

# Inequalities Witnessing Quantum Incompatibility in The Triangle Scenario

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This document is my current working draft of a paper to do with causal inference, inflation, incompatibility inequalities, hypergraph transversals and quantum correlations.

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## I. INTRODUCTION

## II. DEFINITIONS & NOTATION

**Definition 1.** Borrowing the notation from [?], each random variable  $v$  has a set of all possible outcomes called the **outcome space** or **valuation space** and is denoted  $O_v$ . When referencing a *specific* element of  $O_v$  or *valuation* of  $v$ , the notation  $o[v]$  is used. This notation generalizes to set of random variables  $V = \{v_1, \dots, v_{|V|}\}$ ; a specific outcome of  $o[V] \in O_V$  is used to reference a particular tuple or vector of outcomes,

$$o[V] \equiv (o[v_1], o[v_2], \dots, o[v_{|V|}]) = (o[v])_{v \in V} \quad (1)$$

It is important to note that the ordering of events in ?? is irrelevant. Similarly, the outcome space  $O_V$  for a set of random variables  $V$  is the **valuation product** of the individual outcome spaces,

$$O_V \equiv O_{v_1} \times \dots \times O_{v_{|V|}}$$

Where ‘ $\times$ ’ denotes is defined such that,

$$o[A] \times o[B] \equiv (o[a_1], \dots, o[a_{|A|}], o[b_1], \dots, o[b_{|B|}])$$

When referencing the probability that and set of variables  $V$  has outcome  $o[V]$  (say  $v_1 = 0, v_2 = 3$ ), we intend for the following class of notations to be used interchangeably.

$$P_V(o[V]) = P(o[V]) = P(o[v_1] o[v_2]) = P(v_1 = 0, v_2 = 3) = P(v_2 = 3, v_1 = 0) = P_{v_1, v_2}(03)$$

**Definition 2.** An outcome  $o[V]$  is said to be **extendable** to an outcome  $o[W]$  (where  $V \subseteq W$ ) if there exists an outcome  $o[W \setminus V]$  such that:

$$o[W] = o[W \setminus V] \times o[V]$$

The idea being that a *less specific* outcome  $o[V]$  can be made *more specific* by assigning outcomes to the remaining random variables in  $W \setminus V$ . If such an outcome  $o[W \setminus V]$  exists, it is unique.

**Definition 3.** The set of all extendable outcomes of  $o[V]$  in  $O_W$  is called the **extendable set** and can be written as,

$$o[V] \times O_{W \setminus V} \equiv \{o[W] \in O_W \mid \exists o[W \setminus V] : o[W \setminus V] \times o[V] = o[W]\}$$

The extendable set of  $o[V]$  in  $W$  is the set of all outcomes of  $O_W$  that *agree* with  $o[V]$  about valuations for variables in  $V$ . In this language, two outcomes  $o[V]$  and  $o[W]$  are **compatible** if they are both extendable to some outcome  $o[V \cup W]$ . Equivalently,  $o[V]$  and  $o[W]$  agree on their valuations of  $V \cap W$ .

**Example 4.** Consider two sets of random variables  $V = \{a, b\}$  and  $W = \{a, b, c\}$ . Clearly  $V \subseteq W$ ; a prerequisite for extendability. Also take all individual outcome spaces to be finite and of order 3:  $O_a = O_b = O_c = \{1, 2, 3\}$ . Then  $o[V] = o[\{a, b\}] = (a = 1, b = 2)$  is extendable to the outcome  $o[W] = (a = 1, b = 2, c = 1)$ , and the extendable set of  $o[V]$  in  $O_W$  is,

$$o[\{a, b\}] \times O_c = \{(a = 1, b = 2, c = 1), (a = 1, b = 2, c = 2), (a = 1, b = 2, c = 3)\}$$

**Definition 5.** A **graph** is an ordered tuple  $(\mathcal{N}, \mathcal{E})$  of *nodes* and *edges* respectively where the nodes can represent any object and the edges are pairs of nodes. For convenience of notation, one defines an index set over the nodes denoted  $\mathcal{I}_{\mathcal{N}}$ .

$$\mathcal{N} = \{n_i \mid i \in \mathcal{I}_{\mathcal{N}}\} \quad \mathcal{E} = \{\{n_j, n_k\} \mid j, k \in \mathcal{I}_{\mathcal{N}}\}$$

**Definition 6.** A **directed graph**  $\mathcal{G}$  is an ordered tuple  $(\mathcal{N}, \mathcal{E})$  of *nodes* and *edges* respectively where the nodes can represent any object and the edges are *ordered* pairs of nodes. For convenience of notation, one defines an index set over the nodes denoted  $\mathcal{I}_{\mathcal{N}}$ .

$$\mathcal{N} = \{n_i \mid i \in \mathcal{I}_{\mathcal{N}}\} \quad \mathcal{E} = \{n_j \rightarrow n_k \mid j, k \in \mathcal{I}_{\mathcal{N}}\}$$

**Definition 7.** The following definitions are common language in directed graph theory. Let  $n, m \in \mathcal{N}$  be example nodes of the graph  $\mathcal{G}$ .

- The **parents of a node**:  $\text{Pa}_{\mathcal{G}}(n) \equiv \{m \mid m \rightarrow n\}$
- The **children of a node**:  $\text{Ch}_{\mathcal{G}}(n) \equiv \{m \mid n \rightarrow m\}$
- The **ancestry of a node**:  $\text{An}_{\mathcal{G}}(n) \equiv \bigcup_{i \in \mathbb{W}} \text{Pa}_{\mathcal{G}}^i(n)$  where  $\text{Pa}_{\mathcal{G}}^i(n) \equiv \text{Pa}_{\mathcal{G}}(\text{Pa}_{\mathcal{G}}^{i-1}(n))$  and  $\text{Pa}_{\mathcal{G}}^0(n) = n$

All of these terms can be generalized to sets of nodes  $N \subseteq \mathcal{N}$  through union over the elements,

- The **parents of a node set**:  $\text{Pa}_{\mathcal{G}}(N) \equiv \bigcup_{n \in N} \text{Pa}_{\mathcal{G}}(n)$
- The **children of a node set**:  $\text{Ch}_{\mathcal{G}}(N) \equiv \bigcup_{n \in N} \text{Ch}_{\mathcal{G}}(n)$
- The **ancestry of a node set**:  $\text{An}_{\mathcal{G}}(N) \equiv \bigcup_{n \in N} \text{An}_{\mathcal{G}}(n)$

Moreover, an **induced subgraph** of  $\mathcal{G}$  due to a set of nodes  $N \subseteq \mathcal{N}$  is the graph composed of  $N$  and all edges  $e \in \mathcal{E}$  of the original graph that are contained in  $N$ .

