

# Geometry of discrete copulas

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## ABSTRACT

The space of discrete copulas admits a representation as a convex polytope, and this has been exploited in entropy-copula methods used in hydrology and climatology. In this paper, we focus on the class of component-wise convex copulas, i.e., ultramodular copulas, which describe the joint behavior of stochastically decreasing random vectors. We show that the family of ultramodular discrete copulas and its generalization to component-wise convex discrete quasi-copulas also admit representations as polytopes. In doing so, we draw connections to the Birkhoff polytope, the alternating sign matrix polytope, and their generalizations, thereby unifying and extending results on these polytopes from both the statistics and the discrete geometry literature.

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## 1. Introduction

Copulas are widely used for modeling stochastic dependence among random variables [11,34]. 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

$$F_{\mathbf{X}}(x_1, \dots, x_d) = C\{F_{X_1}(x_1), \dots, F_{X_d}(x_d)\}, \quad (1)$$

where the function  $C : [0, 1]^d \rightarrow [0, 1]$  is a  $d$ -dimensional copula [41]. As a result of Sklar's Theorem, the dependence structure of any random phenomenon can be represented by the associated copula which can exhibit different stochastic dependence properties such as exchangeability, positive/negative concordance, or tail dependence. The relation in Eq. (1) uniquely identifies the copula  $C$  associated to  $\mathbf{X}$  on the set  $\text{Ran}(F_{X_1}) \times \dots \times \text{Ran}(F_{X_d})$ . In the particular case of purely discrete random vectors, Sklar's theorem identifies the so-called discrete copulas, i.e., restrictions of copulas on (square or non-square) uniform grid domains.

The subfamily of discrete copulas is particularly useful for constructing the empirical joint distribution of a given multivariate sample. Indeed, the class of discrete copulas includes the so-called empirical copulas, which are the foundation of rank-based (nonparametric) copula approaches to inference [13,40]. Discrete copulas are known to admit a representation as a convex polytope [26], and this geometric property has been exploited in copula-based approaches in various applications

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in the environmental sciences [1,39]. 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

$$a_1x_1 + \dots + a_nx_n \leq b, \quad (2)$$

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 (2) is included in the minimal  $H$ -representation of  $P$ , then the collection of points in  $P$  on which inequality (2) 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 so as to more efficiently solve the associated linear programming problem.

Having a polytopal representation has been particularly helpful for constructing copulas with maximum entropy, i.e., copulas that correspond to the least constrained distributions given the available data [5,6,29]. For instance, the geometric description of discrete copulas has been used to derive checkerboard copulas with maximum entropy that match a given Spearman's rank correlation coefficient [36,37]. In applications with limited data, such as hydrology and climatology, the checkerboard copula with maximum entropy is an important tool to generate synthetic data; see [1] for a comprehensive analysis of entropy-copula methods in hydrology and climatology, and [39] for a particular recent study on rainfall total.

In this paper, we provide polytopal representations of various subfamilies of discrete copulas with desirable stochastic properties. This allows the application of similar convex optimization techniques in the identification of copulas that combine maximum entropy and particular desirable stochastic properties for various applications. We focus on analyzing component-wise convex bivariate copulas, known as ultramodular bivariate copulas [23,24]. As discussed in Chapter 5 of [34], the component-wise convexity has an important probabilistic interpretation as a form of negative dependence for bivariate random vectors known as stochastic decreasingness. This type of negative dependence appears in practice: for example, various parametric families of copulas popular in hydrological applications admit representatives in the class of ultramodular copulas [24]. Notable examples are the families of Farlie–Gumbel–Morgenstern, Ali–Mikhail–Haq, Clayton, and Frank copulas; see, e.g., [43] for an application to rainfall data.

We show here that bivariate discrete copulas with the property of ultramodularity admit polytopal representations. As a consequence, the selection of ultramodular copulas is amenable to techniques from convex geometry and linear optimization. We connect our work with existing entropy-copula methods in hydrology and discuss how to select copulas that have maximum entropy and are ultramodular, a property of interest for example for analyzing rainfall data. In addition, we study the convex space of the more general class of quasi-copulas, i.e., the lattice theoretic completion of the class of copulas [35]; we identify the minimal  $H$ -representation for the family of discrete quasi-copulas on non-square grid domains and the subfamily of discrete quasi-copulas with convex sections residing within. Notably, by doing so, we generalize Theorem 3.3 of Striker [42] by identifying the minimal  $H$ -representation of the well-known alternating transportation polytope [25], a result of independent interest in discrete geometry.

