Non-isomorphic Distribution Supports for Calculating Entropic Vectors

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***Abstract*—A 2^N-1 dimensional vector is said to be entropic if each of its entries can be regarded as the joint entropy of a particular subset of N discrete random variables. The explicit characterization of the closure of the region of entropic vectors $\overline{\Gamma}^*_N$ is unknown for $N \geqslant 4$. A systematic approach is proposed to generate the list of non-isomorphic distribution supports for the purpose of calculating and optimizing entropic vectors. It is shown that a better understanding of the structure of the entropy region can be obtained by constructing inner bounds based on these supports. The constructed inner bounds based on different supports are compared both in full dimension and in a transformed three dimensional space of Csirmaz and Matúš.**

I. INTRODUCTION

The region of entropic vectors $\overline{\Gamma}^*_N$ has been shown to be a key quantity in determining fundamental limits in several contexts in network coding [1], distributed storage [2], group theory [3], and information theory [1]. In Network Coding, to determine the capacity region of every network is essentially equivalent to the characterization of entropy region Γ^*_N, yet the boundaries of the region remain unknown for four or more random variables. Since the first Non-Shannon type information inequality was discovered by Zhang and Yeung in [4], numerous attempts have been made trying to characterize Γ^*_N. More non-Shannon type inequalities had been generated in [5]–[8]. $\overline{\Gamma}^*_N$, the closure of Γ^*_N, is shown to be a non-polyhedral convex cone in [9]. After this, many approaches based on group theory, matroid theory and information geometry has been proposed to help researchers get a better understanding of Γ^*_N. However, the characterization of Γ^*_N is still far from finished.

The goal of this paper is to provide a method for systematically searching for distributions whose entropy vectors may be on the boundary of the region of entropic vectors. In particular, multiple scholars have observed in different ways, both analytical and empirical, that optimized entropic vectors associated with the unknown part of the entropy region are associated with probability mass functions with some values that are identically zero – i.e. whose supports are not expressible with an ordinary cartesian product [3], [10], [11]. For this reason, and because the difficulty of performing global optimization over all probability distributions of a given support grows rapidly in the size of the support, it is of interest to organize numerical studies of the entropic region via the size of the support of the distributions being investigated. In particular, it is desirable to determine all possible supports with a given number of non-zero elements that are distinct up to labeling of the Ω in the finite probability space $(\Omega, \mathcal{F}, \mathbb{P})$ that the discrete random variables are defined on, and the labeling of the random variables themselves, as the associated entropic vector is insensitive to these labels.

In §II, we give some background on the region of entropic vectors and outer bounds for it. In §III, after reviewing inner bounds for the entropy region, we described the gap between the Shannon outer bound and the Ingleton inner bound for 4 random variables, then a slice of it is used to illustrate the relationship among different outer and inner bounds. Next, in §IV, we present our main result. In §IV-A, after introducing the concept of k-atom support and the equivalence of two k-atom supports, the problem of enumerating non-isomorphic k-atom supports is tackled by using tools from abstract algebra, then in §V, distribution supports violate Ingleton inequality are studied, a procedure to generate Ingleton violation points is introduced and inner bounds are generated for different k-atom distributions.

II. THE REGION OF ENTROPIC VECTORS

Consider a set of N discrete random variables $\boldsymbol{X} = (X_1, \dots, X_N)$, $\mathcal{N} = \{1, \dots, N\}$ with joint probability mass function $p_{\boldsymbol{X}}(\boldsymbol{x})$. For every non-empty subset of these random variables $\boldsymbol{X}_{\mathcal{A}} := (X_n \mid n \in \mathcal{A})$, $\mathcal{A} \subset \{1, \dots, N\}$, there is a Shannon entropy $H(\boldsymbol{X}_{\mathcal{A}})$ associated with it, which can be calculated from $p_{\boldsymbol{X}_{\mathcal{A}}}(\boldsymbol{x}_{\mathcal{A}}) = \sum_{\boldsymbol{x}_{\mathcal{N}\setminus\mathcal{A}}} p_{\boldsymbol{X}_{\mathcal{N}}}(\boldsymbol{x})$ via

$$H(\boldsymbol{X}_{\mathcal{A}}) = \sum_{\boldsymbol{x}_{\mathcal{A}}} -p_{\boldsymbol{X}_{\mathcal{A}}}(\boldsymbol{x}_{\mathcal{A}}) \log_2 p_{\boldsymbol{X}_{\mathcal{A}}}(\boldsymbol{x}_{\mathcal{A}}) \tag{1}$$

If we stack these $2^N - 1$ joint entropies associated with all the non-empty subsets into a vector $\boldsymbol{h} = \boldsymbol{h}(p_{\boldsymbol{X}}) = (H(\boldsymbol{X}_{\mathcal{A}}) | \mathcal{A} \subseteq \mathcal{N})$, $\boldsymbol{h}(p_{\boldsymbol{X}})$ is clearly a function of the joint distribution $p_{\boldsymbol{X}}$. A vector $\boldsymbol{h}_? \in \mathbb{R}^{2^N-1}$ is said to be *entropic* if there exist some joint distribution $p_{\boldsymbol{X}}$ such that $\boldsymbol{h}_? = \boldsymbol{h}(p_{\boldsymbol{X}})$. Γ^*_N is then defined as the image of the set $\mathcal{D} = \{p_{\boldsymbol{X}} | p_{\boldsymbol{X}}(\boldsymbol{x}) \geq 0,\ \sum_{\boldsymbol{x}} p_{\boldsymbol{X}}(\boldsymbol{x}) = 1\}$:

$$\Gamma^*_N = \boldsymbol{h}(\mathcal{D}) \subsetneq \mathbb{R}^{2^N-1} \tag{2}$$

The closure of this set $\overline{\Gamma}^*_N$ is a convex cone [1], but surprisingly little else is known about the boundaries of it for $N \geq 4$.

