Integrity Constraints Revisited: From Exact to Approximate Implication

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Abstract

Integrity constraints such as functional dependencies (FD), and multi-valued dependencies (MVD) are fundamental in database schema design. Likewise, probabilistic conditional independences (CI) are crucial for reasoning about multivariate probability distributions. The implication problem studies whether a set of constraints (antecedents) implies another constraint (consequent), and has been investigated in both the database and the AI literature, under the assumption that all constraints hold *exactly*. However, many applications today consider constraints that hold only *approximately*. In this paper we define an approximate implication as a linear inequality between the degree of satisfaction of the antecedents and consequent, and we study the *relaxation problem*: when does an exact implication relax to an approximate implication? We use information theory to define the degree of satisfaction, and prove several results. First, we show that any implication from a set of data dependencies (MVDs+FDs) can be relaxed to a simple linear inequality with a factor at most quadratic in the number of variables; when the consequent is an FD, the factor can be reduced to 1. Second, we prove that there exists an implication between CIs that does not admit any relaxation; however, we prove that every implication between CIs relaxes "in the limit". Finally, we show that the implication problem for differential constraints in market basket analysis also admits a relaxation with a factor equal to 1. Our results recover, and sometimes extend, several previously known results about the implication problem: implication of MVDs can be checked by considering only 2-tuple relations, and the implication of differential constraints for frequent item sets can be checked by considering only databases containing a single transaction.

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1 Introduction

Applications of Big Data require the discovery, or mining, of integrity constraints in a database instance [14, 34, 8, 4, 20]. For example, data cleaning can be done by first learning conditional functional dependencies in some reference data, then using them to identify inconsistencies in the test data [17, 8]. Causal reasoning [35, 28, 31] and learning sum-of-product networks [29, 12, 26] repeatedly discover conditional independencies in the data. Constraints also arise in many other domains, for example in the *frequent itemset problem* (FIS) [22, 6], or as *measure based constraints* [32] in applications like Dempster-Shafer theory, possibilistic theory, and game theory (see discussion in [32]). In all these applications, quite often the constraints are learned from the data, and are not required to hold exactly, but it suffices if they hold only to a certain degree.

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Cone	Relaxation Bounds			
	General	MVDs+FDs $\Rightarrow$ FD	MVDs+FDs $\Rightarrow$ MVD	Disjoint MVDs+FDs $\Rightarrow$ MVD/FD
Γ_n	$(2^n)!$ (Thm. 21)	1 (Thm. 6)	$\frac{n^2}{4}$ (Thm. 6)	1 (Thm. 11)
Γ^*_n	∞ (Thm. 16)	1 (Thm. 6)	$\frac{n^2}{4}$ (Thm. 6)	1 (Thm. 11)
$\mathcal{P}_n$	1 (Thm. 23)	1 (Thm. 23)	1 (Thm. 23)	1 (Thm. 23)

Table 1 Summary of results: relaxation bounds for the implication $\Sigma \Rightarrow \tau$ for the sub-cones of Γ_n under various restrictions. (1) *General*; no restrictions to either Σ or τ (2) Σ is a set of saturated CIs and conditional entropies (i.e., MVDs+FDs in databases), and τ is a conditional entropy. (3) Σ is a set of saturated CIs and conditional entropies, τ is *any* CI (4) *Disjoint* integrity constraints. The terms in Σ are both saturated and *disjoint* (see definition 10 in Sec. 4), and τ is saturated.

The *implication problem* asks whether a set of constraints, called the *antecedents*, logically imply another constraint called the *consequent*. In this setting, both antecedents and consequent are required to hold exactly, hence we refer to it as an *exact implication* (EI). The database literature has extensively studied the EI problem for integrity constraints and shown that the implication problem is decidable and axiomatizable for Functional Dependencies (FDs) and Multivalued Dependencies (MVDs) [23, 19, 1, 3], and undecidable for Embedded Multivalued Dependencies (EMVDs) [16]. The AI community has studied extensively the EI problem for Conditional Independencies (CI), which are assertions of the form $X \perp Y \mid Z$, stating that X is independent of Y conditioned on Z, and has shown that the implication problem is decidable and axiomatizable for saturated CIs [13] (where $XYZ =$ all variables), but not finitely axiomatizable in general [36]. In the FIS problem, a constraint like $X \to Y \vee Z \vee U$ means that every basket that contains X also contains at least one of Y, Z, U, and the implication problem here is also decidable and axiomatizable [33].

The Relaxation Problem. In this paper we consider a new problem, called the *relaxation problem*: if an exact implication holds, does an approximate implication hold too? For example, suppose we prove that a given set of FDs implies another FD, but the input data satisfies the antecedent FDs only to some degree: to what degree does the consequent FD hold on the database? An *approximate implication* (AI) is an inequality that (numerically) bounds the consequent by a linear combination of the antecedents. The relaxation problem asks whether we can convert an EI into an AI. When relaxation holds with a small bound, then any inference system for proving exact implication, e.g. using a set of axioms or some algorithm, can be used to infer approximate implication.

In order to study the relaxation problem we need to measure the degree of satisfaction of a constraint. In this paper we use Information Theory. This is the natural semantics for modeling CIs of multivariate distributions, because $X \perp Y \mid Z$ iff $I(X;Y|Z) = 0$ where I is the *conditional mutual information*. FDs and MVDs are special cases of CIs [21, 9, 38] (reviewed in Sec. 2.1), and thus they are naturally modeled using the information theoretic measure $I(X;Y|Z)$ or $H(Y|X)$; in contrast, EMVDs do not appear to have a natural interpretation using information theory, and we will not discuss them here. Several papers have argued that information theory is a suitable tool to express integrity constraints [21, 9, 38, 24, 14].

An exact implication (EI) becomes an assertion of the form $(\sigma_1 = 0 \wedge \sigma_2 = 0 \wedge \ldots) \Rightarrow (\tau = 0)$, while an approximate implication (AI) is a linear inequality $\tau \le \lambda \cdot \left(\sum \sigma_i\right)$, where $\lambda \ge 0$, and $\tau, \sigma_1, \sigma_2, \ldots$ are information theoretic measures. We say that a class of constraints can be *relaxed* if EI implies AI; we also say that it λ-relaxes, when we want to specify the factor λ in the AI. We notice an AI always implies EI.

Results We make several contributions, summarized in Table 1. We start by showing in Sec. 4 that MVDs+FDs admit an $n^2/4$-relaxation, where n is the number of variables, and when the consequent is an FD, the implication admits a 1-relaxation. Thus, whenever an exact implication holds between MVD+FDs, a simple linear inequality also holds between their associated information theoretic terms. In fact, we prove a stronger result that holds for CIs in general, which imply the result for MVDs+FDs. In addition, under some mild syntactic restrictions to the antecedents, we strengthen the result to 1-relaxation when the consequent is an MVD (i.e., instead of $\frac{n^2}{4}$); we leave open the question whether 1-relaxation exists in general.

So far, we have restricted ourselves to saturated+conditional CIs (which correspond to MVDs+FDs). In Sec. 5 we remove any restrictions, and prove a negative result: there exists an exact implication (Eq. (9), based on an example in [18]) that does not relax. Nevertheless, we show that every EI can be relaxed to an AI plus an error term, which can be made arbitrarily small (at the cost of increasing the factor λ). This result shows that *every* exact implication can be proved from some inequality with an error term. In fact, the proof of the exact implication in Eq. (9), based on an inequality by Matúš [25], is precisely a relaxation plus an arbitrarily small error term; our result shows that every EI can be proven in this style.

Next, we consider two restrictions, which are commonly used in model theory. First, in Sec. 6 we restrict the class of implications to those provable using Shannon's inequalities, i.e. monotonicity and submodularity (reviewed in Sec. 2.2). In general, Shannon's inequalities are sound but incomplete for proving exact and approximate implications that hold for all probability distributions [42, 43], but they are complete for deriving inequalities that hold for all polymatroids [41], and in particular, they are complete for saturated+conditional constraints (as we show in Sec 4), and for measure-based constraints [32]. We prove that every exact implication that holds for all polymatroids relaxes to an approximate implication, and prove an upper bound $\lambda \leq (2^n)!$, and a lower bound $\lambda \geq 3$; the exact bound remains open. Second, in Sec. 7 we restrict the class of models used to check an implication: we only check the implication for uniform probability distributions with 2 tuples (each with probability 1/2); we justify this shortly. We prove that, under this restriction, the implication problem has a 1-relaxation. Restricting the models leads to a complete but unsound method for checking general implication, however this method is sound for saturated+conditional (as we show in Sec 4) and is also sound for checking FIS constraints (as we show in Sec. 7).

Two Consequences While our paper is focused on relaxation, our results have two consequences for the exact implication problem. The first, is a *2-tuple model property*: an exact implication, where the antecedents are saturated+conditional CIs, can be verified on uniform probability distributions with 2 tuples. A similar result is known for MVD+FDs [30]. Geiger and Pearl [13], building on an earlier result by Fagin [11], prove that every set of CIs has an *Armstrong model*: a discrete probability distribution that satisfies only the CIs and their consequences, and no other CI. The Armstrong model is also called a *global witness*, and, in general, can be arbitrarily large. Our result concerns a single witness: for any given set of saturated+conditional antecedents, and any consequent, if the implication holds for all 2-tuple uniform distributions, then it holds in general.

The second consequence concerns the equivalence between the implication problem of saturated+conditional CIs with that of MVD+FDs. It is easy to check that the former implies the latter (Sec. 2). Wong et al. [38] prove the other direction, relying on the sound and complete axiomatization of MVDs [3]. Our 2-tuple model property implies the other direction immediately.

2 Notation and Preliminaries

We denote by $[n] = \{1, 2, \ldots, n\}$. If $\Omega = \{X_1, \ldots, X_n\}$ denotes a set of variables and $U, V \subseteq \Omega$, then we abbreviate the union $U \cup V$ with UV.

2.1 Integrity Constraints and Conditional Independence

A *relation instance* R over signature $\Omega = \{X_1, \ldots, X_n\}$ is a finite set of tuples with attributes Ω. Let $X, Y, Z \subseteq \Omega$. We say that the instance R satisfies the *functional dependency* (FD) $X \to Y$, and write $R \models X \to Y$, if forall $t_1, t_2 \in R$, $t_1[X] = t_2[X]$ implies $t_1[Y] = t_2[Y]$. We say that R satisfies the *embedded multivalued dependency* (EMVD) $X \twoheadrightarrow Y \mid Z$, and write $R \models X \twoheadrightarrow Y \mid Z$, if for all $t_1, t_2 \in R$, $t_1[X] = t_2[X]$ implies $\exists t_3 \in R$ such that $t_1[XY] = t_3[XY]$ and $t_2[XZ] = t_3[XZ]$. One can check that $X \twoheadrightarrow Y \mid Y$ iff $X \to Y$. When $XYZ = \Omega$, then we call $X \twoheadrightarrow Y \mid Z$ a *multivalued dependency*, MVD; notice that X, Y, Z are not necessarily disjoint [3].

A set of constraints Σ *implies* a constraint τ, in notation $\Sigma \Rightarrow \tau$, if for every instance R, if $R \models \Sigma$ then $R \models \tau$. The implication problem has been extensively studied in the literature; Beeri et al. [3] gave a complete axiomatization of FDs and MVDs, while Herrman [16] showed that the implication problem for EMVDs is undecidable.

Recall that two discrete random variables X, Y are called *independent* if $p(X = x, Y = y) = p(X = x) \cdot p(Y = y)$ for all outcomes x, y. Fix $\Omega = \{X_1, \ldots, X_n\}$ a set of n jointly distributed discrete random variables with finite domains $\mathcal{D}_1, \ldots, \mathcal{D}_n$, respectively; let p be the probability mass. For $\alpha \subseteq [n]$, denote by X_α the joint random variable $(X_i : i \in \alpha)$ with domain $\mathcal{D}_\alpha \stackrel{\text{def}}{=} \prod_{i \in \alpha} D_i$. We write $p \models X_\beta \perp X_\gamma | X_\alpha$ when X_β, X_γ are conditionally independent given X_α; in the special case $\beta = \gamma$, then $p \models X_\beta \perp X_\beta | X_\alpha$ iff X_α functionally determines[2] X_β, and we write $p \models X_\alpha \to X_\beta$.

An assertion $Y \perp Z | X$ is called a *Conditional Independence* statement, or a CI; this includes $X \to Y$ as a special case. When $XYZ = \Omega$ we call it *saturated*, and when $Z = \emptyset$ we call it *marginal*. A set of CIs Σ *implies* a CI τ, in notation $\Sigma \Rightarrow \tau$, if every probability distribution that satisfies Σ also satisfies τ. This implication problem has also been extensively studied: Pearl and Paz [27] gave a sound but incomplete set of *graphoid axioms*, Studeny [36] proved that no finite axiomatization exists, while Geiger and Pearl [13] gave a complete axiomatization for saturated, and marginal CIs.

