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Geometry of Discrete Copulas

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Abstract

Multivariate distributions are fundamental to modeling. Discrete copulas can be used to construct diverse multivariate joint distributions over random variables from estimated univariate marginals. The space of discrete copulas admits a representation as a convex polytope which can be exploited in entropy-copula methods relevant to hydrology and climatology. To allow for an extensive use of such methods in a wide range of applied fields, it is important to have a geometric representation of discrete copulas with desirable stochastic properties. In this paper, we show that the families of ultramodular discrete copulas and their generalization to convex discrete quasi-copulas admit representations as polytopes. We draw connections to the prominent Birkhoff polytope, alternating sign matrix polytope, and their most extensive generalizations in the discrete geometry literature. In doing so, we generalize some well-known results on these polytopes from both the statistics literature and the discrete geometry literature.

Keywords: Discrete (quasi-)copulas, ultramodularity, transportation polytope, alternating sign matrix polytope, Birkhoff polytope.

1. Introduction

Multivariate probability distributions with ordinal or interval support are fundamental to a wide range of applications, including health care, weather forecasting, and image analysis. While it is straightforward to estimate univariate marginal distributions, it is often challenging to model multivariate and high-dimensional joint distributions. Copulas (Durante

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and Sempi, 2015; Nelsen, 2006) serve as a general toolbox for constructing multivariate distributions from the estimated univariate marginals and can be equipped with different stochastic dependence properties such as exchangeability, positive/negative association, or tail dependence. Key to the power of copulas is *Sklar's Theorem*, which states that the joint distribution function $F_{\mathbf{X}}$ of *any* d -dimensional random vector $\mathbf{X} = (X_1, \dots, X_d) \in \mathbb{R}^d$ with univariate margins F_{X_1}, \dots, F_{X_d} , can be expressed as

$$F_{\mathbf{X}}(x_1, \dots, x_d) = C(F_{X_1}(x_1), \dots, F_{X_d}(x_d)),$$

where the function $C : \text{Range}(F_{X_1}) \times \dots \times \text{Range}(F_{X_d}) \rightarrow \mathbb{R}$ is uniquely defined and known as *d-dimensional copula* (Sklar, 1959). In the case of purely discrete random vectors, Sklar's theorem identifies the *discrete copulas*.

In view of their probabilistic meaning, it is beneficial to have a wealth of copula functions with application-specific properties. As directly constructing copulas with desirable features is a challenging task, researchers often focus on identifying stochastic properties that may serve as a tool for copula constructions. A property known as *ultramodularity* (Marinacci and Montucchio, 2005) is particularly desirable while aiming at constructing new copulas (Klement et al., 2011, 2014, 2017; Saminger-Platz et al., 2017). In this paper, we show that bivariate discrete copulas with properties such as ultramodularity admit *polytopal representations* and thereby demonstrate that the analysis of stochastic dependence via copulas is amenable to techniques from *convex geometry* and *linear optimization*.

A (*convex*) *polytope* is a bounded convex body in \mathbb{R}^n that consists of the points $(x_1, \dots, x_n) \in \mathbb{R}^n$ satisfying finitely many *affine inequalities*

$$a_1x_1 + a_2x_2 + \dots + a_nx_n \leq b, \tag{1}$$

where $a_1, \dots, a_n, b \in \mathbb{R}$. A collection of such inequalities is called an *H-representation* of the associated polytope. The unique irredundant *H-representation* of a polytope P is called its *minimal H-representation*. If inequality (1) is included in the minimal *H-representation* of P , then the points in P on which (1) achieves equality is the associated *facet* of P . Thus, the size of the minimal *H-representation* of P is the number of facets of P . Polytopes are fundamental objects in the field of *linear optimization*, where a key goal is to decide if a polytope has a small minimal *H-representation* as to more efficiently solve associated linear programming problems.

Discrete copulas are known to admit a representation as a convex polytope (Kolesárová et al., 2006), and such representations have already been

used to apply linear optimization techniques to solve copula-related problems in environmental sciences (AghaKouchak, 2014; Radi et al., 2017). Polytopal representations of discrete copulas are particularly useful when researchers desire copulas with *maximum entropy*; i.e., those copulas that can be used to recover the least prescriptive distributions accounting for the limited data information available. For instance, the geometric description of discrete copulas has been used in hydrology and climatology to derive copulas with maximum entropy that also match a known grade correlation coefficient (Piantadosi et al., 2007, 2012). Here, we extend the families of discrete copulas, and their generalizations, that have known polytopal representations to facilitate the further use of similar linear optimization techniques in the identification of copulas with maximum entropy and desirable stochastic properties such as ultramodularity. Our results allow obtaining simple ultramodular copulas that may serve as a tool for copula construction, and for dependence modeling in applied fields where ultramodularity is a desirable property, such as portfolio risk optimization (Müller and Scarsini, 2001) and risk aversion (Müller and Scarsini, 2012).

The space of discrete copulas in the bivariate setting (i.e., $d = 2$) was studied by Aguiló et al. (2008, 2010); Kolesárová et al. (2006); Mayor et al. (2005); Mesiar (2005); Mordelová and Kolesárová (2007). The results of these papers collectively demonstrate that the space of bivariate discrete copulas constructed from marginal distributions with finite state spaces of sizes p and q correspond to the points within a special polytope known as the *generalized Birkhoff polytope* (Ziegler, 1995). Klement et al. (2011) gave a functional characterization of ultramodular copulas. Here, we use their characterization to identify the minimal H -representation of ultramodular discrete copulas as a *subpolytope* of the generalized Birkhoff polytope.

Bivariate copulas admit an important generalization that in turn results in a natural generalization of the generalized Birkhoff polytope. The bivariate copulas form a *poset* P with partial order \prec defined as $C \prec C'$ whenever $C(u, v) < C'(u, v)$ for all $(u, v) \in [0, 1]^2$ (Durante and Sempi, 2015). However, P fails to admit desirable categorical properties. In particular, P is not a *lattice*, meaning that not all pairs of copulas, C and C' , have both a least upper bound and greatest lower bound with respect to \prec . The family of functions that complete P to a lattice under \prec are known as *quasi-copulas* (Nelsen and Flores, 2005), and in the case where $p = q$, the bivariate discrete quasi-copulas correspond to points within a polytope known as the *alternating sign matrix polytope* (Striker, 2009). In this paper, we identify the minimal H -representations for the family of *discrete quasi-copulas* with $p \neq q$ and the subfamily of *discrete quasi-copulas with convex sections* re-

siding within. Notably, we generalize a theorem of Striker (2009, Theorem 3.3) by showing that the *alternating transportation polytopes* (Knight, 2009) have minimal H -representations whose size is quadratic in p and q , a result of independent interest in discrete geometry.

The remainder of this paper is organized as follows: In Section 2, we provide basic definitions. In Section 3, we present our first main result (Theorem 1), in which we show that the collection of ultramodular bivariate discrete copulas is representable as a polytope, and we identify its minimal H -representation. The statistical significance of this result is that it allows rephrasing the problem of selecting an ultramodular bivariate discrete copula as an efficient linear optimization problem. Similarly, the collection of bivariate discrete quasi-copulas is also representable as a polytope generalizing the alternating sign matrix polytope. In Section 4, we give our second main result (Theorem 3), in which we identify the minimal H -representation of this polytope, thereby generalizing a result in discrete geometry (Striker, 2009). In addition, we identify the minimal H -representation of a subpolytope corresponding to the discrete quasi-copulas with convex sections. In Section 5, we analyze alternative representations of these polytopes; i.e., their sets of *vertices*. Finally, in Section 6, we show that the most extensive generalization of bivariate discrete copulas in the statistical literature admits a characterization in terms of the most extensive generalization of the Birkhoff polytope in the discrete geometry literature, thereby completely unifying these two hierarchies. Collectively, these results provide new and potentially useful geometric perspectives on important families of discrete copulas and quasi-copulas and introduce previously unstudied polytopes that may be of independent interest to researchers in discrete geometry.

2. Copulas and Quasi-copulas in Discrete Geometry

In this section, we present the statistical and geometric preliminaries we will use throughout the paper. We first recall definitions and fundamental results for copulas and quasi-copulas. We then explicitly define the polytopes we will study in the remaining sections. The following defines bivariate copulas by way of functional inequalities.

Definition 1. A function $C : [0, 1]^2 \rightarrow [0, 1]$ is a *copula* if and only if

(C1) for every $u \in [0, 1]$, $C(u, 0) = C(0, u) = 0$ and $C(u, 1) = C(1, u) = u$;

(C2) for every $u_1, u_2, v_1, v_2 \in [0, 1]$ s.t. $u_1 \leq u_2, v_1 \leq v_2$, it holds that

$$C(u_1, v_1) + C(u_2, v_2) \geq C(u_1, v_2) + C(u_2, v_1). \quad (2)$$

Hence, bivariate copulas are functions on the unit square that are uniform on the boundary (C1), *supermodular* (C2), and that capture the joint dependence of random vectors. A (*coordinatewise*) *section* of a bivariate copula is any function given by fixing one of the two variables. A copula is *ultramodular* if and only if all of its coordinatewise sections are convex functions (Klement et al., 2011, 2014). The following generalizes bivariate copulas:

Definition 2. (Genest et al., 1999) A function $Q : [0, 1]^2 \rightarrow [0, 1]$ is a *quasi-copula* if and only if it satisfies condition (C1) of Definition 1,

(Q2) Q is increasing in each component, and

(Q3) Q satisfies the 1-Lipschitz condition, i.e., $\forall u_1, u_2, v_1, v_2 \in [0, 1]$,

$$|Q(u_2, v_2) - Q(u_1, v_1)| \leq |u_1 - v_1| + |u_2 - v_2|.$$

Equivalently, Genest et al. (1999) show that bivariate quasi-copulas are functions that satisfy the boundary condition (C1) and are supermodular on any rectangle with at least one edge on the boundary of the unit square.

2.1. Polytopes for Copulas and Quasi-copulas

In the following, for $p \in \mathbb{Z}_{>0} := \mathbb{N} \setminus \{0\}$ we let $[p] := \{1, \dots, p\}$, $\langle p \rangle := \{0, 1, \dots, p\}$, and $I_p := \{0, \frac{1}{p}, \dots, \frac{p-1}{p}, 1\}$. When the marginal state spaces of a discrete (quasi)-copula $C_{p,q} : I_p \times I_q \rightarrow [0, 1]$ are of sizes p and q , respectively, we can then define it on the domain $I_p \times I_q$. It follows that $C_{p,q}$ is representable with a $(p+1) \times (q+1)$ matrix $C = [c_{ij}]$, where $c_{ij} := C_{p,q}(i/p, j/q)$. We can then define the set of discrete copulas on $I_p \times I_q$, denoted by $\text{DC}_{p,q}$, to be all matrices $[c_{ij}] \in \mathbb{R}^{(p+1) \times (q+1)}$ satisfying the affine inequalities

$$(c1) \quad c_{0j} = 0, \quad c_{pj} = \frac{j}{q}; \quad c_{i0} = 0, \quad c_{iq} = \frac{i}{p} \quad \text{for all } i \in \langle p \rangle, j \in \langle q \rangle;$$

$$(c2) \quad c_{ij} + c_{i-1, j-1} - c_{i, j-1} - c_{i-1, j} \geq 0 \quad \text{for all } i \in [p], j \in [q].$$

Analogously, the polytope of discrete quasi-copulas on $I_p \times I_q$ is denoted by $\text{DQ}_{p,q}$ and it consists of all matrices $[c_{ij}] \in \mathbb{R}^{(p+1) \times (q+1)}$ satisfying

$$(q1) \quad c_{0j} = 0, \quad c_{pj} = \frac{j}{q}; \quad c_{i0} = 0, \quad c_{iq} = \frac{i}{p} \quad \text{for all } i \in \langle p \rangle, j \in \langle q \rangle;$$

$$(q2a) \quad 0 \leq c_{i+1, j} - c_{ij} \leq \frac{1}{p} \quad \text{for all } i \in \langle p-1 \rangle, j \in [q];$$

$$(q2b) \quad 0 \leq c_{i, j+1} - c_{ij} \leq \frac{1}{q} \quad \text{for all } i \in [p], j \in \langle q-1 \rangle.$$

We now recall the definitions of some classically studied polytopes in discrete geometry and show how they relate to the polytopes $\text{DC}_{p,q}$ and $\text{DQ}_{p,q}$. Given two vectors $u := (u_1, \dots, u_p) \in \mathbb{R}_{>0}^p$ and $v := (v_1, \dots, v_q) \in \mathbb{R}_{>0}^q$, the *transportation polytope* $\mathcal{T}(u, v)$ is the convex polytope defined in the pq variables x_{ij} for $i \in [p]$ and $j \in [q]$ satisfying

$$x_{ij} \geq 0, \quad \sum_{h=1}^q x_{ih} = u_i, \quad \text{and} \quad \sum_{\ell=1}^p x_{\ell j} = v_j,$$

for all $i \in [p]$ and $j \in [q]$. The vectors u and v are called the *margins* of $\mathcal{T}(u, v)$. Transportation polytopes capture a number of classically studied polytopes in combinatorics (De Loera and Kim, 2014). For example, the p^{th} *Birkhoff polytope*, denoted by \mathcal{B}_p , is the transportation polytope $\mathcal{T}(u, v)$ with $u = v = (1, 1, \dots, 1)^T \in \mathbb{R}^p$, and the $p \times q$ *generalized Birkhoff polytope*, denoted by $\mathcal{B}_{p,q}$, is the transportation polytope $\mathcal{T}(u, v)$ where $u = (q, q, \dots, q) \in \mathbb{R}^p$ and $v = (p, p, \dots, p) \in \mathbb{R}^q$.

Another combinatorially-well-studied polytope that contains \mathcal{B}_p is given by the convex hull of all *alternating sign matrices*, i.e., square matrices with entries in $\{0, 1, -1\}$ such that the sum of each row and column is 1 and the nonzero entries in each row and column alternate in sign. Striker (2009, Theorem 2.1) proved that this polytope, known as the *alternating sign matrix polytope* and denoted by \mathcal{ASM}_p , is defined by

$$0 \leq \sum_{\ell=1}^i x_{\ell j} \leq 1, \quad 0 \leq \sum_{h=1}^j x_{ih} \leq 1, \quad \sum_{i=1}^n x_{ij} = 1, \quad \sum_{j=1}^n x_{ij} = 1,$$

for all $i, \ell, j, h \in [n]$. Given margins $u \in \mathbb{R}^p$ and $v \in \mathbb{R}^q$, \mathcal{ASM}_p was generalized to the *alternating transportation polytope* $\mathcal{A}(u, v)$ (Knight, 2009, Chapter 5), consisting of all $p \times q$ matrices $[x_{ij}] \in \mathbb{R}^{p \times q}$ satisfying

- (1) $\sum_{\ell=1}^p x_{\ell j} = v_j$; $\sum_{h=1}^q x_{ih} = u_i$ for $i \in [p]$ and $j \in [q]$,
- (2) $0 \leq \sum_{\ell=1}^i x_{\ell j} \leq v_j$ for all $i \in [p]$ and $j \in [q]$,
- (3) $0 \leq \sum_{h=1}^j x_{ih} \leq u_i$ for all $i \in [p]$ and $j \in [q]$.

Analogous to the generalized Birkhoff polytope, we define the *generalized alternating sign matrix polytope*, denoted $\mathcal{ASM}_{p,q}$, to be the alternating transportation polytope $\mathcal{A}(u, v)$ with $u = (q, q, \dots, q)^T \in \mathbb{R}^p$ and $v = (p, p, \dots, p)^T \in \mathbb{R}^q$. As shown in Proposition 1, there is an (invertible) linear transformation taking each discrete copula $[c_{ij}] \in \mathbb{R}^{(p+1) \times (q+1)}$ to a matrix $[b_{ij}] \in \mathcal{B}_{p,q}$ and taking each discrete quasi-copula to a matrix in $\mathcal{ASM}_{p,q}$. In the following result we show that this linear transformation, which is well-known in the statistical literature, is also geometrically nice.

