantifier Elimination for Statistical Problems,” in *Proc. 15th Conf. UAI* (AUAI, 1999) pp. 226–235.

[9] J. Pearl, *Probabilistic Reasoning in Intelligent Systems: Networks of Plausible Inference* (Morgan Kaufmann, 1988).

[10] R. Chaves, L. Luft, T. O. Maciel, D. Gross, D. Janzing, and B. Schölkopf, “Inferring latent structures via information inequalities,” in *Proc. 30th Conf. UAI* (AUAI, 2014) pp. 112–121.

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

[12] M. Weilenmann and R. Colbeck, “Analysing causal structures with entropy,” *Proc. Roy. Soc. A* 473, 20170483 (2017).

[13] M. Weilenmann and R. Colbeck, “Analysing causal structures in generalised probabilistic theories,” *Quantum* 4, 236 (2020).

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

[15] T. Verma and J. Pearl, “Equivalence and synthesis of causal models,” in *Proc. 6th Conf. UAI* (AUAI, 1990).

[16] T. S. Richardson, R. J. Evans, J. M. Robins, and I. Shpitser, “Nested Markov Properties for Acyclic Directed Mixed Graphs,” (2017), Working Paper.

[17] I. Shpitser, T. S. Richardson, and J. M. Robins, “Chapter 41: Multivariate counterfactual systems and causal graphical models,” in *Probabilistic and Causal Inference: The Works of Judea Pearl* (ACM Books, 2021).

[18] J. Tian and J. Pearl, “On the Testable Implications of Causal Models with Hidden Variables,” in *Proc. 18th Conf. UAI* (AUAI, 2002).

[19] R. Bhattacharya, T. Nagarajan, D. Malinsky, and I. Shpitser, “Differentiable Causal Discovery Under Unmeasured Confounding,” (2020), arXiv:2010.06978 .

[20] K. Mohan, J. Pearl, and J. Tian, “Graphical Models for Inference with Missing Data,” in *Advances in Neural Information Processing Systems* (Curran Associates, Inc., 2013) pp. 1277–1285.

[21] F. Gunsilius, “A path-sampling method to partially identify causal effects in instrumental variable models,” (2019), working paper.

[22] A. Balke and J. Pearl, “Nonparametric Bounds on Causal Effects from Partial Compliance Data,” *J. Am. Stat. Ass.* (1993).

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

[24] A. E. Gamal and Y.-H. Kim, *Network Information Theory* (Cambridge University Press, 2011).

[25] D. Janzing, D. Balduzzi, M. Grosse-Wentrup, B. Schölkopf, *et al.*, “Quantifying causal influences,” *Ann. Stat.* 41, 2324 (2013).

[26] P. L. Spirtes, C. N. Glymour, and R. Scheines, *Causation, prediction, and search* (MIT press, 2000).

[27] E. V. Strobl, S. Visweswaran, and P. L. Spirtes, “Fast causal inference with non-random missingness by test-wise deletion,” *Int. J. Data Sci. Anal.* 6, 47 (2018).

[28] D. Bernstein, B. Saeed, C. Squires, and C. Uhler, “Ordering-Based Causal Structure Learning in the Presence of Latent Variables,” in *Proc. 23rd Int. Conf. Art. Intell. Estat.*, Vol. 108 (PMLR, 2020) pp. 4098–4108.
(b) and (c) demonstrate that for a set of variables $D$, the counterfactual random variable $D(D=d)$ is not necessarily equal to the factual $D$. Graph (d) provides an example where the entropic inequality constraints remain relevant even though the counterfactual distribution after intervention on $D$ is identified. This is an illustration of the fact that not every equality restriction featuring non-adjacent variables may be involved in inequality restrictions.