With the convention that $h_\emptyset = 0$, entropy is *sub-modular* [1], [4], meaning that

$$h_{\mathcal{A}} + h_{\mathcal{B}} \geq h_{\mathcal{A}\cap\mathcal{B}} + h_{\mathcal{A}\cup\mathcal{B}} \quad \forall \mathcal{A}, \mathcal{B} \subseteq \mathcal{N}, \tag{3}$$

and is also *non-decreasing* and *non-negative*, meaning that

$$h_{\mathcal{A}} \geq h_{\mathcal{B}} \geq 0 \quad \forall \mathcal{B} \subseteq \mathcal{A} \subseteq \mathcal{N}. \tag{4}$$

The inequalities (3) and (4) together are known as the *polymatroidal axioms* [1] [4], and a function satisfying them is called the *rank function* of a *polymatroid*. If in addition to obeying the polymatroidal axioms (3) and (4), a set function r also satisfies

$$r_{\mathcal{A}} \leq |\mathcal{A}|, \quad r_{\mathcal{A}} \in \mathbb{Z} \quad \forall \mathcal{A} \subseteq \mathcal{N} \tag{5}$$

then it is called the rank function of a *matroid* on the ground set $\mathcal{N}$.

Since an entropic vector must obey the polymatroidal axioms, the set of all valid rank functions of polymatroids forms a natural outer bound for Γ_N^* and is known as the Shannon outer bound Γ_N [1], [4]:

$$\Gamma_N = \left\{ \boldsymbol{h} \;\middle|\; \begin{array}{c} \boldsymbol{h} \in \mathbb{R}^{2^N-1} \\ h_{\mathcal{A}} + h_{\mathcal{B}} \geq h_{\mathcal{A}\cap\mathcal{B}} + h_{\mathcal{A}\cup\mathcal{B}} \ \forall \mathcal{A}, \mathcal{B} \subseteq \mathcal{N} \\ h_{\mathcal{P}} \geq h_{\mathcal{Q}} \geq 0 \quad \forall \mathcal{Q} \subseteq \mathcal{P} \subseteq \mathcal{N} \end{array} \right\} \tag{6}$$

Γ_N is a polyhedron, we have $\Gamma_2 = \Gamma_2^*$ and $\Gamma_3 = \overline{\Gamma}_3^*$, for $N \geq 4$, however, $\Gamma_N \neq \overline{\Gamma}_N^*$. Zhang and Yeung first showed this in [4] by proving a new inequality among 4 variables

$$2I(C;D) \leq I(A;B) + I(A;C,D) + 3I(C;D|A) + I(C;D|B) \tag{7}$$

which held for entropies, but is not implied by the polymatroidal axioms. They called it a *non-Shannon type* inequality to distinguish it from inequalities implied by Γ_N. In the next few years, a few authors have generated new non-Shannon type inequalities [5]–[8]. Then Matúš in [9] showed that $\overline{\Gamma}_N^*$ is not a polyhedron for $N \geq 4$. In this paper, a sequence of non-Shannon inequalities were constructed:

$$\begin{aligned} & s[I(A;B|C) + I(A;B|D) + I(C;D) - I(A;B)] \qquad (8) \\ & + I(B;C|A) + \frac{s(s+1)}{2}[I(A;C|B) + I(A;B|C)] \geq 0 \end{aligned}$$

Notice (8) is the same as Zhang-Yeung inequality (7) when s = 1. Additionally, the infinite sequence of inequalities was used with a curve constructed from a particular form of distributions to prove $\overline{\Gamma}_N^*$ is not a polyhedron. Despite this characterization, even $\overline{\Gamma}_4^*$ is still not fully understand. Since then, many authors has been investigating the properties of $\overline{\Gamma}_N^*$ with the hope of ultimately fully characterizing the region [11]–[17].

III. STRUCTURE OF $\overline{\Gamma}_4^*$: THE GAP BETWEEN INGLETON INNER BOUND $\mathcal{S}_4$ AND SHANNON OUTER BOUND Γ_4

Let's first introduce some basics in linear polymatroids and the Ingeton inner bound. Fix a $N' > N$, and partition the set $\{1, \ldots, N'\}$ into N disjoint sets $\mathcal{I}_1, \ldots, \mathcal{I}_N$. Let $\boldsymbol{U}$ be a length r row vector whose elements are i.i.d. uniform over $GF(q)$, and let $\mathbf{G}$ be a particular $r \times N'$ deterministic matrix with elements in $GF(q)$. Consider the N' dimensional vector

$$\boldsymbol{Y} = \boldsymbol{U}\mathbf{G}, \text{ and define } \boldsymbol{X}_i = \boldsymbol{Y}_{\mathcal{I}_i}, \ i \in \{1, \ldots, N\}.$$

The subset entropies of the random variables $\{\boldsymbol{X}_i\}$ obey

$$H(\boldsymbol{X}_{\mathcal{A}}) = r(\mathcal{A}) \log_2(q) = \text{rank}\left([\mathbf{G}_{\mathcal{I}_i} | i \in \mathcal{A}]\right) \log_2(q). \tag{9}$$

A set function $r(\cdot)$ created in such a manner is called a linear polymatriod or a subspace rank function. It obeys the polymatroidal axioms, and is additionally proportional to an integer valued vector, however it need not obey the cardinality constraint, and therefore is not necessarily the rank function of a matroid.

Such a construction is clearly related to a representable matroid on a larger ground set [18]. Indeed, the subspace rank function vector is merely formed by taking some of the elements from the $2^{N'}-1$ representable matroid rank function vector associated with $\mathbf{G}$. That is, rank function vectors created via (9) are projections of rank function vectors of representable matroids.

Rank functions capable of being represented in the manner for some N', q and $\mathbf{G}$, are called subspace ranks in some contexts [19]–[21], while other papers effectively define a collection of vector random variables created in this manner a subspace arrangement [22].