Proposition 1. *The polytopes $\text{DC}_{p,q}$ and $\frac{1}{pq}\mathcal{B}_{p,q}$ are unimodularly equivalent, as are the polytopes $\text{DQ}_{p,q}$ and $\frac{1}{pq}\mathcal{ASM}_{p,q}$.*

Proof. Recall that two polytopes \mathcal{P} and \mathcal{Q} are unimodularly equivalent if and only if there exists a unimodular transformation L from \mathcal{P} to \mathcal{Q} , i.e., $L : \mathcal{P} \rightarrow \mathcal{Q}$, $x \mapsto \mathbf{A}x'$ is a linear transformation such that $\det(\mathbf{A}) = \pm 1$. It can be seen that there is a linear map $T : \mathbb{R}^{(p+1) \times (q+1)} \rightarrow \mathbb{R}^{p \times q}$ for which $T(c_{ij}) := c_{ij} + c_{i-1,j-1} - c_{i,j-1} - c_{i-1,j}$ for all $i \in [p]$ and $j \in [q]$ that takes a discrete copula to a matrix in $\frac{1}{pq}\mathcal{B}_{p,q}$. Similarly, the linear map T takes a discrete quasi-copula to a matrix in $\frac{1}{pq}\mathcal{A}(u, v)$. Using the boundary condition (c1), the map T is then an invertible transformation on $\mathbb{R}^{p \times q}$, and if we let e_{ij} denote the standard basis vectors for $\mathbb{R}^{p \times q}$ ordered lexicographically (i.e. $e_{ij} < e_{kr}$ if and only if $i < k$ or $i = k$ and $j < r$), then we see that the matrix for the map T is lower triangular and has only ones on the diagonal when the standard basis is chosen with the lexicographic ordering on the columns and rows. Therefore, T is unimodular. \square

Remark 1. Proposition 1 shows that the geometry of $\mathcal{B}_{p,q}$ and $\mathcal{ASM}_{p,q}$ completely describes the geometry of the collection of discrete copulas and discrete quasi-copulas, respectively. In particular, $\text{DC}_{p,q}$ and $\mathcal{B}_{p,q}$ have the same facial structure, and similarly for $\text{DQ}_{p,q}$ and $\mathcal{ASM}_{p,q}$. In addition, for any subpolytopes $P \subset \text{DC}_{p,q}$ and $Q \subset \text{DQ}_{p,q}$ the subpolytopes $T(P) \subset \mathcal{B}_{p,q}$ and $T(Q) \subset \mathcal{ASM}_{p,q}$ have the same facial structure, respectively. \square

The *polytope of ultramodular discrete copulas* is the subpolytope $\text{UDC}_{p,q} \subset \text{DC}_{p,q}$ satisfying the additional constraints

$$2c_{ij} \leq c_{i-1,j} + c_{i+1,j} \quad \text{and} \quad 2c_{ij} \leq c_{i,j-1} + c_{i,j+1}, \quad (3)$$

for all $i \in [p-1]$ and $j \in [q-1]$. These constraints correspond to convexity conditions imposed on the associated copulas, and so we can naturally define a similar subpolytope of $\text{DQ}_{p,q}$. The *polytope of convex discrete quasi-copulas* is the subpolytope $\text{CDQ}_{p,q} \subset \text{DQ}_{p,q}$ satisfying the above constraints (3). Via the transformation T , we will equivalently study the polytopes $\mathcal{UDC}_{p,q} := pqT(\text{UDC}_{p,q}) \subset \mathcal{B}_{p,q}$ and $\mathcal{CDQ}_{p,q} := pqT(\text{CDQ}_{p,q}) \subset \mathcal{ASM}_{p,q}$. We end this section with a second geometric remark.

Remark 2. It is well known that the generalized Birkhoff polytope $\mathcal{B}_{p,q}$ has dimension $(p-1)(q-1)$ (see (De Loera and Kim, 2014) for instance). This is because each of the defining equalities $\sum_{i=1}^p x_{ij} = p$ and $\sum_{j=1}^q x_{ij} = q$ determine precisely one more entry of the matrix. In a similar fashion, the polytopes $\mathcal{UDC}_{p,q}$, $\mathcal{ASM}_{p,q}$, and $\mathcal{CDQ}_{p,q}$ and also the polytopes of discrete (quasi)-copulas $\text{DC}_{p,q}$, $\text{UDC}_{p,q}$, $\text{DQ}_{p,q}$, and $\text{CDQ}_{p,q}$ studied in this paper all have dimension $(p-1)(q-1)$. \square

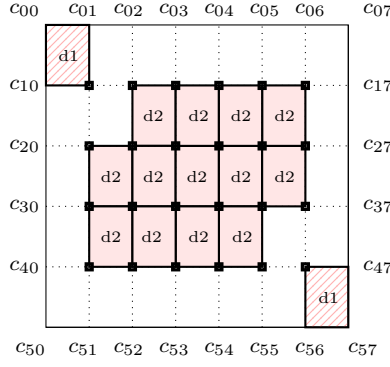


Figure 1: A depiction of the inequalities for the minimal H -representation of $UDC_{5,7}$. The rectangles represent the necessary supermodularity constraints (C2), while the square dots represent the convexity constraints (3).

3. The Polytope of Ultramodular Discrete Copulas

In our first main theorem we identify the minimal H -representation of the polytope of ultramodular discrete copulas $UDC_{p,q}$.

Theorem 1. *The minimal H -representation of the polytope of ultramodular discrete copulas $UDC_{p,q}$ consists of the $(p-2)(q-2) + 2(p-1)(q-1)$ inequalities:*

- (d1) $x_{11} \geq 0$, and $x_{p-1,q-1} \geq \frac{(p-1)(q-1)-1}{pq}$,
- (d2) $x_{ij} + x_{i+1,j+1} - x_{i,j+1} - x_{i+1,j} \geq 0$ for all $i \in [p-2], j \in [q-2]$ with $(i, j) \notin \{(1, 1), (p-2, q-2)\}$,
- (d3a) $x_{ij} + x_{i,j+2} - 2x_{i,j+1} \geq 0$ for all $i \in [p-1], j \in [q-2]$,
- (d3b) $x_{ij} + x_{i+2,j} - 2x_{i+1,j} \geq 0$ for all $j \in [q-1], i \in [p-2]$.

Figure 1 gives a diagrammatic depiction of the inequalities constituting the minimal H -representation of $UDC_{p,q}$. An equivalent statement to Theorem 1 is that the subpolytope $\mathcal{UDC}_{p,q}$ of the generalized Birkhoff polytope $\mathcal{B}_{p,q}$ has minimal H -representation given by the inequalities

- (b1) $x_{11} \geq 0$, and $x_{pq} \geq 0$,
- (b2) $x_{i+1,j+1} \geq 0$ for all $i \in [p-2], j \in [q-2]$ with $(i, j) \notin \{(1, 1), (p-2, q-2)\}$,
- (b3a) $\sum_{\ell=1}^i x_{\ell,j+1} \geq \sum_{\ell=1}^i x_{\ell j}$ for all $i \in [p-1], j \in [q-1]$,

$$(b3b) \quad \sum_{h=1}^j x_{i+1,h} \geq \sum_{h=1}^j x_{ih} \text{ for all } i \in [p-1], j \in [q-1].$$

To prove that the inequalities (d1), (d2), (d3a), and (d3b) constitute the minimal H -representation of $UDC_{p,q}$, we first demonstrate that if $[c_{ij}] \in \mathbb{R}^{(p+1) \times (q+1)}$ satisfies the boundary condition (c1) and all of (d1), (d2), (d3a), and (d3b), then $[c_{ij}] \in UDC_{p,q}$. This is proven in Lemma 9 in the Appendix. Then we show that for each inequality in the list (d1), (d2), (d3a), and (d3b) there exists a point $[c_{ij}] \in \mathbb{R}^{(p+1) \times (q+1)}$ failing to satisfy this inequality that satisfies all the other inequalities. We do this by proving the analogous fact for the subpolytope $UDC_{p,q}$ of $\mathcal{B}_{p,q}$. Since the details of this argument are technical, the complete proof is given in the Appendix.

In the following theorem and remark we show that every point in $UDC_{p,q}$ can be realized as a restriction of some ultramodular bivariate copula on $[0, 1]^2$ and that any restriction of an ultramodular discrete copula is in fact a point in $UDC_{p,q}$. In particular, any point in $UDC_{p,q}$ can be extended to an ultramodular copula on $[0, 1]^2$ known as the *checkerboard extension copula* (Nelsen, 2006). The proof of Theorem 2 is given in the Appendix.

Theorem 2. *Given $p, q \in \mathbb{Z}_{>0}$, the checkerboard extension copula of any $[c_{ij}] \in UDC_{p,q}$ is an ultramodular copula on the unit square.*

Remark 3. The restriction C of any ultramodular copula \tilde{C} on a non-square uniform grid $I_p \times I_q$ of the unit square belongs to $UDC_{p,q}$. Indeed, let us consider a copula \tilde{C} that is ultramodular. Then the restriction C of \tilde{C} to the interval $I_p \times I_q$ is a discrete copula (Kolesárová et al., 2006; Nelsen, 2006). Therefore, C belongs to $DC_{p,q}$ and satisfies (d1), (d2), and (d3). Since \tilde{C} is ultramodular, all of its horizontal and vertical sections are univariate continuous convex functions that fulfill the *Jensen inequality*; i.e., for every $u_1, u_2 \in [0, 1]$, and $a \in [0, 1]$, $\tilde{C}(\frac{u_1}{2} + \frac{u_2}{2}, a) \leq \frac{1}{2}\tilde{C}(u_1, a) + \frac{1}{2}\tilde{C}(u_2, a)$. Inequalities (d3b) can be derived by fixing $a = \frac{j}{q}$, while $u_1 = \frac{i}{p}$, $u_2 = \frac{i+2}{p}$ for $j \in [q-1]$ and $i \in \langle p-2 \rangle$. In an analogous manner, one can obtain conditions (d3a). Hence, $C \in UDC_{p,q}$. \square

Theorem 2 and Remark 3 also provide a statistical interpretation for the polytope $UDC_{p,q}$. In particular, they identify a correspondence between each point in $UDC_{p,q}$, normalized with a multiplicative factor $\frac{1}{pq}$, and the probability mass of an ultramodular bivariate copula on $[0, 1]^2$, which can be constructed via checkerboard extension techniques. This is interesting from a statistical perspective as the checkerboard extension copula plays a crucial role in the entropy-copula approaches presented in Piantadosi et al.

(2007, 2012), and it is at the base of the empirical multilinear copula process recently introduced by Genest et al. (2014, 2017).

4. Polytopes of (Convex) Discrete Quasi-copulas

In this section, we identify the minimal H -representations for the polytope of discrete quasi-copulas $\text{DQ}_{p,q}$ and its subpolytope of convex discrete quasi-copulas $\text{CDQ}_{p,q}$. Recall from Proposition 1 that $\text{DQ}_{p,q}$ is unimodularly equivalent to a dilation of the generalized alternating sign matrix polytope $\mathcal{ASM}_{p,q}$, which was originally studied in (Knight, 2009, Chapter 5). However, while the minimal H -representation for the case $p = q$ (i.e., for the polytope \mathcal{ASM}_p) was identified in (Striker, 2009, Theorem 3.3), it was unknown for $p \neq q$. In this section, we identify the minimal H -representation for $\mathcal{ASM}_{p,q}$ (and hence also for $\text{DQ}_{p,q}$) and also for the polytope $\text{CDQ}_{p,q}$.

It is shown in (Striker, 2009, Theorem 3.3) that for $p \geq 3$ the polytope \mathcal{ASM}_p has $4[(p-2)^2 + 1]$ facets given by the inequalities

- (1) $x_{11} \geq 0$, $x_{1p} \geq 0$, $x_{p1} \geq 0$, and $x_{pp} \geq 0$;
- (2) $\sum_{k=1}^{i-1} x_{kj} \geq 0$, and $\sum_{k=i+1}^p x_{kj} \geq 0$ for $i, j \in \{2, \dots, p-1\}$;
- (3) $\sum_{h=1}^{j-1} x_{ih} \geq 0$, and $\sum_{h=j+1}^p x_{ih} \geq 0$ for $i, j \in \{2, \dots, p-1\}$.

Suppose now that $3 \leq p < q$ and that $q = kp + r$ for $0 \leq r < p$. Our second main theorem of the paper generalizes Theorem 3.3 of Striker (2009).

Theorem 3. *Suppose $3 \leq p < q$ with $q = kp + r$ for $0 \leq r < p$. The minimal H -representation of the generalized alternating sign matrix polytope $\mathcal{ASM}_{p,q}$ consists of the $2((p-1)(q-2) + 2) + 2(p-2)(q-k-1)$ inequalities*

- (a1) $x_{11} \geq 0$, $x_{1q} \geq 0$, $x_{p1} \geq 0$, and $x_{pq} \geq 0$;
- (a2) $\sum_{\ell=1}^{i-1} x_{\ell j} \geq 0$, $\sum_{\ell=i+1}^p x_{\ell j} \geq 0$ for $i \in [p-1]$, $j \in \{2, \dots, q-1\}$;
- (a3) $\sum_{h=1}^{j-1} x_{ih} \geq 0$, $\sum_{h=j+1}^p x_{ih} \geq 0$ for $i \in \{2, \dots, p-1\}$, $j \in [q-k-1]$.

To proof is given in the Appendix and is analogous to the approach taken for proving Theorem 1. The natural functional generalization of ultramodular discrete copulas to the setting of quasi-copulas are *convex* discrete quasi-copulas; i.e., discrete quasi-copulas admitting convex (coordinatewise) sections. These functions are parametrized by the points $[c_{ij}]$ within the polytope $\text{CDQ}_{p,q}$, which has the following H -representation:

Theorem 4. *The minimal H -representation of the polytope of convex discrete quasi-copulas $\text{CDQ}_{p,q}$ consists of the $2[(p-1)(q-1) + 1]$ inequalities*

- (v1) $x_{11} \geq 0, \quad x_{p-1,q-1} \geq \frac{(p-1)(q-1)-1}{pq};$
(v3a) $x_{ij} + x_{i,j+2} - 2x_{i,j+1} \geq 0 \quad \text{for all } i \in [p-1], j \in \langle q-2 \rangle;$
(v3b) $x_{ij} + x_{i+2,j} - 2x_{i+1,j} \geq 0 \quad \text{for all } j \in [q-1], i \in \langle p-2 \rangle.$

The proof is again analogous to the proof of Theorem 1, and is given in the Appendix. In particular, in the proof we show that the unimodularly equivalent subpolytope $\mathcal{CDQ}_{p,q}$ of $\mathcal{ASM}_{p,q}$ has minimal H -representation

- (a1) $x_{11} \geq 0, \quad x_{pq} \geq 0;$
(a3a) $\sum_{\ell=1}^i x_{\ell,j+1} \geq \sum_{\ell=1}^i x_{\ell j} \quad \text{for all } i \in [p-1], j \in [q-1];$
(a3b) $\sum_{h=1}^j x_{i+1,h} \geq \sum_{h=1}^j x_{ih} \quad \text{for all } i \in [p-1], j \in [q-1].$

Since convex discrete quasi-copulas are the natural generalization of ultramodular discrete copulas to the quasi-copula setting, we would hope that the points $[c_{ij}] \in \mathcal{CDQ}_{p,q}$ are, analogously, the family of points that can be extended to convex quasi-copulas on $[0, 1]^2$. Indeed, this is the case:

Theorem 5. *Given $p, q \in \mathbb{Z}_{>0}$, the checkerboard extension of any $[c_{ij}] \in \mathcal{CDQ}_{p,q}$ is a quasi-copula on $[0, 1]^2$ with convex (coordinatewise) sections.*

Remark 4. Following the same considerations as in Remark 3, one can notice that the restriction C of any quasi-copula \tilde{C} on a non-square uniform grid $I_p \times I_q$ of the unit square belongs to $\mathcal{CDQ}_{p,q}$. \square

Analogous to the case of ultramodular copulas, it is useful to notice that Theorem 5 and Remark 4 identify a correspondence between each point in $\mathcal{CDQ}_{p,q}$, normalized with a multiplicative factor $\frac{1}{pq}$, and the signed measure of a bivariate quasi-copula with convex sections. Interestingly, the family of quasi-copulas with convex horizontal and vertical sections has not been studied before. Our findings suggest that further research efforts should be made in understanding the properties of this class of quasi-copulas and its relation to ultramodular copulas.