$$\text{Sub}_{\mathcal{G}}(N) \equiv (N, \{e_i \mid i \in \mathcal{I}_{\mathcal{E}}, e_i \subseteq N\})$$

An **ancestral subgraph** of  $\mathcal{G}$  due to  $N \subseteq \mathcal{N}$  is the induced subgraph due to the ancestry of  $N$ .

$$\text{AnSub}_{\mathcal{G}}(N) \equiv \text{Sub}_{\mathcal{G}}(\text{An}_{\mathcal{G}}(N))$$

**Definition 8.** A **directed acyclic graph** or **DAG**  $\mathcal{G}$  is an directed graph ?? with the additional property that no node  $n$  is in its set of **ancestors**.

$$\forall n \in \mathcal{N} : n \notin \bigcup_{i \in \mathbb{N}} \text{Pa}_{\mathcal{G}}^i(n)$$

Notice the difference between using the natural numbers  $\mathbb{N}$  to distinguish *ancestors* from *ancestry*.

**Definition 9.** A **hypergraph** denoted  $\mathcal{H}$  is an ordered tuple  $(\mathcal{N}, \mathcal{E})$  of *nodes* and *edges* respectively where the nodes can represent any object and the edges are *subsets* of nodes. For convenience of notation, one defines an index set over the nodes and edges of a hypergraph  $\mathcal{H}$  denoted  $\mathcal{I}_{\mathcal{N}}$  and  $\mathcal{I}_{\mathcal{E}}$  respectively.

$$\mathcal{H} = (\mathcal{N}, \mathcal{E}) \quad \mathcal{N} = \{n_i \mid i \in \mathcal{I}_{\mathcal{N}}\} \quad \mathcal{E} = \{e_i \mid i \in \mathcal{I}_{\mathcal{E}}, e_i \subseteq \mathcal{N}\}$$

Note that whenever the index for an edge or node is arbitrary, it will be omitted. There is a dual correspondence between edges  $e \in \mathcal{E}$  and nodes  $n \in \mathcal{N}$  in a Hypergraph. An edge  $e$  is viewed as a set of nodes  $\{n_i\}$ , and a node  $n$  can be viewed as the set of edges  $\{e_i\}$  that contain it.

**Definition 10.** A **hypergraph transversal** (or edge hitting set)  $\mathcal{T}$  of a hypergraph  $\mathcal{H}$  is a set of nodes  $\mathcal{T} \subseteq \mathcal{N}$  that have non-empty intersections with every edge in  $\mathcal{E}$ .

$$\mathcal{T} = \{n_i \in \mathcal{N} \mid i \in \mathcal{I}_{\mathcal{T}}\} \quad \forall e \in \mathcal{E} : \mathcal{T} \cap e \neq \emptyset$$

**Definition 11.** A **minimal hypergraph transversal**  $\mathcal{T}$  is any valid transversal (??) of  $\mathcal{H}$  where every node  $n$  is *necessary* to retain validity. For each node  $n$  in  $\mathcal{T}$ ,  $\mathcal{T} \setminus n$  is no longer a transversal.

$$\mathcal{T} = \{n_i \in \mathcal{N} \mid i \in \mathcal{I}_{\mathcal{T}}\} \quad \forall i \in \mathcal{I}_{\mathcal{T}}, \exists e \in \mathcal{E} : (\mathcal{T} \setminus n_i) \cap e = \emptyset$$

**Definition 12.** A **weighted hypergraph**  $\mathcal{H}_{\mathcal{W}}$  is a regular hypergraph satisfying ?? equipped with a set of weights  $\mathcal{W}$  ascribed to each node such that a weighted hypergraph is written as a triplet  $(\mathcal{W}, \mathcal{N}, \mathcal{E})$ .

$$\mathcal{W} = \{w_i \mid i \in \mathcal{I}_{\mathcal{N}}, w_i \in \mathbb{R}\}$$

One would say that a particular node  $n_i$  carries weight  $w_i$  for each  $i \in \mathcal{I}_{\mathcal{N}}$ .

**Definition 13.** A **bounded transversal** of a weighted hypergraph  $\mathcal{H}_{\mathcal{W}}$  is a transversal  $\mathcal{T}$  of the unweighted hypergraph  $\mathcal{H}$  and a real number  $t$  (denoted  $\mathcal{T}_{\leq t}$ ) such that the sum of the node weights of the transversal is bounded by  $t$ .

$$\mathcal{T}_{\leq t} = \{n_i \mid i \in \mathcal{I}_{\mathcal{T}}\} \quad \text{s.t.} \quad \sum_{j \in \mathcal{I}_{\mathcal{T}}} w_j \leq t$$

One can define analogous **(strictly) upper/lower bounded transversals** by considering modifications of the notation:  $\mathcal{T}_{< t}, \mathcal{T}_{\geq t}, \mathcal{T}_{> t}$ .

**Definition 14.** A **causal structure** is simply a DAG with the extra classification of each node into one of two categories; the **latent nodes** and **observed nodes** denoted  $\mathcal{N}_L$  and  $\mathcal{N}_O$ . The latent nodes correspond to random variables that are either hidden through some fundamental process or cannot/will not be measured. The observed nodes are random variables that are measurable. Every node is either latent or observed and no node is both:

$$\mathcal{N}_L \cap \mathcal{N}_O = \emptyset \quad \mathcal{N}_L \cup \mathcal{N}_O = \mathcal{N}$$

**Definition 15.** The **product distribution** two distributions is denoted as usual with  $\times$  and is defined as,

$$(P_v \times P_w)(o[v], o[w]) \equiv P_v(o[v]) P_w(o[w])$$

A product distribution of  $k$  distributions is defined recursively,

$$\prod_{i=1}^k P_{v_i} \equiv (P_{v_1} \times \cdots \times P_{v_k})$$

**Definition 16.** The **marginalization** of a distribution  $P_{v \cup w}$  to the distribution  $P_v$  is denoted  $\sum_w P_{v \cup w} = P_v$  and is defined such that,

$$\forall o[v] \in O_v : \left( \sum_w P_{v,w} \right)(o[v]) \equiv \sum_{o[w] \in O_w} P_{v,w}(o[v], o[w])$$

Todo (TC Fraser): How many definitions do I need to write??

### III. TRIANGLE SCENARIO

Todo (TC Fraser): Discuss the triangle scenario, previous work done on it, etc. Focusing on the inflation depicted in ??, we obtained the maximally pre-injectable sets through the procedure outlined in [? ].