In Proposition 7, we showed that for graphical models in which the counterfactual $P(A(D=d), B(D=d), D(D=d) = d | C)$ is identified, the entropic constraints of Theorem 5 are weaker than the corresponding Verma constraints. We now illustrate this point with a few examples. In Fig. S6(a) the counterfactual $P(A(D=d), B(D=d), D(D=d) = d | C)$ is identified, and in Fig. S6(b) the counterfactual $P(A(D=d), B(D=d), D(D=d) = d | C)$ is identified. Accordingly, our entropic inequalities are implied by equality constraints, due to Proposition 7. The resulting inequality constraints therefore cannot provide any additional information about whether these causal structures are compatible with observed distributions.

By contrast, in Fig. S6(d) the counterfactual $P(A(D=d), B(D=d), D(D=d) = d | C)$ is not identified, even though $P(A(D=d), B(D=d) | C)$ is. Although Fig. S6(d) implies no equality constraints [29], we find that it does entail the entropic inequality constraint following from the $e$-separation relation $A \perp_e B$ upon $\sim \{D_1, D_2\}$. It is therefore an example of a graph in which our inequality constraints are not made redundant by known equality constraints, despite the fact that intervention on $D$ is identified. This example is also an illustration of the fact that not every equality restriction featuring non-adjacent variables in an identifiable counterfactual distribution implies equality restrictions on the observed data distribution. However, some such non-adjacent variables may be involved in inequality restrictions.

The critical identifiability question for determining whether the entropic constraints are made redundant by equality constraints is $P(A(D=d), B(D=d), D(D=d) = d | C)$. This distribution involves the counterfactual random variable $D(D=d)$. Note that although any single random variable under intervention on itself is equivalent to the random variable under no intervention, the same does not necessarily hold for sets of random variables. Figs. S6(b) and S6(c) demonstrate this point – because $D_2$ is a descendant of $D_1$, after intervention on both, $D_2$ no longer takes its natural value.

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[29] R. J. Evans and T. S. Richardson, “Smooth, identifiable supermodels of discrete DAG models with latent variables,” Bernoulli 25, 848 (2019).

[30] T. Gläßle, D. Gross, and R. Chaves, “Computational tools for solving a marginal problem with applications in Bell non-locality and causal modeling,” J. Phys A 51, 484002 (2018).

[31] E. H. Lieb, “Some convexity and subadditivity properties of entropy,” Bull. Am. Math. Soc. 81, 1 (1975).

[32] G. R. Kumar, C. T. Li, and A. El Gamal, “Exact common information,” in 2014 IEEE International Symposium on Information Theory (2014) pp. 161–165.

[33] D. Geiger and J. Pearl, “On the Logic of Causal Models,” in Proc. 4th Conf. UAI (AUAI, 1998) pp. 136–147.

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A COMPARING ENTRISTIC INEQUALITIES TO GENERALIZED INDEPENDENCE RELATIONS

Figure S6: In graphs (a) and (b), the entropic inequality constraints are logically implied by equality constraints. Graphs (b) and (c) demonstrate that for a set of variables $D$, the counterfactual random variable $D(D=d)$ is not necessarily equal to the factual $D$. Graph (d) provides an example where the entropic inequality constraints remain relevant even though the counterfactual distribution after intervention on $D$ is identified.
B  \( E \)-SEPARATION IN IDENTIFIED COUNTERFACTUAL DISTRIBUTIONS

![Diagrams](image)

Figure S7: In all three graphs, \( A \) and \( B \) are \( e \)-separated by \( D \) after intervention on \( C \). The counterfactual distribution over \( \{A,B,D\} \) after intervention on \( C \) is only identified in graphs (a) and (c), however.

A Single World Intervention Graph (SWIG) \([7]\), which represents the model after intervention on one or more random variables, can be obtained through a node-splitting operation as illustrated in Fig. S6(c). As described in Section 3.2, \( d \)-separation relations that appear under interventions with identified distributions can be used to derive equality constraints on the observed data distribution. In this section, we explore the significance of \( e \)-separation relations in identified counterfactual distributions.

We begin by noting that any \( e \)-separation relation that exists in a SWIG corresponds to an \( e \)-separation in the original DAG.

**Proposition 11.** \((A \perp_C B \mid C \text{ upon } \neg D)\) after intervention on \( E \) only if \((A \perp_C B \mid C \text{ upon } \neg \{D,E\})\).

