A Memory-Efficient Algorithm for Generating Non-Contextuality Inequalities

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This is the abstract.

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A. Definitions

To every random variable[1] v there corresponds a prescribed set of **outcomes** $\mathcal{O}_v$ and a set of **events over** $\boldsymbol{v}$ denoted $\Omega(v)$ corresponding to the set of all functions of the form $\omega : \{v\} \to \mathcal{O}_v$. Evidently, $\Omega(v)$ and $\mathcal{O}_v$ are isomorphic structures and their distinction can be confounding. There is rarely any harm in referring synonymously to either as outcomes. Nonetheless, a sheaf-theoretic treatment of contextuality [1] demands the distinction. Specifically for this work, the distinction becomes essential for the exploitation of marginal symmetries in Section III D. As a natural generalization we define the event over a collection of random variables $V = \{v_1, \ldots, v_n\}$ in a parallel manner:

$$\Omega(V) \equiv \{\omega : V \to \mathcal{O}_V \mid \forall v \in V, \omega(v) \in \mathcal{O}_v\}$$

Furthermore, the **domain** $\boldsymbol{\mathcal{D}(\omega)}$ of an event ω is the set of random variables it valuates, i.e. if $\omega \in \Omega(V)$ then $\mathcal{D}(\omega) = V$.

For every $\omega \in \Omega(V)$ and $V' \subset V$, the **restriction of** $\boldsymbol{\omega}$ **onto** $\boldsymbol{V'}$ (denoted $\omega|_{V'}$) corresponds to the unique event in $\Omega(V')$ that agrees with ω for all valuations of variables in V', i.e. $\forall v' \in V' : \omega|_{V'}(v') = \omega(v')$. Using this notational framework, a probability distribution or simply **distribution** p_V is a probability measure on $\Omega(V)$, assigning to each $\omega \in \Omega(V)$ a real number $\mathsf{p}_V(\omega) \in [0, 1]$ such that $\sum_{\omega\in\Omega(V)} \mathsf{p}_V(\omega) = 1$. The set of all distributions over $\Omega(V)$ is denoted $\mathcal{P}_V$. Moreover, given $\mathsf{p}_V \in \mathcal{P}_V$ and $V' \subset V$, there is an induced distribution $\mathsf{p}_V|_{V'} \in \mathcal{P}_{V'}$ obtained by *marginalizing* p_V:

$$\mathsf{p}_V|_{V'}(\omega') = \sum_{\substack{\omega\in\Omega(V)\\ \omega|_{V'}=\omega'}} \mathsf{p}_V(\omega) \tag{1}$$

Presently, the reader is equipped with sufficient notation and terminology to comprehend the marginal problem.

Definition 1. The Marginal Problem (MP): Given a collection of m distributions $\{\mathsf{p}_{V_1}, \ldots, \mathsf{p}_{V_m}\}$, does there exist a distribution $\mathsf{p}_\Lambda \in \mathcal{P}_\Lambda$ with $\Lambda \equiv \bigcup_{i=1}^m V_m$ such that $\forall i : \mathsf{p}_\Lambda|_{V_i} = \mathsf{p}_{V_i}$?

To facilitate further discussion of this problem, several pieces of nomenclature will be introduced. First, the set $\mathcal{V} = \{V_1, \ldots, V_m\}$ is called the **marginal scenario** while its elements are called the **marginal contexts**. The collection of distributions $\mathsf{p}_{*\mathcal{V}} \equiv \{\mathsf{p}_{V_1}, \ldots, \mathsf{p}_{V_m}\}$[2] is called the

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[1] Throughout this document, it is assumed that all random variables are discrete and have finite cardinality.

[2] The subscript $*$ preceding ${}_*\mathcal{V}$ is added for clarity; $\mathsf{p}_{*\mathcal{V}}$ is *not* a distribution but a set of distributions over $\mathcal{V}$. The ${}_*\mathcal{V}$ convention is adopted throughout this report.

marginal model [2][3]. The distribution p_Λ, if it exists, is termed the **joint distribution**. Strictly speaking, as defined by [2], a marginal scenario forms an *abstract simplicial complex*, meaning it satisfies the supplementary requirement that all subsets of contexts are also contexts, i.e. $\forall V \in \mathcal{V} : V' \subset V \implies V' \in \mathcal{V}$. Throughout this work, we exclusively consider (without loss of generality) *maximal* marginal scenarios, restricting our focus to the contexts which are contained in no others. Finally, a marginal model $\mathsf{p}_{*\mathcal{V}}$ is said to be **non-contextual**, and will be denoted $\mathsf{p}_{*\mathcal{V}} \in \mathcal{N} \subseteq \mathcal{P}_{*\mathcal{V}}$ if it admits a joint distribution and **contextual** otherwise ($\mathsf{p}_{*\mathcal{V}} \in \bar{\mathcal{N}}$). Equipped with this additional terminology and notation, MP now reads: given $\mathsf{p}_{*\mathcal{V}}$, is $\mathsf{p}_{*\mathcal{V}} \in \mathcal{N}$ or not?

B. Linearity

An essential feature of MP is linearity; the marginalization of p_Λ onto the marginal contexts $\{\mathsf{p}_\Lambda|_V \mid V \in \mathcal{V}\}$ is a linear transformation, requiring only the summations pursuant to Eq. (1). Consequently, it is advantageous to consider the statement of MP as a matrix multiplication. To this end, for each marginal scenario $\mathcal{V}$ we define a binary matrix $\mathcal{M}$ called the **incidence matrix** which implements this mapping. The columns of $\mathcal{M}$ are indexed by *joint events* $j \in \Omega(\Lambda)$ and the rows are indexed by *marginal events* $m \in \Omega(V)$ for some $V \in \mathcal{V}$. By deliberate abuse of notation, we will denote the set of all marginal events as $\Omega({}_*\mathcal{V})$ and is defined as the following disjoint union:

$$\Omega({}_*\mathcal{V}) \equiv \coprod_{V \in \mathcal{V}} \Omega(V)$$

The $|\Omega({}_*\mathcal{V})| \times |\Omega(\Lambda)|$ incidence matrix $\mathcal{M}$ is then defined element-wise for $m \in \Omega({}_*\mathcal{V})$ and $j \in \Omega(\Lambda)$:

$$\mathcal{M}^m_j = \begin{cases} 1 & j|_{\mathcal{D}(m)} = m \\ 0 & \text{otherwise} \end{cases} \tag{2}$$