Lee [21] observed the following connection between database constraints and CIs. The *empirical distribution* of a relation R is the uniform distribution over its tuples, in other words, $\forall t \in R$, $p(t) = 1/|R|$. Then:

▶ **Lemma 1.** ([21]) *Forall $X, Y, Z \subset \Omega$ such that $XYZ = \Omega$.*

$$R \models X \to Y \quad \Leftrightarrow \quad p \models X \to Y \qquad \textit{and} \qquad R \models X \twoheadrightarrow Y | Z \quad \Leftrightarrow \quad p \models (Y \perp Z | X) \tag{1}$$

The lemma no longer holds for EMVDs (Appendix A), and for that reason we no longer consider EMVDs in this paper. The lemma immediately implies that if Σ, τ are saturated and/or conditional CIs and the implication $\Sigma \Rightarrow \tau$ holds for all probability distributions, then the corresponding implication holds in databases, where the CIs are interpreted as MVDs or FDs respectively. Wong [38] gave a non-trivial proof for the other direction; we will give a much shorter proof in Corollary 8.

[2] This means: $\forall u \in D_\alpha$, if $p(X_\alpha = u) \neq 0$ then $\exists v \in D_\beta$ s.t. $p(X_\beta = v | X_\alpha = u) = 1$, and v is unique.

2.2 Background on Information Theory

We adopt required notation from the literature on information theory [41, 7]. For $n > 0$, we identify vectors in $\mathbb{R}^{2^n}$ with functions $2^{[n]} \rightarrow \mathbb{R}$.

Polymatroids. A function[3] $h \in \mathbb{R}^{2^n}$ is called a *polymatroid* if $h(\emptyset) = 0$ and satisfies the following inequalities, called *Shannon inequalities*:

1. Monotonicity: $h(A) \leq h(B)$ for $A \subseteq B$
2. Submodularity: $h(A \cup B) + h(A \cap B) \leq h(A) + h(B)$ for all $A, B \subseteq [n]$

The set of polymatroids is denoted $\Gamma_n \subseteq \mathbb{R}^{2^n}$, and forms a polyhedral cone (reviewed in Subsec. 5). For any polymatroid h and subsets $A, B, C \subseteq [n]$, we define[4]

$$h(B|A) \stackrel{\text{def}}{=} h(AB) - h(A) \tag{2}$$

$$I_h(B; C|A) \stackrel{\text{def}}{=} h(AB) + h(AC) - h(ABC) - h(A) \tag{3}$$

Then, $\forall h \in \Gamma_n$, $I_h(B; C|A) \geq 0$ and $h(B|A) \geq 0$. The *chain rule* is the identity:

$$I_h(B; CD|A) = I_h(B; C|A) + I_h(B; D|AC) \tag{4}$$

We call $I_h(B; C|A)$ *saturated* if $ABC = [n]$, and *elemental* if $|B| = |C| = 1$; $h(B|A)$ is a special case of I_h, because $h(B|A) = I_h(B; B|A)$.

Entropic Functions. If X is a random variable with a finite domain $\mathcal{D}$ and probability mass p, then $H(X)$ denotes its entropy

$$H(X) \stackrel{\text{def}}{=} \sum_{x \in \mathcal{D}} p(x) \log \frac{1}{p(x)} \tag{5}$$

For a set of jointly distributed random variables $\Omega = \{X_1, \ldots, X_n\}$ we define the function $h : 2^{[n]} \rightarrow \mathbb{R}$ as $h(\alpha) \stackrel{\text{def}}{=} H(X_\alpha)$; h is called an *entropic function*, or, with some abuse, an *entropy*. The set of entropic functions is denoted Γ_n^*. The quantities $h(B|A)$ and $I_h(B; C|A)$ are called the *conditional entropy* and *conditional mutual information* respectively. The conditional independence $p \models B \perp C \mid A$ holds iff $I_h(B; C|A) = 0$, and similarly $p \models A \rightarrow B$ iff $h(B|A) = 0$, thus, entropy provides us with an alternative characterization of CIs.

2-Tuple Relations and Step functions. 2-tuple relations play a key role for the implication problem of MVDs+FDs: if an implication fails, then there exists a witness consisting of only two tuples [30]. We define a *step function* as the entropy of the empirical distribution of a 2-tuple relation; $R = \{t_1, t_2\}$ and $p(t_1) = p(t_2) = 1/2$. We denote the step function by h_U, where $U \subseteq \Omega$ is the set of attributes where t_1, t_2 agree. One can check:

$$h_U(W) = \begin{cases} 0 & \text{if } W \subseteq U \\ 1 & \text{otherwise} \end{cases} \tag{6}$$

We denote by $\mathcal{S}_n$ the set of step functions; this set is finite and has 2^n elements. We will use the following fact extensively in this paper: $I_{h_U}(Y; Z|X) = 1$ if $X \subseteq U$ and $Y, Z \not\subseteq U$, and $I_{h_U}(Y; Z|X) = 0$ otherwise.

▶ **Example 2.** Consider the relational instance in Fig. 1 (a). It's entropy is the step function $h_{U_1U_2}(W)$, which is 0 for $W \subseteq U_1U_2$ and 1 otherwise. $R \models X_1 \rightarrow X_2$ because

[3] Most authors consider rather the space $\mathbb{R}^{2^n-1}$, by dropping $h(\emptyset)$ because it is always 0.
[4] Recall that AB denotes $A \cup B$.

X_1	X_2	U_1	U_2	Pr
0	0	0	0	1/2
1	1	0	0	1/2

(a)

X	Y	Z	Pr
0	0	0	1/4
0	1	1	1/4
1	0	1	1/4
1	1	0	1/4

(b)

A	B	C	D	Pr
0	0	0	0	$1/2-\varepsilon$
0	1	0	1	$1/2-\varepsilon$
1	0	1	0	ε
1	1	0	0	ε

(c)

Figure 1 Two relations and their empirical distribution (a),(b); a distribution from [18] (c).

$h(X_2|X_1) = h(X_1X_2) - h(X_1) = 1 - 1 = 0$, and $R \not\models U_1 \to X_1$ because $h(X_1|U_1) = h(X_1U_1) - h(U_1) = 1 - 0 \neq 0$.

The relational instance $R = \{(x, y, z) \mid x + y + z \mod 2 = 0\}$ in Fig. 1 (b) is called the *parity function*. It's entropy is $h(X) = h(Y) = h(Z) = 1$, $h(XY) = h(XZ) = h(YZ) = h(XYZ) = 2$. We have that $R \models Y \perp Z$ because $I_h(Y;Z) = h(Y) + h(Z) - h(YZ) = 1 + 1 - 2 = 0$, but $R \not\models Y \perp Z|X$ because $I_h(Y;Z|X) = 1$.

2.3 Discussion

This paper studies exact and approximate implications, expressed as (in)equalities of entropic functions h. For example, the augmentation axiom for MVDs [3] $A \twoheadrightarrow B|CD \Rightarrow AC \twoheadrightarrow B|D$ is expressed as $I_h(B;CD|A) = 0 \Rightarrow I_h(B;D|AC) = 0$, which holds by the chain rule (4). Thus, our golden standard is to prove that (in)equalities hold forall entropic functions, Γ_n^*; for technical reasons we consider it's topological closure, $\mathbf{cl}\left(\Gamma_n^*\right)$, which satsfies the same set of inequalities as Γ_n^*, but not the same class of exact implications[5]. However, characterizing these inequalities is a major open problem in mathematics, which we will not solve in this paper. Therefore, we also consider two restrictions. The first is to restrict the implications to those provable from Shannon inequalities (monotonicity and submodularity); this is a sound but in general incomplete method, and, in fact, every implication derived this way holds not just for $\mathbf{cl}\left(\Gamma_n^*\right)$, but for all polymatroids, Γ_n. The second is to restrict the class of probability distributions to uniform 2-tuple distributions; this leads to a complete but unsound method for checking the implication problem and, in fact, every implication derived this way holds only for the cone closure[6] of the step functions $\mathcal{P}_n \stackrel{\text{def}}{=} \mathbf{conhull}\left(\mathcal{S}_n\right)$. To summarize, this paper discusses three sets of polymatroids: $\mathcal{S}_n \subsetneq \mathbf{cl}\left(\Gamma_n^*\right) \subsetneq \Gamma_n$.

3 Definition of the Relaxation Problem

We now formally define the relaxation problem. We fix a set of variables $\Omega = \{X_1, \ldots, X_n\}$, and consider formulas of the form $\sigma = (Y;Z|X)$, where $X, Y, Z \subseteq \Omega$, which we call a *conditional independence*, CI; when $Y = Z$ then we write it as $X \to Y$ and call it a *conditional*. An *implication* is a formula $\Sigma \Rightarrow \tau$, where Σ is a set of CIs called *antecedents* and τ is a CI called *consequent*. For a CI $\sigma = (B;C|A)$, we define $h(\sigma) \stackrel{\text{def}}{=} I_h(B;C|A)$, for a set of CIs Σ, we define $h(\Sigma) \stackrel{\text{def}}{=} \sum_{\sigma\in\Sigma} h(\sigma)$. Fix a set K s.t. $\mathcal{S}_n \subseteq K \subseteq \Gamma_n$.

▶ **Definition 3.** *The* exact implication *(EI) $\Sigma \Rightarrow \tau$ holds in K, denoted $K \models_{EI} (\Sigma \Rightarrow \tau)$ if, forall $h \in K$, $h(\Sigma) = 0$ implies $h(\tau) = 0$. The* λ-approximate implication *(λ-AI) holds in K,*

[5] See Appendix D and [18]. Our main positive result in Sec. 5 holds only for $\mathbf{cl}\left(\Gamma_n^*\right)$, not for Γ_n^*.
[6] The cone closure of a set $K \subseteq \mathbb{R}^N$ is the set of all vectors of the form $\sum_i c_i x_i$, where $x_i \in K$ and $c_i \geq 0$.

in notation $K \models \lambda \cdot h(\Sigma) \geq h(\tau)$*, if* $\forall h \in K$*,* $\lambda \cdot h(\Sigma) \geq h(\tau)$*. The* approximate implication *holds, in notation* $K \models_{AI} (\Sigma \Rightarrow \tau)$*, if there exist a* $\lambda \geq 0$ *such that the* λ*-AI holds.*

We will sometimes consider an equivalent definition for AI, as $\sum_{\sigma \in \Sigma} \lambda_\sigma h(\sigma) \geq h(\tau)$, where $\lambda_\sigma \geq 0$ are coefficients, one for each $\sigma \in \Sigma$; these two definitions are equivalent, by taking $\lambda = \max_\sigma \lambda_\sigma$. Notice that both EI and AI are preserved under subsets of K in the sense that $K_1 \subseteq K_2$ and $K_2 \models_x (\Sigma \Rightarrow \tau)$ implies $K_1 \models_x (\Sigma \Rightarrow \tau)$, for $x \in \{EI, AI\}$.

AI always implies EI. Indeed, $h(\tau) \leq \lambda \cdot h(\Sigma)$ and $h(\Sigma) = 0$, implies $h(\tau) \leq 0$, which further implies $h(\tau) = 0$, because $h(\tau) \geq 0$ for every CI τ, and every polymatroid h. In this paper we study the reverse.

▶ **Definition 4.** *Let* $\mathcal{I}$ *be a syntactically-defined class of implication statements* $(\Sigma \Rightarrow \tau)$*, and let* $K \subseteq \Gamma_n$*. We say that* $\mathcal{I}$ admits a relaxation *in* K *if, every implication statement* $(\Sigma \Rightarrow \tau)$ *in* $\mathcal{I}$ *that holds exactly, also holds approximately:* $K \models_{EI} \Sigma \Rightarrow \tau$ *implies* $K \models_{AI} \Sigma \Rightarrow \tau$*. We say that* $\mathcal{I}$ *admits a* λ-relaxation *if every EI admits a* λ*-AI.*

▶ **Example 5.** Let $\Sigma = \{(A;B|\emptyset), (A;C|B)\}$ and $\tau = (A;C|\emptyset)$. Since $I_h(A;C|\emptyset) \leq I_h(A;B|\emptyset) + I_h(A;C|B)$ by the chain rule (4), then the exact implication $\Gamma_n \models_{EI} \Sigma \Rightarrow \tau$ admits a 1-AI.

4 Relaxation for FDs and MVDs: Always Possible

In this section we consider the implication problem where the antecedents are either saturated CIs, or conditionals. This is a case of special interest in databases, because the constraints correspond to MVDs, or FDs. Recall that a CI $(B;C|A)$ is *saturated* if $ABC = \Omega$ (i.e., the set of all attributes). Our main result in this section is:

▶ **Theorem 6.** *Assume that each formula in* Σ *is either saturated, or a conditional, and let* τ *be an arbitrary CI. Assume* $\mathcal{S}_n \models_{EI} \Sigma \Rightarrow \tau$*. Then:*

1. $\Gamma_n \models \frac{n^2}{4} h(\Sigma) \geq h(\tau)$*.*
2. *If* τ *is a conditional,* $Z \rightarrow X$*, then* $\Gamma_n \models h(\Sigma) \geq h(\tau)$*.*

Before we prove the theorem, we list two important consequences.