This proposition follows directly from the relationship between the fixing \([16]\) and deletion operations. In particular, fixing and deleting vertices induce the same graphical relationships among the remaining variables in the graph.

It may at first seem that this result indicates that \( e \)-separation relations in SWIGs cannot be used to derive inequality constraints on the observed data distribution that are not already implied by \( e \)-separation relations in the original model. However, entropic inequality constraints on counterfactual distributions have a different form than such constraints on the factual distribution. This is because entropies of counterfactual variables do not in general correspond to entropies of factual variables, so there is no way to express inequality constraints that follow from \( e \)-separation relations in SWIGs as entropic inequalities on the original distribution.

To illustrate this point, consider Fig. S7. In each graph, \((A \perp_C B \mid \text{ upon } \neg D)\) in the SWIG resulting from intervention on \( C \). However, in Fig. S7(b), the distribution after intervention on \( C \) is not identified, whereas in Figs. S7(a) and S7(c) it is identified as \( P(A(c),B(c),D(c)) = \sum_x P(A,B,C=c,D,X=x) \). This means the entropic inequalities \( I(A(c) : B(c)) \leq H(D(c)) \) on this counterfactual distribution (one for each level of \( C \)) imply inequality constraints on the observed data distribution as well. These inequality constraints will be obtained in Figs. S7(a) and S7(c), but not in Fig. S7(b).

Moreover, these inequality constraints can be shown to be nontrivial. Since Figs. S7(a) and S7(b) share the same \( d \)-separation and \( e \)-separation relations it follows that any distributions compatible with Fig. S7(b) cannot be witnessed as incompatible with Fig. S7(a) using non-nested entropic equalities or inequalities. Consider the following structural equation model for Fig. S7(b):

Let \( U_1, U_2 \) and \( U_3 \) be binary and uniformly distributed, and let \( X = U_2 \oplus \epsilon_A, C = X \oplus U_3, B = C \oplus U_3 \oplus \epsilon_B, \) and \( D = \epsilon_D \) where \( \oplus \) indicates addition mod 2 and where \( \epsilon_k \) is a random variable very heavily biased towards zero for \( k \in \{A,B,D\} \). This establishes that \( C \) and \( X \) are uniformly distributed and statistically independent from each-other, and hence that \( P(A,B) = P(A(c=0),B(c=0)) \). This construction also gives \( A \oplus B = U_2 \oplus \epsilon_A \oplus U_3 \oplus \epsilon_B = U_2 \oplus \epsilon_A \oplus X \oplus \epsilon_B = \epsilon_A \oplus \epsilon_B \) and hence \( A \approx B \). This yields \( I(A(c=0) : B(c=0)) \approx H(A) \approx 1 \) whereas \( H(D(c=0)) = H(D) \approx 0 \), strongly violating the entropic inequality \( I(A(c=0) : B(c=0)) \leq H(D(c=0)) \) which applies only to Fig. S7(a).
C  PROOFS

Proof of Theorem 5

Let \( G^\# \) represent the graph in which every node in \( D \) is split, and \( P^* \) denote the distribution over variables in \( G^\# \). We follow the convention established above whereby for each node \( D \) in \( D \), a new node \( D^\# \) is added to the graph, \( D^\# \) is made a parent of all children of \( D \), and all edges outgoing from \( D \) are removed. For notational convenience, we let \( P_{d^\#}(\cdot | \cdot, D^\# = d^\#) \), and \( I_{d^\#} \) and \( H_{d^\#} \) be the mutual information and entropy in this counterfactual distribution. Recall that by Theorem 4, if \( (A \perp B | C \text{ upon } -D) \), then:

4.i. \( I_{d^\#}(A : B | C = c) = 0 \), and
4.ii. \( P(A,B,D=d^\# | C = c) = P_d(\cdot | \cdot, D = d^\#) \).