5. On Vertex Representations

In the previous sections we showed that two special families of discrete copulas and discrete quasi-copulas admit representations as convex polytopes using collections of inequalities. A powerful feature of working with

convex polytopes is that they admit an alternative representation as the convex hull of their vertices (i.e., *extreme points*). If $S \subset \mathbb{R}^p$ then the *convex hull* of S , denoted $\text{conv}(S)$, is the collection of all convex combinations of points in S . A point $x \in S$ is called an *extreme point* of S provided that for any two points $a, b \in S$ for which $(a + b)/2 = x$, we have that $a = b = x$. If $P \subset \mathbb{R}^p$ is a convex polytope, an extreme point of P is called a *vertex* and the collection of all vertices of P is denoted $\mathcal{V}(P)$. The *Krein-Milman Theorem* in convex geometry (Barvinok, 2002, Theorem 3.3) states that P can be represented by its collection of vertices, namely $P = \text{conv}(\mathcal{V}(P))$. The collection of vertices of a convex polytope is known as its *V-representation*.

For example, the vertices of the Birkhoff polytope \mathcal{B}_p are precisely the $p \times p$ permutation matrices (see for instance (Barvinok, 2002, Theorem 5.2)). In Piantadosi et al. (2007), the *V-representation* of the Birkhoff polytope is used to efficiently find a bistochastic matrix B representing a joint density that matches a prescribed grade correlation coefficient and maximizes the entropy. The full-domain checkerboard extension copula of B is the one with maximum entropy, and can be used to conduct further statistical analysis avoiding additional model assumptions. In the setting of discrete copulas, the vertices of DC_p correspond to the *empirical copulas* (Kolesárová et al., 2006; Mesiar, 2005), and thus all bivariate discrete copulas can be constructed by way of convex combinations of empirical copulas. This *V-representation* of DC_p is known in the statistical literature: the empirical copulas are precisely the copulas constructible from observed data (Mesiar, 2005), which has made them fundamental in the development of *rank-based copula methods* (Joe, 2014; Scaillet et al., 2007).

Thus, if a family of discrete copulas or quasi-copulas admits a representation as a polytope, it may be beneficial to identify its *V-representation*. At the same time, polytopes can often have a super-exponential number of vertices, meaning that it may be difficult to learn its *V-representation* in its entirety. Indeed, this appears to be the case for the polytopes $\text{UDC}_{p,q}$ and $\text{CDQ}_{p,q}$, as suggested by the data in Table 5. Although complete *V-representations* of $\text{UDC}_{p,q}$ and $\text{CDQ}_{p,q}$ seem out of reach, we can still benefit from knowing the vertices of $\text{UDC}_{p,q}$ for $(p, q) = \{(3, 3), (4, 4)\}$ to possibly select ultramodular copulas with maximum entropy in a similar fashion as in Piantadosi et al. (2007). Therefore, in the following subsection we provide two constructions to obtain families of vertices for each of these polytopes.

5.1. New Vertices by Way of Symmetry.

In the coming subsections, we will use the following fundamental theorem from convex geometry:

(p, q)	UDC	CDQ	DQ	DC
(3, 3)	7	7	7	6
(3, 4)	52	52	118	96
(3, 5)	166	138	416	360
(4, 4)	115	69	42	24
(4, 5)	3321	2163	7636	3000
(5, 5)	22890	5447	429	120

Table 1: The number of vertices of $\text{UDC}_{p,q}$, $\text{CDQ}_{p,q}$, $\text{DQ}_{p,q}$, and $\text{DC}_{p,q}$ as computed using `polymake` (Gawrilow and Joswig, 2000).

Theorem 6. (*Barvinok, 2002, Theorem 4.2*) Let $P := \{x \in \mathbb{R}^p : \langle a_i, x \rangle \leq \beta_i \text{ for } i \in [m]\}$ be a polyhedron, where $a_i \in \mathbb{R}^p$ and $\beta_i \in \mathbb{R}$ for $i \in [m]$. For $u \in P$ let $I(u) := \{i \in [m] : \langle a_i, u \rangle = \beta_i\}$ be the collection of inequalities that are active on u . Then u is a vertex of P if and only if the set of vectors $\{a_i : i \in I(u)\}$ linearly spans the vector space \mathbb{R}^p . In particular, if u is a vertex of P , then the set $I(u)$ contains at least p indices, i.e., $|I(u)| \geq p$.

The vectors β_i in the above theorem are called the *facet-normals* or *facet-normal vectors* of the polyhedron P . We now apply Theorem 6 to prove a basic symmetry statement about the vertices of $\text{UDC}_{p,q}$ and $\text{CDQ}_{p,q}$. Recall that we think of a bivariate discrete (quasi)-copula $C : I_p \times I_q \rightarrow [0, 1]$ as a $(p+1) \times (q+1)$ matrix $C = [c_{ij}]_{i,j=0}^{p,q}$ whose entries are the values of C . Given this representation for C , we can then consider its transpose C^T .

Proposition 2. Suppose that $C \in \text{UDC}_{p,q}$ ($C \in \text{CDQ}_{p,q}$), then $C^T \in \text{UDC}_{q,p}$ ($C^T \in \text{CDQ}_{q,p}$). Moreover, if C is a vertex of $\text{UDC}_{p,q}$ ($\text{CDQ}_{p,q}$), then C^T is a vertex of $\text{UDC}_{q,p}$ ($\text{CDQ}_{q,p}$).

Proof. We here prove the statement for the polytope $\text{UDC}_{p,q}$. The proof for $\text{CDQ}_{p,q}$ works analogously. Recall that the facet-defining inequalities for $\text{UDC}_{p,q}$ are (d1), (d2), (d3a), and (d3b), which can be reorganized as:

- (1) $x_{11} \geq 0$,
- (2) $x_{p-1,q-1} \geq \frac{(p-1)(q-1)-1}{pq}$,
- (3) $x_{ij} + x_{i+1,j+1} \geq x_{i,j+1} + x_{i+1,j}$ for $i \in [p-2]$ and $j \in [q-2]$,
- (4) $2x_{ij} \leq x_{i-1,j} + x_{i+1,j}$ and $2x_{ij} \leq x_{i,j-1} + x_{i,j+1}$ for $i \in [p-1]$ and $j \in [q-1]$.

By Theorem 1, the minimal H-representation of $\text{UDC}_{p,q}$ is given by the inequalities (1), (2), (3), and (4) with the exception of the two inequalities

$x_{11} + x_{22} \geq x_{12} + x_{21}$ and $x_{p-2,q-2} + x_{p-1,q-1} \geq x_{p-2,q-1} + x_{p-1,q-2}$. From this presentation of the minimal H-representation of $\text{UDC}_{p,q}$, we can see that if $C \in \text{UDC}_{p,q}$ then $C^T \in \text{UDC}_{q,p}$. Moreover, by Theorem 6, it follows that if C is a vertex of $\text{UDC}_{p,q}$ then C^T is a vertex of $\text{UDC}_{q,p}$. \square

The vertex construction technique of Proposition 2 suggests that the most informative extremal discrete copulas of UDC_p are those $\tilde{C} = [c_{ij}]$ such that $c_{ij} \neq c_{ji}$, for some $i, j \in \langle p \rangle$. Indeed, the transpose of any such \tilde{C} is a new distinct vertex of UDC_p . Thus, the checkerboard extension copulas constructed from any such vertex \tilde{C} are asymmetric copulas, i.e. those that describe the stochastic dependence of non-exchangeable random variables. Furthermore, Proposition 2 is an intuitive result whose proof provides a nice example of how Theorem 6 can be used to study extremal discrete copulas. Another example is provided in the following subsection.

5.2. New vertices by way of direct products.

Our second family of vertices arises by taking direct sums of lower-dimensional vertices. Recall from Proposition 1 that there is a linear map $T : \mathbb{R}^{(p+1) \times (q+1)} \rightarrow \mathbb{R}^{p \times q}$ sending a discrete (quasi)-copula to a matrix in $\frac{1}{pq}\mathcal{B}_{p,q}$ (a matrix in $\frac{1}{pq}\mathcal{ASM}_{p,q}$). Further recall that $\mathcal{UDC}_{p,q} = pqT(\text{UDC}_{p,q})$ and $\mathcal{CDQ}_{p,q} = pqT(\mathcal{CDQ}_{p,q})$. Define the direct sum of $B \in \mathcal{UDC}_{p,q}$ ($\mathcal{CDQ}_{p,q}$) and $D \in \mathcal{UDC}_{s,t}$ ($\mathcal{CDQ}_{s,t}$) to be the block matrix

$$B \oplus D := \begin{pmatrix} \mathbf{0}_{p,t} & B \\ D & \mathbf{0}_{s,q} \end{pmatrix} \in \mathbb{R}^{(p+s) \times (q+t)}.$$

Indeed, if we applied the transformation $R : \mathbb{R}^{(p+s) \times (q+t)} \rightarrow \mathbb{R}^{(p+s) \times (q+t)}$ with $e_{ij} \mapsto e_{i(q+t-j+1)}$, then $R(B \oplus D)$ is the direct sum of $R(B)$ and $R(D)$. In the following, we show how to use this operation to identify vertices of $\mathcal{UDC}_{p,q}$ and $\mathcal{CDQ}_{p,q}$ (and equivalently $\text{UDC}_{p,q}$ and $\text{CDQ}_{p,q}$).

Recall from Section 2 that $\mathcal{T}(u, v)$ denotes the transportation polytope with marginals $u \in \mathbb{R}^p$ and $v \in \mathbb{R}^q$, and $\mathcal{A}(u, v)$ denotes the alternating transportation polytope with the same marginals. The subpolytopes $\mathcal{UDC}_{p,q} \subset \mathcal{B}_{p,q}$ and $\mathcal{CDQ}_{p,q} \subset \mathcal{ASM}_{p,q}$ admit a natural geometric generalization to subpolytopes $\mathcal{UDC}(u, v) \subset \mathcal{T}(u, v)$ and $\mathcal{CDQ}(u, v) \subset \mathcal{A}(u, v)$. Namely, we let $\mathcal{UDC}(u, v)$ denote the subpolytope of $\mathcal{T}(u, v)$ satisfying the additional inequalities (b3a) and (b3b), and we let $\mathcal{CDQ}(u, v)$ denote the subpolytope of $\mathcal{A}(u, v)$ satisfying the additional inequalities (a3a) and (a3b). In the following, for $m, k \in \mathbb{Z}$, let $\mathbf{m}_p := (m, m, \dots, m) \in \mathbb{R}^p$, and let $(\mathbf{m}_p, \mathbf{k}_q) \in \mathbb{R}^{p+q}$ denote the concatenation of the vectors \mathbf{m}_p and \mathbf{k}_q . We can then make the following geometric observation.

Theorem 7. *If B is a vertex of $UDC_{p,q}$ ($CDQ_{p,q}$) and D is a vertex of $UDC_{s,t}$ ($CDQ_{s,t}$), then $B \oplus D$ is a vertex of $UDC((\mathbf{q}_p, \mathbf{t}_s), (\mathbf{s}_t, \mathbf{p}_q))$ (and analogously, $CDQ((\mathbf{q}_p, \mathbf{t}_s), (\mathbf{s}_t, \mathbf{p}_q))$).*

The proof of this result is another application of Theorem 6 which is given in the Appendix. In the special case where $p = q$ and $s = t$, then $UDC_{p,q}$ and $UDC_{s,t}$ are dilations of subpolytopes of \mathcal{B}_p and \mathcal{B}_s , respectively. Thus, we can assume that the marginals of $\mathcal{T}(u, v)$ are $u = v = \mathbf{1}_{p+s} \in \mathbb{R}^{p+s}$. Therefore, Theorem 7 produces vertices of UDC_{p+s} . The proof of the following corollary can be found in the Appendix.

Corollary 8. *If B is a vertex of UDC_p (CDQ_p) and D is a vertex of UDC_s (CDQ_s), then $B \oplus D$ is a vertex of UDC_{p+s} (CDQ_{p+s}).*

Remark 5 (Statistical Interpretation of Vertices). Given a copula C , a *patchwork copula* derived from C is any copula whose probability distribution coincides with the one of C up to a finite number of rectangles R_i in $[0, 1]^2$ in which the probability mass is distributed differently (Durante et al., 2013). The vertices obtained via Corollary 8 correspond to a special class of patchwork (quasi)-copulas named *W-ordinal sums*, which are patchworks derived from the Fréchet lower bound of copulas $W(u, v) = \max\{0, u + v - 1\}$ (Mesiar and Szolgay, 2004). The (normalized) direct sum of two vertices $B \in UDC_p$ (CDQ_p) and $D \in UDC_s$ (CDQ_s) is the block matrix $\frac{1}{p+q}B \oplus D$. Any extension (quasi)-copula \tilde{C} on $[0, 1]^2$, whose associated mass is given by $\frac{1}{p+q}B \oplus D$, satisfies $\tilde{C}\left(\frac{p}{p+s}, \frac{s}{p+s}\right) = 0$. Furthermore, any (quasi)-copula C with $C(u_0, 1 - u_0) = 0$ for $0 < u_0 < 1$ can be written as a W-ordinal sum (De Baets and De Meyer, 2007). Thus, any such \tilde{C} associated to $\frac{1}{p+q}B \oplus D$ is a W-ordinal sum. \square

While Corollary 8 is a useful method for constructing vertices of UDC_p and CDQ_p from known, lower-dimensional vertices, it is important to notice that not all vertices of UDC_p and CDQ_p can be captured in this fashion. For example, as we can see in Figure 2, UDC_3 has seven vertices, of which only three arise from this direct sum construction. However, as we show in the following subsection, Corollary 8 can be used to provide lower bounds on the number of vertices of these polytopes.

5.3. Generating Functions for the Number of Vertices.

In this subsection we consider the special case of the polytopes $UDC_{p,q}$ and $CDQ_{p,q}$ for which $p = q$. For convenience, we only discuss the polytope UDC_p . However, the results all hold analogously for CDQ_p . Corollary 8 gives a convenient way by which to partition the collection of vertices

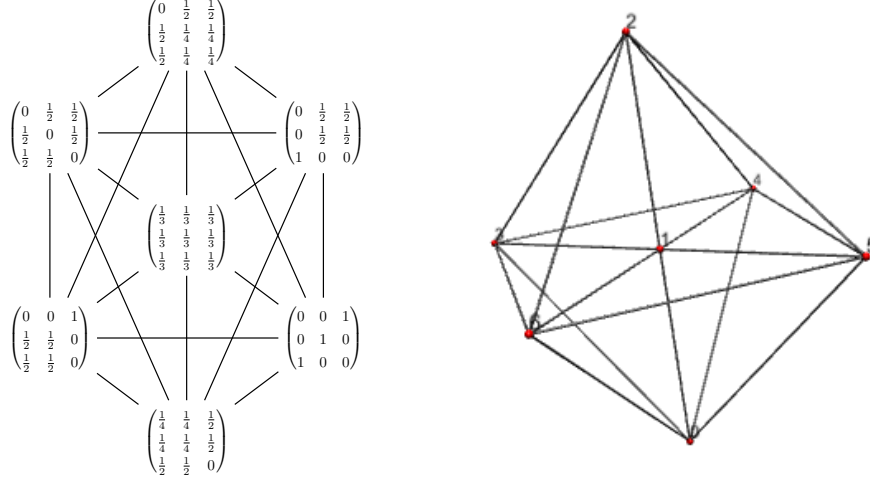


Figure 2: The edge-graph of the polytope UDC_3 , with its seven vertices, is the edge graph of a triangulated octahedron. Indeed, UDC_3 is a four-dimensional polytope, with eight simplicial facets and one octahedral facet. On the right is a *Schlegel diagram* (Ziegler, 1995) of UDC_3 as it appears when projected onto its three-dimensional, octahedral facet.