Define $\mathcal{S}_N$ to be the conic hull of all subspace ranks for N subspaces. It is known that $\mathcal{S}_N$ is an inner bound for $\overline{\Gamma}_N^*$ [19], which we call subspace inner bound. So far $\mathcal{S}_N$ is only known for $N \leq 5$ [21], [22]. More specifically, $\mathcal{S}_2 = \overline{\Gamma}_2^* = \Gamma_2$, $\mathcal{S}_3 = \overline{\Gamma}_3^* = \Gamma_3$. As with most entropy vector sets, things start to get interesting at $N = 4$ variables (subspaces). For $N = 4$, $\mathcal{S}_4$ is given by the Shannon type inequalities (i.e. the polymatroidal axioms) together with six additional inequalities known as *Ingleton*'s inequality [19], [20], [23] which states that for $N = 4$ random variables

$$\begin{aligned} Ingleton_{ij} &= I(X_k;X_l|X_i) + I(X_k;X_l|X_j) \qquad (10) \\ &+ I(X_i;X_j) - I(X_k;X_l) \geq 0 \end{aligned}$$

Thus, $\mathcal{S}_4$ is usually called the Ingleton inner bound. We know Γ_4 is generated by 28 elemental Shannon type information inequalities [1]. As for $\mathcal{S}_4$, in addition to the the 28 Shannon type information inequalities, we also need six Ingleton's inequalities (10), thus $\mathcal{S}_4 \subsetneq \Gamma_4$. In [20] it is stated that Γ_4 is the disjoint union of $\mathcal{S}_4$ and six cones $\{h \in \Gamma_4 | Ingleton_{ij} < 0\}$. The six cones $G_4^{ij} = \{h \in \Gamma_4 | Ingleton_{ij} \leq 0\}$ are symmetric due to the permutation of inequalities $Ingleton_{ij}$, so it sufficient to study only one of the cones. Furthermore, [20] gave the extreme rays of G_4^{ij} in Lemma 1 by using the following functions.

For $N = \{1, 2, 3, 4\}$, with $I \subseteq N$ and $0 \leq t \leq |N \backslash I|$, define

$$r_t^I(J) = \min\{t, |J \backslash I|\} \ with \ J \subseteq N$$

$$g_i^{(2)}(J) = \begin{cases} 2 & \text{if } J = i \\ min\{2, |J|\} & \text{if } J \neq i \end{cases}$$

$$g_i^{(3)}(J) = \begin{cases} |J| & \text{if } i \notin J \\ min\{3, |J|+1\} & \text{if } i \in J \end{cases}$$

$$f_{ij}(K) = \begin{cases} 3 & \text{if } K \in \{ik, jk, il, jl, kl\} \\ min\{4, 2|K|\} & \text{otherwise} \end{cases}$$

Lemma 1: (Matúš) [20] The cone $G_4^{ij} = \{h \in \Gamma_4 | Ingleton_{ij} \leq 0\}$, $i, j \in N$ distinct is the convex hull of 15 extreme rays. They are generated by the 15 linearly independent functions f_{ij}, r_1^{ijk}, r_1^{ijl}, r_1^{ikl}, r_1^{jkl}, $r_1^{\emptyset}$, $r_3^{\emptyset}$, r_1^{i}, r_1^{j}, r_1^{ik}, r_1^{jk}, r_1^{il}, r_1^{jl}, r_2^{k}, r_2^{l}, where $kl = N - ij$.

Note that among the 15 extreme rays of G_4^{ij}, 14 extreme rays r_1^{ijk}, r_1^{ijl}, r_1^{ikl}, r_1^{jkl}, $r_1^{\emptyset}$, $r_3^{\emptyset}$, r_1^{i}, r_1^{j}, r_1^{ik}, r_1^{jk}, r_1^{il}, r_1^{jl}, r_2^{k}, r_2^{l} are also extreme rays of $\mathcal{S}_4$ and thus entropic, which leaves f_{ij} the only extreme ray in G_4^{ij} that is not entropic. It is easily verified that $\overline{\Gamma}_4^*$ is known as long as we know the structure of six cones $\overline{\Gamma}_4^* \cap G_4^{ij}$. Due to symmetry, we only need to focus on one of the six cones $\overline{\Gamma}_4^* \cap G_4^{34}$, thus we define $P_4^{34} = \overline{\Gamma}_4^* \cap G_4^{34}$ and present our results mainly on P_4^{34} in the rest of the paper.

Now we have defined G_4^{ij}, the gap between Ingleton inner bound and Shannon outer bound, we will look at a slice of this gap and plot different outer bounds together with several known entropic vectors on this slice of the entropy region. We consider the hyperplane such that we fix the last 13 dimension of entropic vector to $V = [3\ 2\ 3\ 3\ 4\ 2\ 3\ 3\ 4\ 4\ 4\ 4\ 4]$ and only consider the first two dimensions h_1 and h_2, which is shown in Figure 1. Since Γ_4^* is a 15 dimensional convex cone, if we fixed 13 dimensional to V, only h_1 and h_2 need to be considered, thus we can easily plot the constrained region for visualization.

In Figure 1, f is the one of the 6 bad extreme rays f_{34} (extreme rays of Γ_4 that are not entropic). The rectangle formed by connecting (0, 0), (2, 0), (0, 2) and f is the mapping of Shannon outer bound Γ_4 onto this plane. The green line connecting a and e is the projection of $Ingleton_{34}$ onto the plane. Notice we also plot Zhang-Yeung's inequality (7) and Matúš's sequences of inequalities (8) for some values of s in the figure for the comparison between Ingleton inner bound, Shannon outer bound and non-Shannon outer bound. The red dot point c is the entropic vector of the binary distribution with only four outcomes:

$$\begin{bmatrix} (0,0,0,0) \\ (0,1,1,0) \\ (1,0,1,0) \\ (1,1,1,1) \end{bmatrix} \tag{11}$$

each row in (11) corresponding to one outcome/atom, the number of columns in (11) is the same as the number of random variables this support act on. Point c can be calculated by setting each of the outcomes with probability $\frac{1}{4}$. Following from the convention of [10], we call (11) the 4-atom support and the entropic vector c corresponding to the uniform 4-atom support the 4-atoms uniform point.

Figure 1 shows the relative distance among the bad extreme ray f_{34}, well known non-Shannon type inequalities and the best known entropic points in this specifically hyperplane where we fix the last 13 dimension to V. As it was shown, even though more and more non-Shannon type information inequalities can be generated to get better outer bounds, it is still not very close to the best known entropic point: the 4-atoms uniform point c. In next section, we are going to study the entropic vectors generated by k-atom support, and inner bounds constructed with these supports.