From the latter condition (4.ii.) we readily have that \( H_{d^\#}(\cdot | \cdot, D = d^\#) = H(\cdot | \cdot, D = d^\#) \). This means that for any node set \( Z \), and for any node set \( X \) among the nondescendants of \( D \) in \( G \), we find that

\[
H(Z \mid X=x, D) = \sum_{d^\#} P(D=d^\# \mid X=x) H(Z \mid X=x, D=d^\#) = \sum_{d^\#} P_d(D=d^\# \mid X=x) H_{d^\#}(Z \mid X=x, D=d^\#) = \sum_{d^\#} P_d(D=d^\# \mid X=x) H_{d^\#}(Z \mid X=x, D=d^\#)
\]

(S11)

where the final equality follows from the fact that \( P \) and \( P^* \) agree when referring to nondescendants of \( D^\# \) in \( G^\# \), and that \( D \) is included among the nondescendants of \( D^\# \) in \( G^\# \).

If the counterfactual entropies only involve variables which are nondescendants of \( D^\# \) in \( G^\# \), then they coincide with the observable entropies even without such a weighted summation. This is because by construction \( D^\# \) has no parents, and therefore its nondescendants are marginally independent of \( D^\# \), and cannot be made dependent on it by conditioning on other nondescendants. When \( Y \) are among the nondescendants of \( D^\# \) in \( G^\# \) and further \( X \) are among the nondescendants of \( D \) in \( G \), we find that

\[
H(Y \mid X=x) = H_{d^\#}(Y \mid X=x),
\]

which for later convenience we express as

\[
\left( \sum_{d^\#} P_d(D=d^\# \mid X=x) = 1 \right) \times H_{d^\#}(Y \mid X=x).
\]

(S12)

For \( X \) among the nondescendants of \( D \) in \( G \) we further introduce the notation\(^5\)

\[
h(D=d^\# \mid X=x) = h_{d^\#}(D=d^\# \mid X=x) := -\log(P_d(D=d^\# \mid X=x))
\]

(S13a)

such that

\[
H(D \mid X=x) = H_{d^\#}(D \mid X=x) = \sum_{d^\#} P_d(D=d^\# \mid X=x) h_{d^\#}(D=d^\# \mid X=x)
\]

(S13b)

To find constraints on the observed data distribution that take advantage of the properties of \( P^* \), we can chose a particular node set \( X \) among the nondescendants of \( D \) in \( G \) and then identify entropic inequalities such that all the terms look like either

\[
\begin{align*}
\text{Per (S11):} & \quad H(Z \mid D, X=x) = \sum_{d^\#} P_d(D=d^\# \mid X=x) H_{d^\#}(Z \mid D=d^\#, X=x) & \text{for any } Z, \\
\text{Per (S12):} & \quad H(Y \mid X=x) = \sum_{d^\#} P_d(D=d^\# \mid X=x) H_{d^\#}(Y \mid X=x) & \text{for } Y \text{ among nondescendants of } D^\# \text{ in } G^\# \text{ and } Y \cap D = \emptyset, \\
\text{Per (S13):} & \quad H(D \mid X=x) = \sum_{d^\#} P_d(D=d^\# \mid X=x) h_{d^\#}(D=d^\# \mid X=x).
\end{align*}
\]

Formally, the task of extracting all the implications of a set of linear inequalities on the subset of terms which have suitable form is an instance of polytope projection, and may be solved be means of Fourier-Motzkin elimination or related algorithms [30].\(^6\)

\(^5\)Note that the quantity defined in Eq. (S13a) is a standard unit in information theory, known as “surprisal” or “self-information”.

\(^6\)As the example proofs demonstrate, the equality constraint(s) coming from \( e \)-separation are not in the desired final format. We identify all the undesirable terms, and then cancel them out by combining with subadditivity inequalities, monotonicity inequalities, as well as potentially any zero-mutual-information inequalities associated with \( d \)-separation relations among the visible variables in the original graph \( G \) in order to obtain their testable implications.
To prove the first part of Theorem 5 in this way, suppose \( C \) are among the nondescendants of \( D \) in \( G \). Introducing the shorthand \( c \) to denote \( C = c \) we could derive an inequality of suitable form by summing the four inequalities