▶ **Corollary 7.** *Let* Σ *consist of saturated CIs and/or conditionals, and let* τ *be any CI. Then* $\mathcal{S}_n \models \Sigma \Rightarrow_{EI} \tau$ *implies* $\Gamma_n \models \Sigma \Rightarrow_{EI} \tau$

Proof. If $\mathcal{S}_n \models \Sigma \Rightarrow_{EI} \tau$ then $\forall h \in \Gamma_n$, $h(\tau) \leq \frac{n^2}{4} h(\Sigma)$, thus $h(\Sigma) = 0$ implies $h(\tau) = 0$. ◀

The corollary has an immediate application to the inference problem in graphical models [13]. There, the problem is to check if every probability distribution that satisfies all CIs in Σ also satisfies the CI τ; we have seen that this is equivalent to $\Gamma_n^* \models_{EI} \Sigma \Rightarrow \tau$. The corollary states that it is enough that this implication holds on all of the uniform 2-tuple distributions, i.e. $\mathcal{S}_n \models \Sigma \Rightarrow_{EI} \tau$, because this implies the (even stronger!) statement $\Gamma_n \models \Sigma \Rightarrow_{EI} \tau$. Decidability was already known: Geiger and Pearl [13] proved that the set of graphoid axioms is sound and complete for the case when both Σ and τ are saturated, while Gyssens at al. [15] improve this by dropping any restrictions on τ.

The second consequence is the following:

▶ **Corollary 8.** *Let* Σ, τ *consist of saturated CIs and/or conditionals. Then the following two statements are equivalent:*

1. *The implication* $\Sigma \Rightarrow \tau$ *holds, where we interpret* Σ, τ *as MVDs and/or FDs.*
2. $\Gamma_n \models_{EI} \Sigma \Rightarrow \tau$*.*

Proof. We have shown right after Lemma 1 that (2) implies (1). For the opposite direction, by Th. 6, we need only check $\mathcal{S}_n \models_{EI} \Sigma \Rightarrow \tau$, which holds because on every uniform probability distribution a saturated CI holds iff the corresponding MVD holds, and similarly for conditionals and FDs. Since the 2-tuple relation satisfies the implication for MVDs+FDs, it also satisfies the implication for CIs, proving the claim. ◀

Wong et al. [38] have proven that the implication for MVDs is equivalent to that of the corresponding saturated CIs (called there BMVD); they did not consider FDs. For the proof in the hard direction, they use the sound and complete axiomatization of MVDs in [3]. In contrast, our proof is independent of any axiomatic system, and is also much shorter. Finally, we notice that the corollary also implies that, in order to check an implication between MVDs and/or FDs, it suffices to check it on all 2-tuple databases: indeed, this is equivalent to checking $\mathcal{S}_n \models_{EI} \Sigma \Rightarrow \tau$, because this implies Item (2), which in turn implies item (1). This rather surprising fact was first proven by [30].

We now turn to the proof of Theorem 6. Before proceeding, we note that we can assume w.l.o.g. that Σ consists only of saturated CIs. Indeed, if Σ contains a non-saturated term, then by assumption it is a conditional, $X \to Y$, and we will replace it with two saturated terms: $(Y;Z|X)$ and $XZ \to Y$, where $Z = \Omega \setminus XY$. Denoting Σ' the new set of formulas, we have $h(\Sigma) = h(\Sigma')$, because $h(Y|X) = I_h(Y;Z|X) + h(Y|XZ)$. Thus, we will assume w.l.o.g. that all formulas in Σ are saturated.

Theorem 6 follows from the next result, which is also of independent interest. We say that a CI $(X;Y|Z)$ is *elemental* if $|X| = |Y| = 1$. We say that σ *covers* τ if all variables in τ are contained in σ; for example $\sigma = (abc;d|e)$ covers $\tau = (cd;be)$. Then:

▶ **Theorem 9.** *Let τ be an elemental CI, and suppose each formula in Σ covers τ. Then $\mathcal{S}_n \models_{EI} (\Sigma \Rightarrow \tau)$ implies $\Gamma_n \models h(\tau) \leq h(\Sigma)$.*

Notice that this result immediately implies Item (1) of Theorem 6, because every $\tau = (Y;Z|X)$ can be written as a sum of $|Y| \cdot |Z| \leq n^2/4$ elemental terms (by the chain rule). In what follows we prove Theorem 9, then use it to prove item (2) of Theorem 6.

Finally, we consider whether (1) of Theorem 6 can be strengthened to a 1-relaxation; we give in Th. 11 below a sufficient condition, whose proof uses the notion of I-measure [41] and is included in Appendix, and leave open the question whether 1-relaxation holds in general for implications where the antecedents are saturated CIs and conditionals.

▶ **Definition 10.** *We say that two CIs $(X;Y|Z)$ and $(A;B|C)$ are* disjoint *if at least one of the following four conditions holds: (1) $X \subseteq C$, (2) $Y \subseteq C$, (3) $A \subseteq Z$, or (4) $B \subseteq Z$.*

If $\tau = (X;Y|Z)$ and $\sigma = (A;B|C)$ are disjoint, then for any step function h_W, it cannot be the case that both $h_W(\tau) \neq 0$ and $h_W(\sigma) \neq 0$. Indeed, if such W exists, then $Z, C \subseteq W$ and, assuming (1) $X \subseteq C$ (the other three cases are similar), we have $ZX \subseteq W$ thus $h_W(\tau) = 0$.

▶ **Theorem 11.** *Let Σ be a set of saturated, pairwise disjoint CI terms (Def. 10), and τ be a saturated mutual information. Then, $\mathcal{S}_n \models_{EI} (\Sigma \Rightarrow \tau)$ implies $\Gamma_n \models h(\tau) \leq h(\Sigma)$.*

4.1 Proof of Theorem 9

The following holds by the chain rule (proof in the appendix), and will be used later on.

▶ **Lemma 12.** *Let $\sigma = (A;B|C)$ and $\tau = (X;Y|Z)$ be CIs such that $X \subseteq A$, $Y \subseteq B$, $C \subseteq Z$ and $Z \subseteq ABC$. Then, $\Gamma_n \models h(\tau) \leq h(\sigma)$.*

We now prove theorem 9. We use lower case for single variables, thus $\tau = (x;y|Z)$ because it is elemental. We may assume w.l.o.g. $x, y \notin Z$ (otherwise $I_h(x;y|Z) = 0$ and the lemma holds trivially). The *deficit* of an elemental CI $\tau = (x;y|Z)$ is the quantity $|\Omega - Z|$. We prove by induction on the deficit of τ that $\mathcal{S}_n \models_{EI} \Sigma \Rightarrow \tau$ implies $\Gamma_n \models h(\tau) \leq h(\Sigma)$.

Assume $\mathcal{S}_n \models_{EI} \Sigma \Rightarrow \tau$, and consider the step function at Z. Since $h_Z(\tau) = 1$, there exists $\sigma \in \Sigma$, $\sigma = (A;B|C)$, such that $h_Z(\sigma) = 1$; this means that $C \subseteq Z$, and $A, B \not\subseteq Z$. In particular $x, y \notin C$, therefore $x, y \in AB$, because σ covers τ. If $x \in A$ and $y \in B$ (or vice versa), then $\Gamma_n \models h(\tau) \leq h(\sigma)$ by Lemma 12, proving the theorem. Therefore we assume w.l.o.g. that $x, y \in A$ and none is in B. Furthermore, since $B \not\subseteq Z$, there exists $u \in B - Z$.

Base case: τ is saturated. Then $u \notin xyZ$, contradicting the assumption that τ is saturated; in other words, in the base case, it is the case that $x \in A$ and $y \in B$.

Step: Let $Z_A = Z \cap A$, and $Z_B = Z \cap B$. Since $C \subseteq Z$, and $\sigma = (A;B|C)$ covers τ, then $Z = Z_A Z_B C$. We also write $A = xyA'Z_A$ (since $x, y \in A$) and $B = uB'Z_B$. So, we have that $\sigma = (A;B|C) = (xyA'Z_A; uB'Z_B|C)$, and we use the chain rule to define σ_1, σ_2:

$$h(\sigma) = I_h(xyA'Z_A; uB'Z_B|C) = I_h(\underbrace{xyA'Z_A; uZ_B|C}_{\stackrel{\text{def}}{=}\sigma_1}) + I_h(\underbrace{xyA'Z_A; B'|uCZ_B}_{\stackrel{\text{def}}{=}\sigma_2})$$

We also partition Σ s.t. $h(\Sigma) = h(\sigma_1) + h(\Sigma_2)$, where $\Sigma_2 \stackrel{\text{def}}{=} (\Sigma \setminus \{\sigma\}) \cup \{\sigma_2\}$.
Next, define $\tau' \stackrel{\text{def}}{=} (x;uy|Z)$ and use the chain rule to define τ_1, τ_2:

$$h(\underbrace{x;y|Z}_{\tau}) \leq I_h(\underbrace{x;uy|Z}_{\tau'}) = I_h(\underbrace{x;u|Z}_{\stackrel{\text{def}}{=}\tau_1}) + I_h(\underbrace{x;y|uZ}_{\stackrel{\text{def}}{=}\tau_2}) \tag{7}$$

By Lemma 12, $\Gamma_n \models h(\sigma_1) \geq h(\tau_1)$. We will prove: $\mathcal{S}_n \models_{EI} \Sigma_2 \Rightarrow \tau_2$. This implies the theorem, because Σ_2 is saturated, and by the induction hypothesis $\Gamma_n \models h(\Sigma_2) \geq h(\tau_2)$ (since the deficit of τ_2 is one less than that of τ), and the theorem follows from $h(\Sigma) = h(\sigma_1) + h(\Sigma_2) \geq h(\tau_1) + h(\tau_2) = h(\tau') \geq h(\tau)$. It remains to prove $\mathcal{S}_n \models_{EI} \Sigma_2 \Rightarrow \tau_2$, and we start with a weaker claim:

▷ Claim 13. $\mathcal{S}_n \models_{EI} \Sigma \Rightarrow \tau_2$.

Proof. By Lemma 12 we have that $h(\sigma) = I_h(xyA'Z_A; uB'Z_B|C) \geq I_h(xy;u|Z) = I_h(y;u|Z) + I_h(x;u|yZ)$. Therefore, $\Sigma \Rightarrow (x;u|yZ)$. Since $\Sigma \Rightarrow (x;y|Z)$, then by the chain rule we have that $\Sigma \Rightarrow (x;uy|Z) = \tau'$, and the claim follows from (7). ◀

Finally, we prove $\mathcal{S}_n \models_{EI} \Sigma_2 \Rightarrow \tau_2$. Assume otherwise, and let h_W be a step function such that $h_W(\tau_2) = I_{h_W}(x;y|uZ) = 1$, and $h_W(\Sigma_2) = 0$. This means that $uZ \subseteq W$. Therefore $uZ_B \subseteq W$, implying $I_{h_W}(xyA'Z_A; uZ_B|C) = h_W(\sigma_1) = 0$. Therefore, $h_W(\Sigma) = h_W(\sigma_1) + h_W(\Sigma_2) = 0$, contradicting the fact that $\mathcal{S}_n \models_{EI} \Sigma \Rightarrow \tau_2$.