Maximal Pre-injectable Sets $\Pi$	Ancestral Independences	
$\{A_1, B_1, C_1, A_4, B_4, C_4\}$	$\{A_1, B_1, C_1\} \perp \{A_4, B_4, C_4\}$	
$\{A_1, B_2, C_3, A_4, B_3, C_2\}$	$\{A_1, B_2, C_3\} \perp \{A_4, B_3, C_2\}$	
$\{A_2, B_3, C_1, A_3, B_2, C_4\}$	$\{A_2, B_3, C_1\} \perp \{A_3, B_2, C_4\}$	
$\{A_2, B_4, C_3, A_3, B_1, C_2\}$	$\{A_2, B_4, C_3\} \perp \{A_3, B_1, C_2\}$	
$\{A_1, B_3, C_4\}$	$\{A_1\} \perp \{B_3\} \perp \{C_4\}$	
$\{A_1, B_4, C_2\}$	$\{A_1\} \perp \{B_4\} \perp \{C_2\}$	
$\{A_2, B_1, C_4\}$	$\{A_2\} \perp \{B_1\} \perp \{C_4\}$	
$\{A_2, B_2, C_2\}$	$\{A_2\} \perp \{B_2\} \perp \{C_2\}$	
$\{A_3, B_3, C_3\}$	$\{A_3\} \perp \{B_3\} \perp \{C_3\}$	
$\{A_3, B_4, C_1\}$	$\{A_3\} \perp \{B_4\} \perp \{C_1\}$	
$\{A_4, B_1, C_3\}$	$\{A_4\} \perp \{B_1\} \perp \{C_3\}$	
$\{A_4, B_2, C_1\}$	$\{A_4\} \perp \{B_2\} \perp \{C_1\}$	(2)

As can be counted, there are 12 maximally pre-injectable sets which will be indexed 1 through 12 in the order seen above ( $\Pi = \{\Pi_1, \dots, \Pi_{12}\}$ )

### IV. SUMMARY OF THE INFLATION TECHNIQUE

The causal inflation technique, first pioneered by Wolfe, Spekkens, and Fritz [? ] and inspired by the *do calculus* and *twin networks* of Ref. [? ], is a family of causal inference techniques that can be used to determine if a probability distribution is compatible or incompatible with a given causal structure. As a preliminary summary, the inflation technique begins by *augmenting* a causal structure with additional nodes, producing the *inflated* causal structure, and then exposes how causal inference tasks on the inflated causal structure can be used to make inferences on the original causal structure. Equipped with the common graph-theoretic terminology and notation of ??, an inflation can be formally defined as follows:

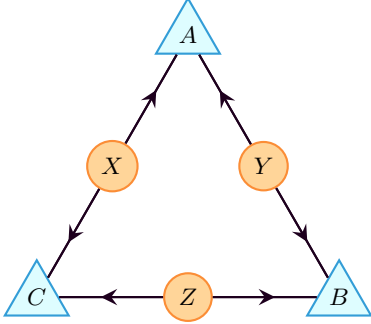


FIG. 1. The casual structure of the triangle scenario. Three variables  $A, B, C$  are observable and illustrated as triangles, while  $X, Y, Z$  are latent variables illustrated as circles.

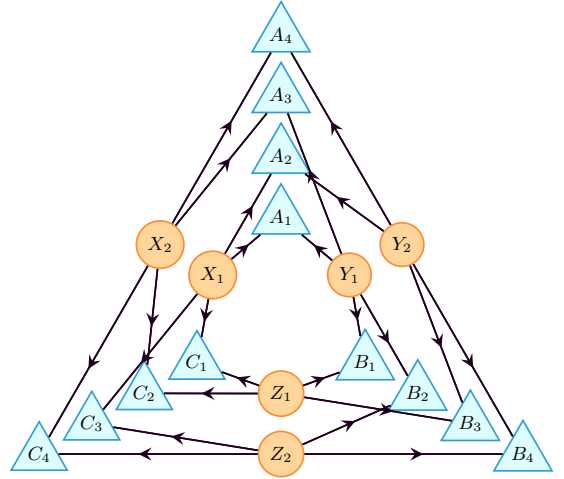


FIG. 2. An inflated causal structure of the triangle scenario ??.

**Definition 17.** An **inflation** of a causal structure  $\mathcal{G}$  is another causal structure  $\mathcal{G}'$  such that:

$$\forall n' \in \mathcal{N}' : \text{AnSub}_{\mathcal{G}'}(n') \sim \text{AnSub}_{\mathcal{G}}(n)$$

Where ‘ $\sim$ ’ is notation for equivalence up to removal of the copy-index. To clarify, each node in an inflated causal structure  $n' \in \mathcal{N}'$  shares a *label* assigned to a node  $n \in \mathcal{N}$  in the original causal structure together with an additional index called the **copy-index**.

**Definition 18.** A set of **causal parameters** for a particular causal structure  $\mathcal{G}$  is the specification of a conditional distribution for every node  $n \in \mathcal{N}$  given it’s parents in  $\mathcal{G}$ .

$$\left\{ P_{n|\text{Pa}_{\mathcal{G}}(n)} \mid n \in \mathcal{N} \right\}$$

Todo (TC Fraser): Clean up what is meant by copy index, example maybe? Todo (TC Fraser): Define injectable sets Todo (TC Fraser): Define pre-injectable sets and then it’s connection to probabilities Todo (TC Fraser): Define pre-injectable sets Todo (TC Fraser): State the main Compatibility lemma of inflation

## V. COMPATIBILITY, CONTEXTUALITY AND THE MARGINAL PROBLEM

In order to determine if a given marginal distribution  $P_V$  or set of marginal distributions  $\{P_{V_1}, \dots, P_{V_k}\}$  is compatible with a causal structure  $\mathcal{G}$ , one should first formalize what is meant by *compatible*.

**Definition 19.** A marginal distribution  $P_V$  is **compatible** with a causal structure  $\mathcal{G}$  (where it is assumed that  $V \subseteq \mathcal{N}_O$ ) if there exists a *choice* of causal parameters  $\left\{ P_{n|\text{Pa}_{\mathcal{G}}(n)} \mid n \in \mathcal{N} \right\}$  such that  $P_V$  can be *recovered* from the following series of operations:

Todo (TC Fraser): Define this notation here

1. First obtain a joint distribution over *all* nodes of of the causal structure,

$$P_{\mathcal{N}} = \prod_{n \in \mathcal{N}} P_{n|\text{Pa}_{\mathcal{G}}(n)}$$

2. Then marginalize over the latent nodes of  $\mathcal{G}$ ,

$$P_{\mathcal{N}_O} = \sum_{\mathcal{N}_L} P_{\mathcal{N}}$$

3. Finally marginalize over the observed nodes not in  $V$  to obtain  $P_V$ ,

$$P_V = \sum_{\mathcal{N}_O \setminus V} P_{\mathcal{N}_O}$$

A set of marginal distributions  $\{P_{V_1}, \dots, P_{V_k}\}$  is compatible with  $\mathcal{G}$  if each of the distributions can be made compatible by the *same* choice of causal parameters. A distribution  $P_V$  or set of distributions  $\{P_{V_1}, \dots, P_{V_k}\}$  is said to be **incompatible** with a causal structure if there *does not exist* a set of causal parameters with the above mentioned property.