\[
0 \leq I(A : D | c) = H(A | c) - H(A | c, D) \\
\therefore \quad 0 \leq -H(A | c, D) + \sum_{d \in \mathcal{D}} P_{d \neq} (D = d^\#) H_{d \neq} (A | c), \quad \text{(S14a)}
\]

\[
0 \leq I(B : D | c) = H(B | c) - H(B | c, D) \\
\therefore \quad 0 \leq -H(B | c, D) + \sum_{d \in \mathcal{D}} P_{d \neq} (D = d^\#) H_{d \neq} (B | c), \quad \text{(S14b)}
\]

\[
0 \leq H(D | A, B, c) = H(D | c) + H(A, B | c, D) - H(A, B | c) \\
\therefore \quad 0 \leq H(D | c) + H(A, B | c, D) - \sum_{d \in \mathcal{D}} P_{d \neq} (D = d^\#) H_{d \neq} (A, B | c), \quad \text{(S14c)}
\]

\[
0 = I_{d \neq} (A : B | c) = -\sum_{d \in \mathcal{D}} P_{d \neq} (D = d^\#) I_{d \neq} (A : B | c) \\
\therefore \quad 0 \leq \sum_{d \in \mathcal{D}} P_{d \neq} (D = d^\#) (H_{d \neq} (A, B | c) - H_{d \neq} (A | c) - H_{d \neq} (B | c)). \quad \text{(S14d)}
\]

Inequalities (S14a) and (S14b) follow from the nonnegativity of conditional mutual information. Subadditivity holds for both discrete and continuously valued variables [31]. Inequality (S14c) follows from monotonicity (the fact that all conditional entropies are nonnegative) and the chain rule. Conditional entropy is only guaranteed to be nonnegative for discrete variables, and this is why Theorem 5 demands that \( D \) be discrete. All but the final inequality implicitly make use of Equation (S11). Inequality (S14d), by contrast, is a consequence of \( I_{d \neq} (A : B | c) = 0 \) per Theorem 4; see condition (4.i.) above. Summing all four inequalities (S14) leads to the derived inequality

\[
0 \leq H(D | c) + H(A, B | c, D) - H(A | c, D) - H(B | c, D), \quad \text{i.e.,} \quad I(A : B | c, D) \leq H(D | c). \quad \text{(S15)}
\]

Now consider the case where we are further promised that \( A \) are nondescendants of \( D \) in \( G \) and hence nondescendants of \( D^\# \) in \( G^\# \). This means that in addition to the above results we also have that \( H_{d \neq} (A | c) = H(A | c) \) per Equation (S12). We proceed as before, but instead of summing all four of the (S14) inequalities we only take the sum of the latter three. This then yields

\[
0 \leq H(D | c) + H(A, B | c, D) - H(A | c) - H(B | c, D) \quad \text{i.e.,} \quad I(A : B, D | c) \leq H(D | c). \quad \text{(S16)}
\]

In both cases, the constraint is maintained after taking the expectation of both sides with respect to \( C \). Because each term in the expectation will satisfy the inequality, so will the sum. That is, in the first case, Eq. (3a) implies Eq. (3b), and in the second case, Eq. (4a) implies Eq. (4b).

\( \square \)

Beyond Theorem 5

Going beyond the result in Theorem 5, even when \( C \) are not entirely among the nondescendants of \( D \) in \( G \) we can nevertheless obtain the nontrivial entropic inequality \( I(A : B | C, D) \leq H(D) \), by noting that

\[
0 \leq I(A : D | C) + I(B : D | C) + H(D | A, B, C) + I(C : D) - \sum_{d \in \mathcal{D}} P_{d \neq} (D = d^\#) I_{d \neq} (A : B | C). \quad \text{(S17)}
\]

One notes that all of the terms introduced by \(- \sum_{d \in \mathcal{D}} P_{d \neq} (D = d^\#) I_{d \neq} (A : B | C)\) are cancelled by judiciously applying Equation (S11) to the other terms, leaving

\[
0 \leq H(D) + H(A, B, C | D) - H(A, C | D) - H(B, C | D) + H(C | D) = H(D) - I(A : B | C, D). \quad \text{(S18)}
\]