$\mathcal{V}(UDC_p)$ into two disjoint collections: we call a vertex of UDC_p *decomposable* if the corresponding vertex in UDC_p admits a decomposition as a direct sum of two lower dimensional vertices as in Corollary 8. All other vertices of UDC_p are called *indecomposable*. Let D_p and ID_p denote the decomposable and indecomposable vertices of UDC_p , respectively, and let

$$V(x) := \sum_{p \geq 0} |\mathcal{V}(UDC_p)| x^p, \quad ID(x) := \sum_{p \geq 0} |ID_p| x^p, \quad \text{and} \quad D(x) := \sum_{p \geq 0} |D_p| x^p,$$

denote the *generating functions* for the values $|\mathcal{V}(UDC_p)|$, $|ID_p|$, and $|D_p|$, respectively. As suggested by the data in Table 5, the size of the set $\mathcal{V}(UDC_p)$ appears to grow super-exponentially in p . The following observation, whose proof is given in the Appendix, may be used to provide lower bounds supporting this observed growth-rate.

Proposition 3. *The number of vertices of UDC_p is computable in terms of its number of decomposable vertices by the relationship*

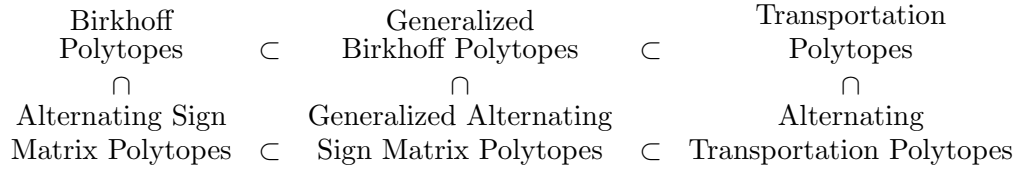
$$V(x) = \frac{D(x)^2 + D(x) - 1}{D(x)}.$$

Moreover, if $M(x) \leq D(x)$, is a lower-bound on the number of decomposable vertices of UDC_p then $V(x) \geq (M(x)^2 + M(x) - 1)/M(x)$.

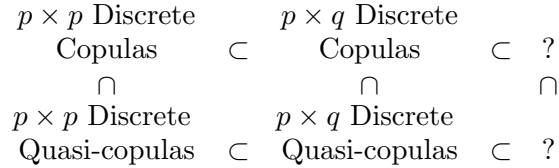
Since a lower bound on the number of decomposable vertices can be achieved by identifying a lower bound on the number of indecomposable vertices in lower dimensions, it is worthwhile to investigate large families of indecomposable *extremal* ultramodular discrete copulas. The identification of sufficiently large families of such copulas could then be used to prove that the size of the vertex representation of UDC_p grows super-exponentially, as well as serve to generate larger families of vertices of these polytopes for statistical use by the construction given in Corollary 8.

6. Aggregation Functions & Alternating Transportation Polytopes

We end this paper with a discussion aimed at completing the evolving parallel story between discrete bivariate copulas, the Birkhoff polytopes and each of their generalizations. In Section 2, we highlighted the following hierarchy of generalizations of Birkhoff polytopes:



Analogously, we have the hierarchy of generalizations of discrete copulas:



The main efforts of this paper were aimed at identifying polyhedral representations of subfamilies of each of these collections of functions (Sections 3 and 4) as well as a polyhedral representation of the family of $p \times q$ discrete quasi-copulas in its entirety (Theorem 3). However, we can also extend the correspondence between these hierarchies of generalizations in terms of a functional generalization of copulas:

Definition 3. (Grabisch et al., 2009) A *(binary) aggregation function* is a function $C : [0, 1]^2 \rightarrow [0, 1]$ that satisfies the following

(A1) $C(0, 0) = 0$ and $C(1, 1) = 1$;

(A2) $C(u_1, v_1) \leq C(u_2, v_2)$, for every $u_1 \leq u_2, v_1 \leq v_2 \in [0, 1]$.

Aggregation functions naturally include copulas and quasi-copulas. In particular, copulas are the supermodular aggregation functions with annihilator 0 and neutral element 1, and quasi-copulas are 1-Lipschitz aggregation functions with annihilator 0 and neutral element 1. Analogous to the case of discrete (quasi)-copulas, we can consider discrete aggregation functions C_{pq} with domain $I_p \times I_q$, which are representable by a matrix $[c_{ij}] \in \mathbb{R}^{(p+1) \times (q+1)}$ where $c_{ij} := C_{p,q}(i/p, j/q)$. By way of the same linear transformation used in Proposition 1, we now observe a correspondence between discrete aggregation functions and the matrices within (alternating) transportation polytopes $\mathcal{A}(u, v)$ with *homogeneous marginals*; i.e., $\sum_i u_i = \sum_j v_j = pq$.

Given two vectors $\tilde{u} := (\tilde{u}_1, \dots, \tilde{u}_p) \in \mathbb{R}_{>0}^p$ and $\tilde{v} := (\tilde{v}_1, \dots, \tilde{v}_q) \in \mathbb{R}_{>0}^q$ with $\tilde{u}_p = \tilde{v}_q = pq$, we define the set $\text{SAF}(\tilde{u}, \tilde{v})$ to be the matrices $[c_{ij}] \in \mathbb{R}^{(p+1) \times (q+1)}$ satisfying

- (AF1a) $c_{0j} = 0, c_{i0} = 0$ with $i \in \langle p \rangle, j \in \langle q \rangle$;
- (AF1b) $c_{p,j-1} = \frac{\tilde{v}_{j-1}}{pq} < \frac{\tilde{v}_j}{pq} = c_{pj}, c_{i-1,q} = \frac{\tilde{u}_{i-1}}{pq} < \frac{\tilde{u}_i}{pq} = c_{iq}$,
- (AF2a) $c_{ij} + c_{i-1,j-1} - c_{i-1,j} - c_{i,j-1} \geq 0$ for every $i \in [p], j \in [q]$.

Note that the elements of $\text{SAF}(\tilde{u}, \tilde{v})$ are discrete aggregation functions. Indeed, given any $i_1 \leq i_2 \in \langle p \rangle$, and $j_1 \leq j_2 \in \langle p \rangle$, property (AF2a) implies that $c_{i_2, j_2} \geq c_{i_1, j_2} \geq c_{i_1, j_1}$. The following proposition links the set $\text{SAF}(\tilde{u}, \tilde{v})$ to a transportation polytope $\mathcal{T}(u, v)$ with homogeneous marginals. The proof of the following two propositions can be found in the Appendix.

Proposition 4. *For a function $C_{pq} : I_p \times I_q \rightarrow [0, 1]$, the following statements are equivalent:*

- (i) $C_{pq} \in \text{SAF}(\tilde{u}, \tilde{v})$.
- (ii) *There is a $(p \times q)$ transportation matrix $[x_{ij}]$ in $\mathcal{T}(u, v)$, with $\sum_{h=1}^q v_h = \sum_{\ell=1}^p u_\ell = pq$, such that for every $i \in \langle p \rangle, j \in \langle q \rangle$*

$$c_{ij} := C_{p,q} \left(\frac{i}{p}, \frac{j}{q} \right) = \frac{1}{pq} \sum_{\ell=1}^i \sum_{h=1}^j x_{\ell h}. \quad (4)$$

A similar construction offers a correspondence between families of aggregation functions and alternating transportation polytopes with homogeneous marginals. Given two vectors $\tilde{u} := (\tilde{u}_1, \dots, \tilde{u}_p) \in \mathbb{R}_{>0}^p$ and $\tilde{v} := (\tilde{v}_1, \dots, \tilde{v}_q) \in \mathbb{R}_{>0}^q$, we define the set $\text{ASA}(\tilde{u}, \tilde{v})$ to be the matrices $[c_{ij}] \in \mathbb{R}^{(p+1) \times (q+1)}$ which satisfy conditions (AF1a), (AF1b), and

- (AF2b) $c_{i_1 j_1} + c_{i_2 j_2} - c_{i_1 j_2} - c_{i_2 j_1} \geq 0$ for every $i_1 \leq i_2 \in \langle p \rangle, j_1 \leq j_2 \in \langle q \rangle$, and $i_1 = 0$, or $i_2 = p$, or $j_1 = 0$, or $j_2 = q$.

It can be shown that the elements of $ASA(\tilde{u}, \tilde{v})$ are discrete aggregation functions by following the same reasoning presented for the set $SAF(\tilde{u}, \tilde{v})$. The following proposition shows the link between the set $ASA(\tilde{u}, \tilde{v})$ and an alternating transportation polytope $\mathcal{A}(u, v)$.

Proposition 5. *For a function $C_{pq} : I_p \times I_q \rightarrow [0, 1]$, the following statements are equivalent:*

- (i) $C_{pq} \in ASA(\tilde{u}, \tilde{v})$.
- (ii) *There is a $(p \times q)$ alternating transportation matrix $[x_{ij}]$ in $\mathcal{A}(u, v)$, with $\sum_{h=1}^q v_h = \sum_{\ell=1}^p u_\ell = pq$, such that for every $i \in \langle p \rangle$, $j \in \langle q \rangle$*

$$c_{ij} := C_{p,q} \left(\frac{i}{p}, \frac{j}{q} \right) = \frac{1}{pq} \sum_{\ell=1}^i \sum_{h=1}^j x_{\ell h}. \quad (5)$$

Remark 6. Propositions 4 and 5 together offer a natural completion for the question marks in our above hierarchy on generalizations of discrete copulas that fits nicely within the current literature on copula functions. We note however, that the correspondence captured in these propositions does not capture all $p \times q$ (alternating) transportation polytopes, but only those with homogeneous marginals. For example, this generalized correspondence does not encompass the (alternating) transportation polytopes containing the polytopes considered in Theorem 7. To the best of the authors' knowledge there is no generalization of discrete copulas in the statistical literature that corresponds to the entire family of $p \times q$ alternating transportation polytopes.

7. Discussion

There has recently been an increasing interest in exploiting tools from the field of discrete geometry to develop new methodology in applied fields (AghaKouchak, 2014; Piantadosi et al., 2007, 2012; Radi et al., 2017) and shed light on well-known stochastic problems (Krause et al., 2017; Embrechts et al., 2016; Fiebig et al., 2017). In this work, we unified the theoretical analysis of discrete copulas and their generalizations with the existing theory on generalizations of the Birkhoff polytope in the discrete geometry literature. Bivariate discrete copulas, and their generalizations discussed in this paper, admit representations as polytopes corresponding to generalizations of the Birkhoff polytope. We identified minimal H -representations of the families of $p \times q$ ultramodular bivariate discrete copulas and of $p \times q$ bivariate convex discrete quasi-copulas as subpolytopes of the $p \times q$ generalized Birkhoff

polytope and the $p \times q$ generalized alternating sign matrix polytope, respectively. Along the way, we also generalized well-known results on alternating sign matrix polytopes by computing the minimal H -representation of the $p \times q$ generalized alternating sign matrix polytope. In addition, we presented new methods for constructing *irreducible* elements of each of these families of $p \times p$ (quasi)-copulas by constructing families of vertices for the associated polytopes. Finally, we ended by connecting the most extensive generalization of discrete copulas in the statistical literature (i.e., aggregation functions) with the most extensive generalization of Birkhoff polytopes in the discrete geometry literature (i.e., alternating transportation polytopes), thereby completely unifying the two hierarchies of generalizations. The geometric findings presented in this paper can be used to determine whether a given arbitrary nonnegative matrix is the probability mass of an ultramodular bivariate copula, thereby providing new tools for entropy-copula approaches in line with Piantadosi et al. (2007, 2012). Moreover, an interesting direction for future research is to build on our results to construct statistical tests of ultramodularity for bivariate copulas in the same fashion as symmetry tests (Genest et al., 2012; Jasson, 2005). The extension results of Theorem 2 and Theorem 5, together with the vertex constructions presented in Section 5, suggest alternative ways to obtain ultramodular bivariate copulas and convex quasi-copulas which could be used as smooth approximators of analytically unfeasible (quasi)-copulas.

A natural follow-up to this research is to define the geometry of multivariate discrete copulas with the property of ultramodularity. This would allow an efficient approximation of popular multivariate families of copulas such as Extreme Value (Capéraà et al., 1997; Gudendorf and Segers, 2010), Archimedean (Genest et al., 2011), and Archimax (Capéraà et al., 2000; Charpentier et al., 2014), which relate to the ultramodular ones (Saminger-Platz et al., 2017). Finally, it would be interesting to consider also other types of stochastic dependence for discrete copulas such as multivariate total positivity (Colangelo et al., 2006; Müller and Scarsini, 2005).

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Appendix A: Proofs for Section 3

Lemma 9. Suppose that $[c_{ij}] \in \mathbb{R}^{(p+1) \times (q+1)}$ satisfies all of (d1), (d2), (d3a), and (d3b) as well as the equalities

$$c_{0k} = 0, c_{pk} = \frac{k}{q}, c_{h0} = 0, c_{hq} = \frac{h}{p} \text{ for all } h \in \langle p \rangle, k \in \langle q \rangle.$$

Then $[c_{ij}] \in \text{UDC}_{p,q}$.

Proof. To prove the result, we consider $C = [c_{ij}] \in \mathbb{R}^{(p+1) \times (q+1)}$ that satisfies all of the inequalities (d1), (d2), (d3a), and (d3b) together with the equalities stated in the lemma. To show $C \in \text{UDC}_{p,q}$, we must check that C satisfies the inequalities (c1). That is, we must show that the following inequalities are valid on C .