Conceptually, the entries of this matrix are populated with ones whenever the marginal event (row) m is the restriction of some joint event (column) j. For a given marginal scenario $\mathcal{V}$, $\mathcal{M}$ represents the tuple of restriction maps $\mathcal{M} : \Omega(\Lambda) \to \prod_{V \in \mathcal{V}} \Omega(V) :: j \mapsto \{j|_V \mid V \in \mathcal{V}\}$ [1]. Furthermore, note that the component indices of $\mathcal{M}$ in Eq. (2) are deliberately separated. Among other reasons, this is done to allow one to denote the m-th row of $\mathcal{M}$ as $\mathcal{M}^m$ and the j-th column as $\mathcal{M}_j$. For further notational convenience, since $\mathcal{M}$ is a binary matrix, we let $\mathcal{M}^m$ and $\mathcal{M}_j$ analogously correspond their respective *supports*[4], e.g. $m \in \sigma(\mathcal{M}_j)$ if and only if $\mathcal{M}^m_j = 1$. Throughout the remainder of this report, the utility of the incidence matrix $\mathcal{M}$ will be indispensable.

To illustrate this concretely, consider the following example. Let Λ be 3 binary variables $\{a, b, c\}$ and $\mathcal{V}$ be the marginal scenario $\mathcal{V} = \{\{a, b\}, \{b, c\}, \{a, c\}\}$. The incidence matrix for $\mathcal{V}$ becomes:

$$\begin{array}{cc}
(a,b,c) \mapsto & \begin{array}{cccccccc} (0,0,0) & (0,0,1) & (0,1,0) & (0,1,1) & (1,0,0) & (1,0,1) & (1,1,0) & (1,1,1) \end{array} \\
\begin{array}{c}
(a \mapsto 0, b \mapsto 0) \\
(a \mapsto 0, b \mapsto 1) \\
(a \mapsto 1, b \mapsto 0) \\
(a \mapsto 1, b \mapsto 1) \\
(b \mapsto 0, c \mapsto 0) \\
(b \mapsto 0, c \mapsto 1) \\
(b \mapsto 1, c \mapsto 0) \\
(b \mapsto 1, c \mapsto 1) \\
(a \mapsto 0, c \mapsto 0) \\
(a \mapsto 0, c \mapsto 1) \\
(a \mapsto 1, c \mapsto 0) \\
(a \mapsto 1, c \mapsto 1)
\end{array} &
\begin{pmatrix}
\mathbf{1} & \mathbf{1} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \mathbf{1} & \mathbf{1} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \mathbf{1} & \mathbf{1} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \mathbf{1} & \mathbf{1} \\
\mathbf{1} & 0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 \\
0 & \mathbf{1} & 0 & 0 & 0 & \mathbf{1} & 0 & 0 \\
0 & 0 & \mathbf{1} & 0 & 0 & 0 & \mathbf{1} & 0 \\
0 & 0 & 0 & \mathbf{1} & 0 & 0 & 0 & \mathbf{1} \\
\mathbf{1} & 0 & \mathbf{1} & 0 & 0 & 0 & 0 & 0 \\
0 & \mathbf{1} & 0 & \mathbf{1} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \mathbf{1} & 0 & \mathbf{1} & 0 \\
0 & 0 & 0 & 0 & 0 & \mathbf{1} & 0 & \mathbf{1}
\end{pmatrix}
\end{array} \tag{3}$$

In addition, for any joint distribution $\mathsf{p}_\Lambda \in \mathcal{P}_\Lambda$ we associate a joint distribution *vector* p_Λ (identically denoted) indexed by $j \in \Omega(\Lambda)$, i.e. $\mathsf{p}^j_\Lambda \equiv \mathsf{p}_\Lambda(j)$. Analogously, for each marginal model $\mathsf{p}_{*\mathcal{V}} \in \mathcal{P}_{*\mathcal{V}}$ there is an associated marginal distribution *vector* $\mathsf{p}_{*\mathcal{V}}$ indexed by $m \in \Omega({}_*\mathcal{V})$ such that $\mathsf{p}^m_{*\mathcal{V}} \equiv \mathsf{p}_{\mathcal{D}(m)}(m)$. Using these vectors, the marginal problem becomes the following linear program:

Definition 2. **The Marginal Linear Program (MLP)**:

$$\begin{aligned} \text{minimize:} \quad & \emptyset \cdot \mathsf{p}_\Lambda{}^{5} \\ \text{subject to:} \quad & \mathsf{p}_\Lambda \succeq 0 \\ & \mathcal{M} \cdot \mathsf{p}_\Lambda = \mathsf{p}_{*\mathcal{V}} \end{aligned} \tag{4}$$

As such, $\mathsf{p}_{*\mathcal{V}} \in \mathcal{N}$ if and only if MLP is a *feasible* linear program. Importantly, if MLP is feasible, it will return the joint distribution p_Λ. To every linear program, there exists a dual linear program that characterizes the feasibility of the original [3]. Constructing the dual linear program is a well-defined procedure [4].

Definition 3. **The Dual Marginal Linear Program (DMLP)**:

$$\begin{aligned} \text{minimize:} \quad & \gamma \cdot \mathsf{p}_{*\mathcal{V}} \\ \text{subject to:} \quad & \gamma \cdot \mathcal{M} \succeq 0 \end{aligned}$$

By construction, DMLP completely determines the whether or not $\mathsf{p}_{*\mathcal{V}} \in \mathcal{N}$ or not. If $\mathsf{p}_{*\mathcal{V}} \in \mathcal{N}$, then MLP is feasible and the following holds,

$$\gamma \cdot \mathsf{p}_{*\mathcal{V}} = \gamma \cdot (\mathcal{M} \cdot \mathsf{p}_\Lambda) \geq 0 \tag{5}$$

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[3] In [1], $\mathsf{p}_{*\mathcal{V}}$ is instead called an *empirical model*.