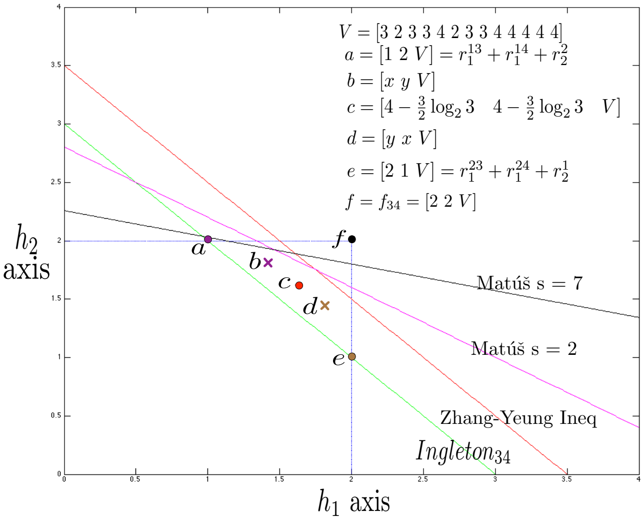

Fig. 1. Entropic vector hyperplane with only h_1 and h_2 coordinate not fixed

IV. LISTING CANONICAL k-ATOM SUPPORTS

To begin, we must formally introduce the concept of k-atom support and define the equivalence of two k-atom supports. Consider the probability distributions for a random vector $\boldsymbol{X} = (X_1, \ldots, X_N)$ taking values on the Cartesian product $\boldsymbol{\mathcal{X}} = \mathcal{X}_1 \times \mathcal{X}_2 \times \cdots \times \mathcal{X}_N$, where $\mathcal{X}_n$ is a finite set with values $i \in \{0, \ldots, |\mathcal{X}_n| - 1\}$. To a particular probability mass function $p_{\boldsymbol{X}}$ we can associate a length $\prod_{n=1}^{N} |\mathcal{X}_n| - 1$ vector by listing the probabilities of all but one of the outcomes in $\boldsymbol{\mathcal{X}}$ into a vector

$$\boldsymbol{\eta} = \left[p_{\mathbf{X}}(i_1, \ldots, i_N) \left| \begin{array}{c} i_k \in \{0, 1, \ldots, |\mathcal{X}_k| - 1\}, \\ k \in \{1, \ldots, N\}, \\ \sum_k i_k \neq 0. \end{array} \right. \right]. \tag{12}$$

Notice we are only listing outcomes such that $\sum_k i_k \neq 0$, $p_{\mathbf{X}}(\mathbf{0}) = p_{\mathbf{X}}(i_1 = 0, \ldots, i_N = 0)$ will be the only outcome that is left out. $\boldsymbol{\eta}$ in (12) can be determined uniquely from the probability mass function $p_{\boldsymbol{X}}$, and owing to the fact that the probability mass function must sum to one, the omitted probability $p_{\mathbf{X}}(\mathbf{0})$ can be calculated, and hence the probability mass function can be determined from $\boldsymbol{\eta}$.

A probability distribution support defined by $\boldsymbol{\eta}$ assume all outcomes have nonzero probability, however, entropic vectors are often extremized by selecting some of the elements of $\mathcal{X}_1 \times \cdots \times \mathcal{X}_N$ to have zero probability. For this reason, rather than specifying some probabilities in their cartesian product to be zero, it is of interest to instead specify a support $\boldsymbol{\mathcal{X}}$, no longer a cartesian product, on which the probabilities will be non-zero. Thus we may consider only those probability spaces $(\Omega, \mathcal{F}, \mathbb{P})$ with $|\Omega| = k$ to define the random variables $\boldsymbol{X} : \Omega \to \boldsymbol{\mathcal{X}}$ on. A probability support $\boldsymbol{\mathcal{X}}$ satisfying $|\boldsymbol{\mathcal{X}}| = k$ is called a k-atom support, and a joint distribution created this way will be called a k-atom distribution.

Two k-atom supports $\boldsymbol{\mathcal{X}}, \boldsymbol{\mathcal{X}}'$, $|\boldsymbol{\mathcal{X}}| = |\boldsymbol{\mathcal{X}}'| = k$, will be said to be *equivalent*, for the purposes of tracing out the entropy region, if they yield the same set of entropic vectors, up to a permutation of the random variables. In other words, $\boldsymbol{\mathcal{X}}$ and $\boldsymbol{\mathcal{X}}'$ are equivalent, if, for every probability mass function $p_{\mathbf{X}} : \boldsymbol{\mathcal{X}} \to [0, 1]$, there is another probability mass function $p_{\mathbf{X}'} : \boldsymbol{\mathcal{X}}' \to [0, 1]$ and a bijection $\pi : \mathcal{N} \to \mathcal{N}$ such that

$$h_{\mathcal{A}}(p_{\mathbf{X}}) = h_{\pi(\mathcal{A})}(p_{\mathbf{X}'}) \quad \forall \mathcal{A} \subseteq \mathcal{N}.$$

Take $N = 4$ and $|\boldsymbol{\mathcal{X}}| = 1$ as a trivial example, since we only have one outcome/atom, it will have the probability of 1. In this way, different 1-atom supports like $[(0, 0, 0, 0)]$, $[(0, 0, 1, 2)]$, $[(0, 1, 2, 3)]$ and $[(2, 5, 7, 9)]$ are equivalent because they all map to the same 15 dimensional entropic vector with all zero elements.

The goal of this section is to formalize this notion of equivalent supports with the use of tools from abstract algebra, then describe some methods for enumerating and listing one representative from each equivalence class of supports.

Before moving on to the next section, we will need to first introduce some basic abstract algebra concepts that will be used in the algorithm to enumerate non-isomorphic distribution supports for entropic vector calculations.

Definition 1: Let G be a finite group acting on a finite set X, a *group action* is a mapping

$$G \times X \to X : (g, x) \mapsto gx$$

such that if e is the identity in G, $ex = x \ \forall x \in X$ and for any $g_1, g_2 \in G$, $g_2 g_1 x = (g_2 g_1)x$ for all $x \in X$. For $x \in X$, the *orbit* of x under G is defined as

$$G(x) = \{gx \mid g \in G\}$$

the *stabilizer* subgroup of x in X is defined as

$$G_x = \{g \in G \mid gx = x\}$$

Suppose there is some ordering of X, and let x be the element of $G(x)$ that is least under this ordering, i.e. the *canonical representative* of the orbit $G(x)$. For another $y \in G(x)$, an element $g \in G$ is called a *transporter element* for y if $gy = x$.

Definition 2: (orbit data structure [24]) Let G be a group which acts on the finite set X. The triple

$$orbit(G, X) = (\mathcal{T}, \sigma, \varphi)$$

is the *orbit data structure* for G acting on X provided that

1. $\mathcal{T}$ is a transversal of the G-orbits on X
2. $\sigma : X \to L(G) : x \mapsto G_x$
3. $\varphi : X \to G : x \mapsto g$ with $gx \in \mathcal{T}$

Here, $L(G)$ denotes the lattice of subgroups of G, we call σ the *stabilizer map* and φ the *transporter map*.