- i.** $c_{11} + c_{22} - c_{12} - c_{21} \geq 0$;
- ii.** $c_{p-2,q-2} + c_{p-1,q-1} - c_{p-2,q-1} - c_{p-1,q-2} \geq 0$;
- iii.** (a) $c_{1,j+1} - c_{1j} \geq 0$, (b) $c_{i+1,1} - c_{i1} \geq 0$;
for all $i \in \langle p-1 \rangle$, $j \in \langle q-1 \rangle$
- iv.** (a) $c_{p-1,j+1} - c_{p-1,j} \leq \frac{1}{q}$, (b) $c_{i+1,q-1} - c_{i,q-1} \leq \frac{1}{p}$;
for all $i \in \langle p-1 \rangle$, $j \in \langle q-1 \rangle$

C satisfies conditions (d3a) and (d3b), respectively for $(i, j) = (2, 0)$ and $(i, j) = (0, 2)$. Moreover, $c_{11} \geq 0$. Therefore, inequality **i.** can be obtained from

$$2(c_{11} + c_{22}) \geq 2c_{22} \geq 2(c_{12} + c_{21}).$$

From inequalities (d1), it holds that $c_{p-1,q-1} \geq -\frac{1}{p} + \frac{q-1}{q}$. Assuming $q \geq p$, we then have that

$$c_{p-1,q-1} \geq \max\left\{-\frac{1}{q} + \frac{q-1}{q}, -\frac{1}{p} + \frac{p-1}{p}\right\} = \max\left\{\frac{q-2}{q}, \frac{p-2}{p}\right\}.$$

From (d3a) and (d3b) for $(i, j) = (p-2, q-2)$, we recover inequality **ii.**

$$2 \left(c_{p-2,q-2} + c_{p-1,q-1} \right) \geq 2 c_{p-2,q-2} + \frac{p-2}{p} + \frac{q-2}{q} \geq 2 \left(c_{p-2,q-1} + c_{p-1,q-2} \right).$$

The inequalities **iii.(a)** and **iv.(a)** can be obtained by combining conditions (d1) and (d3a). Indeed, for **iii.(a)** we have that

$$c_{1,j+2} - c_{1,j+1} \stackrel{(d3a)}{\geq} c_{1,j+1} - c_{1j} \geq \dots \geq c_{12} + c_{11} \geq c_{11} \stackrel{(d1)}{\geq} 0.$$

Similarly, for **iv.(a)** we have that

$$\frac{1}{q} \stackrel{(d1)}{\geq} c_{p-1,q} - c_{q-1,q-1} \stackrel{(d3a)}{\geq} c_{p-1,j+2} - c_{p-1,j+1} \geq c_{p-1,j+1} - c_{p-1,j}.$$

In an analogous manner one can derive **iii.(b)** and **iv.(b)**. \square

7.1. Proof of Theorem 1.

We here prove that the inequalities in the list (b1), (b2), (b3a), and (b3b) are the minimal H-representation of the polytope $\mathcal{UDC}_{p,q}$. To do this, we identify $(p \times q)$ -matrices $M_{pq}^{(ij)} = [b_{ij}]$, and $H_{pq}^{(ij)} = [h_{ij}]$ for $i \in [p]$ and $j \in [q]$ such that

Case (b1). for every p and q , $M_{pq}^{(11)}$ satisfies all inequalities in the list (b1), (b2), (b3a), and (b3b) except for inequality of the type $b_{11} \geq 0$.

Case (b2). for every $i = 2, \dots, p-1$ and $j = 2, \dots, q-1$, except for $(i, j) = \{(2, 2), (p-1, q-1)\}$, $M_{pq}^{(ij)}$ satisfies all inequalities in the list (b1), (b2), (b3a), and (b3b) but one of the type $b_{ij} \geq 0$.

Case (b3a). for every $i \in [p-1]$ and $1 \leq j \leq \lfloor \frac{q+1}{2} \rfloor$, $H_{pq}^{(ij)}$ satisfies all inequalities in the list (b1), (b2), (b3a), and (b3b) except for one of the type $\sum_{h=1}^j b_{i+1,h} \geq \sum_{h=1}^j b_{ih}$.

The matrices that we shall identify satisfying each of these cases are, collectively, sufficient to prove that every inequality in the list (b1), (b2), (b3a), and (b3b) is needed to bound the polytope $\mathcal{UDC}_{p,q}$. Indeed, let us assume $M_{pq}^{(ij)} = (b_{ij})$ to be a matrix that satisfies (b1), (b2), (b3a), and (b3b), but for $b_{\hat{i}\hat{j}} \geq 0$ with $\hat{i} \in \{2, \dots, \lfloor \frac{p+1}{2} \rfloor\}$ and $\hat{j} \in \{2, \dots, \lfloor \frac{q+1}{2} \rfloor\}$. Then the matrix $M_{pq}^{(p-\hat{i}+1, q-\hat{j}+1)} = (b_{p-\hat{i}+1, q-\hat{j}+1})$ obtained by flipping the original matrix $M_{pq}^{(ij)} = (b_{ij})$ as follows

$$M_{pq}^{(p-\hat{i}+1, q-\hat{j}+1)} = \begin{pmatrix} b_{pq} & b_{p,q-1} & \dots & b_{p1} \\ b_{p-1,q} & b_{p-1,q-1} & \dots & b_{p-1,1} \\ \vdots & & & \vdots \\ b_{1q} & b_{1,q-1} & \dots & b_{11} \end{pmatrix}$$

satisfies all of the constraints but for $b_{p-\hat{i}+1, q-\hat{j}+1} \geq 0$. We indicate this transformation with b_{ij}^F . In an analogous manner, one can obtain all of the remaining cases among inequalities (b3a). Moreover, matrices that satisfy all the inequalities of $\mathcal{UDC}_{p,q}$ except for one of the (b3b)-type can be obtained by transposing the ones of case (b3a) above.

We now present the matrices corresponding to cases (b1), (b2), and (b3a) listed above. The inequalities considered in each of these three cases are further subdivided into the following subcases. Following the list of subcases

for each case, we present the matrices satisfying all inequalities in the list (b1), (b2), (b3a), and (b3b) with the exception of the inequality corresponding to the given subcase. When considered together with Lemma 9, these subcases and their corresponding matrices complete the proof.

The subcases of case (b1) are the following:

A. $b_{11} < 0$ with $p, q \geq 4$.

The following is the associated list of matrices for the subcases of case (b1) listed above.

$$\mathbf{A.} \begin{pmatrix} -1 & 1 & 1 & 2 & 2 \\ 1 & 0 & 1 & 1 & 2 \\ p-4 \left[\begin{array}{ccccc} 1 & 1 & 1 & 1 & 1 \\ 2 & 1 & 1 & 1 & 0 \\ 2 & 2 & \underbrace{1}_{q-4} & 0 & 0 \end{array} \right. \end{pmatrix}.$$

The subcases of case (b2) are the following:

B1. $b_{23} < 0$ with $p = 4$ and $q = 5$;

B2. $b_{2j} < 0$ with $3 \leq j \leq \lfloor \frac{q}{2} \rfloor$, for $p \geq 4, q \geq 6$;

B3. $b_{2 \lfloor \frac{q+1}{2} \rfloor} < 0$, with $p \geq 4, q \geq 7, q$ odd;

B4. $b_{32} < 0$, with $p = 5, q \geq 4$;

B5. $b_{3j} < 0$, with $3 \leq j \leq \lfloor \frac{q}{2} \rfloor$, and $p = 4, q \geq 4$;

B6. $b_{3j} < 0$, with $3 \leq j \leq \lfloor \frac{q}{2} \rfloor$, and $p = 5, q \geq 6$;

B7. $b_{3 \lfloor \frac{q+1}{2} \rfloor} < 0$, with $p = 5, q \geq 5, q$ odd;

B8. $b_{ij} < 0$, with $3 \leq i \leq \lfloor \frac{p}{2} \rfloor, 3 \leq j \leq \lfloor \frac{q}{2} \rfloor$, and $p \geq 6, q \geq 6$;

B9. $b_{i \lfloor \frac{q+1}{2} \rfloor} < 0$, with $3 \leq i \leq \lfloor \frac{p}{2} \rfloor$, and $p \geq 6, q \geq 7, q$ odd;

B10. $b_{\lfloor \frac{p+1}{2} \rfloor j} < 0$, with $3 \leq j \leq \lfloor \frac{q}{2} \rfloor$, and $p \geq 7, q \geq 6, p$ odd;

B11. $b_{\lfloor \frac{p+1}{2} \rfloor \lfloor \frac{q+1}{2} \rfloor} < 0$, with $p, q \geq 7, p$ and q odd;

B12. $b_{42} < 0$, with $p = 5, q \geq 5$;

B13. $b_{p-1,2} < 0$, with $p \geq 6, q \geq 6$;

B14. $b_{p-1,j} < 0$, with $3 \leq j \leq \lfloor \frac{q}{2} \rfloor$, $p \geq 5, q \geq 6$, and p odd;

B15. $b_{p-i+1,j} < 0$, with $2 \leq i \leq \lfloor \frac{p}{2} \rfloor$, $2 \leq j \leq \lfloor \frac{q}{2} \rfloor$, $p \geq 6, q \geq 6$, p odd;

The following is the associated list of matrices for the subcases of case (b2) listed above.

$$\mathbf{B1.} \begin{pmatrix} 0 & 0 & 1 & 2 & 2 \\ \frac{2}{3} & \frac{2}{3} & -\frac{1}{3} & 2 & 2 \\ \frac{4}{3} & \frac{4}{3} & \frac{7}{3} & 0 & 0 \\ 2 & 2 & 1 & 0 & 0 \end{pmatrix}$$

$$\mathbf{B2.} \begin{pmatrix} 0 & 0 & 0 & 1 & 1 & 1 & 2 \\ 0 & \frac{2}{3} & \frac{2}{3} & -\frac{1}{3} & 1 & 1 & 2 \\ p-4 \left[\begin{array}{ccccccc} 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 2 & \frac{4}{3} & \frac{4}{3} & \frac{4}{3} & 1 & 2 & 0 \\ \underbrace{2}_{j-3} & 2 & 2 & 2 & \underbrace{1}_{q-2j} & 0 & \underbrace{0}_{j-1} \end{array} \right. \end{pmatrix}$$

$$\mathbf{B3.} \begin{pmatrix} 0 & 0 & 0 & 1 & 2 & 2 & 2 \\ 0 & \frac{2}{3} & \frac{2}{3} & -\frac{1}{3} & 2 & 2 & 2 \\ p-4 \left[\begin{array}{ccccccc} 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 2 & \frac{4}{3} & \frac{4}{3} & \frac{7}{3} & 0 & 0 & 0 \\ \underbrace{2}_{j-3} & 2 & 2 & 1 & 0 & 0 & \underbrace{0}_{j-3} \end{array} \right. \end{pmatrix}$$

$$\mathbf{B4.} \begin{pmatrix} 0 & 1 & 1 & 1 & 2 \\ 0 & 1 & 1 & 1 & 2 \\ \frac{3}{2} & -\frac{1}{2} & 1 & 2 & 1 \\ \frac{3}{2} & \frac{3}{2} & 1 & 1 & 0 \\ 2 & 2 & \underbrace{1}_{q-4} & 0 & 0 \end{pmatrix}$$

$$\mathbf{B5.} \left(\begin{array}{cccccc} 0 & 1 & 1 & 1 & 2 & 2 \\ 0 & 1+y & 1+y & 1+y & 1 & 2 \\ 2 & -y & x & 1+x & 1 & 0 \\ \underbrace{2}_{j-1} & 2 & \underbrace{1}_{q-2j} & 0 & 0 & \underbrace{0}_{j-2} \end{array} \right) \text{ where}$$

$$y = \frac{1}{q-2j+2} \quad \text{and} \quad x = \frac{q-2j+1}{q-2j+2}.$$

$$\mathbf{B6.} \left(\begin{array}{cccccc} 0 & 0 & 1 & 1 & 1 & 2 \\ 0 & 0 & 1 & 1 & 1 & 2 \\ 1 & \frac{3}{2} & -\frac{1}{2} & 1 & 2 & 1 \\ 2 & \frac{3}{2} & \frac{3}{2} & 1 & 1 & 0 \\ \underbrace{2}_{j-2} & 2 & 2 & \underbrace{1}_{q-2j} & 0 & \underbrace{0}_{j-1} \end{array} \right)$$

$$\mathbf{B7.} \left(\begin{array}{cccccc} 0 & 0 & 0 & 1 & 2 & 2 \\ 0 & 0 & 0 & 2 & 1 & 2 \\ 1 & 1 & 2 & -1 & 2 & 1 \\ 1 & 2 & 2 & 2 & 0 & 0 \\ 3 & \underbrace{2}_{j-3} & 1 & 1 & 0 & \underbrace{0}_{j-2} \end{array} \right)$$

$$\mathbf{B8.} \left(\begin{array}{cccccc} i-3 \left[\begin{array}{cccccc} 0 & 0 & 1 & 2 & 2 & 2 \\ 0 & \frac{2}{3} & 1 & \frac{4}{3} & 2 & 2 \\ 0 & \frac{2}{3} & 1 & \frac{4}{3} & 2 & 2 \\ 1 & -\frac{1}{3} & 1 & \frac{4}{3} & 1 & 2 \end{array} \right. \\ p-2i \left[\begin{array}{cccccc} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 2 & 1 & 0 \end{array} \right. \\ i-1 \left[\begin{array}{cccccc} \underbrace{2}_{j-1} & 2 & \underbrace{1}_{q-2j} & 0 & \underbrace{0}_{j-2} & 0 \end{array} \right. \end{array} \right)$$

$$\begin{aligned}
\mathbf{B9.} & \left(\begin{array}{c} i-1 \left[\begin{array}{ccccc} 0 & 0 & 0 & 1 & 2 \\ 0 & \frac{2}{3} & \frac{2}{3} & -\frac{1}{3} & 2 \end{array} \right] \\ p-2i \left[\begin{array}{ccccc} 1 & 1 & 1 & 1 & 1 \\ 2 & \frac{4}{3} & \frac{4}{3} & \frac{7}{3} & 0 \end{array} \right] \\ i-1 \left[\underbrace{2}_{j-3} \quad 2 \quad 2 \quad 1 \quad \underbrace{0}_{j-1} \right] \end{array} \right) \\
\mathbf{B10.} & \left(\begin{array}{c} i-3 \left[\begin{array}{ccccc} 0 & 0 & 1 & 2 & 2 \\ 0 & \frac{2}{3} & 1 & \frac{4}{3} & 2 \\ 0 & \frac{2}{3} & 1 & \frac{4}{3} & 2 \\ 1 & -\frac{1}{3} & 1 & \frac{7}{3} & 1 \end{array} \right] \\ i-1 \left[\underbrace{2}_{j-1} \quad 2 \quad \underbrace{1}_{q-2j} \quad 0 \quad \underbrace{0}_{j-1} \right] \end{array} \right) \\
\mathbf{B11.} & \left(\begin{array}{c} i-2 \left[\begin{array}{cccccc} 0 & 0 & 0 & 1 & 2 & 2 & 2 \\ 0 & 1 & 1 & 1 & 1 & 1 & 2 \\ 1 & 1 & 1 & -1 & 2 & 2 & 1 \\ 2 & 1 & 1 & 3 & 0 & 0 & 0 \end{array} \right] \\ i-2 \left[\underbrace{2}_{j-3} \quad 2 \quad 2 \quad 1 \quad 0 \quad 0 \quad \underbrace{0}_{j-3} \right] \end{array} \right) \\
\mathbf{B12.} & \left(\begin{array}{c} 0 \quad 1 \quad 1 \quad 1 \quad 1 \quad 2 \\ 0 \quad 1 \quad 1 \quad 1 \quad 1 \quad 2 \\ 0 \quad 1 \quad 1 \quad 1 \quad 2 \quad 1 \\ \frac{5}{2} \quad -\frac{1}{2} \quad 1 \quad 2 \quad 1 \quad 0 \\ \frac{5}{2} \quad \frac{5}{2} \quad \underbrace{1}_{q-5} \quad 0 \quad 0 \quad 0 \end{array} \right)
\end{aligned}$$

$$\mathbf{B13.} \begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1 & 2 \\ 0 & 1 & 1 & 1 & 1 & 1 & 2 \\ 0 & 1 & 1 & 1 & 1 & 2 & 1 \\ 0 & 1 & 1 & 1 & 1 & 2 & 1 \\ p-6 \left[\begin{array}{cccccc} 1 & 1 & 1 & 1 & 1 & 1 \\ 3 & -1 & 1 & 2 & 2 & 0 & 0 \\ 3 & 3 & \underbrace{1}_{q-6} & 0 & 0 & 0 & 0 \end{array} \right. \end{pmatrix}$$

$$\mathbf{B14.} \begin{pmatrix} 0 & 0 & 1 & 1 & 1 & 2 & 2 \\ 0 & 1 & 1 & 1 & 1 & 1 & 2 \\ 1 & 0 & 1+y & 1+y & 1+y & 1 & 1 \\ p-5 \left[\begin{array}{cccccc} 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 2 & 2 & -y & x & 1+x & 1 & 0 \\ \underbrace{2}_{j-2} & 2 & 2 & \underbrace{1}_{q-2j} & 0 & \mathbf{0} & \underbrace{0}_{j-2} \end{array} \right. \end{pmatrix} \text{ where}$$

$$y = \frac{1}{q-2j+2} \quad \text{and} \quad x = \frac{q-2j+1}{q-2j+2}.$$

$$\mathbf{B15.} \begin{pmatrix} i-2 \left[\begin{array}{cccc} 0 & 0 & 1 & 2 & 2 \\ 0 & 1 & 1 & 1 & 2 \\ 0 & 1+x & 1 & 1+y & 2 \end{array} \right. \\ p-2i \left[\begin{array}{ccccc} 1 & x & 1 & 1+y & 1 \\ 2 & -y & 1 & 1+y & 1 \end{array} \right. \\ i-1 \left[\begin{array}{cccc} \underbrace{2}_{j-1} & 2 & \underbrace{1}_{q-2j} & 0 & \underbrace{0}_{j-1} \end{array} \right. \end{pmatrix} \text{ where}$$

$$y = \frac{1}{p-2i+2} \quad \text{and} \quad x = \frac{p-2i+1}{p-2i+2}.$$

The subcases for case (b3a) are the following:

$$\mathbf{C1.} \sum_{h=1}^j b_{2h} < \sum_{h=1}^j b_{1h} \quad 1 \leq j \leq \left\lfloor \frac{q-1}{2} \right\rfloor,$$