[4] The *support* $\sigma(f)$ of a mapping f is the subset of its domain $\mathcal{D}(f)$ that is not mapped to a zero element: $\sigma(f) = \{x \in \mathcal{D}(f) \mid f(x) \neq 0\}$.

[5] Note that the primal value of the linear program is of no interest, all that matters is its *feasibility*. Here $\emptyset$ denotes a null vector of all zero entries.

because both $\gamma\cdot\mathcal{M}\succeq 0$ and $\mathsf{p}_{\Lambda}\succeq 0$. If however, $\gamma\cdot\mathsf{p}_{*\mathcal{V}}<0$, then Eq. (5) is violated and $\mathsf{p}_{*\mathcal{V}}\notin\mathcal{N}$[6]. In summary, the sign of $d\equiv\min(\gamma\cdot\mathsf{p}_{*\mathcal{V}})$ answers the marginal program; $\mathsf{p}_{*\mathcal{V}}\in\mathcal{N}$ if and only if $d\geq 0$[7].

Corollary 1. *All linear, homogeneous constraints* $\gamma\cdot\mathsf{p}_{*\mathcal{V}}\geq 0$ *constraining non-contextual marginal models* $\mathcal{N}\subseteq\mathcal{P}_{*\mathcal{V}}$ *satisfy* $\gamma\cdot\mathcal{M}\succeq 0$. *Moreover, all vectors* γ *satisfying* $\gamma\cdot\mathcal{M}\succeq 0$ *correspond to valid constraints* $\gamma\cdot\mathsf{p}_{*\mathcal{V}}\geq 0$ *for* $\mathcal{N}\subseteq\mathcal{P}_{*\mathcal{V}}$.

In light of Defs. 2 and 3, when supplied with a particular marginal model $\mathsf{p}_{*\mathcal{V}}$, the marginal problem can be solved computationally by evaluating DMLP to determine the feasibility of MLP. A more difficult variant of the marginal problem is one wherein no particular marginal model is supplied.

Definition 4. The General Marginal Problem (GMP): Given a marginal scenario $\mathcal{V}$ find a set of independent constraints Γ which completely constraint $\mathcal{N}\subseteq\mathcal{P}_{*\mathcal{V}}$; i.e. $\mathsf{p}_{*\mathcal{V}}\in\mathcal{N}$ if and only if it satisfies all constraints in Γ.

The remainder of this paper is concerned with methods for solving (or partially solving) GMP. Specifically, Section II C discusses existing methods for completely solving GMP and outlines some of their disadvantages. Section II D summarizes an existing method for completely solving a possibilistic variant of GMP. Sections II C and II D motivate Section III, wherein a new method for completely solving GMP is presented.

C. Marginal Polytopes

The complete space of marginal models over $\mathcal{V}$ (denoted $\mathcal{P}_{*\mathcal{V}}$) can be partitioned into two spaces: the contextual marginal models ($\bar{\mathcal{N}}$) and the non-contextual marginal models ($\mathcal{N}\equiv\mathcal{P}_{*\mathcal{V}}\setminus\bar{\mathcal{N}}$). Pitowsky [7] demonstrates that $\mathcal{N}$ forms a *convex* polytope commonly referred to as the **marginal polytope** for $\mathcal{V}$. When embedded in $\mathbb{R}^{|\Omega(*\mathcal{V})|}$, the extremal rays of the marginal polytope correspond to the columns of $\mathcal{M}$ which further correspond to all *deterministic* joint distributions $\mathsf{p}_{\Lambda}\in\mathcal{P}_{\Lambda}$[8]. The normalization of p_{Λ} ($\sum_j\mathsf{p}_{\Lambda}^{j}=1$) defines the convexity of the polytope; each marginal model $\mathsf{p}_{*\mathcal{V}}\in\mathcal{P}_{*\mathcal{V}}$ must be a convex mixture of the deterministic marginal models pursuant to Eq. (4). Consequently, characterizing the contextuality of marginal models is manifestly a problem of polytope description. Notably, the **facets** of a marginal polytope correspond to a finite set of linear inequalities that are complete in the sense that all contextual distributions violate at least one facet inequality [8]. From the perspective of a marginal polytope, convex hull algorithms or linear quantifier elimination can be used to compute a representation of the complete set of facet inequalities and consequently completely solve the GMP. A popular tool for linear quantifier elimination is *Fourier-Motzkin elimination* [9–12]. In this report, we will avoid expounding upon the Fourier-Motzkin procedure and instead recall a few of its notable features and consequences.[9]

Definition 5. [3, Section 12.2] Given a system of linear inequality constraints $\mathcal{S}=\{A\cdot x\leq b\}$ constraining some free variables x, the **Fourier-Motzkin elimination** procedure eliminates some of the variables in x and returns a system of linear inequality constraints $\mathcal{S}'=\{A'\cdot x'\leq b'\}$ over $x'\subset x$ such that any solution x' of $\mathcal{S}'$ will permit at least one compatible solution x of $\mathcal{S}$ (and vice versa).

$$\exists x' : A'\cdot x'\leq b' \iff \exists x : A\cdot x\leq b \tag{6}$$

In particular, the following system of linear inequalities defines the marginal polytope for $\mathcal{V}$:

$$\begin{aligned}
\forall m\in\Omega(*\mathcal{V}) : &\quad \mathsf{p}_{*\mathcal{V}}^{m}-\sum\nolimits_j\mathcal{M}_j^m\mathsf{p}_{\Lambda}^{j}\geq 0\\
\forall m\in\Omega(*\mathcal{V}) : &\quad -\mathsf{p}_{*\mathcal{V}}^{m}+\sum\nolimits_j\mathcal{M}_j^m\mathsf{p}_{\Lambda}^{j}\geq 0\\
\forall j\in\Omega(\Lambda) : &\quad \mathsf{p}_{\Lambda}^{j}\geq 0\\
&\quad \sum\nolimits_j\mathsf{p}_{\Lambda}^{j}\geq 1\\
&\quad -\sum\nolimits_j\mathsf{p}_{\Lambda}^{j}\geq -1
\end{aligned}\tag{7}$$

Using the Fourier-Motzkin elimination procedure, it is possible to eliminate the variables p_{Λ}^{j} relating to joint events and obtain a system of linear inequalities constraining only marginal events $\mathsf{p}_{*\mathcal{V}}^{m}$ which completely characterizes the set of non-contextual marginal models $\mathcal{N}\subseteq\mathcal{P}_{*\mathcal{V}}$.