In next section, we will show listing non-isomorphic distribution supports is equivalent to calculate orbit data structure of symmetry group on some finite set.

A. Non-isomorphic k-atom supports via Snakes and Ladders

Let $\mathbb{N}_1^k = \{1, \ldots, k\}$. The key to enumerate non-isomorphic distribution supports is to realize that for each random variable, all possible outcomes for k-atom support can be encoded as the list of all *set partitions* [25]. A *set partition* of $\mathbb{N}_1^k$ is a set $\mathcal{B} = \{B_1, \ldots, B_t\}$ consisting of t subsets $B_1, \ldots, B_t$ of $\mathbb{N}_1^k$, called the *blocks* of the partition, that are pairwise disjoint $B_i \cap B_j = \emptyset, \forall i \neq j$, and whose union is $\mathbb{N}_1^k$, so that $\mathbb{N}_1^k = \bigcup_{i=1}^t B_i$. Let $\Pi(\mathbb{N}_1^k)$ denote the set of all set partitions of $\mathbb{N}_1^k$. The cardinality of $\Pi(\mathbb{N}_1^k)$ is commonly known as *Bell numbers*. For instance, there are 5 different set partitions for $k = 5$, that is $|\Pi(\mathbb{N}_1^3)| = 5$ and

$$\Pi(\mathbb{N}_1^3) = \{\{\{1,2,3\}\}, \{\{1,2\},\{3\}\}, \{\{1,3\},\{2\}\}, \{\{2,3\},\{1\}\}, \{\{1\},\{2\},\{3\}\}\},$$

$|\Pi(\mathbb{N}_1^4)| = 15$ and $\Pi(\mathbb{N}_1^4)$ is the set

$$\{\{\{1,2,3,4\}\}, \{\{1,2,3\},\{4\}\}, \{\{1,2,4\},\{3\}\}, \{\{1,3,4\},\{2\}\}, \{\{2,3,4\},\{1\}\}, \{\{1,2\},\{3,4\}\}, \{\{1,3\},\{2,4\}\}, \{\{1,4\},\{2,3\}\}, \{\{1,2\},\{3\},\{4\}\}, \{\{1,3\},\{2\},\{4\}\}, \{\{1,4\},\{2\},\{3\}\}, \{\{2,3\},\{1\},\{4\}\}, \{\{2,4\},\{1\},\{3\}\}, \{\{3,4\},\{1\},\{2\}\}, \{\{1\},\{2\},\{3\},\{4\}\}\}.$$

A set partition $\mathcal{B} \in \Pi(\mathbb{N}_1^k)$ is said to *refine* a set partition $\mathcal{B}' \in \Pi(\mathbb{N}_1^k)$ if all of the blocks in $\mathcal{B}'$ can be written as the union of some blocks in $\mathcal{B}$. The *meet* of two partitions $\mathcal{B}, \mathcal{B}' \in \Pi(\mathbb{N}_1^k)$, denoted by $\mathcal{B} \wedge \mathcal{B}'$ is the partition of $\mathbb{N}_1^k$ formed by all of the non-empty intersections of a block from $\mathcal{B}$ and a block from $\mathcal{B}'$:

$$\mathcal{B} \wedge \mathcal{B}' = \left\{ B_i \cap B_j' \,\middle|\, B_i \in \mathcal{B}, B_j' \in \mathcal{B}', B_i \cap B_j' \neq \emptyset \right\}$$

Refinement and meet set up a partial order on $\Pi(\mathbb{N}_1^k)$ which enable it to be identified as a *lattice*, the lattice of $\Pi(\mathbb{N}_1^4)$ is shown in Figure 2

Let Ξ_N be the collection of all sets of N set partitions of $\mathbb{N}_1^k$ whose meet is the finest partition (the set of singletons),

$$\Xi_N := \left\{ \xi \,\middle|\, \xi \subseteq \Pi(\mathbb{N}_1^k),\ |\xi| = N,\ \bigwedge_{\mathcal{B} \in \xi} \mathcal{B} = \bigcup_{i=1}^{N} \{\{i\}\} \right\}. \tag{13}$$

The symmetric group $\mathbb{S}_k$ induces a natural group action on a set partition $\mathcal{B} \in \Pi(\mathbb{N}_1^k)$, $\mathcal{B} = \{B_1, \ldots, B_t\}$: representing an element $\pi \in \mathbb{S}_k$ as a permutation $\pi : \mathbb{N}_1^k \to \mathbb{N}_1^k$, we have

$$\pi(\mathcal{B}) := \{\pi(B_1), \ldots, \pi(B_t)\}. \tag{14}$$

This action on set partitions induces, again in a natural manner, a group action of $\mathbb{S}_k$ on the set Ξ_N of subsets of N partitions from $\Pi(\mathbb{N}_1^k)$ whose meet is the singletons: $\pi \in \mathbb{S}_k$ acts on a set of partitions $\xi \in \Xi_N$, $\xi = \{\mathcal{B}_1, \ldots, \mathcal{B}_N\}$ via

$$\pi(\xi) := \{\pi(\mathcal{B}_1), \ldots, \pi(\mathcal{B}_N)\}. \tag{15}$$

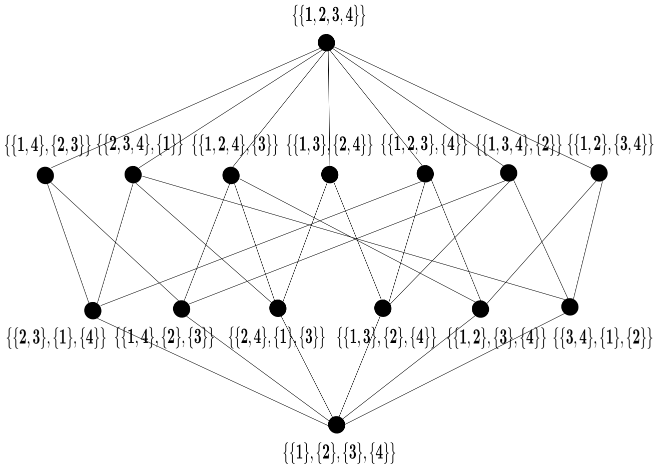

Fig. 2. Lattice of $\Pi(\mathbb{N}_1^4)$: the set of all set partitions for $k = 4$

The group action (14) on set partition and group action (15) on sets of set partitions enable us to enumerate the non-isomorphic k-atom supports by calculating the orbit data structure of symmetry group acting on a well defined set, the result is summarized in Theorem 1.