- C2.** $\sum_{h=1}^{\hat{j}} b_{2h} < \sum_{h=1}^{\hat{j}} b_{1h}$ $\hat{j} = \lfloor \frac{q+1}{2} \rfloor$, q odd;
- C3.** $\sum_{h=1}^{\hat{j}} b_{2h} < \sum_{h=1}^{\hat{j}} b_{1h}$ with $\hat{j} = \lfloor \frac{q}{2} \rfloor$, q even;
- C4.** $\sum_{h=1}^i b_{i+1,h} < \sum_{h=1}^j b_{ih}$ with $1 \leq j \leq \lfloor \frac{q-1}{2} \rfloor$, $2 \leq i \leq p-2$
- C5.** $\sum_{h=1}^{\hat{j}} b_{i+1,h} < \sum_{h=1}^{\hat{j}} b_{ih}$ $\hat{j} = \lfloor \frac{q+1}{2} \rfloor$, $2 \leq i \leq p-2$; q odd;
- C6.** $\sum_{h=1}^{\hat{j}} b_{i+1,h} < \sum_{h=1}^{\hat{j}} b_{ih}$ $\hat{j} = \lfloor \frac{q}{2} \rfloor$, $2 \leq i \leq p-2$; q even;
- C7.** $\sum_{h=1}^i b_{ph} < \sum_{h=1}^j b_{p-1,h}$ with $1 \leq j \leq \lfloor \frac{q-1}{2} \rfloor$, $q, p \geq 4$;
- C8.** $\sum_{h=1}^{\hat{j}} b_{ph} < \sum_{h=1}^{\hat{j}} b_{p-1,h}$ with $\hat{j} = \lfloor \frac{q+1}{2} \rfloor$, $q, p \geq 4$ q odd;
- C9.** $\sum_{h=1}^{\hat{j}} b_{ph} < \sum_{h=1}^{\hat{j}} b_{p-1,h}$ with $\hat{j} = \lfloor \frac{q}{2} \rfloor$, $q, p \geq 4$ q even.

The following is the associated list of matrices for the subcases of case (b3a) listed above.

$$\begin{array}{l}
\mathbf{C1.} \left(\begin{array}{cccccc}
0 & \frac{1}{2} & \frac{1}{2} & 1 & 2 \\
0 & 0 & 1 & 1 & 2 \\
p-4 \left[\begin{array}{ccccc}
1 & 1 & 1 & 1 & 1 \\
2 & \frac{3}{2} & \frac{3}{2} & 1 & 0 \\
\underbrace{2}_{j-1} & 2 & 1 & \underbrace{1}_{q-2j-1} & \underbrace{0}_j
\end{array} \right. \\
\mathbf{C2.} \left(\begin{array}{cccccc}
0 & 0 & 1 & 1 & 1 & 2 \\
0 & 1 & 0 & 0 & 2 & 2 \\
p-4 \left[\begin{array}{ccccc}
1 & 1 & 1 & 1 & 1 & 1 \\
2 & 1 & 1 & 2 & 1 & 0 \\
\underbrace{2}_{\hat{j}-3} & 2 & 2 & 1 & 0 & \underbrace{0}_{\hat{j}-2}
\end{array} \right.
\end{array} \right)
\end{array}$$

$$\begin{aligned}
\mathbf{C3.} & \left(\begin{array}{cccc} 0 & 1 & 1 & 2 \\ 0 & 0 & 2 & 2 \\ p-4 \left[\begin{array}{cccc} 1 & 1 & 1 & 1 \\ 2 & 1 & 1 & 0 \end{array} \right. \\ \underbrace{2}_{\hat{j}-1} & 2 & 0 & \underbrace{0}_{\hat{j}-1} \end{array} \right) \\
\mathbf{C4.} & \left(\begin{array}{ccccc} 0 & \frac{1}{2} & \frac{1}{2} & 1 & 2 \\ i-1 \left[\begin{array}{cccc} 1 & 1 & 1 & 1 \\ 1 & \frac{1}{2} & \frac{3}{2} & 1 \end{array} \right. \\ p-i-2 \left[\begin{array}{cccc} 1 & 1 & 1 & 1 \\ 2 & 2 & 1 & 1 \end{array} \right. \\ \underbrace{2}_{j-1} & 2 & 1 & \underbrace{1}_{q-2j-1} & \underbrace{0}_j \end{array} \right) \\
\mathbf{C5.} & \left(\begin{array}{ccccc} 0 & 0 & 2 & 2 & 3 \\ i-2 \left[\begin{array}{cccc} 1 & 1 & 1 & 1 \\ 1 & 2 & 0 & 1 \end{array} \right. \\ p-i-2 \left[\begin{array}{cccc} 1 & 1 & 1 & 1 \\ 1 & 1 & 2 & 1 \end{array} \right. \\ \underbrace{2}_{\hat{j}-1} & 1 & 0 & \underbrace{0}_{\hat{j}-3} & 0 \end{array} \right) \\
\mathbf{C6.} & \left(\begin{array}{cccc} 0 & 0 & 2 & 2 \\ i-2 \left[\begin{array}{cccc} 1 & 1 & 1 & 1 \\ 1 & 2 & 0 & 1 \end{array} \right. \\ p-i-1 \left[\begin{array}{cccc} 1 & 1 & 1 & 1 \\ 2 & 1 & 1 & 0 \end{array} \right. \\ \underbrace{2}_{\hat{j}-1} & 1 & 1 & \underbrace{0}_{\hat{j}-1} \end{array} \right) \\
\mathbf{C7.} & \left(\begin{array}{ccccc} 0 & 0 & 1 & 1 & 2 \\ 0 & 0 & 1 & 1 & 2 \\ p-4 \left[\begin{array}{cccc} 1 & 1 & 1 & 1 \\ 2 & \frac{5}{2} & \frac{1}{2} & 1 \end{array} \right. \\ \underbrace{2}_{j-1} & \frac{3}{2} & \frac{3}{2} & \underbrace{1}_{q-2j-1} & \underbrace{0}_j \end{array} \right)
\end{aligned}$$

$$\begin{array}{l}
\mathbf{C8.} \\
\mathbf{C9.}
\end{array}
\left(\begin{array}{cccc}
0 & 1 & 2 & 2 \\
0 & \frac{3}{2} & \frac{3}{2} & 2 \\
p-4 \left[\begin{array}{cccc} 1 & 1 & 1 & 1 \\ 2 & 1 & 0 & 0 \end{array} \right. \\
\underbrace{2}_{\hat{j}-1} & \frac{1}{2} & \frac{1}{2} & \underbrace{0}_{\hat{j}-2} \\
0 & 0 & 2 & 2 \\
0 & 1 & 1 & 2 \\
p-4 \left[\begin{array}{cccc} 1 & 1 & 1 & 1 \\ 2 & 2 & 0 & 0 \end{array} \right. \\
\underbrace{2}_{\hat{j}-1} & 1 & 1 & \underbrace{0}_{\hat{j}-1}
\end{array} \right)$$

Together with Lemma 9, these subcases and their corresponding matrices complete the proof of the theorem. \square

7.2. Proof of Theorem 2.

Every $C \in \text{UDC}_{p,q}$ is a discrete copula on $I_p \times I_q$. Thus, according to (Nelsen, 2006, Lemma 2.3.5), the checkerboard extension \tilde{C} of C which is defined as

$$\tilde{C}(u, v) = (1 - \lambda_u)(1 - \mu_v)c_{ij} + (1 - \lambda_u)\mu_v c_{i,j+1} + \lambda_u(1 - \mu_v)c_{i+1,j} + \lambda_u\mu_v c_{i+1,j+1}$$

where $\frac{i}{p} \leq u \leq \frac{i+1}{p}$, $\frac{j}{q} \leq v \leq \frac{j+1}{q}$, and

$$\lambda_u = \begin{cases} (u - \frac{i}{p})p & u > \frac{i}{p} \\ 1 & u = \frac{i}{p} \end{cases} \quad \text{and} \quad \mu_v = \begin{cases} (v - \frac{j}{q})q & v > \frac{j}{q} \\ 1 & v = \frac{j}{q} \end{cases}$$

is a copula on $[0, 1]^2$, whose restriction on $I_p \times I_q$ is C . We now show that for any $C \in \text{UDC}_{p,q}$, \tilde{C} is an ultramodular copula; i.e., \tilde{C} has convex horizontal and vertical (coordinatewise) sections. We here focus on any arbitrary horizontal section $C_a : u \mapsto \tilde{C}(u, a)$ with $a \in [0, 1]$ and prove that it is a convex function. The same argument can be used to prove the convexity of an arbitrary vertical section. C_a is a p -piecewise continuous function. Therefore, to prove its convexity it is sufficient to show the *Jensen convexity*, i.e., for $u_1, u_2 \in [0, 1]$

$$C_a\left(\frac{u_1}{2} + \frac{u_2}{2}\right) \leq \frac{1}{2}C_a(u_1) + \frac{1}{2}C_a(u_2). \quad (6)$$

Without loss of generality, we assume $\frac{j}{q} < a < \frac{j+1}{q}$ and define $\mu_a = (a - \frac{j}{q})q$. We then proceed by induction on the number M of intervals that contain $[u_1, u_2]$. To do this, we consider a few cases.

CASE M=1. Let us consider $\frac{i}{p} < u_1, u_2 < \frac{i+1}{p}$, and $u_3 = \frac{u_1}{2} + \frac{u_2}{2}$, for $i \in \langle p-1 \rangle$. By definition, $\lambda_1 = pu_1 - i$ and $\lambda_2 = pu_2 - i$. Hence,

$$\lambda_3 = \frac{pu_1}{2} + \frac{pu_2}{2} - i = \frac{\lambda_1}{2} + \frac{\lambda_2}{2}$$

By construction, we can then express Eq.(6) as follows.

$$\begin{aligned} C_a(u_3) &= (1 - \lambda_3)(1 - \mu_a)c_{ij} + (1 - \lambda_3)\mu_a c_{i,j+1} \\ &\quad + \lambda_3(1 - \mu_a)c_{i+1,j} + \lambda_3\mu_a c_{i+1,j+1} \\ &= \frac{C_a(u_1)}{2} + \frac{C_a(u_2)}{2} \end{aligned}$$

CASE M=2. Let us consider $\frac{i}{p} < u_1 < \frac{i+1}{p} < u_2 < \frac{i+2}{p}$ for $i \in \langle p-1 \rangle$. Then, $\frac{C_a(u_1)}{2} + \frac{C_a(u_2)}{2}$ can be written as

$$\begin{aligned} \frac{C_a(u_1)}{2} + \frac{C_a(u_2)}{2} &= (1 - \mu_a) \left(\frac{1}{2} - \frac{\lambda_1}{2} \right) c_{ij} + \left(\frac{1}{2} - \frac{\lambda_1}{2} \right) \mu_a c_{i,j+1} \\ &\quad + \frac{\lambda_1}{2} (1 - \mu_a) c_{i+1,j} + \mu_a \frac{\lambda_1}{2} c_{i+1,j+1} \\ &\quad + \frac{1}{2} (1 - \mu_a) c_{i+1,j} + \frac{1}{2} (1 - \mu_a) c_{i+1,j+1} \\ &\quad + (1 - \mu_a) \frac{\lambda_2}{2} (c_{i+2,j} - c_{i+1,j}) \\ &\quad + \mu_a \frac{\lambda_2}{2} (c_{i+2,j+1} - c_{i+1,j+1}) \end{aligned}$$

If $\frac{i}{p} < u_3 < \frac{i+1}{p}$, then $\lambda_3 = \frac{pu_1}{2} + \frac{pu_2}{2} - i = \frac{\lambda_1}{2} + \frac{\lambda_2}{2} + \frac{1}{2}$. Thus, from inequalities (d3a) and (d3b), we have that

$$c_{i+2,j+1} - c_{i+1,j+1} \geq c_{i+1,j+1} - c_{i,j+1} \geq c_{i+1,j} - c_{ij}.$$

Thus, it follows that

$$\begin{aligned} \frac{C_a(u_1)}{2} + \frac{C_a(u_2)}{2} &\geq \left[(1 - \mu_a) \left(\frac{1}{2} - \frac{\lambda_1}{2} \right) - (1 - \mu_a) \frac{\lambda_2}{2} \right] c_{ij} \\ &\quad + \left[\mu_a \left(\frac{1}{2} - \frac{\lambda_1}{2} \right) - \mu_a \frac{\lambda_2}{2} \right] c_{i,j+1} \\ &\quad + \left[(1 - \mu_a) \frac{\lambda_1}{2} + \frac{1}{2} (1 - \mu_a) + (1 - \mu_a) \frac{\lambda_2}{2} \right] \cdot c_{i+1,j} \\ &\quad + \left[\mu_a \frac{\lambda_1}{2} + \frac{1}{2} \mu_a + \mu_a \frac{\lambda_2}{2} \right] c_{i+1,j+1} \\ &= C_a \left(\frac{u_1}{2} + \frac{u_2}{2} \right) \end{aligned}$$

Assuming $\frac{i+1}{p} < u_3 < \frac{i+2}{p}$. One has $\lambda_3 = \frac{pu_1}{2} + \frac{pu_2}{2} - i = \frac{\lambda_1}{2} + \frac{\lambda_2}{2} - \frac{1}{2}$. Conditions (d3a) and (d3b) imply the following inequalities for $k \in \{j, j+1\}$

$$c_{i,k} \geq 2 c_{i+1,k} - c_{i+2,k}$$

The result can therefore be derived as follows.

$$\begin{aligned} \frac{C_a(u_1)}{2} + \frac{C_a(u_2)}{2} &\geq \left[(1 - \mu_a) \left(1 - \lambda_1 + \frac{\lambda_1}{2} + \frac{1}{2} - \frac{\lambda_2}{2} \right) \right] c_{i+2,j+1} \\ &\quad + \left[(1 - \mu_a) \left(-\frac{1}{2} + \frac{\lambda_1}{2} + \frac{\lambda_2}{2} \right) \right] c_{i+2,j} \\ &\quad + \left[\mu_a \left(1 - \lambda_1 + \frac{\lambda_1}{2} + \frac{1}{2} - \frac{\lambda_2}{2} \right) \right] c_{i+1,j+1} \\ &\quad + \left[\mu_a \left(-\frac{1}{2} + \frac{\lambda_1}{2} + \frac{\lambda_2}{2} \right) \right] c_{i+2,j+1} \\ &= C_a \left(\frac{u_1}{2} + \frac{u_2}{2} \right) \end{aligned}$$

CASE $M = N \leq p$. Let us assume the result is true for $N - 1$ intervals. In order to prove that C_a is convex, we only need to show that the last two intervals of the partition attach in a convex way. Therefore, we can restrict ourselves to the situation where $\frac{N-2}{p} < u_1 < \frac{N-1}{p} < u_2 < \frac{N}{p}$. The thesis follows from case $M=2$. \square

Appendix B: Proofs for Section 4

Lemma 10. *Suppose that $3 \leq p < q$ with $q = kp + r$ for $0 \leq r < p$ and that $[c_{ij}] \in \mathbb{R}^{(p+1) \times (q+1)}$ satisfies all of (a1), (a2), and (a3). Then $[c_{ij}] \in \mathcal{ASM}_{p,q}$.*

Proof. Recall that for $p < q$ with $q = pk + r$ with $0 \leq r < p$ the alternating sign matrix polytope $\mathcal{ASM}_{p,q}$ is defined by the collection of inequalities

1. $\sum_{\ell=1}^p x_{\ell j} = p$; $\sum_{h=1}^q x_{ih} = q$ for $i \in [p]$ and $j \in [q]$,
2. $0 \leq \sum_{\ell=1}^i x_{\ell j} \leq p$ for all $i \in [p]$ and $j \in [q]$,
3. $0 \leq \sum_{h=1}^j x_{ih} \leq q$ for all $i \in [p]$ and $j \in [q]$.