Lemma 1. [10] *There exists a finite set of integral vectors* Γ *such that for all* $\mathsf{p}_{*\mathcal{V}}\in\mathcal{P}_{*\mathcal{V}}$:

$$\mathsf{p}_{*\mathcal{V}}\in\mathcal{N} \iff \forall\gamma\in\Gamma : \gamma\cdot\mathsf{p}_{*\mathcal{V}}\geq 0 \tag{8}$$

Proof. The finiteness and existence of Γ is a fundamental property of polytopes [9, 11–14]. The fact that each vector $\gamma\in\Gamma$ need only be integer-valued follows from

[6] These observations are collectively a consequence of Farkas's Lemma [5].

[7] In particular, if $d\geq 0$, then $d=0$ due to the existence of the trivial solution $\gamma=\emptyset$. This observation is an instance of the *Complementary Slackness Property* [6]. Alternatively, if $d<0$, then it is unbounded $d=-\infty$ due to the *Unbounded Property* [6].

[8] A deterministic distribution p_{Λ} is a distribution in which a singular event $j\in\Omega(\Lambda)$ occurs with certainty, i.e. $\mathsf{p}_{\Lambda}^{j}=1$ and $\forall j'\neq j:\mathsf{p}_{\Lambda}^{j'}=0$.

[9] Applying the Fourier-Motzkin procedure to completely solve GMP is discussed in more detail in Fritz and Chaves [2].

[10] This is a stronger variant of [11, Proposition 7].

the integer-valued coefficients that constrain Eq. (7). Finally, the homogeneity of the constraints in Eq. (8) follows from the assumption that each $\mathsf{p}_{*\mathcal{V}} \in \mathcal{P}_{*\mathcal{V}}$ a priori satisfies normalization constraints context-wise; i.e. $\forall V \in \mathcal{V} : \sum_{m\in\Omega(V)} \mathsf{p}_V^m = 1$[11]. □

D. Logical Contextuality

Let $a \in \Omega(_*\mathcal{V})$ be *any* marginal event and $C = \{c_1, \dots, c_n\} \subseteq \Omega(_*\mathcal{V})$ be a subset of marginal events such that the following logical implication holds for *all* marginal models $\mathsf{p}_{*\mathcal{V}} \in \mathcal{P}_{*\mathcal{V}}$:

$$a \implies c_1 \vee \dots \vee c_n = \bigvee_{c\in C} c \tag{9}$$

Which can be dictated: *whenever the event a occurs, at least one event in C occurs.* In accordance with the logical form of Eq. (9), a will be referred to as the **antecedent** and C as the **consequent set**. To clarify, a marginal model $\mathsf{p}_{*\mathcal{V}} \in \mathcal{P}_{*\mathcal{V}}$ satisfies Eq. (9) if there always at least one $c \in C$ that is *possible* ($\mathsf{p}_{*\mathcal{V}}^c > 0$) whenever a is possible. A marginal model violates Eq. (9) whenever *none* of events in c are possible while a remains possible. Marginal models that violate logical statements such as Eq. (9) are known as **Hardy Paradoxes** [10, 15, 16]. Motivated by a greater sense of robustness compared to possibilistic constraints, the concept of witnessing quantum contextuality on a logical level has be analyzed thoroughly for decades [11, 17].

All logical implications of the form of Eq. (9) can be derived by first selecting am antecedent marginal event a, then constructing a consequent set C such that Eq. (9) holds. This is accomplished by making use of Lemma 2.

Lemma 2. *Let $m \in \Omega(_*\mathcal{V})$ be a marginal event. Then for all non-contextual marginal models $\mathsf{p}_{*\mathcal{V}} \in \mathcal{N}$,*

$$m \iff \bigvee_{j\in\sigma(\mathcal{M}^m)} j$$

Essentially, if a joint distribution does exist ($\mathsf{p}_{*\mathcal{V}} \in \mathcal{N}$), then event m represents partial knowledge of the entire system of variables Λ; whenever m occurs, exactly one joint event j has occurred in reality and m must be a restriction of j. Applying Lemma 2 to the antecedent $a \in \Omega(_*\mathcal{V})$ and consequent set $C \subseteq \Omega(_*\mathcal{V})$,

$$\begin{aligned} a &\iff \bigvee_{j\in\sigma(\mathcal{M}^a)} j \\ \bigvee_{c\in C} c &\iff \bigvee_{c\in C} \bigvee_{j\in\sigma(\mathcal{M}^c)} j \end{aligned} \tag{10}$$

[11] Specifically, any inhomogeneous constraint $\gamma \cdot \mathsf{p}_{*\mathcal{V}} \geq \alpha$ can be *homogenized* by replacing α with $\sum_{m\in\Omega(V)} \alpha \mathsf{p}_V^m$.

Therefore, if a subset C of $\Omega(_*\mathcal{V})$ (preferably excluding a) can be found such that,

$$\sigma(\mathcal{M}^a) \subseteq \bigcup_{c\in C} \sigma(\mathcal{M}^c) \tag{11}$$

then Eq. (9) follows from Eqs. (10,11).

It is possible to show that for each logical constraint of the form Eq. (9), there exists a corresponding probabilistic constraint that is tighter. Corollary 2[12] generalizes Lemma 2.