The remainder of this paper is organized as follows. In Section 2, we provide basic definitions and known results connecting copulas and discrete geometry. 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. We then discuss how to apply our findings to select ultramodular copulas with maximum entropy. In Section 4, we give our second main result (Theorem 3), in which we identify the minimal  $H$ -representation of the polytope of discrete quasi-copulas, thereby generalizing a result in discrete geometry [42]. 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 the polytopes introduced here; namely, we study their sets of vertices. Finally, in Section 6, we show that bivariate discrete (quasi-)copulas defined on non-uniform grid domains admit a characterization in terms of the most extensive generalization of the Birkhoff polytope known in the discrete geometry literature, thereby completely unifying these two hierarchies.

## 2. Copulas and quasi-copulas in discrete geometry

In this section, we present the statistical and geometric preliminaries to be used 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)  $C(u, 0) = C(0, u) = 0$  and  $C(u, 1) = C(1, u) = u$  for every  $u \in [0, 1]$ ;
- (C2)  $C(u_1, v_1) + C(u_2, v_2) \geq C(u_1, v_2) + C(u_2, v_1)$  for every  $u_1, u_2, v_1, v_2 \in [0, 1]$  such that  $u_1 \leq u_2, v_1 \leq v_2$ .

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 (coordinate-wise) 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 coordinate-wise sections are convex functions [23,24].

The bivariate copulas form a poset  $P$ , called the concordance ordering or PQD ordering with partial order  $\prec$  defined as  $C \prec C'$  whenever  $C(u, v) \leq C'(u, v)$  for all  $(u, v) \in [0, 1]^2$ ; see Definition 2.8.1 and Example 5.13 in [34]. 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 [35], and are defined as follows by Genest et al. [21].

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

(Q2)  $Q$  is increasing in each component.

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

Equivalently, Genest et al. [21] show that bivariate quasi-copulas are functions that satisfy 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

The space of discrete copulas and quasi-copulas in the bivariate setting was studied by [2,3,26,28,30,32,38]. These papers collectively demonstrate that the space of bivariate discrete copulas constructed from marginal distributions with finite state spaces of size  $p$  and  $q$  corresponds to a polytope known as the generalized Birkhoff polytope [9]. Furthermore, the bivariate discrete quasi-copulas in the case  $p = q$  correspond to points within a polytope known as the alternating sign matrix polytope [42]. We now review these results by formally introducing discrete copulas and quasi-copulas on (rectangular) uniform discrete domains, recalling the definitions of some classically studied polytopes in discrete geometry, and showing how they relate to the set of discrete copulas and quasi-copulas.

In the following, for  $p \in \mathbb{Z}_{>0}$  we let  $[p] = \{1, \dots, p\}$ ,  $\langle p \rangle = \{0, \dots, p\}$ , and  $I_p = \{0, 1/p, \dots, (p-1)/p, 1\}$ . 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  $C = (c_{i,j})$ , where  $c_{i,j} = C_{p,q}(i/p, j/q)$ . The set of discrete copulas on  $I_p \times I_q$ , denoted by  $DC_{p,q}$ , can be defined to be all matrices  $(c_{i,j}) \in \mathbb{R}^{(p+1) \times (q+1)}$  satisfying the affine inequalities

(c1)  $c_{0,j} = 0, c_{p,j} = j/q, c_{i,0} = 0$ , and  $c_{i,q} = i/p$  for all  $i \in \langle p \rangle$  and  $j \in \langle q \rangle$ ;

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

Analogously, the polytope of discrete quasi-copulas on  $I_p \times I_q$  is denoted by  $DQ_{p,q}$  and it consists of all matrices  $(c_{i,j}) \in \mathbb{R}^{(p+1) \times (q+1)}$  satisfying:

(q1)  $c_{0,j} = 0, c_{p,j} = j/q, c_{i,0} = 0, c_{i,q} = i/p$  for all  $i \in \langle p \rangle$  and  $j \in \langle q \rangle$ ;

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

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

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  $x_{i,j}$  satisfying, for all  $i \in [p]$  and  $j \in [q]$ ,

$$x_{i,j} \geq 0, \quad \sum_{h=1}^q x_{i,h} = u_i, \quad \sum_{\ell=1}^p x_{\ell,j} = v_j.$$

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 [9]. For example, the  $p$ th Birkhoff polytope, denoted by  $\mathcal{B}_p$ , is the transportation polytope  $\mathcal{T}(u, v)$  with  $u = v = (1, \dots, 1) \in \mathbb{R}^p$ , and the  $p \times q$  generalized Birkhoff polytope, denoted by  $\mathcal{B}_{p,q}$ , is the transportation polytope  $\mathcal{T}(u, v)$  where  $u = (q, \dots, q) \in \mathbb{R}^p$  and  $v = (p, \dots, p) \in \mathbb{R}^q$ .