Todo (TC Fraser): Source this?

Operations 2 and 3 of ?? are related to the *marginal problem*.

**Definition 20. The Marginal Problem:** Given a set of distributions  $\{P_{V_1}, \dots, P_{V_k}\}$  where  $V_i \subseteq \mathcal{V}$  for some set of random variables  $\mathcal{V}$  and  $k \geq 2$ , does there exist a joint distribution  $P_{\mathcal{V}}$  such that each given distribution  $P_{V_i}$  can be obtained from marginalizing  $P_{\mathcal{V}}$ ?

$$\forall i \in \{1, \dots, k\} : P_{V_i} = \sum_{\mathcal{V} \setminus V_i} P_{\mathcal{V}}$$

Typically (although not strictly necessary),  $\mathcal{V}$  is taken to mean the union of all  $V_i$ 's.

$$\mathcal{V} = V_1 \cup \dots \cup V_k = \bigcup_{i=1}^k V_i \quad (3)$$

**Definition 21.** A reoccurring motif of these discussions will be the set of distributions  $\{P_{V_1}, \dots, P_{V_k}\}$  mentioned in ??. In agreement with [?] we will call this set of distributions a **marginal model** and denote it  $P^{\mathcal{M}}$  provided that they are *compatible*:

$$\forall i \neq j \text{ if } V_i \cap V_j \neq \emptyset \text{ then } \sum_{V_i \setminus V_j} P_{V_i} = \sum_{V_j \setminus V_i} P_{V_j}$$

We call the set of subsets  $\{V_1, \dots, V_k\}$  the marginal contexts or the **maximal marginal scenario** and an individual  $V_i$  a **marginal context**. Finally we will denote the union of all contexts  $\mathcal{V}$  and define it exactly as in ??

Todo (TC Fraser): Discuss Compatibility, connection to cooperative games/resources, bell incompatibility? Todo (TC Fraser): Connection between contextuality and Compatibility via the marginal problem for causal parameters Todo (TC Fraser): Discuss what is meant by a 'complete' solution to the marginal problem Todo (TC Fraser): Maybe define the possibilistic marginal problem for later

## VI. THE FRITZ DISTRIBUTION

The **Fritz distribution**  $P_F$  is a quantum-accessible distribution known to be incompatible with the triangle scenario. Explicitly,  $P_F$  is a three-party  $(A, B, C)$ , four-outcome  $(1, 2, 3, 4)$  distribution that has form as follows:

$$\begin{aligned} P_F(111) &= P_F(221) = P_F(412) = P_F(322) = P_F(233) = P_F(143) = P_F(344) = P_F(434) = \frac{1}{32} (2 + \sqrt{2}) \\ P_F(121) &= P_F(211) = P_F(422) = P_F(312) = P_F(243) = P_F(133) = P_F(334) = P_F(444) = \frac{1}{32} (2 - \sqrt{2}) \end{aligned}$$

Here the notation  $P_F(abc) = P_{ABC}(abc) = P(A=a, B=b, C=c)$  is used. The Fritz distribution  $P_F$  can be realized with the following quantum configuration:

$$\begin{aligned} \rho_{AB} &= |\Psi^+\rangle \langle \Psi^+| \quad \rho_{BC} = \rho_{CA} = |\Phi^+\rangle \langle \Phi^+| \\ M_A &= \{|0\psi_0\rangle \langle 0\psi_0|, |0\psi_\pi\rangle \langle 0\psi_\pi|, |1\psi_{-\pi/2}\rangle \langle 1\psi_{-\pi/2}|, |1\psi_{\pi/2}\rangle \langle 1\psi_{\pi/2}|\} \\ M_B &= \{|\psi_{\pi/4}0\rangle \langle \psi_{\pi/4}0|, |\psi_{5\pi/4}0\rangle \langle \psi_{5\pi/4}0|, |\psi_{3\pi/4}1\rangle \langle \psi_{3\pi/4}1|, |\psi_{-\pi/4}1\rangle \langle \psi_{-\pi/4}1|\} \\ M_C &= \{|00\rangle \langle 00|, |01\rangle \langle 01|, |10\rangle \langle 10|, |11\rangle \langle 11|\} \end{aligned}$$

Where for convenience of notation  $\psi_x$  is used to denote the superposition,

$$|\psi_x\rangle = \frac{1}{\sqrt{2}} (|0\rangle + e^{ix} |1\rangle)$$

Additionally  $|\Psi^+\rangle = \frac{1}{\sqrt{2}} (|01\rangle + |10\rangle)$  and  $|\Phi^+\rangle = \frac{1}{\sqrt{2}} (|00\rangle + |11\rangle)$  are two maximally entangled Bell states. Fritz first proved it's incompatibility [?] by showing  $C$  acts a moderator to ensure measurement pseudo-settings for  $A$  and  $B$  are independent, satisfying non-broadcasting requirements for the standard Bell scenario. In fact, by coarse-graining outcomes for  $A$  and  $B$  and treating  $C$  as a measurement-setting moderator,  $P_F$  maximally violates the CHSH inequality. To illustrate this, begin with the CHSH inequality [?],

$$\langle AB|S_A = 1, S_B = 1\rangle + \langle AB|S_A = 1, S_B = 2\rangle + \langle AB|S_A = 2, S_B = 1\rangle - \langle AB|S_A = 2, S_B = 2\rangle \leq 2 \quad (4)$$

Where  $\langle AB|S_A = i, S_B = j\rangle$  is the correlation between  $A$  and  $B$  given the measurement settings for  $A$  ( $B$ ) is  $i$  ( $j$ ) respectively. Next, each of  $C$ 's outcomes become the condition settings in ??,

$$\langle AB|C = 2\rangle + \langle AB|C = 3\rangle + \langle AB|C = 4\rangle - \langle AB|C = 1\rangle \leq 2$$

Finally, specifying the correlation between  $A$  and  $B$  to be defined in terms of a  $\{1, 2, 3, 4\} \rightarrow \{(1, 4), (2, 3)\}$  coarse-graining,

$$\frac{\sqrt{2}}{2} + \frac{\sqrt{2}}{2} + \frac{\sqrt{2}}{2} - \frac{-\sqrt{2}}{2} \leq 2$$

$$2\sqrt{2} \leq 2$$

Which corresponds to the maximum quantum violation of the CHSH inequality ??