4.2 Proof of Theorem 6 Item 2

▶ **Lemma 14.** *Suppose $\mathcal{S}_n \models_{EI} \Sigma \Rightarrow \tau$, where $\tau = (X;Y|Z)$. Let $\sigma \in \Sigma$ such that τ, σ are disjoint (Def. 10). Then: $\mathcal{S}_n \models_{EI} \big(\Sigma \setminus \{\sigma\}\big) \Rightarrow \tau$.*

Proof. Let $\Sigma' \stackrel{\text{def}}{=} \Sigma \setminus \{\sigma\}$. Assume by contradiction that there exists a step function h_W such that $h_W(\Sigma') = 0$ and $h_W(\tau) = 1$. Since σ, τ are disjoint, $h_W(\sigma) = 0$. Then $h_W(\Sigma) = 0$, contradicting the assumption $\mathcal{S}_n \models_{EI} \Sigma \Rightarrow \tau$. ◀

▶ **Lemma 15.** *Let Σ be a set of saturated CIs s.t. $\mathcal{S}_n \models_{EI} \Sigma \Rightarrow \tau$. Suppose $\tau = (Z \to uX)$ (which, recall, is a shorthand for $(uX; uX|Z)$), and define $\tau_1 = (Z \to u)$, $\tau_2 = (uZ \to X)$; thus, $h(\tau) = h(\tau_1) + h(\tau_2)$. Then there exists Σ_1 and Σ_2 such that: (1) $h(\Sigma) = h(\Sigma_1) + h(\Sigma_2)$; we say that Σ_1, Σ_2 form a parition of Σ. (2) Σ_1 covers τ_1 and $\mathcal{S}_n \models_{EI} \Sigma_1 \Rightarrow \tau_1$. (3) Σ_2 is saturated and $\mathcal{S}_n \models \Sigma_2 \Rightarrow \tau_2$.*

Proof. We partition Σ into Σ_1 and Σ_2 as follows. For every $\sigma = (A; B|C) \in \Sigma$, if $u \in C$ then we place σ in Σ_2. Otherwise, assume w.l.o.g that $u \in A$, and we write $A = uA_ZA_XA'$ where $A_Z = A \cap Z$, $A_X = A \cap X$, and $A' = A \backslash \{uA_ZA_X\}$. We use the chain rule to define σ_1, σ_2:

$$I_h(A; B|C) = I_h(uA_ZA_XA'; B|C) = I_h(\underbrace{uA_Z; B|C}_{\stackrel{\text{def}}{=}\sigma_1}) + I(\underbrace{A_XA'; B|uA_ZC}_{\stackrel{\text{def}}{=}\sigma_2}) \tag{8}$$

We place σ_1 in Σ_1, and σ_2 in Σ_2. We observe that σ_1 covers τ_1 (because $Z = A_ZB_ZC_Z \subseteq A_ZBC$) and σ_2 is saturated. Furthermore, $h(\Sigma_1) + h(\Sigma_2) = h(\Sigma)$. We prove $\Sigma_1 \models_{EI} \tau_1$. By assumption, $\Sigma \models_{EI} \tau_1 = (Z \to u)$. Let any $\sigma_2 = (A; B|C) \in \Sigma_2$; since $u \in C$, by Lemma 14 we can remove it, obtaining $\Sigma \setminus \{\sigma_2\} \models_{EI} \tau_1$; repeating this process proves $\Sigma_1 \models_{EI} \tau_1$. Finally, we prove $\Sigma_2 \models_{EI} \tau_2$. By assumption, $\Sigma \models_{EI} \tau_2 = (uZ \to X)$. Let any $\sigma_1 = (uA_Z; B|C) \in \Sigma_1$; since $uA_Z \subseteq uZ$, by Lemma 14 we can remove it, obtaining $\Sigma \setminus \{\sigma_1\} \models_{EI} \tau_2$; repeating this process proves $\Sigma_2 \models_{EI} \tau_2$. ◀

We now complete the proof of Theorem 6 item 2. Let $\tau = (Z \to X)$, and Σ be saturated. We show, by induction on $|X|$, that if $\mathcal{S}_n \models_{EI} \Sigma \Rightarrow \tau$ then $\Gamma_n \models h(\tau) \leq h(\Sigma)$. If $|X| = 1$, then $X = \{x\}$, $h(x|Z) = I(x; x|Z)$ is elemental, and the claim follows from Th. 9. Otherwise, let u be any variable in X, write $\tau = (Z \to uX')$, and apply Lemma 15 to $\tau_1 = (Z \to u)$, $\tau_2 = (Zu \to X')$, which gives us a partition of Σ into Σ_1, Σ_2. On one hand, $\mathcal{S}_n \models_{EI} \Sigma_1 \Rightarrow \tau_1$, and from Th. 9 we derive $h(\tau_1) \leq h(\Sigma_1)$ (because τ_1 is elemental, and covered by Σ_1); on the other hand $\mathcal{S}_n \models_{EI} \Sigma_2 \Rightarrow \tau_2$ where Σ_2 is saturated, which implies, by induction, $h(\tau_2) \leq h(\Sigma_2)$. The result follows from $h(\tau) = h(\tau_1) + h(\tau_2) \leq h(\Sigma_1) + h(\Sigma_2) = h(\Sigma)$, completing the proof.

5 Relaxation for General CIs: Sometimes Impossible

We consider the relaxation problem for arbitrary Conditional Independence statements. Recall that our golden standard is to check (in)equalities forall entropic functions, $h \in \Gamma_n^*$. As we saw, for MVD+FDs, these (in)equalities coincide with those satisfied by $\mathcal{S}_n$, and with those satisfied by Γ_n. In general, however, they differ. We start with an impossibility result, then prove that relaxation with an arbitrarily small error term always exists. Both results are for the topological closure, $\mathbf{cl}(\Gamma_n^*)$. This makes the negative result stronger, but the positive result weaker; it is unlikely for the positive result to hold for Γ_n^*, see [18, Sec.V.(A)] and Appendix D.

▶ **Theorem 16.** *There exists Σ, τ with four variables, such that $\mathbf{cl}(\Gamma_4^*) \models_{EI} (\Sigma \Rightarrow \tau)$ and $\mathbf{cl}(\Gamma_4^*) \not\models_{AI} (\Sigma \Rightarrow \tau)$.*

For the proof, we adapt an example by Kaced and Romashchenko [18, Inequality $(\mathcal{I}5')$ and Claim 5], built upon an earlier example by Matúš [25]. Let Σ and τ be the following:

$$\Sigma = \{(C; D|A), (C; D|B), (A; B), (B; C|D)\} \qquad \tau = (C; D) \tag{9}$$

We first prove that, for any $\lambda \geq 0$, there exists an entropic function h such that:

$$I_h(C;D) >\lambda \cdot (I_h(C;D|A) + I_h(C;D|B) + I_h(A;B) + I_h(B;C|D)) \tag{10}$$

Indeed, consider the distribution shown in Fig. 1 (c) (from [18]). By direct calculation, $I_h(C;D) = \varepsilon + O(\varepsilon^2) = \Omega(\varepsilon)$, while $I_h(C;D|A) = I_h(C;D|B) = I_h(A;B) = 0$ and $I_h(B;C|D) = O(\varepsilon^2)$ and we obtain Eq.(10) by choosing ε small enough. Next, we prove $\mathbf{cl}(\Gamma_n^*) \models_{EI} (\Sigma \Rightarrow \tau)$. Matúš [25] proved the following[7] $\forall h \in \Gamma_n^*$ and $\forall k \in \mathbb{N}$:

$$I_h(C;D) \leq I_h(C;D|A) + \frac{k+3}{2} I_h(C;D|B) + I_h(A;B) + \frac{k-1}{2} I_h(B;C|D) + \frac{1}{k} I_h(B;D|C) \tag{11}$$

The inequality obviously holds for $\mathbf{cl}(\Gamma_n^*)$ too. The EI follows by taking $k \to \infty$. Inequality (11) is almost a relaxation of the implication (9): the only extra term is the last term, which can be made arbitrarily small by increasing k. Our second result generalizes this:

▶ **Theorem 17.** *Let Σ, τ be arbitrary CIs, and suppose $\mathbf{cl}(\Gamma_n^*) \models \Sigma \Rightarrow \tau$. Then, for every $\varepsilon > 0$ there exists $\lambda > 0$ such that, forall $h \in \mathbf{cl}(\Gamma_n^*)$:*

$$h(\tau) \leq \lambda \cdot h(\Sigma) + \varepsilon \cdot h(\Omega) \tag{12}$$

Intuitively, the theorem shows that every EI can be relaxed in $\mathbf{cl}(\Gamma_n^*)$, if one allows for an error term, which can be made arbitrarily small. We notice that the converse of the theorem always holds: if $h(\Sigma) = 0$, then (12) implies $h(\tau) \leq \varepsilon \cdot h(\Omega)$, $\forall \varepsilon > 0$, which implies $h(\tau) = 0$.

Proof of Theorem 17. For the proof we need a brief review of cones [37, 5]. A set $C \subseteq \mathbb{R}^N$ is *convex* if, for any two points $x_1, x_2 \in C$ and any $\theta \in [0,1]$, $\theta x_1 + (1-\theta)x_2 \in C$; and it is called a *cone*, if for every $x \in C$ and $\theta \geq 0$ we have that $\theta x \in C$. The *conic hull* of C, $\mathbf{conhull}(C)$, is the set of vectors of the form $\theta_1 x_1 + \cdots + \theta_k x_k$, where $x_1, \ldots, x_k \in C$ and $\theta_i \geq 0, \forall i \in [k]$. A cone K is *finitely generated* if $K = \mathbf{conhull}(L)$ for some finite set $L \subset \mathbb{R}^N$, and is *polyhedral* if there exists $u_1, \ldots, u_r \in \mathbb{R}^N$ s.t. $K = \{x \mid u_i \cdot x \geq 0, i \in [r]\}$; a cone is finitely generated iff it is polyhedral. For any $K \subseteq \mathbb{R}^N$, the *dual* is the set $K^* \subseteq \mathbb{R}^N$ defined as:

$$K^* \stackrel{\text{def}}{=} \{y \mid \forall x \in K, x \cdot y \geq 0\} \tag{13}$$

K^* represents the linear inequalities that hold for all $x \in K$, and is always a closed, convex cone (it is the intersection of closed half-spaces). We warn that the $*$ in Γ_n^* does *not* represent the dual; the notation Γ_n^* for entropic functions is by now well established, and we adopt it here too, despite it's clash with the standard notation for the dual cone. The following are known properties of cones (reviewed and proved in the Appendix):

(A) For any set K, $\mathbf{cl}(\mathbf{conhull}(K)) = K^{**}$.
(B) If L is a finite set, then $\mathbf{conhull}(L)$ is closed.
(C) If K_1 and K_2 are closed, convex cones then: $(K_1 \cap K_2)^* = \Big(\mathbf{cl}\left(\mathbf{conhull}(K_1^* \cup K_2^*)\right)\Big)$.

Theorem 17 follows from a more general statement about cones:

▶ **Theorem 18.** *Let $K \subseteq \mathbb{R}^N$ be a closed, convex cone, and let $y_1, \ldots, y_m, y$ be $m+1$ vectors in $\mathbb{R}^N$. The following are equivalent:*
(a) *For every $x \in K$, if $x \cdot y_1 \leq 0, \ldots, x \cdot y_m \leq 0$ then $x \cdot y \leq 0$.*

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[7] Matus [25] proved $I(C;D) \leq I(C;D|A) + I(C;D|B) + I(A;B) + I(C;E|B) + \frac{1}{k} I(B;E|C) + \frac{k-1}{2}(I(B;C|D) + I(C;D|B))$. Inequality (11) follows by setting $E = D$.

(b) *For every $\varepsilon > 0$ there exists $\theta_1, \ldots, \theta_m \geq 0$ and an error vector $e \in \mathbb{R}^N$ such that $||e||_\infty < \varepsilon$ and, for every $x \in K$, $x \cdot y \leq \theta_1 x \cdot y_1 + \cdots + \theta_m x \cdot y_m + x \cdot e$.*

Proof. Let $L \stackrel{\text{def}}{=} \{-y_1, -y_2, \ldots, -y_m\}$. Statement (a) is equivalent to $-y \in (K \cap L^*)^*$; Statement (b) is equivalent[8] to $-y \in \mathbf{cl}\left(\mathbf{conhull}\,(K^* \cup L)\right)$. We prove their equivalence:

$$\begin{aligned}
(K \cap L^*)^* =& \mathbf{cl}\left(\mathbf{conhull}\,(K^* \cup L^{**})\right) && \text{Item (C)}\\
=& \mathbf{cl}\left(\mathbf{conhull}\left(K^* \cup \mathbf{cl}\left(\mathbf{conhull}\,(L)\right)\right)\right) && \text{Item (A)}\\
=& \mathbf{cl}\left(\mathbf{conhull}\left(K^* \cup \mathbf{conhull}\,(L)\right)\right) && \text{Item (B)}\\
=& \mathbf{cl}\left(\mathbf{conhull}\,(K^* \cup L)\right) && \text{Def. of } \mathbf{conhull}\,(-)
\end{aligned}$$

◀

We now prove Theorem 17, using the fact that $K \stackrel{\text{def}}{=} \mathbf{cl}\,(\Gamma_n^*)$ is a closed cone [41]. Let $\Sigma = \{\sigma_1, \ldots, \sigma_m\}$. Associate to each term $\sigma_i = (B_i; C_i | A_i)$ the vector $y_i \in \mathbb{R}^{2^n}$ such that, forall $h \in \mathbb{R}^{2^n}$, $h \cdot y_i = I_h(B_i; C_i | A_i) = h(A_i B_i) + h(A_i C_i) - h(A_i B_i C_i) - h(X_i)$ (i.e. y_i has two dimensions equal to $+1$, and two equal to -1), for $i = 1, m$. Denote by y the similar vector associated to τ. Then, $\mathbf{cl}\,(\Gamma_n^*) \models \Sigma \Rightarrow \tau$ becomes condition (a) of Th. 18, and it implies condition (b). Define $\lambda = \max_i \theta_i$, and $\varepsilon \stackrel{\text{def}}{=} 2^n \cdot ||e||_\infty$. Then the error term in (b) is:

$$x \cdot e = \sum_{W \subseteq [n]} e_W h(W) \leq \sum_{W \subseteq [n]} |e_W| h(W) \leq 2^n \cdot ||e||_\infty \cdot h(\Omega)$$

6 Restricted Axioms

The characterization of the entropic cone $\mathbf{cl}\,(\Gamma_n^*)$ is currently an open problem [41]. In other words, there is no known decision procedure capable of deciding whether an exact or approximate implication holds for all entropic functions. In this section, we consider implications that can be inferred using only the Shannon inequalities (e.g., (2), and (3)), and thus hold for all polymatroids $h \in \Gamma_n$. Several tools exists (e.g. ITIP or XITIP [40]) for checking such inequalities.