Theorem 1: The problem of generating the list of all non-isomorphic k-atom, N-variable supports, that is, selecting one representative from each equivalence class of isomorphic supports, is equivalent to obtaining a transversal of the orbits $\Xi_N // \mathbb{S}_k$ of $\mathbb{S}_k$ acting on Ξ_N, the set of all subsets of N set partitions of the set $\mathbb{N}_1^k$ whose meets are the set of singletons $\{\{1\}, \{2\}, \dots, \{N\}\}$.

Proof (sketch): A random variable introduces a partition on the sample space based on its inverse image. The joint distributions of several random variables is created from the meet of these partitions. The joint entropy is insensitive to the labeling of elements in the sample space, as well as the labeling of the outcomes of the random variable, hence it is only the partitions and their meets that matter in determining the joint entropies. Since an appropriate notion of isomorphism between supports also recognizes that it does not matter which random variable is labeled as the first random variable and so on, and there is no need to duplicate random variables when enumerating supports, rather than a N tuple of partitions, the support of a collection of random variables is best thought of, then, as a set of such set-partitions. The requirement that the meet is the singletons follows from the fact that if it is not, there is a k' atom distribution with $k' < k$ whose atoms are the sets in the meet partition, which gives equivalent entropies, and hence such a situation is better labelled as a k'-atom distribution. ■

Theorem 1 set up the theoretical framework for obtaining the list of non-isomorphic k-atom, N-variable supports for the purpose of calculating entropic vector, that is to calculate the orbits data structure of symmetry group $\mathbb{S}_k$ on Ξ_N, the set of N element subsets of Ξ_1. One way to carry out the computation is to directly calculate the orbit data structure on Ξ_N using the default subroutine in GAP. However, this approach become intractable when k and N are larger than four, both CPU time and memory usage go beyond the capacity of a single computer. Alternatively, one can use a recursive breadth-first search style algorithm called the algorithm of Snake and Ladder [26] to efficiently calculate the orbit data structure.

$N \backslash k$	3	4	5	6	7
2	2	8	18	48	112
3	2	31	256	2437	25148
4	1	75	2665	105726	5107735
5	0	132	22422	3903832	
6	0	187	161118		

TABLE I
OF NON-ISOMORPHIC k-ATOM, N-VARIABLE SUPPORTS.

Suppose we have a group G acting on a set X, the algorithm Snakes and Ladders, see e.g. [24] pp. 709–710, is an algorithm which enables one to compute orbit data structure of group G on the set $\mathcal{P}_i(X)$ of all subsets of the set X of cardinality i. For a given set X, the algorithm first computes the orbit data structure on the set of subsets of size $i = 1$, then it recursively increase the subsets size i, where the computation to determine the orbit data structure for subsets of size i is created from manipulations with the orbit data structure on subsets of size $i - 1$.

To apply this problem to the non-isomorphic support enumeration problem, one selects the set X to be the set of all set partitions of the set $\mathbb{N}_1^k$, ordered lexicographically, and the group G to be the symmetric group $\mathbb{S}_k$. Once the step in Snakes and Ladders associated with subsets (of set partitions) of size N is reached, each element of the transversal is checked to determine if the meet of its partitions is the set of singletons, and the resulting sets of N set partitions yield the non-isomorphic supports.

The snakes and ladders algorithm was applied to enumerating non-isomorphic supports in this manner, and the resulting numbers of non-isomorphic supports obtained are displayed in Table I. As shown, for $N = 4$ variables, only one support is needed for calculating entropic vectors of 3-atom distribution, however, there are 75 non-isomorphic supports for $k = 4$, and the number of non-isomorphic supports grow rapidly in the number of atoms k.

In the next section, we will utilize these non-isomorphic k-atom supports together with numerical optimization to obtain inner bounds for entropy.

V. MAPPING THE ENTROPY REGION WITH k-ATOM DISTRIBUTIONS

With the list of canonical k supports obtained through the method described in the previous section in hand, the matter turns to how to exploit them to better numerically map out the unknown parts of the entropy region. In this section, we

number of atoms k	3	4	5	6	7
all supports	1	75	2665	105726	5107735
Ingleton violating	0	1	29	1255	60996

TABLE II
OF NON-ISOMORPHIC k-ATOM, 4-VARIABLE SUPPORTS THAT CAN VIOLATE THE INGLETON INEQUALITY.

study this problem from two angles, the first, in §V-A, aims to solely focus on optimizing the Ingleton score, while the second, in §V-B describes a process for obtaining numerically optimized inner bounds to the entropy region.

A. Maximal Ingleton Violation and the Four Atom Conjecture

Given that the unknown part of $\bar{\Gamma}^*_4$ is associated with violating the Ingleton inequality, substantial research effort has been exerted towards determining distributions on $N = 4$ random variables that violate the Ingleton inequality (10). Dougherty, Freiling, and Zeger [10] defined a normalized function called the *Ingleton score* to measure the degree of Ingleton violation for 4 random variables, and they also make the *Four-Atom Conjecture* which states that the Ingleton score of 4 random variables can not be lower than -0.08937. After the Four-Atom conjecture was proposed, Ingleton violation was been studied extensively with finite groups [13], [14], [17], then in [11], the conjecture was refuted by transforming a distribution obtaining Ingleton score of -0.078277 through a operation which preserves the property of almost entropic to a vector with Ingleton score -0.09243. In this section, we study the number of k atom supports that can, for some probability distribution, violate Ingleton, as well as the Ingleton scores they can attain.

For a particular k atom support for N variables, the Ingleton score can be numerically optimized via fine grid search and numerical gradient optimization. Doing so for each four variable support with 7 or fewer atoms yielded the results in Table II, which shows that only a small fraction of the canonical supports can violate Ingleton.