Note that this proof technique can be adapted to derive stronger entropic inequalities for graphs which exhibit multiple different \( c \)-separation relations involving the same \( D \) set. If \((A_1 \perp B_1 | C_1 \text{ upon } \neg D)\) and \((A_2 \perp B_2 | C_2 \text{ upon } \neg D)\) and so forth, then Theorem 4 still demands the existence of a single \( P_{d \neq} \) whose various margins must now satisfy multiple distinct zero conditional mutual informational equalities. We can accommodate multiple entropic equality constraints on \( P_{d \neq} \) just as easily as we can accommodate a single equality constraint: The translation between constraints on \( P_{d \neq} \) and \( P \) will continue to be governed by conditions (S11), (S12), and (S13b).
Proof of Proposition 6
If conditioning on some variables \( D \) is sufficient to close a path, then that path must go through \( D \), and therefore deletion of \( D \) eliminates the path. By construction, the deletion operation can never open a path, unlike the conditioning operation. If \((A \perp_B C \mid D)\), then all paths from \( A \) to \( B \) go through \( C \) or \( D \), or through colliders that are not in \( \{C, D\} \), nor have any descendants therein. It follows that \((A \perp_B C \mid \neg D)\), as after deletion of \( D \) all paths through \( C \) remain blocked through conditioning, all paths through \( D \) are eliminated, and all other paths remain blocked by colliders.

Proof of Proposition 8
Firstly, we note that the data processing inequality
\[
I(A : B \mid C = c) \geq I(A : B \mid C = c) \quad \text{whenever} \quad A \perp_B \{C, U\} \tag{S19}
\]
holds for continuous variables, since it is merely a consequence of the fact that the chain rule can by applied to \( I(A : B \mid C = c) \) in either of two ways, i.e.
\[
I(A : B \mid C = c) = I(A : B \mid C = c) + I(A : U \mid B, c),
\]
and also that
\[
I(A : B \mid C = c) = I(A \mid U = c) + I(A : B \mid U, c).
\]
The data processing inequality, then, follows from the nonnegativity of \( I(A : B \mid c) \) and from \( I(A : B \mid U, c) = 0 \) being an implication of \( A \perp_B \{C, U\} \). Recognizing that \( I(A : U \mid c) = H(U \mid c) - (H(A, U \mid c) - H(A \mid c)) \), and that by weak monotonicity \( H(A, U \mid c) - H(A \mid c) \geq 0 \), we then have that
\[
H(A \mid C = c) \geq I(A : U \mid C = c).
\]
To obtain Corollary 8.1 simply note that the constraint is maintained after taking the expectation of both sides with respect to \( C \): because each term in the expectation will satisfy the inequality whenever the cardinality of \( U \) is finite, so will the sum.

Proof of Corollary 10.1
Per Definition 10, \( \text{MME}_{X \rightarrow Y} \) is defined as the smallest entropy \( H(W) \) over all structural equations models over \( G'_{X \rightarrow W \rightarrow Y} \) in which \( W \) has finite cardinality and which reproduce the observed data distribution over \( \{A, B, C, D\} \). Let \( P'(A, B, C, D, W) \) be the distribution over \( \{A, B, C, D, W\} \) associated with some structural equation model which minimizes \( H(W) \). Since the premises of Corollary 10.1 stipulate that \( G'_{X \rightarrow W \rightarrow Y} \) exhibits the \( e \)-separation relation \((A \perp_B C \mid \neg \{D, W\})\), and that no element of \( \{A, C\} \) is a descendant of any in \( \{D, W\} \), it follows from Equation (4b) in our main theorem that \( P' \) must satisfy \( I(A : B, W \mid C, D) \leq H(D, W \mid C) \). Indeed, one can confirm the following sequence of inequalities which \( P' \) must satisfy:
\[
I(A : B \mid C, D) \leq I(A : B, W \mid C, D) \leq I(A : B, W \mid C) \leq H(D, W \mid C) \leq H(D \mid C) + H(W) \leq H(D \mid C) + \text{MME}_{X \rightarrow Y}
\]
where all the steps above are consequences of subadditivity except for the step from Equation (S21a) to Equation (S21b), which is just the application of Equation (4b) as noted above.