Corollary 2. *Let $m \in \Omega(_*\mathcal{V})$ be a marginal event. Then for all non-contextual marginal models $\mathsf{p}_{*\mathcal{V}} \in \mathcal{N}$,*

$$\mathsf{p}_{*\mathcal{V}}^m = \sum_{j\in\sigma(\mathcal{M}^m)} \mathsf{p}_\Lambda^j$$

III. AN OBSERVATION

A. An Antecedent Hierarchy

B. The Antecedent Hypergraph

Given an antecedent multi-set γ where $\gamma \preceq 0$, we identify the **inhibiting set** of joint events $\mathcal{I}(\gamma) \subseteq \Omega(\Lambda)$ preventing $\gamma \cdot \mathcal{M}$ from being positive semi-definite:

$$\mathcal{I}(\gamma) \equiv \left\{ j \in \Omega(\Lambda) \mid (\gamma \cdot \mathcal{M})_j < 0 \right\}$$

The inhibiting set $\mathcal{I}(\gamma)$ of γ completely characterizes the **antecedent hypergraph** $\mathcal{H}(\gamma)$ whose edges $\mathcal{E}_j$ are indexed by the inhibiting events $j \in \mathcal{I}(\gamma)$. Each edge $\mathcal{E}_j \subseteq \Omega(_*\mathcal{V})$ corresponds to the set of the marginal events $m \in \Omega(_*\mathcal{V})$ which are restrictions of j. Specifically,

$$\begin{gathered} \mathcal{H}(\gamma) \equiv \{\mathcal{E}_j \mid j \in \mathcal{I}(\gamma)\} \\ \mathcal{E}_j \equiv \left\{ m \in \Omega(_*\mathcal{V}) \mid m = j|_{\mathcal{D}(m)}, \gamma_m = 0 \right\} \end{gathered}$$

Todo (TC Fraser): Incorporate weights

$$\omega(\gamma) = \left\{ \omega_j = -(\gamma \cdot \mathcal{M})_j \mid j \in \mathcal{I}(\gamma) \right\}$$

Todo (TC Fraser): Define set of right-minimal inequalities

$$I(\gamma) = \left\{ (\gamma + \tilde{\gamma}) \cdot \mathsf{p}_{*\mathcal{V}} \geq 0 \mid \tilde{\gamma} \in \mathrm{Tr}_{\omega(\gamma)}(\mathcal{H}(\gamma)) \right\}$$

[12] Corollary 2 is simply the m-th row of Eq. (4).

C. Irreducibility

D. Marginal Symmetries

E. Curated Inequalities

F. Targeted Searches

G. Relaxations

IV. HYPERGRAPH TRANSVERSALS

A. Preliminaries

[18] [19] [20] [21] Todo (TC Fraser): Numerous computational problems can be casted as a hypergraph transversal problem Todo (TC Fraser): w,t-transversals are not the same thing

Definition 6. A **hypergraph** $\mathcal{H}$ is defined by a set of nodes $\mathbf{N}(\mathcal{H})$ whos $\mathcal{H} = (\mathcal{N}, \mathcal{E})$ where $\mathcal{N} = \{n_1, \ldots, n_p\}$ is some finite set and $\mathcal{E}$ is a finite collection of non-empty subsets $\mathcal{E} = \{\mathcal{E}_1, \ldots, \mathcal{E}_q\}$ of $\mathcal{N}$. The elements of $\mathcal{N}$ are called **nodes** while the elements of $\mathcal{E}$ are called **hyperedges** of the hypergraph $\mathcal{H}$.

A hypergraph generalizes the notion of a *graph* in that each hyperedge has the capacity to contain more (or possibly less) than two nodes. This generalization is illustrated by Fig. 1a, in which the hyperedges enclose their corresponding nodes. For large hypergraphs, this graphical representation can be cumbersome to draw. Alternatively, a hypergraph can be represented by a $p \times q$ binary matrix wherein non-zero entries indicate node-hyperedge membership. The matrix representation of Fig. 1a is depicted in Fig. 1b. Representing $\mathcal{H}$ as a matrix, the two conditions of Def. 6 ensure that no row or column of $\mathcal{H}$ is completely filled with zeros. Henceforth, $\mathcal{H}$ will be used to denote both a hypergraph and its corresponding matrix representation.

Definition 7. A **weighted hypergraph** is an ordered pair $\mathcal{W} = (\mathcal{H}, \omega)$ consisting of a hypergraph $\mathcal{H}$ and corresponding *weighting* $\omega \in \mathbb{Z}^{\mathcal{E}}_{\geqslant 1}$ over the edges of $\mathcal{H}$.

Definition 8. A **transversal** of a weighted hypergraph $\mathcal{W} = (\mathcal{H}, \omega)$ is a positive-integer solution $t \in \mathbb{Z}^{\mathcal{N}}_{\geqslant 0}$ of the following system of linear inequalities:

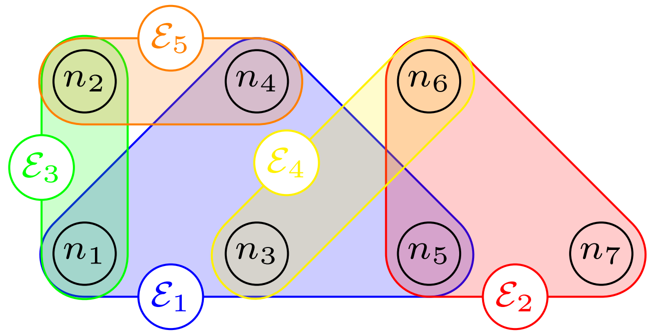
$$t \cdot \mathcal{H} \succcurlyeq \omega \iff \forall \mathcal{E} \in \mathcal{H}, \sum_{n \in \mathcal{E}} t_n \equiv t \cdot \mathcal{E} \geqslant \omega_{\mathcal{E}} \tag{12}$$

The space of all transversals will be denoted $\mathscr{T}_{\succcurlyeq}(\mathcal{W})$.

Definition 9. A transversal $t \in \mathscr{T}_{\succcurlyeq}(\mathcal{W})$ is **minimal** if

$$\nexists t' \in \mathscr{T}_{\succcurlyeq}(\mathcal{W}),\ t' \neq t \text{ and } t' \preccurlyeq t.$$

The space of all minimal transversals will be denoted $\mathscr{T}^*_{\succcurlyeq}(\mathcal{W})$.