**Todo (TC Fraser): Discuss non-uniqueness and relabeling** **Todo (TC Fraser): Summarize Problem 2.17 in fritz BBT, make it more formal**

## VII. CERTIFICATE INEQUALITIES

### A. Casting the Inflated Marginal Problem as a Linear Program

After obtaining the maximal pre-injectable sets associated with a particular inflation, one can write the marginal problem of ?? as a linear program. The key observation is that marginalization is a *linear* operator that can be performed via a matrix multiplication. To do this, we will define the *marginalization matrix*.

**Definition 22.** The **marginalization matrix**  $M$  for a marginal scenario  $\{V_1, \dots, V_k\}$  is a bit-wise matrix where the columns are indexed by *joint* outcomes  $o[\mathcal{V}] \in O_{\mathcal{V}}$  and the rows are indexed by *marginal* outcomes corresponding to all outcomes  $o[V_i] \in O_{V_i}$  of the marginal contexts  $V_i$ . The entries of  $M$  are populated whenever a row index is extendable to a column index.

$$M_{(o[V_i], o[\mathcal{V}])} = \begin{cases} 1 & \exists o[\mathcal{V} \setminus V_i] \text{ such that } o[V_i] \times o[\mathcal{V} \setminus V_i] = o[\mathcal{V}] \\ 0 & \text{otherwise} \end{cases}$$

The marginalization matrix has  $|O_{\mathcal{V}}|$  columns and  $\sum_{i=1}^k |O_{V_i}|$  rows. The number of non-zero entries of  $M$  is a simple expression,

$$\sum_{i=1}^k |O_{V_i}| |O_{\mathcal{V} \setminus V_i}| = \sum_{i=1}^k |O_{\mathcal{V}}| = k |O_{\mathcal{V}}|$$

Each of the  $k$  elements of  $\{V_1, \dots, V_k\}$  contributes a single non-zero entry to each column of  $M$ , resulting in  $k |O_{\mathcal{V}}|$  total non-zero entries.

Note that the row and column indices of the marginalization matrix will be referred to very frequently. We will refer to the

Todo (TC Fraser): Computationally Efficient generation?

To illustrate this concretely, consider the following example:

**Example 23.** Suppose one has 4 binary random variables  $\mathcal{V} = \{a, b, c\}$  in mind and 2 subsets  $\{\{a, c\}, \{b\}\}$ . Then the marginalization matrix is:

$$M = \begin{matrix} & \begin{matrix} (a,b,c)= \\ (a=0,c=0) \\ (a=0,c=1) \\ (a=1,c=0) \\ (a=1,c=1) \\ (b=0) \\ (b=1) \end{matrix} & \begin{matrix} (0,0,0) & (0,0,1) & (0,1,0) & (0,1,1) & (1,0,0) & (1,0,1) & (1,1,0) & (1,1,1) \end{matrix} \\ \begin{pmatrix} 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 \end{pmatrix} \end{matrix}$$

In order to describe how marginalization can be written as matrix multiplication  $M \cdot x = b$ , we need to describe how to define two more quantities:

**Definition 24.** The **joint distribution vector**  $\mathcal{P}_{\mathcal{V}}$  for a probability distribution  $P_{\mathcal{V}}$  is the vector whose entries are the positive, real-valued probabilities that  $P_{\mathcal{V}}$  assigns to each outcome of  $o[\mathcal{V}]$  of  $O_{\mathcal{V}}$ .  $\mathcal{P}_{\mathcal{V}}$  shares the same indices as the *column* indices of  $M$ .

$$\mathcal{P}_{\mathcal{V}}^T = [P_{\mathcal{V}}(o[\mathcal{V}])]_{o[\mathcal{V}] \in O_{\mathcal{V}}}$$

**Definition 25.** The **marginal distribution vector**  $\mathcal{P}_{\{V_1, \dots, V_k\}}$  for a marginal model  $\{P_{V_1}, \dots, P_{V_k}\}$  is the vector whose entries are probabilities over the set of **marginal outcomes**  $\bigcup_{j=1}^k O_{V_j}$ .  $\mathcal{P}_{\{V_1, \dots, V_k\}}$  shares the same indices as the *row* indices of  $M$ .

$$\mathcal{P}_{\{V_1, \dots, V_k\}}^T = [P_{V_i}(o[V_i])]_{o[V_i] \in \bigcup_{j=1}^k O_{V_j}}$$

The marginal and joint distribution vectors are related via the marginalization matrix  $M$ . Given a joint distribution vector  $\mathcal{P}_{\mathcal{V}}$  one can obtain the marginal distribution vector  $\mathcal{P}_{\{V_1, \dots, V_k\}}$  by multiplying  $M$  by  $\mathcal{P}_{\mathcal{V}}$ .

$$\mathcal{P}_{\{V_1, \dots, V_k\}} = M \cdot \mathcal{P}_{\mathcal{V}} \quad (5)$$

Todo (TC Fraser): Discuss non-unique but consistent ordering of  $M$ ,  $\mathcal{P}_{\mathcal{V}}$  and  $\mathcal{P}_{\{V_1, \dots, V_k\}}$

The marginal problem can now be rephrased in the language of the marginalization matrix. Suppose one obtains a marginal distribution vector  $\mathcal{P}_{\{V_1, \dots, V_k\}}$ . The marginal problem becomes equivalent to the question: *Does there exist a joint distribution vector  $\mathcal{P}_{\mathcal{V}}$  such that ?? holds?*

**Definition 26.** The **Marginal Linear Program** is the following linear program:

$$\begin{aligned} & \text{minimize: } \emptyset \cdot x \\ & \text{subject to: } x \succeq 0 \\ & \quad M \cdot x = \mathcal{P}_{\{V_1, \dots, V_k\}} \end{aligned}$$

If this “optimization”<sup>1</sup> is *feasible*, then there exists a vector  $x$  than can satisfy ?? and is a valid joint distribution vector. Therefore feasibility implies that  $P_{\mathcal{V}} = x$ , solving the marginal problem with positive result. Moreover if the marginal linear program is *infeasible*, then there *does not* exist a joint distribution  $P_{\mathcal{V}}$  over all random variables.

**Definition 27.** The **Dual Marginal Linear Program** is the dual of ?? formulated via a procedure similar to [? ]:

$$\begin{aligned} & \text{minimize: } y \cdot \mathcal{P}_{\{V_1, \dots, V_k\}} \\ & \text{subject to: } y \cdot M \succeq 0 \end{aligned}$$

Where  $y$  is a real valued vector with the same length as  $\mathcal{P}_{\{V_1, \dots, V_k\}}$ .