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. Theorem 2.1 of Striker [42] states that this polytope, known as the alternating sign matrix polytope and denoted by  $\mathcal{ASM}_p$ , is defined, for all  $i, \ell, j, h \in [n]$ , by

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

Given margins  $u \in \mathbb{R}^p$  and  $v \in \mathbb{R}^q$ ,  $\mathcal{ASM}_p$  was generalized to the alternating transportation polytope  $\mathcal{A}(u, v)$  [25, Chapter 5], consisting of all  $p \times q$  matrices  $(x_{i,j}) \in \mathbb{R}^{p \times q}$  satisfying

(1)  $\sum_{\ell=1}^p x_{\ell,j} = v_j$  and  $\sum_{h=1}^q x_{i,h} = u_i$  for all  $i \in [p]$  and  $j \in [q]$ ;

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

$$(3) \quad 0 \leq \sum_{h=1}^j x_{i,h} \leq u_i \text{ for all } i \in [p] \text{ and } j \in [q].$$

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  $u = (q, \dots, q) \in \mathbb{R}^p$  and  $v = (p, \dots, p) \in \mathbb{R}^q$ . As shown in Proposition 1, there is an (invertible) linear transformation taking each discrete copula  $(c_{i,j}) \in \mathbb{R}^{(p+1) \times (q+1)}$  to a matrix  $(b_{i,j}) \in \mathcal{B}_{p,q}$  and taking each discrete quasi-copula to a matrix in  $\mathcal{ASM}_{p,q}$ . The following result shows that this linear transformation, which is well-known in the statistical literature, is also geometrically significant.

**Proposition 1.** *The polytopes  $DC_{p,q}$  and  $\{1/(pq)\}\mathcal{B}_{p,q}$  are unimodularly equivalent, as are  $DQ_{p,q}$  and  $\{1/(pq)\}\mathcal{ASM}_{p,q}$ .*

**Proof.** 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.,  $L: \mathcal{P} \rightarrow \mathcal{Q}$ ,  $x \mapsto \mathbf{A}x^\top$  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  $T(c_{i,j}) = c_{i,j} + c_{i-1,j-1} - c_{i,j-1} - c_{i-1,j}$  for all  $i \in [p]$  and  $j \in [q]$  that takes a discrete copula to a matrix in  $\{1/(pq)\}\mathcal{B}_{p,q}$ . Similarly, the linear map  $T$  takes a discrete quasi-copula to a matrix in  $\{1/(pq)\}\mathcal{ASM}_{p,q}$ . Using the boundary condition (c1), the map  $T$  can be interpreted as an invertible transformation on  $\mathbb{R}^{p \times q}$ , and if we let  $e_{i,j}$  denote the standard basis vectors for  $\mathbb{R}^{p \times q}$  ordered lexicographically (i.e.,  $e_{i,j} < e_{k,r}$  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,  $DC_{p,q}$  and  $\mathcal{B}_{p,q}$  have the same facial structure, and similarly for  $DQ_{p,q}$  and  $\mathcal{ASM}_{p,q}$ . In addition, for any subpolytopes  $P \subset DC_{p,q}$  and  $Q \subset DQ_{p,q}$  the subpolytopes  $T(P) \subset \mathcal{B}_{p,q}$  and  $T(Q) \subset \mathcal{ASM}_{p,q}$  have the same facial structure, respectively.