Using the equalities (1), we can transform the inequalities (2) and (3) into the two families

- 2(a). $0 \leq \sum_{\ell=1}^i x_{\ell j}$ for all $i \in [p]$ and $j \in [q]$,
- 2(b). $0 \leq \sum_{\ell=i+1}^p x_{\ell j}$ for all $i \in [p]$ and $j \in [q]$,
- 3(a). $0 \leq \sum_{h=1}^j x_{ih}$ for all $i \in [p]$ and $j \in [q]$, and
- 3(b). $0 \leq \sum_{h=j+1}^q x_{ih}$ for all $i \in [p]$ and $j \in [q]$.

By symmetry, it suffices to determine which inequalities among 2(a) and 3(a) are necessary and then take their symmetric opposites from among 2(b) and 3(b) as well.

Notice first that since the full column sums are always equal to $q > 0$, then the equality $\sum_{\ell=1}^p x_{\ell j} = 0$ yields the empty set. Thus, the case when $i = p$ for $j \in [q]$ is not facet-defining. Similarly, this is true for the case when $j = q$ and $i \in [p]$. Next notice that the inequalities $x_{\ell 1} \geq 0$ for all $\ell \in [p]$ imply that $\sum_{\ell=1}^i x_{\ell j} \geq 0$ for $i \in \{2, \dots, p-1\}$. Thus, the inequalities of type 2(a) are not facet-defining when $i \in \{2, \dots, p-1\}$ and $j = 1$. Similarly, the inequalities of type 3(a) are not facet-defining when $i = 1$ and $j \in \{2, \dots, q-1\}$. Thus, we now know that the minimal H representation of $\mathcal{ASM}_{p,q}$ is contained within the collection of inequalities

- 2(a). $0 \leq \sum_{\ell=1}^i x_{\ell j}$ for all $i \in \{1, \dots, p-1\}$ and $j \in \{2, \dots, q-1\}$,
- 2(b). $0 \leq \sum_{\ell=i+1}^p x_{\ell j}$ for all $i \in \{1, \dots, p-1\}$ and $j \in \{2, \dots, q-1\}$,
- 3(a). $0 \leq \sum_{h=1}^j x_{ih}$ for all $i \in \{2, \dots, p-1\}$ and $j \in \{1, \dots, q-1\}$, and
- 3(b). $0 \leq \sum_{h=j+1}^q x_{ih}$ for all $i \in \{2, \dots, p-1\}$ and $j \in \{1, \dots, q-1\}$.

To complete the proof, it remains to show that the inequalities of type 3(a) $\sum_{h=1}^j x_{ih} \geq 0$ are redundant (i.e. not facet-defining) whenever $i \in \{2, \dots, p-1\}$ and $j \in \{q-k, \dots, q-1\}$. Notice first that when $p \leq q$ and $[c_{ij}] \in \mathcal{ASM}_{p,q}$ then $c_{ij} \leq p$ for all $i \in [p]$ and $j \in [q]$. To see this fact, recall that $\mathcal{ASM}_{p,q}$ is defined by the inequalities listed in (1), (2), and (3) above. So, if there existed some $c_{ij} > p$, then since $0 \leq \sum_{\ell=1}^{i-1} c_{\ell j}$, it would follow that $\sum_{\ell=1}^i c_{\ell j} > p$, which contradicts the above inequalities defining $\mathcal{ASM}_{p,q}$.

Now, let $i \in \{2, \dots, p-1\}$. Since $x_{ih} \leq q = pk + r$ for all $h \in [q]$ then $\sum_{h=j+1}^q x_{ih} \leq q$ for all $j \in \{q-k, \dots, q-1\}$. Thus, since $\sum_{h=1}^q x_{ih} = q$, it follows that $\sum_{h=1}^j x_{ih} \geq 0$, as desired.

Notice that for the symmetry argument to work, we must not apply it to the corner inequalities; i.e., $x_{11} \geq 0$, $x_{1p} \geq 0$, $x_{1q} \geq 0$ and $x_{pq} \geq 0$. Thus, these inequalities are counted separately from the rest within (a1). This completes the proof. \square

Given Lemma 10, to prove Theorem 3 it remains to show that for each inequality in the list (a1), (a2), and (a3), there exists a point $[c_{ij}] \in \mathbb{R}^{p \times q}$ satisfying all inequalities in the list with the exception of the chosen one.

Proof of Theorem 3.

By Lemma 10, we know that the minimal H -representation of $\mathcal{ASM}_{p,q}$ for $p \neq q$ is contained within the collection of inequalities (a1), (a2) and

(a3). We here prove that inequalities (a1), (a2) and (a3) are exactly the minimal H -representation of $\mathcal{ASM}_{p,q}$ for $p \neq q$. To do this, it suffices to show that for each inequality in the list there exists a matrix $[c_{ij}] \in \mathbb{R}^{p \times q}$ that does not satisfy the chosen inequality but satisfies all other inequalities among (a1), (a2), and (a3). The matrices are given as follows. The matrix P

$$P = \begin{pmatrix} -1 & 1 & 1 & 3 \\ p-3 \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 2 & 0 \\ 3 & \underbrace{1}_{q-3} & 0 & 0 \end{bmatrix} \end{pmatrix} \in \mathbb{R}^{p \times q}$$

can be seen to satisfy all inequalities among (a1), (a2), and (a3) except for $x_{11} \geq 0$. By permuting the columns of this matrix and flipping the matrix horizontally, we see the desired matrices for the other inequalities listed in (a1). For the conditions listed in (a1), the analogous matrix for the inequality $\sum_{\ell=1}^i x_{\ell 2} \geq 0$ is the matrix

$$\begin{pmatrix} A & \mathbf{1}_{i \times (q-i-2)} \\ \mathbf{1}_{(p-i-1) \times (i+2)} & \mathbf{1}_{(p-i-1) \times (q-i-2)} \end{pmatrix} \in \mathbb{R}^{p \times q},$$

where A is the block matrix $(B \ C) \in \mathbb{R}^{(i+1) \times (i+2)}$, with B, C as follows

$$B = \begin{pmatrix} \mathbf{1}_{(i-1) \times 1} & \mathbf{0}_{(i-1) \times 1} \\ 2 & -1 \\ 0 & i+2 \end{pmatrix} \in \mathbb{R}^{(i+1) \times 2}, \quad C = \begin{pmatrix} \mathbf{1}_{i \times i} + I_i \\ \mathbf{0}_{1 \times i} \end{pmatrix} \in \mathbb{R}^{(i+1) \times i}.$$

Permuting the columns and flipping this matrix horizontally then recovers the matrices for the other inequalities listed in (a2). Similarly, for the inequality $\sum_{h=1}^j x_{2h} \geq 0$ listed in (a3), we use the matrix

$$\begin{pmatrix} A & \mathbf{1}_{3 \times (q-2j+2)} \\ \mathbf{1}_{(p-3) \times (2j-2)} & \mathbf{1}_{(p-3) \times (q-2j+2)} \end{pmatrix} \in \mathbb{R}^{p \times q},$$

where A is the block matrix $(B \ C \ D) \in \mathbb{R}^{3 \times (2j-2)}$, where B, C , and D are

$$B = \begin{pmatrix} 2 & 2 & \cdots & 2 \\ 0 & 0 & \cdots & 0 \\ 1 & 1 & \cdots & 1 \end{pmatrix}, \quad D = \begin{pmatrix} 0 & 0 & \cdots & 0 \\ 2 & 2 & \cdots & 2 \\ 1 & 1 & \cdots & 1 \end{pmatrix} \in \mathbb{R}^{3 \times (j-2)}, \quad \text{and } C = \begin{pmatrix} 2 & 0 \\ -1 & 3 \\ 2 & 0 \end{pmatrix}$$

Here, permuting the rows and flipping the matrix along its vertical axis produces the remaining desired matrices. Collectively, these matrices combined with Lemma 10 complete the proof. \square

Lemma 11. *Suppose that $[c_{ij}] \in \mathbb{R}^{(p+1) \times (q+1)}$ satisfies all of (v1), (v3a), and (v3b) as well as the equalities*

$$c_{0k} = 0, c_{pk} = \frac{k}{q}, c_{h0} = 0, c_{hq} = \frac{h}{p} \text{ for all } h \in \langle p \rangle, k \in \langle q \rangle.$$

Then $[c_{ij}] \in \text{CDQ}_{p,q}$.

Proof. Let us consider $C = [c_{ij}] \in \mathbb{R}^{(p+1) \times (q+1)}$ that satisfies all of the inequalities (v1), (v3a), and (v3b) as well as those equalities stated in the lemma. Then C satisfies the equalities (q1). The proof of Lemma 9 also shows that C meets the following requirements for $i \in \langle p-1 \rangle$ and $j \in \langle q-1 \rangle$.

$$\begin{aligned} \mathbf{a} \quad (1) \quad & c_{1,j+1} - c_{1,j} \geq 0, & (2) \quad & c_{i+1,1} - c_{ij} \geq 0 \\ \mathbf{b} \quad (1) \quad & c_{p-1,j+1} - c_{p-1,j} \leq \frac{1}{q}, & (2) \quad & c_{i+1,q-1} - c_{i+1,q-1} \leq \frac{1}{p} \end{aligned}$$

Conditions **iv.(a)** and **(b)** of Lemma 9 are equivalent to

$$c_{p,j+1} - c_{p-1,j+1} \geq c_{p,j} - c_{p-1,j} \quad \text{and} \quad c_{i+1,p} - c_{i+1,p-1} \geq c_{i,p} - c_{i,p-1}.$$

Hence, from **iv.(b)** of Lemma 9 it results the following chain of inequalities.

$$c_{p-1,q} - c_{p-1,q-1} \geq \dots \geq c_{i+2,q} - c_{i+2,q-1} \geq c_{i,q} - c_{i,q-1} \geq \dots \geq c_{1,q} - c_{1,q-1}.$$

Now, combining the last relationships with (v1) and (v3b), one obtains that for every $i \in [p-1], j \in [q-1]$

$$\begin{aligned} \frac{1}{q} & \stackrel{(v1)}{\geq} c_{p-1,q} - c_{p-1,q-1}, \\ & \geq \stackrel{\text{iv.(b)}}{c_{i,q} - c_{i,q-1}}, \\ & \geq \stackrel{(v3b)}{c_{i,j+1} - c_{ij}}, \\ & \geq c_{ij} - c_{i,j-1}, \\ & \geq \stackrel{(v1)}{0}, \end{aligned}$$

which proves (q2b). Conditions (q2a) can be derived analogously. Therefore, $C \in \text{CDQ}_{p,q}$. \square

7.3. Proof of Theorem 4.

By Lemma 11, we know that the minimal H -representation of $\text{CDQ}_{p,q}$ is contained within the collection of inequalities (a1),(a3a), and (a3b). We here show that the inequalities in the list (a1),(a3a), and (a3b) are exactly the minimal H -representation of $\text{CDQ}_{p,q}$. In particular, we identify $(p \times q)$ -matrices $M_{pq}^{(ij)} = [b_{ij}]$, and $H_{pq}^{(ij)} = [h_{ij}]$ for $i \in [p]$ and $j \in [q]$ such that

Case (a1). for every p and q , $M_{pq}^{(11)}$ satisfies all inequalities in the list (a1), (a3a), and (a3b) except for inequality of the type $b_{11} \geq 0$.

Case (a3a). for every $i \in [p-1]$ and $1 \leq j \leq \lfloor \frac{q+1}{2} \rfloor$, $H_{pq}^{(ij)}$ satisfies all inequalities in the list (a1), (a3a), and (a3b) except for one inequality of the type $\sum_{h=1}^j b_{i+1,h} \geq \sum_{h=1}^j b_{ih}$.

As shown in Theorem 1's proof, the matrices we shall identify suffice to prove the thesis as the other inequalities of (a1), (a3a), and (a3b) can be obtained from $M_{pq}^{(11)}$ and $H_{pq}^{(ij)}$ via suitable transformations.

To obtain the thesis it is sufficient to notice that the polytope \mathcal{CDQ}_{pq} contains \mathcal{UDC}_{pq} . Thus, the matrices **A** and **C1** to **C9** of Theorem 1's proof are of the type $M_{pq}^{(11)}$ and $H_{pq}^{(ij)}$ for every $i \in [p-1]$ and $1 \leq j \leq \lfloor \frac{q+1}{2} \rfloor$. Hence the inequalities (a1), (a3a), and (a3b) are all needed to bound \mathcal{CDQ}_{pq} . \square

7.4. Proof of Theorem 5.

Lemma 11 shows each $C \in \mathcal{CDQ}_{p,q}$ to be a discrete quasi-copula. According to (Quesada Molina and Sempi, 2005, Theorem 2.3) the checkerboard extension \tilde{C} of C defined as

$$\tilde{C}(u, v) = (1 - \lambda_u)(1 - \mu_v)c_{ij} + (1 - \lambda_u)\mu_v c_{i,j+1} + \lambda_u(1 - \mu_v)c_{i+1,j} + \lambda_u\mu_v c_{i+1,j+1}$$

where $\frac{i}{p} \leq u \leq \frac{i+1}{p}$, $\frac{j}{q} \leq v \leq \frac{j+1}{q}$, and

$$\lambda_u = \begin{cases} (u - \frac{i}{p})p & u > \frac{i}{p} \\ 1 & u = \frac{i}{p} \end{cases} \quad \text{and} \quad \mu_v = \begin{cases} (v - \frac{j}{q})q & v > \frac{j}{q} \\ 1 & v = \frac{j}{q} \end{cases}$$

is a quasi-copula on $[0, 1]^2$ whose restriction on $I_p \times I_q$ is C . Following the same arguments of the proof of Theorem 2, one can check that any arbitrary horizontal section $C_a : u \mapsto \tilde{C}(u, a)$, with $a \in [0, 1]$, is a convex function. This also works analogously for any arbitrary vertical section. \square

Appendix C: Proofs for Section 5

Lemma 12. Let $\tau : \mathbb{R}^{p \times q} \rightarrow \mathbb{R}^{p \times q}$ denote the linear map taking the standard basis vectors $\{e_{ij} : i \in [p], j \in [q]\}$ to

$$\tau(e_{ij}) := \begin{cases} \sum_{\ell=1}^i e_{k\ell} - \sum_{k=1}^i e_{k,j+1} & \text{for } i \in [p-1], j \in [q-1], \\ \sum_{k=1}^q e_{ik} - \sum_{k=1}^q e_{i+1,k} & \text{for } i \in [p-1], j = q, \\ \sum_{k=1}^j e_{p-1,k} - \sum_{k=1}^j e_{pk} & \text{for } i = p, j \in [q-1], \\ e_{pq} & \text{for } i = p, j = q. \end{cases}$$

Then τ is an invertible map with determinant $(-1)^{q-1} q^{p-2}$.