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<sup>1</sup> “Optimization” is presented in quotes here because the minimization objective is trivially always zero ( $\emptyset$  denotes the null vector of all zero entries). The primal value of the linear program is of no interest, all that matters is its *feasibility*.



## B. Infeasibility Certificates

The dual marginal linear program also provides an answer to the marginal problem. To prove this, first notice that the dual problem is *never infeasible*; by choosing  $y$  to be trivially the null vector  $\emptyset$  of appropriate size, all constraints are satisfied. Secondly if  $y \cdot M \succeq 0$  and  $x \succeq 0$ , then the following must hold if the primal is feasible:

$$y \cdot \mathcal{P}_{\{V_1, \dots, V_k\}} = y \cdot M \cdot x \geq 0 \quad (6)$$

Therefore the *sign* of the dual value  $d \equiv \min (y \cdot \mathcal{P}_{\{V_1, \dots, V_k\}})$  solves the marginal problem. If  $d < 0$  then ?? is violated and therefore the marginal problem has negative result. Likewise if  $d$  satisfies ??, then a joint distribution  $P_{\mathcal{V}}$  exists. Before continuing, an important observation needs to be made. If  $d \geq 0$ , then it is exactly  $d = 0$ , due to the existence of the trivial  $y = \emptyset$ . This observation is an instance of the *Complementary Slackness Property* of [? ]. **Comment (TC Fraser): Is this really the CSP?** Moreover, if  $d < 0$ , then it is unbounded  $d = -\infty$ . This latter point becomes clear upon recognizing that for any  $y$  such that  $d < 0$ , another  $y'$  can be constructed by multiplying  $y$  by a real constant  $\alpha$  greater than one such that,

$$y' = \alpha y \mid \alpha > 1 \implies d' = \alpha d < d$$

Since a more negative  $d'$  can always be found, it must be that  $d$  is unbounded. This is a demonstration of the fundamental *Unboundedness Property* of [? ]; if the dual is unbounded, then the primal is infeasible.

**Comment (TC Fraser): Farkas's lemma here?**

**Definition 28.** An **infeasibility certificate** is any vector  $y$  that satisfies the constraints of ?? and also permits violation of ?? for some marginal distribution vector  $\mathcal{P}_{\{V_1, \dots, V_k\}}$ .

$$y \in \mathbb{R}^{\sum_{i=1}^k |O_{V_i}|} : y \cdot M \succeq 0, \quad y \cdot \mathcal{P}_{\{V_1, \dots, V_k\}} < 0$$

Furthermore, any  $y$  satisfying  $y \cdot M \succeq 0$  induces a **certificate inequality** that constraints the space of marginal distribution vectors which takes the symbolic form of ??,

$$y \cdot \mathcal{P}_{\{V_1, \dots, V_k\}} \geq 0$$

Where the entries of the certificate  $y$  act as coefficients for the entries of  $\mathcal{P}_{\{V_1, \dots, V_k\}}$ .

**Todo (TC Fraser): Discuss Infeasibility Certificates basis**

**Example 29.** The marginal problem for the inflated causal structure  $\mathcal{G}'$  depicted in ?? concerns itself with whether or not distributions over the pre-injectable sets  $\{P_{\Pi_1}, \dots, P_{\Pi_{12}}\}$  admit a joint distribution  $P_{\mathcal{N}'}$  over all nodes of  $\mathcal{G}'$  where  $\mathcal{N}' = \bigcup_{i=1}^{12} \Pi_i$ . The marginalization matrix  $M$  has 16,896 rows and 16,777,216 columns.

$$\begin{aligned} \# \text{ Rows} &= \sum_{i=1}^{12} |O_{\Pi_i}| = \sum_{i=1}^{12} 4^{|\Pi_i|} = 4 \cdot 4^6 + 8 \cdot 4^3 = 16,896 \\ \# \text{ Columns} &= |O_{\mathcal{N}'}| = 4^{|\mathcal{N}'|} = 4^{12} = 16,777,216 \end{aligned}$$

With  $12 \cdot 4^{12} = 201,326,592$  non-zero entries.

**Todo (TC Fraser): Discuss the certificate inequalities we found.**

## VIII. LOGICAL IMPLICATIONS OF NON-CONTEXTUALITY

Following the definition of contextuality given as Definition 2.3 in [? ] **Todo (TC Fraser): Motivate why certificates are not enough, want many solutions**

### A. Logical Implications & Inequalities

Following the work conducted by Mansfield and Fritz [? ], we consider a possibilistic implications of the **(1, n)-type** to be all implications of the form,

$$A \implies C_1 \vee \dots \vee C_n = \bigvee_{i=1}^n C_i \quad (7)$$

Where  $A$  and each of the  $C_i$ 's are simply events or outcomes of a particular set of variables. The letter ' $A$ ' is chosen for the event  $A$  since it takes the place of the logical **antecedent** of  $??$ . Likewise, the letter ' $C$ ' is chosen to represent logical **consequents**. We refer to the set of all  $C_i$ 's simply as  $C = \{C_i \mid i \in 1, \dots, n\}$ . The implication  $??$  can be read as *whenever  $A$  occurs, at least one element of  $C$  also occurs*.

It is possible to turn possibilistic  $(1, n)$ -type implications into probabilistic inequalities by recognizing that the logical implication of  $??$  induces the inequality,

$$P(A) \leq P\left(\bigvee_{i=1}^n C_i\right)$$

Furthermore utilizing Boole's inequality,

$$P\left(\bigvee_{i=1}^n C_i\right) \leq \sum_{i=1}^n P(C_i) \quad (8)$$

Gives,

$$P(A) \leq \sum_{i=1}^n P(C_i) \quad (9)$$

Such that whenever the inequality  $??$  is violated, the implication in  $??$  is violated as well. Note that the converse is *not* true; if the inequality  $??$  holds true, it is still possible for there to be a violation of  $??$ .

*Remark 30.* An important result of Boole's inequality is that  $??$  becomes an exact *equality* whenever elements of  $C$  are pairwise disjoint. Therefore, finding a set  $C$  of pairwise disjoint events satisfying  $??$  will give rise to tighter inequalities.

## B. Implications in the Marginal Problem

The question then remains, *how does non-contextuality give rise to implications of the form of  $??$ ?* We begin by making the principle assumption that a joint distribution *does* exist for a family of marginal distributions  $\{P_{V_1}, \dots, P_{V_k}\}$ . We can then derive logical *tautologies* under this assumption that are of  $(1, n)$ -type, which we call **marginal implications**, using the following train of logic.