The polytope of ultramodular discrete copulas is the subpolytope  $UDC_{p,q} \subset DC_{p,q}$  satisfying, for all  $i \in [p-1]$  and  $j \in [q-1]$ , the constraints

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

These constraints correspond to convexity conditions imposed on the associated copulas, and so we can naturally define a similar subpolytope of  $DQ_{p,q}$ . The polytope of convex discrete quasi-copulas is the subpolytope  $CDQ_{p,q} \subset DQ_{p,q}$  satisfying the above constraints (3). Via the transformation  $T$ , we will equivalently study the polytopes  $\mathcal{UDC}_{p,q} = pqT(UDC_{p,q}) \subset \mathcal{B}_{p,q}$  and  $\mathcal{CDQ}_{p,q} = pqT(CDQ_{p,q}) \subset \mathcal{ASM}_{p,q}$ . 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 [9]. This is because each of the defining equalities  $x_{1,j} + \dots + x_{p,j} = p$  and  $x_{i,1} + \dots + x_{i,q} = q$  determines 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  $DC_{p,q}$ ,  $UDC_{p,q}$ ,  $DQ_{p,q}$ , and  $CDQ_{p,q}$  studied in this paper all have dimension  $(p-1)(q-1)$ .

### 3. The polytope of ultramodular discrete copulas $UDC_{p,q}$

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

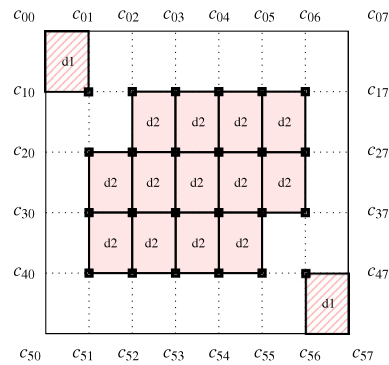
**Theorem 1.** *The minimal  $H$ -representation of the polytope of ultramodular discrete copulas  $UDC_{p,q}$  consists of the  $(p-2)(q-2) + 2(p-1)(q-1)$  inequalities:*

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

Fig. 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)  $x_{1,1} \geq 0$  and  $x_{p,q} \geq 0$ ;
- (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)  $\sum_{h=1}^j x_{i+1,h} \geq \sum_{h=1}^j x_{i,h}$  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  $(c_{i,j}) \in \mathbb{R}^{(p+1) \times (q+1)}$  satisfies the boundary condition (c1) and all of (d1), (d2), (d3a), and (d3b), then  $(c_{i,j}) \in UDC_{p,q}$ . This is proven in Lemma A in the Appendix. Then we show that for each inequality in the list (d1), (d2), (d3a),



**Fig. 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).

and (d3b) there exists a point  $(c_{i,j}) \in \mathbb{R}^{(p+1) \times (q+1)}$  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  $[0, 1]^2$  via bilinear extension techniques; see Lemma 2.3.5 in [34]. We refer to this full-domain copula as the bilinear extension copula of any discrete copula  $C = (c_{i,j})$ . Note that in the special case when  $p$  equals  $q$ , the bilinear extension copula is the well-known checkerboard approximation copula; see Definition 4.1.4 in [11].

**Theorem 2.** Given  $p, q \in \mathbb{Z}_{>0}$ , the bilinear extension copula of any  $(c_{i,j}) \in UDC_{p,q}$  is an ultramodular copula on the unit square.

We now give a simple intuition for the proof of [Theorem 2](#). For each bilinear extension copula, the density is constant on each rectangle of the partition. Thus, the conditional distributions of  $Y$  given  $X$ , and vice versa, are piecewise linear functions. As a consequence, each horizontal and vertical section of any bilinear extension is also a piecewise linear function. To complete the proof of [Theorem 2](#) it is hence sufficient to show that convexity of the piecewise linear sections of the bilinear extension follows from the convexity of the ultramodular discrete copula. We relegate this last step of the proof in the [Appendix](#).

**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  $UDC_{p,q}$ . 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 [26,34]. 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 Jensen's inequality; i.e., for all  $u_1, u_2 \in [0, 1]$ , and  $a \in [0, 1]$ ,

$$\tilde{C}(u_1/2 + u_2/2, a) \leq \tilde{C}(u_1, a)/2 + \tilde{C}(u_2, a)/2.$$

Inequalities (d3b) can be derived by fixing  $a = j/q$ , while  $u_1 = i/p$ ,  $u_2 = (i+2)/p$  for  $j \in [q-1]$  and  $i \in [p-2]$ . 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 of the polytope  $UDC_{p,q}$ . In particular, they identify a correspondence between each point in  $UDC_{p,q}$ , and the density of an ultramodular bivariate copula on  $[0, 1]^2$ , which can be constructed via bilinear extension techniques. These techniques are at the base of the empirical multilinear copula process [19,20]. In the next subsection, we also connect our results on the polytope of ultramodular discrete copulas with previous work by [36] related to checkerboard copulas, showing that our geometric results can be used to select ultramodular copulas with maximum entropy.