This study is important for several reasons. First, by restricting to Shannon inequalities we obtain a sound, but in general incomplete method for deciding implications. All axioms for reasoning about MVD, FD, or semi-graphoid axioms[9] [3, 27, 13] are, in fact, based on Shannon inequalities. Second, under some syntactic restrictions, they are also complete; as we saw, they are complete for MVD and/or FDs, for saturated constraints and/or conditionals, and also for marginal constraints [13]. Third, Shannon inequalities are complete for reasoning for a different class of constraints, called *measure-based constraints*, which were introduced by Sayrafi et al. [32] (where Γ_n is denoted by $\mathcal{M}_{\mathtt{SI}}$) and shown to have a variety of applications.

We start by showing that every exact implication of CIs can be relaxed over Γ_n. This result was known, e.g. [18]; we re-state and prove it here for completeness.

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[8] To see this, notice that $\forall x \in K, x \cdot y \leq x \cdot (\sum \theta_i y_i + e)$ iff $-y + \sum \theta_i y_i + e \in K^*$; the latter holds for some $\theta_1, \ldots, \theta_m \geq 0$ iff $-y + e \in \mathbf{conhull}\left(K^* \cup L\right)$; and finally the latter holds for arbitrarily small e iff $-y \in \mathbf{cl}\left(\mathbf{conhull}\left(K^* \cup L\right)\right)$.

[9] Semi-graphoid axioms restricted to "strictly positive" distributions, which fail Γ_n^*.

▶ **Theorem 19.** *Let Σ, τ be arbitrary CIs. If $\Gamma_n \models_{EI} \Sigma \Rightarrow \tau$, then there exist $\lambda \geq 0$, s.t. $\Gamma_n \models h(\tau) \leq \lambda \cdot h(\Sigma)$. In other words, CIs admit relaxation over Γ_n.*

Proof. (Sketch) We set $K = \Gamma_n$ in Th. 18. Then K is polyhedral, hence K^* is finitely generated. Therefore, in the proof of Th. 18, the set $K^* \cup L$ is finitely generated, hence $\mathbf{conhull}\,(K^* \cup L)$ is closed, therefore there is no need for an error vector e in Statement (b) of Th. 18, and, hence, no need for ε in AI (12) ◀

It follows that Shannon inequalities are incomplete for proving the implication $\Sigma \Rightarrow \tau$, where Σ, τ are given by Eq. (9). This is a "non-Shannon" exact implication, i.e. it holds only in $\mathbf{cl}\,(\Gamma_n^*)$, but fails in Γ_n, otherwise it would admit a relaxation. The explanation is that Matus' inequality (11) is a non-Shannon inequality. (The first example of a non-Shannon inequality is due to Yeung and Zhang [43].) Next, we turn our attention to the size of the factor λ. We prove a lower bound of 3:

▶ **Theorem 20** ([10]). *The following inequality holds for all polymatroids $h \in \Gamma_n$:*

$$h(Z) \leq I_h(A;B|C) + I_h(A;B|D) + I_h(C;D|E) + I_h(A;E) + 3h(Z|A) + 2h(Z|B) \tag{14}$$

but the inequality fails if any of the coefficients $3, 2$ are replaced by smaller values. In particular, denoting τ, Σ the terms on the two sides of Eq.(26), the exact implication $\Gamma_n \models_{EI} \Sigma \Rightarrow \tau$ holds, and does not have a 1-relaxation.

We have checked the two claims in the theorem using the ITIP[10] tool. For the positive result, we also provide direct (manual) proof in the Appendix. Since some EIs relax only with $\lambda \geq 3$, the next question is, how large does λ need to be? We give here an upper bound:

▶ **Theorem 21.** *If $\Gamma_n \models \Sigma \Rightarrow \tau$ then $\Gamma_n \models \tau \leq (2^n)! \cdot h(\Sigma)$. In other words, every implication of CIs admits a $(2^n)!$-relaxation over Γ_n.*

7 Restricted Models

In this section we restrict ourselves to models of uniform 2-tuple distributions, which are equivalent to the step functions $\mathcal{S}_n$. We prove that, under this restriction, all exact implications admit a 1-relaxation and, in fact, this result holds on the conic closure, $\mathcal{P}_n = \mathbf{conhull}\,(\mathcal{S}_n)$. This study also has two motivations. First, it leads to a complete, but unsound procedure for implication; in other words, it can be used to disprove implications. A simple example where it is unsound is the inequality $I_h(X;Y|Z) \leq I_h(X;Y)$, which holds for every step function, but fails for the "parity function" in Fig. 1 (b). Second, this restriction leads to a sound and complete procedure for checking *differential constraints* in market basket analysis [33]. These are more general than the CIs we discussed so far, yet we prove that they, too, admit a 1-relaxation in $\mathcal{P}_n$. Thus, our relaxation result has immediate application to market basket constraints.

Consider a set of items $\Omega = \{X_1, \ldots, X_n\}$, and a set of baskets $\mathcal{B} = \{b_1, \ldots, b_N\}$ where every basket is a subset $b_i \subseteq \Omega$. The *support function* $f : 2^\Omega \to \mathbb{N}$ assigns to every subset $W \subseteq \mathcal{B}$ the number of baskets in $\mathcal{B}$ that contain all items in W: $f(W) = |\{b \mid W \subseteq b \in \mathcal{B}\}|$. A constraint $f(W) = f(WX)$ asserts that every basket that contains W also contains X. Sayrafi and Van Gucht [33] define the *density* as $d_f(W) = \sum_{Z:W\subseteq Z}(-1)^{|Z-W|}f(Z)$ (which we show

[10] http://user-www.ie.cuhk.edu.hk/ ITIP/

below equals the number of baskets $b \in \mathcal{B}$ s.t. $W = b$), then study the implication problem of *differential constraints*, which are certain sums of densities. For example, $f(W) = f(WX)$ is a differential constraint, because $f(W) - f(WX) = \sum_{Z:W\subseteq Z, X\not\subseteq Z} d_f(Z)$.

We now explain the connection to step functions $\mathcal{S}_n$. Fix a single basket $b \in \mathcal{B}$ and define f_b to be the support function for the singleton set $\{b\}$, that is $f_b(W) = 1$ if $W \subseteq b$ and 0 otherwise. It follows that $h_b(W) \stackrel{\text{def}}{=} 1 - f_b(W)$ is precisely the step function at b. Then, we can write the support function as $f = \sum_{b\in\mathcal{B}} f_b = N - h$, where $h = \sum_{b\in\mathcal{B}} h_b \in \mathcal{P}_n$, and $N = |\mathcal{B}|$. Note that the densities are also related, by[11] $d_f(W) = -d_h(W)$. Conversely, any positive combination of step functions $h = \sum_{U\subseteq\Omega} c_U h_U \in \mathcal{P}_n$ with integer coefficients c_U is the negation of the support function for the set $\mathcal{B}$ that contains exactly c_U copies of U, forall $U \subseteq \Omega$. It follows that an implications of differential constraints (i.e. sum of densities) holds for all $h \in \mathcal{P}_n$ iff it holds for all support functions f. We now formalize.

▶ **Lemma 22.** *Any function $h : 2^\Omega \to \mathbb{R}$ s.t. $h(\emptyset) = 0$ can be uniquely written as a linear combination of step functions $h = \sum_{Z\subseteq\Omega} \delta_h(Z) \cdot h_Z$, where $\delta_h(W) \stackrel{def}{=} -\sum_{Z:W\subseteq Z}(-1)^{|Z-W|}h(Z)$ for $W \neq \Omega$ and*[12] *$\delta_h(\Omega) = 0$. Notice that δ_h is equals the density of the associated support function, $\delta_h = d_f$.*

Proof. The following two identities are equivalent, representing Möbius' inversion formula:

$$\forall W : h(\Omega|W) = \sum_{Z:W\subseteq Z} \delta_h(Z) \quad \iff \quad \forall W : \delta_h(W) = \sum_{Z:W\subseteq Z} (-1)^{|Z-W|} h(\Omega|Z) \tag{15}$$

We first derive an expression for $h(W)$ from the left part of Eq.(15):

$$h(W) = h(\Omega|\emptyset) - h(\Omega|W) = \sum_{Z} \delta_h(Z) - \sum_{Z:W\subseteq Z} \delta_h(Z) = \sum_{Z:W\not\subseteq Z} \delta_h(W) = \sum_{Z} \delta_h(Z) \cdot h_Z(W)$$

Second, we derive an expression for δ_h from the right part of Eq.(15):

$$\delta_h(W) = h(\Omega)(\sum_{Z:W\subseteq Z} (-1)^{|Z-W|}) - \sum_{Z:W\subseteq Z} (-1)^{|Z-W|} h(Z)$$

and the claim follows from $\sum_{Z:W\subseteq Z}(-1)^{|Z-W|} = 0$ whenever $W \neq \Omega$. ◀

The lemma says that the step functions $(h_W)_{W\subset\Omega}$ form a basis for the vector space $\mathbb{R}^{2^n}$ (where $|\Omega| = n$), and the coordinates of h are differentials of the support function, $\delta_h(W) = d_f(W)$. If $h = h_b$ (the step function at b), then it belongs to the basis, hence $\delta_h(W) = 1$ iff $W = b$ otherwise it is 0; this explains why $d_f(W)$ is the number of baskets b s.t. $b = W$. In information theory the quantity $I_h(y_1; y_2; \cdots ; y_m|W) \stackrel{\text{def}}{=} -\sum_{Z:W\subseteq Z\subseteq\{y_1,\ldots,y_m\}}(-1)^{|Z-W|}h(Z)$ is called the *conditional multivariate mutual information*, thus, $\delta_h(W)$ is a saturated conditional multivariate mutual information. We also show in the Appendix that $\delta_h(W)$ is precisely the I-measure of an atom in I-measure theory [41].

Once we have motivated the critical role of the negated differentials $\delta_h(W)$, we define an *I-measure constraint* to be an arbitrary sum $\sigma = \sum_i \delta_h(W_i)$; the exact constraint is the assertion $\sigma = 0$, while an approximate constraint asserts some bound, $\sigma \leq c$. The differential constraints [33] are special cases of I-measure constraints. Any CI constraint is also a special case of an I-measure, for example $h(Y|X) = \sum_{W:X\subseteq W, Y\not\subseteq W} \delta_h(W)$, and

[11] This holds forall $W \neq \Omega$. For $W = \Omega$, $d_h(\Omega) = 0$, while $d_f(\Omega) =$ number of baskets equal to Ω.
[12] Recall that the step function h_Ω is identically 0; hence it suffices to define $\delta_h(\Omega) = 0$.

$I_h(Y;Z|X) = \sum_{W:X\subseteq W, X\not\supseteq W, Y\not\supseteq W} \delta_h(W)$. If $h \in \mathcal{P}_n$ then all coordinates are positive, $\delta_h(W) \geq 0$ (this is precisely the definition of $\mathcal{P}_n$), and this implies that all I-measure constraints are ≥ 0. We prove:

▶ **Theorem 23.** *Exact implications of I-measure constraints admit a 1-relaxation in $\mathcal{P}_n$.*

Proof. Consider an implication $\Sigma \Rightarrow \tau$ where all constraints in Σ, τ are I-measure constraints. Let $\tau = \sum_i \delta_h(W_i)$. Then, for every i, there exists some constraint $\sigma = \sum_j \delta_h(W_j) \in \Sigma$ such that $W_i = W_j$ for some j, proving the theorem. If not, then for the step function $h \stackrel{\text{def}}{=} h_{W_i}$ we have $h(\sigma) = 0$ forall $\sigma \in \Sigma$, yet $h(\tau) = 1$, contradicting the assumption $P_n \models \Sigma \Rightarrow \sigma$. ◀

▶ **Example 24.** Consider Example 4.3 in [33]: $d_1 = f(A) + f(ABCD) - f(ABC) - f(ACD)$, $d_2 = f(C) - f(CD)$, and $d = f(AB) - f(ABD)$. Sayrafi and Van Gucht prove $d_1 = d_2 = 0$ implies $d = 0$ for all support functions f. The quantity d_1 represents the number of baskets that contain A, but do not contain BC nor CD, while d_2 is the number of baskets that contain C but not D. Our theorem converts the exact implication into an inequality as follows. Denote by $\sigma_1 \stackrel{\text{def}}{=} I_h(BC;CD|A), \sigma_2 \stackrel{\text{def}}{=} h(D|C), \tau \stackrel{\text{def}}{=} h(D|AB)$, $P_n \models (\sigma_1 = \sigma_2 = 0 \Rightarrow \tau = 0)$ relaxes to $P_n \models \sigma_1 + \sigma_2 \geq \tau$, which translates into $d_1 + d_2 \leq d$ forall support functions f.