Additionally, in keeping with the findings of the four atom conjecture and the attempts to refute it, no k-atom support with $k \leq 7$ is capable of directly violating the Ingleton score. Among all the 75 non-isomorphic 4-atom distribution supports, including any cardinality and any distribution value, only one have distributions violate Ingleton, that is the famous 4-atom support (11). Among the 29 5-atom supports, 28 of them obtain the minimal Ingleton score of -0.08937 where one atom have probability zero, which means it shrink to 4-atom support and achieve the same Ingleton score as 4-atom support in (11), and the remaining one support

$$\begin{bmatrix} (0,0,0,0) \\ (0,0,1,1) \\ (0,1,1,0) \\ (1,0,1,0) \\ (1,1,1,0) \end{bmatrix} \tag{16}$$

only achieves a minimal Ingleton score of -0.02423. For the 1255 6-atom supports, 58 of them get a minimal Ingleton score strictly less than -0.08937, while the remainder of the supports yield minimal scores of -0.08937. These exhaustive results substantiate findings from other researchers that suggest that if it is indeed possible to give a probability distribution which directly (without any almost entropic preserving transformation on the entropic vectors as utilized in [11]) violates the four atom conjecture, at least a large support will be required.

B. Optimizing Inner Bounds to Entropy from k-Atom Distributions

For the purpose of generating better inner bounds for the region of entropic vector, minimizing only the Ingleton score is far from enough, since it is only optimizing the distribution to a cost function of certain hyperplane defined by Ingleton inequality. Bearing this in mind, one can define cost functions different from the Ingleton score, but still yielding optimized points that are in the unknown part of the entropy region associated with violating Ingleton. We will first describe a simple procedure to randomly generate such cost functions, and then their numerical optimization over each of the Ingleton violating 4,5, and 6 atom supports. The resulting entropic vectors are then collected to generate inner bounds to $\bar{\Gamma}^*_4$ based on distributions with 4,5, and 6 atom supports.

Lemma 1 defined the 15 extreme rays of the pyramid G^{ij}_4, and without loss of generality, it suffices to consider G^{34}_4. Among these 15 rays, the 14 extreme rays lie on the hyperplane of $Ingleton_{34} = 0$ are r^{134}_1, r^{234}_1, r^{123}_1, r^{124}_1, $r^{\emptyset}_1$, $r^{\emptyset}_3$, r^3_1, r^4_1, r^{13}_1, r^{14}_1, r^{23}_1, r^{24}_1, r^1_2, r^2_2, the only extreme ray in G^{34}_4 that is not entropic is f_{34}. For generating a cost function, a random vector $\Lambda = \{\lambda_1, \lambda_2, \cdots \lambda_{14}\}$ of 14 dimension is generated, where λ_i takes value from 0 to a large positive value. Then for each of the 14 extreme rays on the hyperplane of $Ingleton_{34} = 0$, one new ray is generated through the following equation

$$r^{new}_i = \frac{r^{base}_i + \lambda_i f_{34}}{1 + \lambda_i} \tag{17}$$

where $r^{base}_i \in \{r^{134}_1$, r^{234}_1, r^{123}_1, r^{124}_1, $r^{\emptyset}_1$, $r^{\emptyset}_3$, r^3_1, r^4_1, r^{13}_1, r^{14}_1, r^{23}_1, r^{24}_1, r^1_2, $r^2_2\}$. After obtaining the 14 new rays $\mathbf{r^{new}} = \{r^{new}_1, \cdots, r^{new}_{14}\}$, the hyperplane defined by these new rays, which in turn defines a new cost function, can be easily calculated. Notice if we let $\lambda_i = 0$ for $i = 1, 2, \cdots 14$, we will get the hyperplane of $Ingleton_{34} = 0$.

Computer experiments were run to generate more than 1000 cost functions in this manner by random selection of the λ_is. For each of these cost functions, numerical optimization of the distribution for each Ingleton violating k-atom support was performed, and a k-atom inner bound was generated by taking the convex hull of the entropic vectors corresponding to the optimized distribution.

The progress of characterizing Γ^*_4 while performing these experiments was in part estimated by the volume of the inner bound as compare to the total volume of the pyramid

inner and outer bounds	percent of pyramid
Shannon	100
Outer bound from [21]	96.5
4,5,6 atoms inner bound	57.8
4,5 atoms inner bound	57.1
4 atoms inner bound	55.9
4 atom conjecture point only	43.5
3 atoms inner bound	0

TABLE III
THE VOLUME INCREASE WITHIN PYRAMID G_4^{34} AS MORE ATOMS ARE INCLUDED

G_4^{34}. For comparison purpose, we also list the calculated volume ratio of the best outer bound in [10], the result is shown in Table III. Note the volume of the k-atom inner bound obtained through the process describe above is only a estimated value and a lower bound to the true volume fraction, because only a finite number of cost functions and a finite number of entropic vectors were generated through the random cost function generation process. In principle one can generate as much entropic vectors as one wants through this process by growing the number of random cost functions selected, however calculating volume for many extreme points in high dimension can become computationally intractable. A key observation from the process is that while growing the support helps, from a volume standpoint the improvement after four atoms is somewhat small.

However, volume is just one metric for an inner bound, which can also be hard to visualize in high dimensions. For this reason, similar to what we did in Figure 1 of §III, we would like to visualize the k-atom inner bound in lower dimension. Here instead of viewing it in two dimensions, we follow the procedure of [11] to transform the 15 dimensional pyramid into 3 dimension. Each numerically obtained 15 dimensional vector $h \in G_4^{34}$ is first transformed into its *tight* component by subtracting its *modular* component which is defined by

$$h^m(I) = \sum_{i \in I} [h(N) - h(N \backslash i)] \quad I \subseteq N$$

Next h^{ti} was pushed onto the hyperplane such that $I(X_3, X_4) = 0$ and $I(X_1, X_2 | X_3, X_4) = 0$ through linear mapping

$$\begin{aligned} h_{AB} = A_{34} B_{34,1} h^{ti} = h^{ti} + (h_3^{ti} + h_4^{ti} - h_{34}^{ti})(r_1^3 - r_1^{\emptyset}) \\ +(h_{123}^{ti} + h_{124}^{ti} - h_{34}^{ti} - h_{1234}^{ti})(r_2^1 - r_3^{\emptyset}) \end{aligned}$$