Proof. To prove this lemma we will use the matrix representation of τ and observe that it has a desirable block form from which we can deduce the claimed statements. Let $M = [m_{ij}]$ denote that matrix representation of τ with respect to the standard basis vectors ordered lexicographically from smallest-to largest along both the rows and columns. (Recall that the lexicographic ordering states that $e_{ij} < e_{st}$ if and only if $i < s$ or $i = s$ and $j < t$.) Define the matrices D_n, F_n, R_n, K_n and L_n by

$$\begin{aligned} d_{ij} &:= \begin{cases} 1 & \text{if } i = j \text{ or } j = n, \\ -1 & \text{if } i + 1 = j, \\ 0 & \text{otherwise,} \end{cases} & r_{ij} &:= \begin{cases} 1 & \text{if } i = j \text{ and } j < n, \\ -1 & \text{if } i + 1 = j, \\ 0 & \text{otherwise,} \end{cases} \\ k_{ij} &:= \begin{cases} 1 & \text{if } i \leq j \text{ and } j < n, \\ 0 & \text{otherwise,} \end{cases} & f_{ij} &:= \begin{cases} 1 & \text{if } i = j = n, \\ -1 & \text{if } i \leq j \text{ and } j < n, \\ 0 & \text{otherwise,} \end{cases} \\ \ell_{ij} &:= \begin{cases} -1 & \text{if } j = n, \\ 0 & \text{otherwise,} \end{cases} \end{aligned}$$

Let M_k denote the block matrix consisting of rows $kq + 1, \dots, (k+1)q$ for $k \in \langle p-1 \rangle$. Then, for $k \in [p-3]$

$$M_k = \begin{pmatrix} \underbrace{\mathbf{0}_q \cdots \mathbf{0}_q}_{k-1 \text{ times}} & L_q & D_q & \underbrace{R_q \cdots R_q}_{p-k-2 \text{ times}} & \mathbf{0}_q \end{pmatrix},$$

and for $k \in \{0, p-2, p-1\}$

$$\begin{aligned} M_0 &= \begin{pmatrix} D_q & R_q & \cdots & R_q & \mathbf{0}_q \end{pmatrix}, \\ M_{p-2} &= \begin{pmatrix} \mathbf{0}_q & \mathbf{0}_q & \cdots & \mathbf{0}_q & L_q & D_q & K_q \end{pmatrix}, \\ M_{p-1} &= \begin{pmatrix} \mathbf{0}_q & \mathbf{0}_q & \cdots & \mathbf{0}_q & L_q & F_q \end{pmatrix}. \end{aligned}$$

Now define the matrices \tilde{D}_n , \tilde{R}_n , \tilde{K}_n , and \tilde{F}_n where

$$\tilde{d}_{ij} := \begin{cases} 1 & \text{if } i = j \text{ and } j < n, \\ i & \text{if } j = n, \\ 0 & \text{otherwise,} \end{cases} \quad \tilde{r}_{ij} := \begin{cases} 1 & \text{if } i = j \text{ and } j < n, \\ 0 & \text{otherwise,} \end{cases}$$

$$\tilde{k}_{ij} := \begin{cases} j & \text{if } i \geq j \text{ and } j < n, \\ i & \text{if } i < j \text{ and } j < n, \\ 0 & \text{otherwise,} \end{cases} \quad \tilde{f}_{ij} := \begin{cases} -1 + \frac{j}{q} & \text{if } i \geq j \text{ and } j < n, \\ \frac{j}{q} & \text{if } i < j \text{ and } j < n, \\ 1 & \text{if } i = j = n, \\ 0 & \text{otherwise.} \end{cases}$$

Via row reduction, we can reduce M_0 to

$$\tilde{M}_0 := \left(\tilde{D}_q \quad \tilde{R}_q \quad \cdots \quad \tilde{R}_q \quad \mathbf{0}_q \right),$$

and so we can use the final row of \tilde{M}_0 to reduce M_1 to

$$\tilde{M}_1 := \left(\mathbf{0}_q \quad \tilde{D}_q \quad \tilde{R}_q \quad \cdots \quad \tilde{R}_q \quad \mathbf{0}_q \right).$$

It then follows by induction that for $k = 2, \dots, p-3$ the matrix M_k is reducible to

$$\tilde{M}_k := \left(\mathbf{0}_q \quad \cdots \quad \mathbf{0}_q \quad \tilde{D}_q \quad \tilde{R}_q \quad \cdots \quad \tilde{R}_q \quad \mathbf{0}_q \right),$$

and that the blocks M_{p-2} and M_{p-1} , respectively, are reducible to

$$\tilde{M}_{p-2} := \left(\mathbf{0}_q \quad \cdots \quad \mathbf{0}_q \quad \tilde{D}_q \quad \tilde{K}_q \right), \text{ and}$$

$$\tilde{M}_{p-1} := \left(\mathbf{0}_q \quad \cdots \quad \mathbf{0}_q \quad \tilde{F}_q \right).$$

From here, basic row reductions can be applied to reduce the block \tilde{F}_q to the upper triangular matrix

$$\begin{pmatrix} -1 & -1 & \cdots & -1 & -1 & -1 \\ 0 & -1 & & -1 & -1 & -1 \\ \vdots & \ddots & \ddots & & \vdots & \vdots \\ & & \ddots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & -1 & -1 \\ 0 & 0 & \cdots & 0 & 0 & \frac{1}{q} \end{pmatrix}.$$

We may then compute the determinant of M to be

$$\det(M) = \det(\tilde{F}_q) \cdot \prod_{k=0}^{p-2} \det(\tilde{D}_q) = (-1)^{q-1} q^{p-2}.$$

In particular, since $\det(M) \neq 0$, we conclude that τ is invertible. \square

7.5. Proof of Theorem 7.

In the following, we work with the polytope $\mathcal{UDC}_{p,q}$. However, the same argument works for $\mathcal{CDQ}_{p,q}$. So as to apply Theorem 6, we must show that $(p+s)(q+t)$ facet-defining inequalities of $\mathcal{UDC}((\mathbf{q}_p, \mathbf{t}_s), (\mathbf{s}_t, \mathbf{p}_q))$ with linearly independent facet-normals are active on $B \oplus D$. Notice that since B and D are submatrices of $B \oplus D$, then the pq and st (respectively) inequalities that are active on each of B and D and have linearly independent normal vectors all yield active inequalities on $B \oplus D$ that have linearly independent normal vectors. There are also pt inequalities of the form

$$\sum_{k=1}^i e_{kj} - \sum_{k=1}^i e_{kj-1} \geq 0$$

that are active on the submatrix $\mathbf{0}_{p,t}$ of $B \oplus D$, and there are sq inequalities contained in the list

- (1) $\sum_{k=1}^i e_{ki} - \sum_{k=1}^i e_{k,j+1} \leq 0$ for $i \in [p+s-1], j \in [q+t-1]$,
- (2) $\sum_{k=1}^q e_{ik} - \sum_{k=1}^q e_{i+1,k} \leq 0$ for $i \in [p+s-1]$,
- (3) $\sum_{k=1}^j e_{p+s-1,k} - \sum_{k=1}^j e_{p+s,k} \leq 0$ for $j \in [q+t-1]$,
- (4) $e_{pq} \geq 0$,

that are active on the submatrix $\mathbf{0}_{s,q}$ of $B \oplus D$. These can be seen to have linearly independent facet-normals from those given by the submatrices B and D . Moreover, by Lemma 12, all such inequalities have linearly independent facet-normals from one another. Thus, we conclude that $B \oplus D$ is a vertex of $\mathcal{UDC}((\mathbf{q}_p, \mathbf{t}_s), (\mathbf{s}_t, \mathbf{p}_q))$. \square

7.6. Proof of Corollary 3.

To prove this corollary, we first recall that a (weak) composition of a positive integer $p \in \mathbb{Z}_{>0}$ with k parts is a sum $c_1 + c_2 + \cdots + c_k = p$, in which the order of the summands $c_1, \dots, c_k \in \mathbb{Z}_{>0}$ matters. It follows that if $C \in \mathbb{R}^{p \times p}$ is a decomposable vertex of \mathcal{UDC}_p , then there exists a

composition $c_1 + c_2 + \dots + c_k = p$ such that there are indecomposable matrices $C_1 \in \text{ID}_{c_1}, \dots, C_k \in \text{ID}_{c_k}$ such that

$$C = C_1 \oplus \dots \oplus C_k.$$

It then follows that

$$\begin{aligned} \text{D}(x) &= \sum_{k \geq 0} \left(\sum_{\ell \geq 0} |\text{ID}_\ell| x^\ell \right)^k, \\ &= \sum_{k \geq 0} (\text{ID}(x))^k, \\ &= \sum_{k \geq 0} (V(x) - \text{D}(x))^k, \\ &= \frac{1}{1 + \text{D}(x) - V(x)}. \end{aligned}$$

From this it is quick to conclude that

$$V(x) = \frac{\text{D}(x)^2 + \text{D}(x) - 1}{\text{D}(x)}.$$

In a similar fashion, the inequality follows. \square

Appendix D: Proofs for Section 6

7.7. Proof of Proposition 4.

(i) \Rightarrow (ii) We consider $C_{pq} \in \text{SAF}(\tilde{u}, \tilde{v})$. For every $i \in \langle p \rangle, j \in \langle q \rangle$, we can take C_{pq} to a $(p \times q)$ matrix $[x_{ij}]$ through the following linear transformation

$$x_{ij} = pq(c_{ij} + c_{i-1,j-1} - c_{i-1,j} - c_{i,j-1}).$$

We here show that the new constructed matrix $[x_{ij}]$ lies in the transportation polytope $\mathcal{T}(u, v)$ whose margins are the vectors $u \in \mathbb{R}^p$ and $v \in \mathbb{R}^q$, such that for every $i \in [p], u_i := \tilde{u}_i - \tilde{u}_{i-1}$, and $j \in [q], v_j := \tilde{v}_j - \tilde{v}_{j-1}$. Indeed, condition (AF2) implies that $x_{ij} \geq 0$ for every $i \in \langle p \rangle, j \in \langle q \rangle$. By construction, one has that $\sum_{h=1}^q x_{ih} = pq(c_{iq} - c_{i-1,q}) = \tilde{u}_i - \tilde{u}_{i-1} = u_i$. Similarly, it follows that $\sum_{\ell=1}^p x_{\ell j} = v_j$. Hence, the thesis.

(i) \Leftarrow (ii) We here verify that every C_{pq} defined as in equation (4) belongs to the set $\text{SAF}(\tilde{u}, \tilde{v})$, with margins given by the vectors $\tilde{u} \in \mathbb{R}^p$ and $\tilde{v} \in \mathbb{R}^q$, whose values are defined for every $i \in [p]$, as $\tilde{u}_i := \sum_{\ell=1}^i u_\ell$, and for $j \in [q]$,

as $\tilde{v}_j := \sum_{h=1}^j v_h$. Clearly, any such matrix C_{pq} satisfies condition (AF2). Since the empty sum equals zero by convention, (AF1a) holds as well. It remains to show the validity of (AF1b). From equation (4), one has that

$$c_{pj} = \frac{1}{pq} \sum_{\ell=1}^p \sum_{h=1}^j x_{\ell h} = \frac{1}{pq} \sum_{h=1}^j v_h < \frac{1}{pq} \sum_{h=1}^{j+1} v_h = c_{p,j+1}$$

A similar argument applied to the columns completes the proof. \square

7.8. Proof of Proposition 5.

(i) \Rightarrow (ii) We consider $C_{pq} \in \text{ASA}(\tilde{u}, \tilde{v})$. For every $i \in \langle p \rangle$, $j \in \langle q \rangle$, we can take C_{pq} to a $(p \times q)$ matrix $[x_{ij}]$ through the following linear transformation

$$x_{ij} = pq(c_{ij} + c_{i-1,j-1} - c_{i-1,j} - c_{i,j-1}).$$

The new constructed matrix $[x_{ij}]$ lies in the alternating transportation polytope $\mathcal{A}(u, v)$ whose margins are the vectors $u \in \mathbb{R}^p$ and $v \in \mathbb{R}^q$, such that for every $i \in [p]$, $u_i := \tilde{u}_i - \tilde{u}_{i-1}$, and $j \in [q]$, $v_j := \tilde{v}_j - \tilde{v}_{j-1}$. According to Proposition 4's proof, one can derive the marginal constraints of $[x_{ij}]$ from (AF1a) and (AF1b). It remains to verify that $0 \leq \sum_{\ell=1}^i x_{\ell j} \leq v_j$, and $0 \leq \sum_{h=1}^j x_{ih} \leq u_i$, for every $i \in \langle p \rangle$, $j \in \langle q \rangle$. It is useful to observe that $\sum_{\ell=1}^i x_{\ell j} = pq \sum_{\ell=1}^i (c_{\ell j} + c_{\ell-1,j-1} - c_{\ell-1,j} - c_{\ell,j-1}) = pq(c_{ij} - c_{i,j-1})$. We now notice that for every $i \in \langle p \rangle$ and $j \in \langle q \rangle$, one has $(c_{ij} - c_{i,j-1} - c_{0j} + c_{0,j-1}) \geq 0$, from (AF2b) and (AF1a). Hence $\sum_{\ell=1}^i x_{\ell j} \geq 0$. Moreover, from (AF2b) and (AF1b), one has $(c_{i,j-1} - c_{ij} - c_{p,j-1} + c_{pj}) \geq 0$. Thus, $c_{ij} - c_{i,j-1} \leq c_{pj} - c_{p,j-1}$ and $\sum_{\ell=1}^i x_{\ell j} \leq \tilde{v}_j - \tilde{v}_{j-1} = v_j$. The remaining conditions on the row sums can be derived in a similar fashion.

(i) \Leftarrow (ii) We now prove that every C_{pq} defined as in equation (5) belongs to the set $\text{ASA}(\tilde{u}, \tilde{v})$, with margins given by the vectors $\tilde{u} \in \mathbb{R}^p$ and $\tilde{v} \in \mathbb{R}^q$, whose values are defined for every $i \in [p]$, as $\tilde{u}_i := \sum_{\ell=1}^i u_\ell$, and for $j \in [q]$, as $\tilde{v}_j := \sum_{h=1}^j v_h$. Conditions (AF1a) and (AF1b) can be derived according to Proposition 4's proof. We notice that $c_{i_1 j_1} + c_{i_2 j_2} - c_{i_1 j_2} - c_{i_2 j_1}$ can be expressed as

$$\sum_{\ell=1}^{i_1} \sum_{h=1}^{j_1} x_{\ell h} + \sum_{\ell=1}^{i_2} \sum_{h=1}^{j_2} x_{\ell h} - \sum_{\ell=1}^{i_1} \sum_{h=1}^{j_2} x_{\ell h} - \sum_{\ell=1}^{i_2} \sum_{h=1}^{j_1} x_{\ell h}.$$

Hence, the above formulation becomes $\sum_{\ell=1}^{i_2} (x_{\ell, j_1+1} + \dots + x_{\ell, j_2})$, when $i_1 = 0$, and $\sum_{\ell=i_1+1}^p (x_{\ell, j_1+1} + \dots + x_{\ell, j_2})$, if $i_2 = p$. In either case, the sums are nonnegative. In similar way, one can derive the cases $j_2 = q$ and $j_1 = 0$. \square