1. Suppose a particular marginal outcome  $A \in \bigcup_{i=1}^k O_{V_i}$  happens to occur. For reference, take  $A = o[V_j] \in O_{V_j}$  to belong to the outcome space of  $V_j$  for some index  $j$ .
2. Since a joint distribution exists, then  $A$  refers to some *incomplete* knowledge about some *joint* event  $J$  that actually occurred. In fact,  $J$  is required to belong to the extendable set of  $A$  in  $O_{\mathcal{V}}$ .

$$J \in A \times O_{\mathcal{V} \setminus V_j}$$

3. Therefore whenever  $A$  occurs, one of the elements  $J$  of  $A \times O_{\mathcal{V} \setminus V_j}$  has to occur.

$$A \implies J_1 \vee \dots \vee J_l = \bigvee_{J \in A \times O_{\mathcal{V} \setminus V_j}} J \quad (10)$$

4. Now suppose we could obtain a set of marginal outcomes  $C = \{C_1, \dots, C_n\}$  each different from  $A$  such that every  $J$  is in the extendable set of at least one element  $C$ . If such a  $C$  can be found, then the possibility of at least one  $J$  occurring implies the possibility of at least one  $C$  occurring.

$$J_1 \vee \dots \vee J_l \implies C_1 \vee \dots \vee C_n \quad (11)$$

5. Combing  $??$  with  $??$ , one obtains  $??$ .

Todo (TC Fraser): Talk about why this is called hardy paradox

Finding all marginal implications for a chosen marginal outcome  $A$  corresponds to finding a set of marginal outcomes  $C = \{C_1, \dots, C_n\}$  whose extendable sets *cover* the extendable set of  $A$ . Formally this corresponds to a **set covering** problem Todo (TC Fraser): cite which we elected to cast as the equivalent **hypergraph transversal problem**.

Todo (TC Fraser): Mention sufficient solution to the possibilistic marginal problem Todo (TC Fraser): Illustrate how it can distinguish more than possibilistic differences

Given an antecedent  $A$ , we can construct a hypergraph  $\mathcal{H}_A$  with nodes  $\mathcal{N}_A$  and  $\mathcal{E}_A$ . The edges are labeled by outcomes in  $A$ 's extendable set  $A \times O_{\mathcal{V} \setminus V_j}$ , namely  $o[\mathcal{V}]$ , and contain all marginal outcomes compatible with  $o[\mathcal{V}]$ . The nodes are the subset of marginal outcomes compatible with  $A$ ; equivalently the union of all edges. Todo (TC Fraser): Notation for compatible and extendable?

$$\mathcal{E}_A = \{o[\mathcal{V}] \mid o[\mathcal{V}] \in A \times O_{\mathcal{V} \setminus V_j}\}$$

The nodes are all marginal outcomes  $C$  compatible with  $A$ .

$$\mathcal{N}_A = \left\{ n \in \bigcup_{i=1}^k O_{V_i} \mid n \neq A, n \right\}$$

And edges  $\mathcal{E}_A$  labeled by elements of  $A$ 's extendable set  $o[\mathcal{V} \setminus V_j] \times$

Todo (TC Fraser): Discuss  $(m, n)$  - type implications and the non-triviality Todo (TC Fraser): Link to logical bell inequalities/completeness or not?

### C. Hypergraph Transversals

Todo (TC Fraser): Convince one how marginal implications are a hypergraph transversal or covering problem Todo (TC Fraser): Existing algorithms Todo (TC Fraser): Discuss the Inequalities Derived/ Trivial and non-trivial Todo (TC Fraser): Weighted transversals and Optimizations Todo (TC Fraser): Seeding inequalities (huge advantage here)

## IX. DERIVING SYMMETRIC INEQUALITIES

Todo (TC Fraser): Identify the desired symmetry group Todo (TC Fraser): How we obtained the desired symmetry group Todo (TC Fraser): Group orbits to symmetric marginal description matrix Todo (TC Fraser): Infeasibility on symmetric marginal problem Todo (TC Fraser): Hardy Transversals can't work on the symmetric marginal problem Todo (TC Fraser): Symmetrizing non-symmetric inequalities through avoiding orbits Todo (TC Fraser): higher order transversals on mutually impossible events

## X. NON-LINEAR OPTIMIZATIONS

Compatibility inequalities for a given causal structure are fantastic for finding incompatible distributions. In the inflation technique, this is no exception. Parameterizing a space distributions using a set of real-valued parameters  $\lambda$ , enables us to perform numerical optimizations against these inequalities in hopes that a particular set of parameters  $\lambda$  is able to generate an incompatible distribution  $P$ . To illustrate this generic procedure and it's reliability, we will first examine the popular CHSH inequality.

### A. Numerical Violations of The CHSH Inequality

The CHSH inequality [?] can be viewed as a causal compatibility inequality for iconic the Bell Scenario (Fig. 19 of [?], Fig. 11 of [?], Fig. 1 a) of [?], etc.) corresponding to Bell's notion of local causality [?]. It constrains the set of 2-outcome bipartite distributions over local binary measurement settings for each party  $P_{AB|S_A S_B} \equiv \{P_{AB|00}, P_{AB|01}, P_{AB|10}, P_{AB|11}\}$ . Numerical optimization *should* obtain the algebraic violation associated with the PR-Box correlations [?]. Maintaining full generality, we simply need to parameterize these 4 distributions using ??, each requiring 4 real-valued parameters.

Todo (TC Fraser): Demonstrate Quantum, Convexity

Todo (TC Fraser): Why Inequalities are great for optimizations Todo (TC Fraser): Non-linearity Todo (TC Fraser): Techniques Used Todo (TC Fraser): Finding maximum violation of CHSH easily Todo (TC Fraser): Unreliance when number of parameters increases Todo (TC Fraser): Issues with local minimum Todo (TC Fraser): Using initial conditions close to fritz, obtain greater violation Todo (TC Fraser): Greater violation shares possibilistic structure of fritz and violates CHSH under definition Todo (TC Fraser): Not realizable with maximally entangled qubit states Todo (TC Fraser): Not realizable with separable measurements Todo (TC Fraser): Many non-trivial inequalities to be tested Todo (TC Fraser): inequality  $\rightarrow$  dist  $\rightarrow$  inequality evolution

## XI. CONCLUSIONS

Todo (TC Fraser): Inflation technique allows one to witness fritz incompatibility Todo (TC Fraser): Linear optimization induces certificates which are incompatibility witnesses Todo (TC Fraser): There are quantum distributions in the triangle scenario that are incompatible and different from fritz in terms of entanglement but not possibilistic structure