(a) Graphical representation of $\mathcal{H}$.

$$\begin{array}{c c}
 & \begin{array}{ccccc} \mathcal{E}_1 & \mathcal{E}_2 & \mathcal{E}_3 & \mathcal{E}_4 & \mathcal{E}_5 \end{array} \\
\begin{array}{c} n_1 \\ n_2 \\ n_3 \\ n_4 \\ n_5 \\ n_6 \\ n_7 \end{array} &
\left(\begin{array}{ccccc}
\mathbf{1} & 0 & \mathbf{1} & 0 & 0 \\
0 & 0 & \mathbf{1} & 0 & \mathbf{1} \\
\mathbf{1} & 0 & 0 & \mathbf{1} & 0 \\
\mathbf{1} & 0 & 0 & 0 & \mathbf{1} \\
\mathbf{1} & \mathbf{1} & 0 & 0 & 0 \\
0 & \mathbf{1} & 0 & \mathbf{1} & 0 \\
0 & \mathbf{1} & 0 & 0 & 0
\end{array}\right)
\end{array}$$

(b) Matrix representation of $\mathcal{H}$.

FIG. 1: Two different representations of a hypergraph $\mathcal{H}$ which has 5 hyperedges and 7 nodes.

In the special case where $\omega = \mathbf{1}$[13], one recovers the notion of a transversal $t \in \{0,1\}^{\mathcal{N}}$ of an *unweighted* hypergraph; $t \cdot \mathcal{H} \succeq \mathbf{1}$ if and only if the support of t intersects every hyperedge of $\mathcal{H}$, i.e. $\forall \mathcal{E},\ t \cdot \mathcal{E} \neq 0$.

The purpose of Section IV C is to provide an algorithm which, when given a weighted hypergraph $\mathcal{W}$, outputs all minimal transversals $\mathscr{T}^*_{\succcurlyeq}(\mathcal{W})$. Procedurally, the algorithm operates inductively over an arbitrary ordering of the hyperedges in $\mathcal{W}$. It begins by minimally solving the first inequality $t \cdot \mathcal{E}_1 \geqslant \omega_{\mathcal{E}_1}$ of Eq. (12) and then subsequently solving the the $(k+1)$-th inequality $t \cdot \mathcal{E}_{k+1} \geqslant \omega_{\mathcal{E}_{k+1}}$ given a minimal solution for first k inequalities. By construction, these *partial* solutions are transversals of a partial weighted hypergraph.

Definition 10. The **partial weighted hypergraph** $\mathcal{W}_k$ of $\mathcal{W} = (\mathcal{H}, \omega)$ is a weighted hypergraph consisting of the first k hyperedges of $\mathcal{H}$ and corresponding weights from ω.

$$\mathcal{W} = (\mathcal{H}, \omega) = \big(\{\mathcal{E}_1, \ldots, \mathcal{E}_q\}, \{\omega_{\mathcal{E}_1}, \ldots, \omega_{\mathcal{E}_q}\}\big)$$
$$\mathcal{W}_k = (\{\mathcal{E}_1, \ldots, \mathcal{E}_k\}, \{\omega_{\mathcal{E}_1}, \ldots, \omega_{\mathcal{E}_k}\}) \qquad 1 \leq k \leq q$$

In the special case of $\omega = \mathbf{1}_{\mathcal{E}}$, it is customary to identify a class of hypergraphs known as *simple* or *Sperner* hypergraphs wherein $\forall i, j : \mathcal{E}_i \subseteq \mathcal{E}_j \Rightarrow j = i$ [22]. Non-simple

[13] Here $\mathbf{1}$ denotes the vector containing all ones.

hypergraphs possess a redundancy: whenever $\mathcal{E}_i \subset \mathcal{E}_j$, any $t \subseteq \mathcal{N}$ which satisfies $t \cap \mathcal{E}_i \neq 0$ automatically satisfies $t \cap \mathcal{E}_j \neq 0$ and hence any such $\mathcal{E}_j$ can be ignored by any transversal generation algorithm. Analogous redundancies are absent from the ω-transversal generation problem because $\omega \in \mathbb{Z}^{\mathcal{E}}_{\geq 1}$ is arbitrary.

B. Generalized Nodes

In the original algorithm of Kavvadias and Stavropoulos [18], the concept of a *generalized node* was introduced in order to improve the total running time and reduce memory requirements. The algorithm presented in Section IV C also utilizes these generalized nodes and benefits significantly by reducing the number of intermediate partial transversals.

Let $\mathcal{X}_k$ be the generalized nodes of $\mathcal{H}_k$. The generalized nodes $\mathcal{X}_{k+1}$ of $\mathcal{H}_{k+1} = \mathcal{H}_k \cup \{\mathcal{E}_{k+1}\}$ can be computed using only $\mathcal{X}_k$ and $\mathcal{E}_{k+1}$. The following procedure accomplishes this as well as classifies each

(α) If $X \cap \mathcal{E}_{k+1} = \emptyset$, then $X \in \mathcal{X}^{\alpha}_{k+1}$.

(β) If $X \subseteq \mathcal{E}_{k+1}$, then $X \in \mathcal{X}^{\beta}_{k+1}$.

(γ) If $X \cap \mathcal{E}_{k+1} \neq \emptyset$ and $X \not\subseteq \mathcal{E}_{k+1}$, then

- (γ_1) $X \setminus (X \cap \mathcal{E}_{k+1}) \in \mathcal{X}^{\gamma_1}_{k+1}$,
- (γ_2) $X \cap \mathcal{E}_{k+1} \in \mathcal{X}^{\gamma_2}_{k+1}$.

As a special case, if $\mathcal{E}_{k+1}$ introduces any new nodes not captured by $\mathcal{X}_k$, these nodes form a unique type δ in $\mathcal{X}_{k+1}$.

(δ) If $\delta X \equiv \mathcal{E}_{k+1} \cap \left(\bigcup_{X \in \mathcal{X}_k} X\right)$, then $\delta X \in \mathcal{X}^{\delta}_{k+1}$.