8 Discussion and Future Work

Number of Repairs A natural way to measure the degree of a constraint in a relation instance R is by the number of repairs needed to enforce the constraint on R. In the case of a key constraint, $X \to Y$, where $XY = \Omega$, our information-theoretic measure is naturally related to the number of repairs, as follows. If $h(Y|X) = c$, where h is the entropy of the empirical distribution on R, then one can check $|R|/|\Pi_X(R)| \leq 2^c$. Thus, the number of repairs $|R| - |\Pi_X(R)|$ is at most $(2^c - 1)|\Pi_X(R)|$. We leave for future work an exploration of the connections between number of repairs and information theoretic measures.

Small Model Property. We have proven in Sec. 4 that several classes of implications (including saturated CIs, FDs, and MVDs) have a "small model" property: if the implication holds for all uniform, 2-tuple distributions, then it holds in general. In other words, it suffices to check the implication on the step functions $\mathcal{S}_n$. One question is whether this small model property continues to hold for other tractable classes of implications in the literature. For example, Geiger and Pearl [13] give an axiomatization (and, hence, a decision procedure) for *marginal* CIs. However, marginal CIs do not have the same small model property. Indeed, the implication $(X \perp Y)\&(X \perp Z) \Rightarrow (X \perp YZ)$ holds for all uniform 2-tuple distributions (because $I_h(X;YZ) \leq I_h(X;Y) + I_h(X;Z)$ holds for all step functions), however it fails for the "parity distribution" in Fig.1(b). We leave for future work an investigation of the small model property for other classes of constraints.

Proof Techniques. Since we had to integrate concepts from both database theory and information theory, we had to make a choice of which proof techniques to favor. In particular, $\mathcal{P}_n$, the cone closure of the step functions, is better known in information theory as the *set of entropic functions with a non-negative I-measure*. After trying both alternatives, we have chosen to favor the step functions in most of the proofs, because of their connection to 2-tuple relations. We explain in the Appendix the connection to the I-measure, and include the proof of Th. 11, which is easier to express in that language.

Bounds on the factor λ. In the early stages of this work we conjectured that all CIs in Γ_n admit 1-relaxation, until we discovered the counterexample in Th. 20, where $\lambda = 3$. On the other hand, the only general upper bound is $(2^n)!$. None of them is likely to be tight. We leave for future work the task of finding tighter bounds for λ.

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APPENDIX

A EMVDs and CIs

Equation (1) holds only for MVDs and not for EMVDs, as illustrated in Table 2. To the best of our knowledge, EMVD's have not been characterized using information theory; we do not discuss them further in the paper.

X_1	X_2	X_3
a	c	e
b	c	e
a	d	e
b	d	e
b	d	f

Table 2 The relation $R[X_1, X_2, X_3]$ satisfies the EMVD $\emptyset \twoheadrightarrow X_1|X_2$, yet for the empirical distribution, $I_h(X_1; X_2) \neq 0$ because X_1, X_2 are dependent: $p(X_1 = a) = 2/5 \neq p(X_1 = a|X_2 = c) = 1/2$.

B The I-measure

The I-measure [39, 41] is a theory which establishes a one-to-one correspondence between Shannon's information measures and set theory. We use the I-measure in order to prove Theorems 11, and 23. In Section H we characterize $\mathcal{P}_n$, the conic hull of step functions, using this notion.

Let $h \in \Gamma_n$ denote a polymatroid defined over the variable set $\{X_1, \dots, X_n\}$. Every variable X_i is associated with a set $\mathrm{m}(X_i)$, and it's complement $\mathrm{m}^c(X_i)$. The universal set is $\Lambda \stackrel{\text{def}}{=} \bigcup_{i=1}^{n} \mathrm{m}(X_i)$, and we consider only atoms in which at least one set appear in positive form (i.e., the atom $\bigcap_{i=1}^{n} \mathrm{m}^c(X_i) \stackrel{\text{def}}{=} \emptyset$ is defined to be empty). Let $\mathcal{I} \subseteq [n]$. We denote by $X_{\mathcal{I}} \stackrel{\text{def}}{=} \{X_j \mid j \in \mathcal{I}\}$, and $\mathrm{m}(X_{\mathcal{I}}) \stackrel{\text{def}}{=} \bigcup_{i \in \mathcal{I}} \mathrm{m}(X_i)$.

▶ **Definition 25.** *The field $\mathcal{F}_n$ generated by sets $\mathrm{m}(X_1), \dots, \mathrm{m}(X_n)$ is the collection of sets which can be obtained by any sequence of usual set operations (union, intersection, complement, and difference) on $\mathrm{m}(X_1), \dots, \mathrm{m}(X_n)$.*

The *atoms* of $\mathcal{F}_n$ are sets of the form $\bigcap_{i=1}^{n} Y_i$, where Y_i is either $\mathrm{m}(X_i)$ or $\mathrm{m}^c(X_i)$. We denote by $\mathcal{A}$ the atoms of $\mathcal{F}_n$. There are $2^n - 1$ non-empty atoms and 2^{2^n-1} sets in $\mathcal{F}_n$ expressed as the union of its atoms. A function $\mu : \mathcal{F}_n \to \mathbb{R}$ is *set additive* if for every pair of disjoint sets A and B it holds that $\mu(A \cup B) = \mu(A) + \mu(B)$. A real function μ defined on $\mathcal{F}_n$ is called a *signed measure* if it is set additive, and $\mu(\emptyset) = 0$.

The *I*-measure μ^* on $\mathcal{F}_n$ is defined by $\mu^*(m(X_{\mathcal{I}})) = h(X_{\mathcal{I}})$ for all nonempty subsets $\mathcal{I} \subseteq \{1, \dots, n\}$. Table 3 summarizes the extension of this definition to the rest of the Shannon measures. Theorem 26 [39, 41] establishes the one-to-one correspondence between Shannon's information measures and μ^*.

▶ **Theorem 26.** ([39, 41]) *μ^* is the unique signed measure on $\mathcal{F}_n$ which is consistent with all Shannon's information measures (i.e., entropies, conditional entropies, and mutual information).*

Information Measures	μ^*
$h(X)$	$\mu^*(\mathrm{m}(X))$
$h(XY)$	$\mu^*\left(\mathrm{m}(X) \cup \mathrm{m}(Y)\right)$
$h(X\|Y)$	$\mu^*\left(\mathrm{m}(X) \cap \mathrm{m}^c(Y)\right)$
$I_h(X;Y)$	$\mu^*\left(\mathrm{m}(X) \cap \mathrm{m}(Y)\right)$
$I_h(X;Y\|Z)$	$\mu^*\left(\mathrm{m}(X) \cap \mathrm{m}(Y) \cap \mathrm{m}^c(Z)\right)$

Table 3 Information measures and associated I-measure

In particular, μ^* can be negative. If $\mu^*(a) \geq 0$ for all atoms $a \in \mathcal{A}$ then it is called a *positive measure*. A polymatroid is said to be positive if its I-measure is positive, and $\mathcal{P}_n$ is the cone of positive polymatroids. Theorem 27, that will be used later on, states that any i-measure assigning a non-negative value to its atoms is a polymatroid.

▶ **Theorem 27.** ([41]) *If there is no constraint on $X_1, \ldots, X_n$, then μ^* can take any set of nonnegative values on the nonempty atoms of $\mathcal{F}_n$.*

Let $\sigma = I(X;Y|Z)$. We denote by $\mathrm{m}(\sigma) = \mathrm{m}(X) \cap \mathrm{m}(Y) \cap \mathrm{m}^c(Z)$ the set associated with σ (see also Table 3). For a set of mutual information and entropy terms Σ, we let:

$$\mathrm{m}(\Sigma) \stackrel{\text{def}}{=} \bigcup_{\sigma \in \Sigma} \mathrm{m}(\sigma).$$

Theorem 28, that will be used later on, shows that a necessary condition for the implication $\Gamma_n \models_{EI} \Sigma \Rightarrow \tau$ is that $\mathrm{m}(\tau) \subseteq \mathrm{m}(\Sigma)$.

▶ **Theorem 28.** *Let Σ denote a set of mutual information terms. If $\Gamma_n \models_{EI} \Sigma \Rightarrow \tau$ then $\mathrm{m}(\tau) \subseteq \mathrm{m}(\Sigma)$.*

Proof. Assume, by contradiction, that $\mathrm{m}(\tau) \not\subseteq \mathrm{m}(\Sigma)$, and let $b \in \mathrm{m}(\tau) \backslash \mathrm{m}(\Sigma)$. By Theorem 27 the I-measure μ^* can take the following non-negative values:

$$\mu^*(a) = \begin{cases} 1 & \text{if } a = b \\ 0 & \text{otherwise} \end{cases}$$

It is evident that $\mu^*(\Sigma) = 0$ while $\mu^*(\tau) \geq 1$, which contradicts the implication. ◀

C Proofs from Section 4

Lemma 12. *Let $\sigma = (A;B|C)$ and $\tau = (X;Y|Z)$ be CIs such that $X \subseteq A$, $Y \subseteq B$, $C \subseteq Z$ and $Z \subseteq ABC$. Then, $\Gamma_n \models h(\tau) \leq h(\sigma)$.*

Proof. Since $Z \subseteq ABC$, we denote by $Z_A = A \cap Z$, $Z_B = B \cap Z$, and $Z_C = C \cap Z$. Also, denote by $A' = A \backslash (Z_A \cup X)$, $B' = B \backslash (Z_B \cup Y)$. So, we have that: $I(A;B|C) = I(Z_A A' X; Z_B B' Y|C)$. By the chain rule, we have that:

$$\begin{aligned} I(Z_A A' X; Z_B B' Y|C) &= I(Z_A; Z_B|C) + I(A'X; Z_B|CZ_A) + I(Z_A; B'Y|Z_B C) \\ &\quad + I(X;Y|CZ_A Z_B) + I(X; B'|CZ_A Z_B Y) + I(A'; B'Y|CZ_A Z_B X) \end{aligned}$$

Noting that $Z = CZ_A Z_B$, we get that $I(X;Y|Z) \leq I(A;B|C)$ as required. ◀

Theorem 11. *Let Σ be a set of saturated, pairwise disjoint CI terms (Def. 10), and τ be a saturated mutual information. Then, $\mathcal{S}_n \models_{EI} (\Sigma \Rightarrow \tau)$ implies $\Gamma_n \models h(\tau) \leq h(\Sigma)$.*

The proof of Theorem 11 relies on the i-measure presented in Section B, and in particular, on theorem 28.

Proof. From Theorem 7 we have that $\Gamma_n \models \Sigma \Rightarrow \tau$. Let $\tau = I(A;B|C)$ be the saturated implied CI, and let $\sigma = I(X;Y|Z) \in \Sigma$ be a saturated CI. Noting that $\mathrm{m}(\tau) = \mathrm{m}^c(C)\mathrm{m}(A)\mathrm{m}(B)$ we get that:

$$\mathrm{m}^c(\tau) = \mathrm{m}(C) \cup \mathrm{m}^c(C)\mathrm{m}^c(A) \cup \mathrm{m}^c(C)\mathrm{m}(A)\mathrm{m}^c(B) \tag{16}$$

Furthermore, since $\sigma = I(X;Y|Z)$ is saturated, we get that $C = C_X C_Y C_Z$ where $C_X = C \cap X$, $C_Y = C \cap Y$, and $C_Z = C \cap Z$. From this, we get that:

$$\mathrm{m}(C) = \mathrm{m}(C_X) \cup \mathrm{m}^c(C_X)\mathrm{m}(C_Y) \cup \mathrm{m}^c(C_X)\mathrm{m}^c(C_Y)\mathrm{m}(C_Z) \tag{17}$$

Then, from (16), and the set-additivity of μ^*, we get that:

$$\begin{aligned}
&\mu^*\left(\mathrm{m}(\sigma) \cap \mathrm{m}^c(\tau)\right) \\
&= \mu^*(\mathrm{m}(\sigma) \cap \mathrm{m}(C)) + \mu^*(\mathrm{m}(\sigma) \cap \mathrm{m}^c(C)\mathrm{m}^c(A)) + \mu^*(\mathrm{m}(\sigma) \cap \mathrm{m}^c(C)\mathrm{m}(A)\mathrm{m}^c(B))
\end{aligned} \tag{18}$$

We consider each one of the terms in (18) separately. By (17), we have that:

$$\begin{aligned}
&\mu^*(\mathrm{m}(\sigma) \cap \mathrm{m}(C)) \\
&= \mu^*(\mathrm{m}(\sigma)\mathrm{m}(C_X)) + \mu^*(\mathrm{m}(\sigma)\mathrm{m}^c(C_X)\mathrm{m}(C_Y)) + \mu^*(\mathrm{m}(\sigma)\mathrm{m}^c(C_X)\mathrm{m}^c(C_Y)\mathrm{m}(C_Z)) \\
&= \mu^*(\mathrm{m}(C_X)\mathrm{m}(Y)\mathrm{m}^c(Z)) + \mu^*(\mathrm{m}(X \backslash C_X)\mathrm{m}(C_Y)\mathrm{m}^c(ZC_X)) + \\
&\mu^*(\mathrm{m}(X \backslash C_X)\mathrm{m}(Y \backslash C_Y)\mathrm{m}(C_Z)\mathrm{m}^c(ZC_XC_Y)) \\
&= \mu^*(\mathrm{m}(C_X)\mathrm{m}(Y)\mathrm{m}^c(Z)) + \mu^*(\mathrm{m}(X \backslash C_X)\mathrm{m}(C_Y)\mathrm{m}^c(ZC_X)) && (19) \\
&= I_h(C_X;Y|Z) + I_h(X \backslash C_X; C_Y|ZC_X) && (20)
\end{aligned}$$

where transition (19) is because $C_Z \subseteq Z$ and thus $\mathrm{m}(C_Z)\mathrm{m}^c(ZC_XC_Y) = \emptyset$, and $\mu^*(\emptyset) = 0$. We now consider the second term of (18).