Note that we have elected to define \( \text{MME} := \min_{\text{SEM} G'} H(W) \), i.e. Definition 10 minimizes \( H(W) \) over all structural equations models over \( G'_{X \rightarrow W \rightarrow Y} \). One may also consider distinct but related entropic measures of causal influence to \( Y \) from \( X \), such as
\[
\text{MME}' := \max_{Z, z} \min_{\text{SEM} G'} H(W \mid \text{do } Z = z), \tag{S22}
\]
which involves recomputing (or at least lower bounding) \( \text{MME} \) under different external intervention choices (\( Z \) being any subset of the variables in \( G \) excluding \( X \) and \( Y \), and \( z \) being any value tuple for \( Z \) and retaining the largest of all the lower bounds. Plainly \( \text{MME}' \geq \text{MME} \). However, we can exploit Equation (4a) to obtain a slightly stronger lower bound on \( \text{MME}' \) than just \( \text{MME}_{X \rightarrow Y} \geq I(A : B \mid C, D) - H(D \mid C) \) when the premises of Corollary 10.1 hold, namely
\[
\text{MME}' \geq \max_c I(A : B \mid D, \text{do } C = c) - H(D \mid \text{do } C = c). \tag{S23}
\]
D RELATION BETWEEN COMMON ENTROPY AND MME

The MME bears some resemblance to a concept called common entropy \([32]\), which is defined for a distribution \(P(X,Y)\) as the smallest possible entropy of an unobserved variable \(W\) such that \(X \perp Y \mid W\). Unlike the MME, the common entropy is a function only of the probability distribution \(P(X,Y)\), and not of the graph \(G\). Any \(W\) that renders \(X\) and \(Y\) conditionally independent must also fully mediate the effect of \(X\) on \(Y\), which at first glance might be taken to mean that the common entropy is an upper bound on the MME, because it implies that the MME can search over a larger set of distributions to obtain a low-entropy mediator. Indeed in the simple \(X \rightarrow Y\) model, it is the case that \(\text{MME}_{X \rightarrow Y}\) is bounded from above by the common entropy between \(X\) and \(Y\) for precisely this reason.

However, the common entropy is not an upper bound on the MME in general. To see this, consider the graph presented in Fig. 1(c). This model contains distributions in which \(A\) and \(B\) are highly correlated, but \(D\) and \(B\) are entirely uncorrelated. For such distributions, the common entropy of \(B\) and \(D\) would be 0, as they are already marginally independent. However, by Corollary 10.1, the MME would be bounded from below by \(I(A : B)\), which can be larger than 0. The intuition for this phenomenon is that if the edge \(D \rightarrow B\) were missing, \(A\) and \(B\) would be marginally independent, so a high mutual information between them is evidence for the causal significance of the edge.
E  AN INVERSE OF THEOREM 5

The goal of this appendix is to establish that

**Proposition 12.** If a graph \( \mathcal{G} \) has the feature \( \{A \not\rightarrow_{\mathcal{G}} B \mid C \uparrow \neg D\} \), then there exists a distribution in the marginal model of \( \mathcal{G} \) with discrete \( D \) such that \( (A : B \mid C, D) = I(A : B \mid C) \geq H(D) \).

We begin by simply noting that

**Lemma 13.** The marginal model of any graph \( \mathcal{G} \) whose nodes include \( \{A, B, C, D\} \) contains all conditional distributions \( P(A, B \mid C, D) \) wherein

1. \( P(A, B \mid C, D) = P(A, B \mid C) \), and
2. \( P(A, B \mid C) \) is within the marginal model of the graph \( \mathcal{G}' \) defined by removing outgoing edges from \( D \) in \( \mathcal{G} \).