C. An Algorithm

$$
\begin{array}{c|cccccc}
 & \mathcal{E}_1 & \mathcal{E}_2 & \mathcal{E}_3 & \mathcal{E}_4 & \mathcal{E}_5 & \mathcal{E}_6 \\
\hline
n_1 & \mathbf{1} & 0 & 0 & \mathbf{1} & 0 & 0 \\
n_2 & 0 & \mathbf{1} & \mathbf{1} & \mathbf{1} & \mathbf{1} & 0 \\
n_3 & \mathbf{1} & 0 & 0 & 0 & 0 & \mathbf{1} \\
n_4 & \mathbf{1} & 0 & 0 & 0 & \mathbf{1} & 0 \\
n_5 & \mathbf{1} & \mathbf{1} & 0 & 0 & \mathbf{1} & \mathbf{1} \\
n_6 & 0 & \mathbf{1} & \mathbf{1} & \mathbf{1} & 0 & \mathbf{1} \\
n_7 & 0 & 0 & \mathbf{1} & 0 & \mathbf{1} & 0
\end{array}
$$

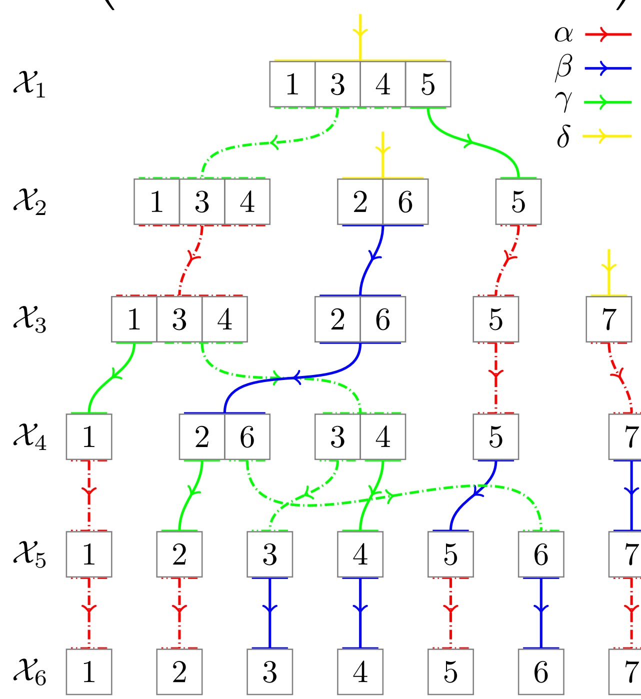


FIG. 2: The Generalized Node Tree of a hypergraph $\mathcal{H}$ which has 6 hyperedges and 7 nodes.

Algorithm 1: Generation of Minimal Solutions

Procedure `WKS`($\mathcal{G}$, U, ϵ):
  Input : An instruction set $\mathcal{G}$, a unitary U, and accuracy $\epsilon > 0$
  Output: $S \in \langle \mathcal{G} \rangle$ such that $d(S_\times, U) < \epsilon$
Choose $\eta \geq \mathcal{O}\left(\frac{d^2-1}{\log|\mathcal{G}|}\log(1/\epsilon)\right)$
$T \leftarrow \bigcup_{\ell=0}^{\eta} \mathcal{G}^\ell$
for $S \in T$ **do**
  $S_\times \leftarrow \prod_{g \in S} g$
  if $d(S_\times, U) < \epsilon$ **then**
    return S
  end
end

Algorithm 2: Canonical Minimalization Procedure

Procedure `CanonicalMinimal`($\mathcal{W}$, t):
  Input : A weighted hypergraph $\mathcal{W} = (\mathcal{H}, \omega)$ and a transversal $t \in \mathscr{T}_{\succcurlyeq}(\mathcal{W})$.
  Output: A minimal transversal $\Gamma_{\mathcal{W}}(t) \in \mathscr{T}^*_{\succcurlyeq}(\mathcal{W})$ such that $\Gamma_{\mathcal{W}}(t) \preccurlyeq t$.
for $n \in \sigma(t)$ **do**
  if $(t - \delta_n) \in \mathscr{T}_{\succcurlyeq}(\mathcal{W})$ **then**
    return `CanonicalMinimal`($\mathcal{W}$, $t - \delta_n$)
  end
end
return t

Algorithm 3: Solving the k-th Inequality

```
Procedure kSolve(t, W^g_{k-1}, X_k):
  Input : A minimal transversal t ∈ 𝒯*_⪰(W^g_{k-1}), the
          associated generalized partial hypergraph
          W^g_{k-1}, and generalized nodes X_k for W^g_k.
  Output: The set of all minimal transversals of.
for n ∈ σ(t) do
    if (t − δ_n) ∈ 𝒯_⪰(W) then
        return CanonicalMinimal(W, t − δ_n)
    end
end
return t
```

Definition 11. Given a set of generalized nodes $\mathcal{X}$ for $\mathcal{N}$, define the **unpacking operation** $\mathrm{U}_{\mathcal{X}}$ which takes any vector $t \in \mathbb{Z}_{\geq 0}^{\mathcal{X}}$ to a family of vectors $\mathrm{U}_{\mathcal{X}}(t) \subset \mathbb{Z}_{\geq 0}^{\mathcal{N}}$:

$$\mathrm{U}_{\mathcal{X}}(t) \equiv \left\{ t' \in \mathbb{Z}_{\geq 0}^{\mathcal{N}} \middle| \forall X \in \mathcal{X}, \sum\nolimits_{n \in X} t'_n = t_X \right\}$$

$$|\mathrm{U}_{\mathcal{X}}(t)| = \prod_{X \in \mathcal{X}} \binom{t_X + |X| - 1}{t_X}$$

$$\widetilde{\mathcal{T}}_{\succeq \omega_{k]}}\left(\mathcal{H}_{k]}\right) = \mathrm{U}_{\mathcal{X}_k}\left(\widetilde{\mathcal{T}}^{\mathcal{X}_k}_{\succeq \omega_{k]}}\left(\mathcal{H}_{k]}\right)\right)$$

$$\mathcal{X}_k = \mathcal{X}_k^{\alpha} \sqcup \mathcal{X}_k^{\beta} \sqcup \mathcal{X}_k^{\gamma_1} \sqcup \mathcal{X}_k^{\gamma_2} \sqcup \mathcal{X}_k^{\delta}$$

$$\mathcal{X}_k \equiv \mathcal{X}_k^{\alpha,\beta,\gamma_1,\gamma_2,\delta}$$

Definition 12.