$$\begin{aligned}
\mu^*(\mathrm{m}(\sigma) \cap \mathrm{m}^c(C)\mathrm{m}^c(A)) &= \mu^*(\mathrm{m}(X)\mathrm{m}(Y)\mathrm{m}^c(Z)\mathrm{m}^c(C)\mathrm{m}^c(A)) \\
&= \mu^*(\mathrm{m}(X)\mathrm{m}(Y)\mathrm{m}^c(ZCA)) \\
&= I_h(X;Y|ZCA)
\end{aligned} \tag{21}$$

Finally, we consider the third term of (18). Since $I(X;Y|Z)$ is saturated, we get that $A = A_X A_Y A_Z$ where $A_X = A \cap X$, $A_Y = A \cap Y$, and $A_Z = A \cap Z$. Therefore:

$$\mathrm{m}(A) = \mathrm{m}(A_X) \cup \mathrm{m}^c(A_X)\mathrm{m}(A_Y) \cup \mathrm{m}^c(A_X)\mathrm{m}^c(A_Y)\mathrm{m}(A_Z) \tag{22}$$

From (22), and the set-additivity of μ^*, we get that:

$$\begin{aligned}
&\mu^*(\mathrm{m}(\sigma) \cap \mathrm{m}^c(C)\mathrm{m}(A)\mathrm{m}^c(B)) \\
&= \mu^*(\mathrm{m}(X)\mathrm{m}(Y)\mathrm{m}^c(Z)\mathrm{m}^c(C)\mathrm{m}(A)\mathrm{m}^c(B)) \\
&= \mu^*(\mathrm{m}(X)\mathrm{m}(Y)\mathrm{m}(A)\mathrm{m}^c(ZCB)) \\
&= \mu^*(\mathrm{m}(A_X)\mathrm{m}(Y)\mathrm{m}^c(ZCB)) + \mu^*(\mathrm{m}(X \backslash A_X)\mathrm{m}(A_Y)\mathrm{m}^c(ZCBA_X)) \\
&+ \mu^*(\mathrm{m}(X \backslash A_X)\mathrm{m}(Y \backslash A_Y)\mathrm{m}(A_Z)\mathrm{m}^c(ZCBA_XA_Y)) \\
&= \mu^*(\mathrm{m}(A_X)\mathrm{m}(Y)\mathrm{m}^c(ZCB)) + \mu^*(\mathrm{m}(X \backslash A_X)\mathrm{m}(A_Y)\mathrm{m}^c(ZCBA_X)) && (23) \\
&= I_h(A_X;Y|ZCB) + I_h(X \backslash A_X; A_Y|ZCBA_X) && (24)
\end{aligned}$$

where transition (23) is because $A_Z \subseteq Z$, and thus $\mathrm{m}(A_z) \cap \mathrm{m}^c(ZCBA_X) = \emptyset$, and $\mu^*(\emptyset) = 0$. By (20), (21), and (24) we get that:

$$\mu^*(\mathrm{m}(\sigma) \cap \mathrm{m}^c(\tau)) = I_h(C_X; Y|Z) + I_h(X \backslash C_X; C_Y|ZC_X) \\ + I_h(X; Y|ZCA) + I_h(A_X; Y|ZCB) + I_h(X \backslash A_X; A_Y|ZCBA_X) \quad (25)$$

Therefore, by (25), we get that: $\mu^*\left(\mathrm{m}(\sigma) \cap \mathrm{m}^c(\tau)\right) \geq 0$ for every $\sigma \in \Sigma$. By theorem 28 we have that $\mathrm{m}(\tau) \subseteq \mathrm{m}(\Sigma)$. And since Σ is disjoint then $\mu^*(\mathrm{m}(\tau)) = \sum_{\sigma\in\Sigma} \mu^*(\mathrm{m}(\tau) \cap \mathrm{m}(\sigma))$. The result then follows from noting that due to the set-additivity of μ^* then:

$$h(\Sigma) = \sum_{\sigma\in\Sigma} \mu^*(\mathrm{m}(\sigma)) = \sum_{\sigma\in\Sigma} \mu^*(\mathrm{m}(\sigma) \cap \mathrm{m}(\tau)) + \sum_{\sigma\in\Sigma} \mu^*(\mathrm{m}(\sigma) \cap \mathrm{m}^c(\tau)).$$

◀

D Example for Section 5

[18] gave an example of a conditional inequality that holds in Γ_n^* but fails in $\mathbf{cl}\left(\Gamma_n^*\right)$. They also gave several examples of conditional inequalities that are "essentially conditional", i.e. are not derived from other inequalities: our example of an EI that is not and AI (Theorem 16) is based on one of their essentially conditional inequalities. To give a better intuition and geometric interpretation of these phenomena, we give here a much simpler example, albeit unrelated to information theory.

Let K denote the cone of semi-positively defined 2×2 matrices with non-negative elements. We extend it with one other matrix $-Y$ and take the convex hull:

$$K \stackrel{\text{def}}{=} \left\{ \begin{pmatrix} a & b \\ b & c \end{pmatrix} \mid a, b, c \in \mathbb{R}_+, ac \geq b^2 \right\}$$

$$Y \stackrel{\text{def}}{=} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

$$K' \stackrel{\text{def}}{=} \mathbf{conhull}\left(K \cup \{-Y\}\right)$$

Equivalently:

$$K' \stackrel{\text{def}}{=} \left\{ \begin{pmatrix} a-d & b \\ b & c \end{pmatrix} \mid a, b, c, d \in \mathbb{R}_+, ac \geq b^2 \right\}$$

This example illustrates several things:

- Even though K is a closed and convex cone, K' $(= \mathbf{conhull}\left(K \cup \{-y\}\right))$ is not closed; this justifies the condition used in Theorem 18. To see why it is not closed, consider the following sequence of matrices is in K':

$$A_n = \begin{pmatrix} 0 & 1 \\ 1 & 1/n \end{pmatrix}$$

We have $A_n \in K'$ because we can set $a = d = n$, $b = 1$, $c = 1/n$. The limit of this sequence is:

$$\lim_n A_n = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

This matrix is not in K', thus proving that K' is not closed.

- K satisfies the following EI: $a = 0 \Rightarrow b = 0$. However, there is no corresponding AI: for no $\lambda > 0$ does it hold that $K \models (b \leq \lambda \cdot a)$. However, by Theorem 18, there exists an AI with an error term. Indeed, $K \models (b \leq (k \cdot a + 1/k \cdot c)/2)$ forall $k \geq 1$, because $b \leq \sqrt{ac} \leq (k \cdot a + 1/k \cdot c)/2$.
- There exists an EI that holds in the cone K' but not in the topological closure $\mathbf{cl}\left(K'\right)$. Indeed, $K' \models_{EI} (c = 0 \Rightarrow b = 0)$, however this EI does not hold in $\mathbf{cl}\left(K\right)$ because it fails for the matrix $\lim_{n\to\infty} A_n$, which has $c = 0$ but $b = 1$; in other words, $\mathbf{cl}\left(K\right) \not\models_{EI} (c = 0 \Rightarrow b = 0)$.

E Proof of Cone Properties and Identities from Section 5

The required identities are proved in Theorem 30. We require the following simple Lemma.

▶ **Lemma 29.** *Let $A \subset \mathbb{R}^n$ be a finite set and $K = \mathbf{conhull}\left(A\right)$ a finitely generated cone. Then $K^* = A^*$.*

Proof. Let $A = \{a_1, \ldots, a_n\}$. Then
$A^* = \{y \in \mathbb{R}^n, \mid a \cdot y \geq 0 \; \forall a \in A\}$. We show that $A^* = K^*$ by mutual inclusion. Let $v \in K$ then v is a conic combination of vectors in A. That is $v = \sum_{a_i \in A} \alpha_i a_i$ where $\alpha_i \geq 0$. For any $y \in A^*$ we have that $y \cdot v = \sum_{a_i \in A} \alpha_i (y \cdot a_i) \geq 0$. Therefore, $y \in K^*$ proving that $A^* \subseteq K^*$. Now let $y \in K^*$. That is $y \cdot x \geq 0$ for any conic combination x of vectors in A. Since every $a_i \in A$ is, trivially, a conic combination of vectors in A, then $y \in A^*$. Therefore, $K^* \subseteq A^*$, and we get that $K^* = A^*$. ◀

▶ **Theorem 30.** *Let $K, K_1, K_2 \subseteq \mathbb{R}^n$. The following holds.*

1. $K_1 \subseteq K_2 \Rightarrow K_2^* \subseteq K_1^*$
2. *If $K \neq \emptyset$ then $\mathbf{cl}\left(\mathbf{conhull}\left(K\right)\right) = K^{**}$.*
3. $K_1 \subseteq K_2^*$ *iff*[13] $K_1^* \supseteq K_2$.
4. $K^* = \left(\mathbf{cl}\left(\mathbf{conhull}\left(K\right)\right)\right)^*$.
5. *If L is a finite set, then $\mathbf{conhull}\left(L\right)$ is closed.*
6. *If K_1 and K_2 are closed, convex cones then: $(K_1 \cap K_2)^* = \left(\mathbf{cl}\left(\mathbf{conhull}\left(K_1^* \cup K_2^*\right)\right)\right)$.*
7. *A cone K is finitely generated iff K^* is finitely generated.*

Proof. Proof of (1)
Let $x \in K_2^*$, and let $y \in K_1$. Since $x \cdot z \geq 0$ for every vector $z \in K_2$, and since $K_2 \supseteq K_1$ then $x \cdot y \geq 0$ as well. Therefore, $x \in K_1^*$.

Proof of (6)
By definition of union we have that:
$K_i^* \subseteq \mathbf{cl}\left(\mathbf{conhull}\left(K_1^* \cup K_2^*\right)\right)$ for $i \in \{1, 2\}$. By item (1) we have that $K_i^{**} \supseteq \left(\mathbf{cl}\left(\mathbf{conhull}\left(K_1^* \cup K_2^*\right)\right)\right)^*$ for $i \in \{1, 2\}$. Since K_1 and K_2 are closed convex cones then by item (2) it holds that $K_1^{**} =$

[13] Both statements assert $\forall x \in K_1, \forall y \in K_2, x \cdot y \geq 0$.

K_1 and $K_2^{**} = K_2$. Therefore, for $i \in \{1,2\}$ we have that $K_i \supseteq \left(\mathbf{cl}\left(\mathbf{conhull}\left(K_1^* \cup K_2^*\right)\right)\right)^*$. From the above we get that $K_1 \cap K_2 \supseteq \left(\mathbf{cl}\left(\mathbf{conhull}\left(K_1^* \cup K_2^*\right)\right)\right)^*$. By property (1) we get that:
$(K_1 \cap K_2)^* \subseteq \left(\mathbf{cl}\left(\mathbf{conhull}\left(K_1^* \cup K_2^*\right)\right)\right)^{**}$. By property (2) we have that

$$\left(\mathbf{cl}\left(\mathbf{conhull}\left(K_1^* \cup K_2^*\right)\right)\right)^{**} = \mathbf{cl}\left(\mathbf{conhull}\left(K_1^* \cup K_2^*\right)\right).$$

Overall, we get that $(K_1 \cap K_2)^* \subseteq \mathbf{cl}\left(\mathbf{conhull}\left(K_1^* \cup K_2^*\right)\right)$.

Proof of (7).
Let $K = \mathbf{conhull}(A)$ where A is finite. By Lemma 29 it holds that $K^* = A^*$, making K^* a polyhedral cone. By the Minkowski-Weyl Theorem, K^* is also finitely generated. ◀

F Proofs from Section 6

THEOREM 20. *The following inequality holds for all polymatroids $h \in \Gamma_n$:*

$$h(Z) \leq I_h(A;B|C) + I_h(A;B|D) + I_h(C;D|E) + I_h(A;E) + 3h(Z|A) + 2h(Z|B) \tag{26}$$

but the inequality fails if any of the coefficients $3, 2$ are replaced by smaller values. In particular, denoting τ, Σ the terms on the two sides of Eq.(26), the exact implication $\Gamma_n \models_{EI} \Sigma \Rightarrow \tau$ holds, and does not have a 1-relaxation.