## XII. OPEN QUESTIONS & FUTURE WORK

Todo (TC Fraser): Lots of stuff

### Appendix A: Computationally Efficient Parametrization of the Unitary Group

Spengler, Huber and Hiesmayr [?] suggest the parameterization of the unitary group  $\mathcal{U}(d)$  using a  $d \times d$ -matrix of real-valued parameters  $\lambda_{n,m}$

$$U = \left[ \prod_{m=1}^{d-1} \left( \prod_{n=m+1}^d \exp(iP_n \lambda_{n,m}) \exp(i\sigma_{m,n} \lambda_{m,n}) \right) \right] \cdot \left[ \prod_{l=1}^d \exp(iP_l \lambda_{l,l}) \right] \quad (\text{A1})$$

Where  $P_l$  are one-dimensional projective operators,

$$P_l = |l\rangle \langle l| \quad (\text{A2})$$

and the  $\sigma_{m,n}$  are generalized anti-symmetric  $\sigma$ -matrices,

$$\sigma_{m,n} = -i |m\rangle \langle n| + i |n\rangle \langle m|$$

Where  $1 \leq m < n \leq d$ . For the sake of reference, let us label the matrix exponential terms in ?? in a manner that corresponds to their affect on a orthonormal basis  $\{|1\rangle, \dots, |d\rangle\}$ .

$$\begin{aligned} GP_l &= \exp(iP_l \lambda_{l,l}) \\ RP_{n,m} &= \exp(iP_n \lambda_{n,m}) \\ R_{n,m} &= \exp(i\sigma_{m,n} \lambda_{m,n}) \end{aligned} \quad (\text{A3})$$

It is possible to remove the reliance on matrix exponential operations in ?? by utilizing the explicit form of the exponential terms in ?. As a first step, recognize the defining property of the projective operators ??,

$$P_l^k = (|l\rangle \langle l|)^k = |l\rangle \langle l| = P_l$$

This greatly simplifies the global phase terms  $GP_l$ ,

$$GP_l = \exp(iP_l \lambda_{l,l}) = \sum_{k=0}^{\infty} \frac{(iP_l \lambda_{l,l})^k}{k!} = \mathbb{I} + \sum_{k=1}^{\infty} \frac{(i\lambda_{l,l})^k}{k!} P_l^k = \mathbb{I} + P_l \left[ \sum_{k=1}^{\infty} \frac{(i\lambda_{l,l})^k}{k!} \right] = \mathbb{I} + P_l (e^{i\lambda_{l,l}} - 1)$$

Analogously for the relative phase terms  $RP_{n,m}$ ,

$$RP_{n,m} = \dots = \mathbb{I} + P_n (e^{i\lambda_{n,m}} - 1)$$

Finally, the rotation terms  $R_{n,m}$  can also be simplified by examining powers of  $i\sigma_{n,m}$ ,

$$R_{n,m} = \exp(i\sigma_{n,m}\lambda_{m,n}) = \sum_{k=0}^{\infty} \frac{(|m\rangle\langle n| - |n\rangle\langle m|)^k \lambda_{m,n}^k}{k!}$$

One can verify that the following properties hold,

$$\begin{aligned} (|m\rangle\langle n| - |n\rangle\langle m|)^0 &= \mathbb{I} \\ \forall k \in \mathbb{N}, k \neq 0 : (|m\rangle\langle n| - |n\rangle\langle m|)^{2k} &= (-1)^k (|m\rangle\langle m| + |n\rangle\langle n|) \\ \forall k \in \mathbb{N} : (|m\rangle\langle n| - |n\rangle\langle m|)^{2k+1} &= (-1)^k (|m\rangle\langle n| - |n\rangle\langle m|) \end{aligned}$$

Revealing the simplified form of  $R_{n,m}$ ,

$$R_{n,m} = \mathbb{I} + (|m\rangle\langle m| + |n\rangle\langle n|) \sum_{j=1}^{\infty} (-1)^j \frac{\lambda_{n,m}^{2j}}{(2j)!} + (|m\rangle\langle n| - |n\rangle\langle m|) \sum_{j=0}^{\infty} (-1)^j \frac{\lambda_{n,m}^{2j+1}}{(2j+1)!}$$

$$R_{n,m} = \mathbb{I} + (|m\rangle\langle m| + |n\rangle\langle n|) (\cos \lambda_{n,m} - 1) + (|m\rangle\langle n| - |n\rangle\langle m|) \sin \lambda_{n,m}$$

Todo (TC Fraser): Explanation of Computational Complexity  $\mathcal{O}(d^3)$  vs.  $\mathcal{O}(1)$  using [?] Todo (TC Fraser): Pre-Caching for Fixed dimension  $d$

## Appendix B: Parametrization of Quantum States & Measurements

### Appendix C: Convex Parametrization of Finite Probability Distributions

As discussed in ??, there is a need to parameterize the family of all probability distributions  $P_V$  over a given set of variables  $V = (v_1, \dots, v_{|V|})$ . If the cardinality of  $O_V$  is finite, then this is computationally feasible. The space of probability distributions over  $n = |O_V|$  distinct outcomes forms a  $n - 1$  dimensional convex polytope naturally embedded in  $\mathbb{R}_{\geq 0}^n$  [?] that is parameterizable by  $n - 1$  real value parameters; normalization  $\sum_{o[V] \in O_V} P_V(o[V]) = 1$  accounts for the ‘-1’. An example of a non-degenerate parameterization of  $P_V$  consists of  $n - 1$  parameters  $\lambda = (\lambda_1, \dots, \lambda_{n-1})$ ,  $\lambda_i \in [0, \pi/2]$  which generate the probabilities  $n$  probability values  $p_j$  using hyperspherical coordinates [? ?],

$$\begin{aligned} p_j &= \cos^2 \lambda_j \prod_{i=1}^{j-1} \sin^2 \lambda_i \quad \forall j \in 1, \dots, n-1 \\ p_n &= \prod_{i=1}^{n-1} \sin^2 \lambda_i \end{aligned} \tag{C1}$$

Furthermore due to the periodicity of the parameter space  $\lambda$ , ?? can be used for either constrained or unconstrained optimization problems.

Although non-degenerate, this parameterization suffers from uniformity; a randomly sampled vector of parameters  $\lambda$  *does not* translate to a randomly sampled probability  $P_V$ . An easy-to-implement, degenerate parameterization of  $P_V$  can be constructed by simply beginning with  $n$  real parameters  $\lambda = (\lambda_1, \dots, \lambda_n)$ , then making them positive and normalized by their sum<sup>2</sup>.

$$p_j = \frac{|\lambda_j|}{\sum_{i=1}^n |\lambda_i|} \quad \forall j \in 1, \dots, n \tag{C2}$$

For various convex optimization tasks sensitive to initial conditions outlined ??, the latter parameterization of ?? generally performed better than former ??.

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<sup>2</sup> Strictly speaking, ?? *also* suffers from non-uniformity; being biased toward uniform probability distributions  $P_V$ . Todo (TC Fraser): Discuss rejection sampling simplex algorithms