### 3.1. Statistical relevance of our results for entropy-copula methods

In applications such as to hydrology or climatology, data are often limited and choosing a suitable parametric copula model can therefore be challenging. In such applications, practitioners often seek to use “simple” copulas that make minimal assumptions. As discussed in [1] and references therein, a practical solution to this problem is to derive a copula  $C_h$ , with density  $h$ , such that the entropy of  $h$  is maximal and the degree of association such as Spearman's  $\rho$  between the margins is matched with the observed values. In [36], the authors propose to select such a copula  $C_h$  among the family of checkerboard copulas, and show how to obtain any such  $C_h$  from the solution of a convex optimization problem on the Birkhoff polytope. Following the steps of [36], we show here how the correspondence between discrete copulas and the generalized Birkhoff

polytope  $\mathcal{B}_{p,q}$  can be used to obtain elementary forms for the joint density, and formulate the maximum entropy problem for copulas.

Let  $X$  and  $Y$  be random variables on  $\mathbb{R}$  with corresponding cumulative probability distributions  $F$  and  $G$ , and probability density functions  $f$  and  $g$ . As a consequence of Sklar's Theorem [41], the joint probability density  $c$  of  $(X, Y)$  can be expressed as  $c(x, y) = h\{F(x), G(y)\}f(x)g(y)$ , where  $h$  is the joint density of a copula function  $C_h$ . We consider two partitions  $I_p$  and  $I_q$  on the unit interval, and fix  $u_i = (i - 1)/p$  and  $v_j = (j - 1)/q$ , for each  $i \in [p + 1]$  and  $j \in [q + 1]$ . We note that our problem formulation extends that of [36] as it also allows for the case  $p \neq q$ .

Given any arbitrary matrix  $H = (h_{i,j}) \in \mathcal{B}_{p,q}$ , the joint density  $h$  of a full-domain copula can be defined as  $h(u, v) = h_{i,j}$ , for  $(u, v) \in (u_i, u_{i+1}) \times (v_j, v_{j+1})$ . The joint density  $h$  is a step function on the unit square, and is the density of the bilinear extension copula of the unique discrete copula  $C_H$  associated with  $H$  through the unimodular map defined in Proposition 1. For copulas with any such density function  $h$ , the entropy function  $J(h)$  and Spearman's rank correlation coefficient  $\rho$  can be expressed as follows:

$$J(h) = (-1) \left\{ \frac{1}{pq} \sum_{i=1}^p \sum_{j=1}^q h_{i,j} \ln(h_{i,j}) \right\}, \quad \rho = 12 \left\{ \frac{1}{(pq)^2} \sum_{i=1}^p \sum_{j=1}^q h_{i,j} (i - 1/2)(j - 1/2) - \frac{1}{4} \right\}. \quad (4)$$

We refer to Chapter 5 in Nelsen [34] and to [36] for the technical details.

As discussed in [36,37], a simple (checkerboard) copula that maximizes the entropy  $J(h)$  and matches a given Spearman's rank correlation coefficient  $\tilde{\rho}$ , can be found as the solution to the following optimization problem on the polytope  $\mathcal{B}_{p,q}$ :

$$\text{maximize } J(h) \quad (5a)$$

$$\text{subject to } \rho = \tilde{\rho}, \quad (5b)$$

$$H = (h_{i,j}) \in \mathcal{B}_{p,q}. \quad (5c)$$

By substituting the linear constraints of Eq. (5c) with the  $H$ -representation of the polytope  $\mathcal{UDC}_{p,q}$ , the results presented in Section 3 can be used to determine an ultramodular copula with maximum entropy and prescribed Spearman's rank correlation coefficient. Note that as a consequence of Theorem 2, the bilinear extension copula of any (approximate) solution to this optimization problem on  $\mathcal{UDC}_{p,q}$  is ultramodular. This provides a construction technique for obtaining maximum entropy ultramodular copulas and generating, for example, bivariate synthetic rainfall data in the case of negative dependence [39,43]. In Section 5, we consider the maximum entropy problem on  $\mathcal{UDC}_{p,q}$  and show through a simple example how to calculate approximate solutions.