$$\mathcal{T}(\mathcal{H}, \omega) \equiv \left\{ t \in \mathbb{Z}_{\geq 0}^{\mathcal{N}} \mid t \cdot \mathcal{H} \succeq \omega \right\}$$

$$\widetilde{\mathcal{T}}(\mathcal{H}, \omega) \equiv \{ t \in \mathcal{T}(\mathcal{H}, \omega) \mid \nexists t' \in \mathcal{T}(\mathcal{H}, \omega), t' \neq t, t' \preceq t \}$$

$$\mathcal{T}_k(\mathcal{H}, \omega) \equiv \left\{ t \in \mathbb{Z}_{\geq 0}^{\mathcal{N}} \mid t \cdot \mathcal{E}_i \geq \omega_i, 1 \leq i \leq k \right\}$$

$$\mathcal{T}_k(\mathcal{H}, \omega) \equiv \left\{ t \in \mathbb{Z}_{\geq 0}^{\mathcal{N}} \mid t \cdot \mathcal{H} \succeq_k \omega \right\}$$

$$\mathcal{T}_k^{\mathcal{X}}\left(\mathcal{H}_{k]}, \omega_{k]}\right) \equiv \left\{ t \in \mathbb{Z}_{\geq 0}^{\mathcal{X}} \mid t \cdot \mathcal{H} \succeq_k \omega \right\}$$

$$\mathcal{T}\left(\mathcal{H}_{k]}^{g}, \omega_{k]}\right) \equiv \left\{ t \in \mathbb{Z}_{\geq 0}^{\mathcal{N}\left(\mathcal{H}_{k]}^{g}\right)} \mid t \cdot \mathcal{H}_{k]}^{g} \succeq \omega_{k]} \right\}$$

Shorthand,

$$\mathcal{X}_k \equiv \mathcal{N}\left(\mathcal{H}_{k]}^{g}\right)$$

Begin with $\mathcal{T}\left(\mathcal{H}_{1]}^{g}, \omega_{1]}\right) = \{t\}$ which corresponds to a single generalized transversal $t \in \mathbb{Z}_{\geq 0}^{\mathcal{X}_1}$. Since $\mathcal{X}_k$ only contains one generalized node $\mathcal{X}_1 = \{\mathcal{E}_1\}$, the initial generalized transversal has $t_{\mathcal{X}_1} = \omega_1$,

$$\mathcal{T}_k^{\mathcal{X}}(, \omega) \equiv \left\{ t \in \mathbb{Z}_{\geq 0}^{\mathcal{X}} \mid t \cdot \mathcal{H} \succeq_k \omega \right\}$$

$$\mathcal{T}_q(\mathcal{H}, \omega) = \mathcal{T}(\mathcal{H}, \omega)$$

$$\mathcal{T}_1(\mathcal{H}, \omega) = \left\{ t \in \mathbb{Z}_{\geq 0}^{\mathcal{N}} \mid t \cdot \mathcal{E}_1 \geq \omega_1 \right\}$$

$$\mathcal{T}_1(\mathcal{H}, \omega) = \left\{ t \in \mathbb{Z}_{\geq 0}^{\mathcal{N}} \mid t \cdot \mathcal{E}_1 \geq \omega_1 \right\}$$

$$\mathcal{T}(\mathcal{H}, \omega) \equiv \left\{ t \in \mathbb{Z}_{\geq 0}^{\mathcal{N}} \mid t \cdot \mathcal{E}_i \leq \omega_i, 1 \leq i \leq q \right\}$$

Given the minimal solutions $\widetilde{\mathcal{T}}\left(\mathcal{H}_{k]}, \omega_{k]}\right)$, how does one find the minimal solutions $\widetilde{\mathcal{T}}\left(\mathcal{H}_{k+1]}, \omega_{k+1]}\right)$? Given a particular partial solution $t \in \widetilde{\mathcal{T}}\left(\mathcal{H}_{k]}, \omega_{k]}\right)$

Definition 13. Given $t \in \widetilde{\mathcal{T}}^{\mathcal{X}_k}_{\succeq \omega_{k]}}\left(\mathcal{H}_{k]}\right)$, the **offspring** $\mathcal{O}(t)$ of t are all minimal $\omega_{k]}$-transversals of $\mathcal{H}_{k]}$ in terms of the generalized nodes $\mathcal{X}_{k+1}$. $\mathcal{O}(t)$ is the set of all $t' \in \mathbb{Z}_{\geq 0}^{\mathcal{X}_{k+1}}$

- $\forall X \in \mathcal{X}_{k+1}^{\alpha} \cup \mathcal{X}_{k+1}^{\beta}, t'_X = t_X$ and
- $\forall X_1 \in \mathcal{X}_{k+1}^{\gamma_1}, X_2 \in \mathcal{X}_{k+1}^{\gamma_2}$ such that $X_1 \cup X_2 \in \mathcal{X}_k$

$$\mathcal{E}_{k+1} = \mathcal{X}_{k+1}^{\beta} \sqcup \mathcal{X}_{k+1}^{\gamma_2} \sqcup \mathcal{X}_{k+1}^{\delta}$$

Given transversal t, each offspring $t' \in \mathcal{O}(t)$ already covers edge $\mathcal{E}_{k+1}$ an amount η.

$$\eta \equiv t' \cdot \mathcal{E}_{k+1} = \sum_{X \in \mathcal{X}_{k+1}^{\beta} \sqcup \mathcal{X}_{k+1}^{\gamma_2}} t_X$$

If $\eta < \omega_{k+1}$ then the offspring t' needs to be supplemented by $s \in \mathbb{Z}_{\geq 0}^{\mathcal{X}_{k+1}}$ such that s covers the remaining weight for edge $\mathcal{E}_{k+1}$. Explicitly, s needs to be constructed such that,

$$s \cdot \mathcal{E}_{k+1} = \sum_{X \in \mathcal{X}_{k+1}^{\beta,\gamma_2,\delta}} s_X = \omega_{k+1} - \eta$$

$$\mathcal{S}(t') \equiv t_X$$

V. CONCLUSIONS

A. Unsolved

Consider γ_1, γ_2 and $\gamma_1 + \gamma_2$.

$$I(\gamma_a) = \left\{ (\gamma_a + \tilde{\gamma}_a) \cdot \mathsf{p}_* \mathcal{V} \geq 0 \mid \tilde{\gamma}_a \in \mathrm{Tr}_{\omega(\gamma_a)}(\mathcal{H}(\gamma_a)) \right\} \quad a = 1, 2$$

ACKNOWLEDGMENTS

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