The sorts of \( P(A, B \mid C, D) \) described in Lemma 13 arise by considering causal models wherein every child of \( D \) always ignores the values of \( D \), treating \( D \) as if it has no descendants. We next invoke the completeness of \( d \)-separation. That is,

**Lemma 14.** If \( \{A \not\rightarrow_{\mathcal{G}} B \mid C\} \) in \( \mathcal{G} \), then there exists a distribution in the marginal model of \( \mathcal{G} \) for which \( I(A : B \mid C) \geq 0 \).

We note that Lemma 14 follows from

**Lemma 15.** If \( \{A \not\rightarrow_{\mathcal{G}} B \mid C\} \) in \( \mathcal{G} \) for singleton nodes \( A \) and \( B \), then there exists a distribution in the marginal model of \( \mathcal{G} \) for which \( \exists_c \) s.t. \( I(A : B \mid C=c) \geq 0 \).

After all, \( I(A : B \mid C) = 0 \) if and only if \( I(A : B \mid C) = 0 \) for all singleton nodes \( A \in A \) and \( B \in B \). Moreover, \( I(A : B \mid C) = 0 \) if and only if \( I(A : B \mid C=e) = 0 \) for all \( e \) having positive support. We believe that Lemma 15 explicitly follows from Theorem 3 in Ref. [33], but we provide an explicit proof of it below for completeness.

By combining Lemmas 13 and 14 we obtain Proposition 12. This follows by noting that whenever a graph \( \mathcal{G} \) has the feature \( \{A \not\rightarrow_{\mathcal{G}} B \mid C \uparrow \neg D\} \), then by definition the graph \( \mathcal{G}' \) defined by removing outgoing edges from \( D \) in \( \mathcal{G} \) exhibits \( \{A \not\rightarrow_{\mathcal{G}} B \mid C\} \). To violate the basic inequality in Theorem 5 we apply Lemma 14 while keeping \( H(D) \leq I(A : B \mid C) \). We can make \( H(D) \) arbitrarily small by heavily biasing \( P(D) \) towards one value.

**Proof of Lemma 15**

The following construction yields \( I(A : B \mid C=1) = \log(2) \) whenever \( \mathcal{G} \) exhibits \( \{A \not\rightarrow_{\mathcal{G}} B \mid C\} \) for singleton nodes \( A \) and \( B \).

If \( \{A \not\rightarrow_{\mathcal{G}} B \mid C\} \) in \( \mathcal{G} \) then there exists some path in \( \mathcal{G} \) with end nodes \( A \) and \( B \) such that all colliders in the path are elements of \( C \) and no element in \( C \) is present in the path except as a collider. We classify the nodes within the path into three distinct types:

**Two Incoming Edges from the Path** These are the colliders in the path, elements of \( C \). We take each such node to act as a Kronecker delta function over its two in-path parents. That is, it will return the value 1 iff the two in-path parents have coinciding values. That is,

\[
y(x_1, x_2) = \begin{cases} 
0, & \text{with unit probability iff } x_1 \neq x_2, \\
1, & \text{with unit probability iff } x_1 = x_2.
\end{cases} \tag{S24}
\]

**One Incoming Edge from the Path** These are the mediaries in the path, as well as at least one (perhaps both) of the end nodes of the path. Let these variables act as an identity functions of its single in-path parent. That is,

\[
y(x) = \begin{cases} 
0, & \text{with unit probability iff } x = 0, \\
1, & \text{with unit probability iff } x = 1.
\end{cases} \tag{S25}
\]

**Zero Incoming Edges from the Path** These are the bases of forks in the path, as well as potentially one of the end nodes of the path. Let these variable act as uniformly random variables with cardinality 2. That is,

\[
y() = \begin{cases} 
0, & \text{with probability } \frac{1}{2}, \\
1, & \text{with probability } \frac{1}{2}.
\end{cases} \tag{S26}
\]
This construction results in every non-collider being uniformly distributed over \( \{0,1\} \) and always taking the same value as every other non-collider in the path upon postelecting all colliders in the path to take the value 1. That is, this construction explicitly ensures that \( I(A:B | C=1) = \log(2) \).