After that, another linear mapping C_{34}(refer to page 14 of [11])

$$h_C = C_{34} h_{AB}$$

is used to further reduce the dimension of G_4^{34} to 4. If we further normalize the last dimension to equal to one, that is $g = h_C \backslash h_{C_{1234}}$, the resulting polytope is three dimensional. Define $\alpha = \frac{1}{4} f_{34}$, $\beta = \frac{1}{2}(r_1^3 + r_1^4)$, $\gamma = \frac{1}{4}(r_2^1 + r_2^2)$ and $\delta = \frac{1}{4}(r_1^{13} + r_1^{14} + r_1^{23} + r_1^{24})$, for any given transformed g, we can write

$$g = \bar{\alpha}_h \alpha + \bar{\beta}_h \beta + \bar{\gamma}_h \gamma + \bar{\delta}_h \delta$$

where $\bar{\alpha}_h + \bar{\beta}_h + \bar{\gamma}_h + \bar{\delta}_h = 1$. So in three dimensional space, we consider α to be (0, 0, 1), β to be (1, 0, 0), γ to be (0, 1, 0), δ to be (1, 1, 0), so we can make the plot using $\bar{\beta}_h + \bar{\delta}_h$, $\bar{\gamma}_h + \bar{\delta}_h$ and $\bar{\alpha}_h$ as the three coordinate.

See Figure 3 for a surface plot of the inner bound generated by 4-atom supports, where we also plot the extremal points of 5-atom(red X) and 6-atom(black squares) inner bounds for comparison. Since we are transforming entropic vector from 15 dimension to 3 dimension, lots of extreme points of our 15 dimensional inner bound actually become redundant in this three dimensional space, so the number of points we can plot is significantly less than the number of extreme points we get from numerical optimization. As can be seen in Figure 3, the extreme points of 4-atom inner bound mostly lies in a curve, where there are some 5-atom extreme points away from the curve, and some of 6-atom extreme points get even further away.

In order to better visualize the difference between different inner bound, we also compared the contour of inner bound generated by $\leq k$ atom supports for $k \in \{4, 5, 6\}$, see Figure 4 for this comparison plot where *blue* line is $k = 4$, *red* line is $k = 5$ and *black* line is $k = 6$. As you can see, the contour is larger as more atoms are involved, meaning we can constantly get better inner bound by increasing the number of atoms, this is because more types of distribution supports can be found to have distribution violate Ingleton inequality.

VI. CONCLUSIONS

In this paper, we reviewed the region of entropic vector, including the best known inner and outer bounds for it, and the gap between Shannon outer bound and Ingleton inner bound. We proposed and solved the problem of listing non-isomorphic distribution supports for the purpose of calculating entropic vectors. This is carried out by fixing k, the number of atoms and N, the number of random variables, so we can grow in k or N to see the progress we make towards the characterization of entropy region. Along the way, a recursive algorithm, Snakes and Ladders, was used to efficiently enumerate the unique supports. The concept of inner bounds based on k-atom distributions was introduced to aid understanding the structure of the entropic vector region. We experimentally generated k-atom inner bounds for k = 4, 5, and 6, calculated the volume of these inner bounds, and visualized them via a certain three dimensional projection.

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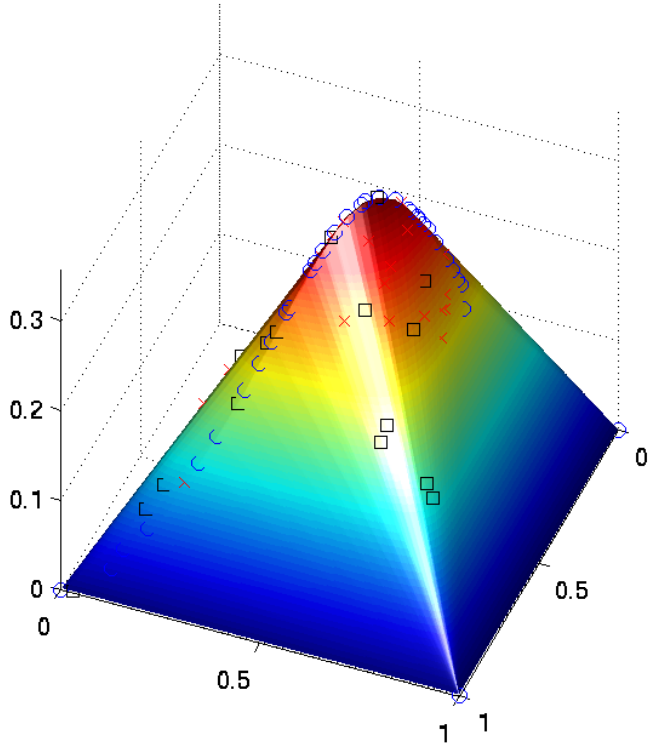

Fig. 3. The surface is a projection of a 3D face of the inner bound to $\bar{\Gamma}_4^*$ created with the numerical process described in the text with 4-atom distributions. The blue circles are the from the entropic vectors from the extremal optimized four atom distributions, while the red Xs and the black squares are the additional extremal optimized k distributions for $k \in \{5, 6\}$, respectively.

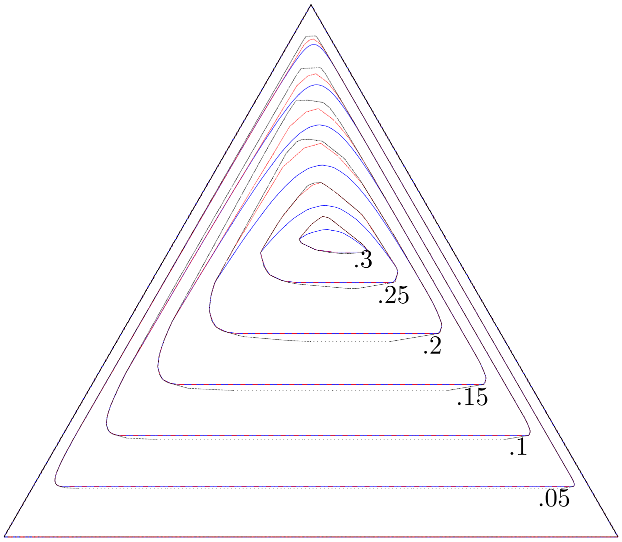

Fig. 4. Comparison of contour plots of inner bound created from $\leq k$ atom distributions for $k \in \{4, 5, 6\}$. For each contour value, the inner most line is $k = 4$ while the outermost line is $k = 6$. The numerical inner bounds generated from only four atom distributions are quite good in this space.

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