Proof. We show that (26) does not admit UAI by proving that the following inequality holds for all polymatroids:

$$H(Z) \leq I(A;B|C) + I(A;B|D) + I(C;D|E) + I(A;E) + 3H(Z|A) + 2H(Z|B)$$

This inequality can be verified using known tools for testing whether an inequality holds for all polymatroids (e.g., ITIP[14], and XITIP[15]). We can apply these same tools to verify that the coefficients 3 and 2 (for $H(Z|A)$ and $H(Z|B)$, respectively), cannot be reduced. In particular, they cannot be reduced to 1. For completeness, we provide the analytical proof as well.

We make use the following inequality that was proved in Lemma 1 in [10].

$$H(Z|R) + I(R;S|T) \geq I(Z;S|T) \tag{27}$$

We apply (27) three times:
1. $H(Z|A) + I(A;B|C) \geq I(Z;B|C)$
2. $H(Z|A) + I(A;B|D) \geq I(Z;B|D)$
3. $H(Z|A) + I(A;E) \geq I(Z;E)$

Plugging back into the formula we get that:

$$\begin{aligned} &I(A;B|C) + I(A;B|D) + I(C;D|E) + I(A;E) + 3H(Z|A) + 2H(Z|B) \\ &\geq I(Z;B|C) + I(Z;B|D) + I(Z;E) + I(C;D|E) + 2H(Z;B) \end{aligned} \tag{28}$$

We now apply this identity twice more:

[14] http://user-www.ie.cuhk.edu.hk/ ITIP/
[15] http://xitip.epfl.ch/

1. $H(Z|B) + I(Z;B|C) \geq I(Z;Z|C) = H(Z;C)$
2. $H(Z|B) + I(Z;B|D) \geq I(Z;Z|D) = H(Z|D)$

Plugging back into (28) we get that:

$$\begin{aligned}
&I(Z;B|C) + I(Z;B|D) + I(Z;E) + I(C;D|E) + 2H(Z|B)\\
&\geq H(Z|C) + H(Z|D) + I(Z;E) + I(C;D|E)\\
&= H(ZC) - H(C) + H(ZD) - H(D) + H(Z) + H(E) - H(ZE) + H(CE) + H(DE) - H(E) - H(CDE)\\
&= I(Z;E|C) + H(ZEC) + I(Z;E|D) + H(ZED) + H(Z) - H(ZE) - H(CDE)\\
&= I(Z;E|C) + I(Z;E|D) + I(C;D|ZE) + H(CDZE) - H(CDE) + H(Z)\\
&= I(Z;E|C) + I(Z;E|D) + I(C;d|ZE) + H(CDE) + H(Z)\\
&\geq H(Z)
\end{aligned}$$

◀

THEOREM 21. *If $\Gamma_n \models \Sigma \Rightarrow \tau$ then $\Gamma_n \models \tau \leq (2^n)! \cdot h(\Sigma)$. In other words, every implication of CIs admits a $(2^n)!$-relaxation over Γ_n.*

Proof. Since $\Gamma \models \Sigma \Rightarrow \tau$ we have, by Theorem 21, that for every polymatroid $h \in \Gamma$: $0 \leq -\tau + \lambda_1\sigma_1 + \cdots + \lambda_m\sigma_m$ for some finite, positive λ_i. We may assume, without loss of generality, that all CIs in Σ appear in elemental form, and that $\tau = \tau_1 + \cdots + \tau_k$ where τ_i are elemental as well. It is easy to see that the number of elemental constraints for an n-variable polymatroid is $M = n + \binom{n}{2}2^{n-2}$. Let us denote by $\boldsymbol{b}$ the M-dimensional vector of coefficients corresponding to $\tau_1, \ldots, \tau_k, \sigma_1, \ldots, \sigma_m$. That is $\boldsymbol{b}^T = [0, \ldots, 0, \lambda_1, \ldots, \lambda_m, -1, \ldots, -1, 0, \ldots, 0]$ where the λ_i are the positive coefficients of the elemental forms in Σ, and the -1 correspond to the elemental forms in τ.

Let $h \in \Gamma_n$, and let h^e be an M-dimensional vector whose ith entry corresponds to the value of the ith elemental form of h (e.g., $h^e[(a;b)] = h(a) + h(b) - h(ab)$). Note the one-to-one correspondence between h and h^e. By our assumption, we have that the inequality $\boldsymbol{b}^T \cdot h^e \geq 0$ holds for all $h \in \Gamma_n$. This, in turn, means that $\boldsymbol{b}$ is a positive linear combination of the elemental forms [41]. Let $\boldsymbol{G}$ denote the $(2^n - 1) \times M$ matrix whose columns represent the elemental forms, and let $\boldsymbol{G}^i$ represent the ith column. Since $\boldsymbol{b}$ is a positive linear combination of the elemental forms then: $\boldsymbol{b} = \sum_{i=1}^{M} x_i \boldsymbol{G}^i$ where $x_i \geq 0$. In other words, for every polymatroid $h \in \Gamma_n$, it holds that: $\boldsymbol{b}^T \cdot h^e - \boldsymbol{x}^T \cdot h^e = 0$ for some positive M-dimensional vector $\boldsymbol{x}$.

Since the coefficients for the CIs in Σ are unknown, we can always assume that the vector $\boldsymbol{x}$ contains 0 in the entries corresponding to $\tau_1, \ldots, \tau_k, \sigma_1, \ldots, \sigma_m$. Indeed, if the coefficient x_σ of the elemental $\sigma \in \Sigma$ is greater than 0, then we may assume that x_α cancels out with λ_α.

So let $\boldsymbol{c}^T = (\boldsymbol{b}^T - \boldsymbol{x}^T)$. By the previous discussion we can assume that $\boldsymbol{c}^T$ is an M-dimensional vector that takes the following form. For every elemental $\sigma_i \in \Sigma$ it holds that $\boldsymbol{c}^T[\sigma_i] = c_i \geq 0$, for every τ_i, it holds that $\boldsymbol{c}^T[\tau_i] = -1$, and there is some set of l elemental forms $\alpha_1, \ldots, \alpha_l$ such that $\boldsymbol{c}^T[\alpha_j] = -d_j$ where $d_j \geq 0$.

The identity $\boldsymbol{c}^T \cdot h^e = 0$ holds for every $h \in \Gamma_n$ if and only if $\boldsymbol{G}\boldsymbol{c} = 0$ where $\boldsymbol{G}$ is the $(2^n - 1) \times M$ matrix where each column corresponds to an elemental positivity constraint. Clearly, all entries in $\boldsymbol{G}$ are either 0, 1, or -1.

Since, by our assumption, the equation $\boldsymbol{G}\boldsymbol{c} = 0$ has a solution, then it has a non-zero determinant. Specifically, there must exist $2^n - 1$ columns in $\boldsymbol{G}$, denoted $i_1, \ldots, i_{2^n-1}$ such that the minor $M_{i_1,\ldots,i_{2^n-1}}$ is nonzero. (The entry $a_{j,k}$ in $M_{i_1,\ldots,i_{2^n-1}}$ is the determinant of the $(2^n-2)\times(2^n-2)$ square matrix whose columns are $i_1,\dots i_{k-1},i_{k+1},\dots,i_{2^n-1}$, and rows are $1,\dots,j-1,j+1,\dots,2^n-1$). We denote by $\boldsymbol{G}'$ the augmented matrix whose last (i.e., 2^nth) column is the 2^n-1-dimensional $\vec{0}$. We apply the generalized Cramer's rule from linear algebra [2] to get that:

$$c_j = \frac{M_{i_1,\dots,i_{j-1},2^n,i_{j+1},\dots,i_{2^n-1}}}{M_{i_1},\dots,i_{2^n-1}} \leq M_{i_1,\dots,i_{j-1},2^n,i_{j+1},\dots,i_{2^n-1}} \leq (2^n)!$$

The final inequality results from the fact that all entries in $\boldsymbol{G}$ are 0, 1, or -1, and that the 2^nth column is comprised of 0s, giving us the required result. ◀

G I-measure proof for unit relaxation in $\mathcal{P}_n$

THEOREM 23. *Exact implications of I-measure constraints admit a 1-relaxation in $\mathcal{P}_n$.*

Proof. By Theorem 28 we have that $\mathrm{m}(\tau)\subseteq \mathrm{m}(\Sigma)$. This means that $\mathrm{m}(\tau)=\cup_{\sigma\in\Sigma}\big(\mathrm{m}(\tau)\cap\mathrm{m}(\sigma)\big)$. By the assumption that the I-measure μ^* is nonnegative, we get that:

$$\mu^*(\mathrm{m}(\tau)) = \mu^*\left(\cup_{\sigma\in\Sigma}\big(\mathrm{m}(\tau)\cap\mathrm{m}(\sigma)\big)\right) \leq \sum_{\sigma\in\Sigma}\mu^*((\mathrm{m}(\tau)\cap\mathrm{m}(\sigma)) \tag{29}$$

By the set-additivity of μ^* we get that:

$$\sum_{\sigma\in\Sigma}\mu^*(\mathrm{m}(\sigma)) = \sum_{\sigma\in\Sigma}\mu^*(\mathrm{m}(\sigma)\cap\mathrm{m}(\tau)) + \sum_{\sigma\in\Sigma}\mu^*(\mathrm{m}(\sigma)\cap\mathrm{m}^c(\tau)) \tag{30}$$

From (30), (29), and non-negativity of μ^* we get that:

$$\begin{aligned}\mu^*(\mathrm{m}(\tau)) &\leq \sum_{\sigma\in\Sigma}\mu^*(\mathrm{m}(\sigma)) - \sum_{\sigma\in\Sigma}\mu^*(\mathrm{m}(\sigma)\cap\mathrm{m}^c(\tau))\\ &\leq \sum_{\sigma\in\Sigma}\mu^*(\mathrm{m}(\sigma)).\end{aligned}$$

◀

H $\mathcal{P}_n$ coincides with the cone of step functions

We describe the structure of the I-measure of a step function, and prove that the conic hull of step functions and positive polymatroids coincide. That is, $\Delta_n=\mathcal{P}_n$. We let $U\subseteq[n]$, and let s_U denote the step function at U. In the rest of this section we prove Theorem 31.

▶ **Theorem 31.** *It holds that $\Delta_n=\mathcal{P}_n$.*

▶ **Lemma 32.** *Let s_U be the step function at $U\subseteq[n]$, and $R=[n]\setminus U$. The unique i-measure for any step function s_U is:*

$$\mu^*(a) = \begin{cases}1 & \text{if } a = \big(\cap_{X\in R}\mathrm{m}(X)\big)\cap\big(\cap_{X\in U}\mathrm{m}^c(X)\big)\\ 0 & \text{otherwise}\end{cases} \tag{31}$$

Proof. We define the atom a^* by:

$$a^* \stackrel{\text{def}}{=} \big(\cap_{X \in R} \mathrm{m}(X)\big) \cap \big(\cap_{X \in U} \mathrm{m}^c(X)\big)$$

Let $S \subseteq U$. We show that $h(S) = \mu^*(\mathrm{m}(S)) = 0$. By definition, $\mathrm{m}(S) = \cup_{Y \in S} \mathrm{m}(Y)$. Therefore, every atom $a \in \mathrm{m}(S)$ has at least one set $\mathrm{m}(Y)$, where $Y \in S$, that appears in positive form. In particular, $a^* \notin \mathrm{m}(S)$. Therefore, by (31), we have that $h(S) = \mu^*(\mathrm{m}(S)) = 0$ as required.

Now, let $T \not\subseteq U$, and let $X \in T \setminus U$. Since $\mathrm{m}(X)$ appears in positive form in a^*, and since $\mathrm{m}(X) \subseteq \mathrm{m}(T)$, then we have that $h(T)=1$. Therefore, μ^* as defined in (31) is the i-measure for s_U. By Theorem 26, the i-measure μ^* is *unique*, and is therefore the only i-measure for s_U. ◀

By Lemma 32, every step function has a nonnegative i-measure. As a consequence, any conic combination of step functions has a positive i-measure, proving that $\Delta_n \subseteq \mathcal{P}_n$.

Now, let μ^* denote any nonnegative i-measure. For every atom a, we let $\mathbf{neg}(a)$ denote the set of variables whose sets appear in negated form (e.g., if $a = \big(\cap_{X \in R} \mathrm{m}(X)\big) \cap \big(\cap_{X \in U} \mathrm{m}^c(X)\big)$, then $\mathbf{neg}(a) = U$). Let $\mathcal{A}$ denote the atoms of $\mathcal{F}_n$. We define the mapping $f : \mathcal{A} \mapsto \Delta_n$ as follows.

$$f(a) = \mu^*(a) \cdot s_{\mathbf{neg}(a)}$$

where $s_{\mathbf{neg}(a)}$ is the step function at $\mathbf{neg}(a)$. Since the i-measure of $s_{\mathbf{neg}(a)}$ is 1 at atom a and 0 everywhere else we get that:

$$\mu^* = \sum_{a \in \mathcal{A}} f(a) = \sum_{a \in \mathcal{A}} \mu^*(a) \cdot s_{\mathbf{neg}(a)}$$

proving that $\mu^* \in \Delta_n$, and that $\mathcal{P}_n \subseteq \Delta_n$.