#### 4. Polytopes of (component-wise convex) discrete quasi-copulas $CDQ_{p,q}$

In this section, we identify the minimal  $H$ -representations for the polytope of discrete quasi-copulas  $DQ_{p,q}$  and its subpolytope of convex discrete quasi-copulas  $CDQ_{p,q}$ . Recall from Proposition 1 that  $DQ_{p,q}$  is unimodularly equivalent to a dilation of the generalized alternating sign matrix polytope  $\mathcal{ASM}_{p,q}$ , which was originally studied in Chapter 5 of [25]. However, while the minimal  $H$ -representation for the case  $p = q$  (i.e., for the polytope  $\mathcal{ASM}_p$ ) was identified in Theorem 3.3 of [42], it was not identified for  $p \neq q$ . In this section, we identify the minimal  $H$ -representation for  $\mathcal{ASM}_{p,q}$  (and hence also for  $DQ_{p,q}$ ) as well as that of the polytope  $CDQ_{p,q}$ .

It is shown in Theorem 3.3 of [42] that for  $p \geq 3$  the polytope  $\mathcal{ASM}_p$  has  $4\{(p - 2)^2 + 1\}$  facets given by

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

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 [42].

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

The 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 (coordinate-wise) sections. These functions are parametrized by the points  $(c_{i,j})$  within the polytope  $CDQ_{p,q}$ , which has the following  $H$ -representation:



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

- (v1)  $x_{1,1} \geq 0, x_{p-1,q-1} \geq 1 - 1/p - 1/q$ ;  
 (v3a)  $x_{i,j} + x_{i,j+2} - 2x_{i,j+1} \geq 0$  for all  $i \in [p-1], j \in [q-2]$ ;  
 (v3b)  $x_{i,j} + x_{i+2,j} - 2x_{i+1,j} \geq 0$  for all  $j \in [q-1], i \in [p-2]$ .

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  $CDQ_{p,q}$  of  $ASM_{p,q}$  has minimal  $H$ -representation

- (a1)  $x_{1,1} \geq 0, x_{p,q} \geq 0$ ;  
 (a3a)  $\sum_{\ell=1}^i x_{\ell,j+1} \geq \sum_{\ell=1}^i x_{\ell,j}$  for all  $i \in [p-1], j \in [q-1]$ ;  
 (a3b)  $\sum_{h=1}^j x_{i+1,h} \geq \sum_{h=1}^j x_{i,h}$  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  $(c_{i,j}) \in CDQ_{p,q}$  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 bilinear extension of any  $(c_{i,j}) \in CDQ_{p,q}$  is a quasi-copula on  $[0, 1]^2$  with convex (coordinate-wise) 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  $CDQ_{p,q}$ .

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  $CDQ_{p,q}$ , normalized with a multiplicative factor  $1/(pq)$ , and the signed doubly stochastic measure of a bivariate quasi-copula with convex sections. The family of quasi-copulas with convex sections introduced in this paper has not been studied before and our results lead to interesting new open questions: For instance, does every component-wise convex quasi-copula assign a signed doubly stochastic measure on the unit square? And more generally, what are the properties of component-wise convex quasi-copulas and how do they relate to ultramodular copulas in the continuous setting?

## 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 [4, 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.

While having efficiently-sized minimal  $H$ -representations of convex polytopes is beneficial from a linear optimization perspective, it can also be useful to have a  $V$ -representation of the same polytope. For example, the vertices of the Birkhoff polytope  $\mathcal{B}_p$  are precisely the  $p \times p$  permutation matrices; see, e.g., Theorem 5.2 in Barvinok [4]. In the setting of discrete copulas, this means that the vertices of  $DC_p$  correspond to the empirical copulas [26,30], and thus all bivariate discrete copulas can be constructed by way of convex combinations of empirical copulas. This property is used in [36] to solve the convex optimization problem in (5) on  $\mathcal{B}_p$ , and as demonstrated by the following example, a similar approach can be taken in the ultramodular case.

**Example 1.** Consider  $p = q = 3$ , and Spearman's rank correlation  $\tilde{\rho} = -0.8$ . We aim to determine an approximate solution to the optimization problem in (5), subject to the constraints  $\rho = -0.8$  and  $H = (h_{i,j}) \in \mathcal{UDC}_3$ . As noted in [36], we can turn this optimization problem into a minimization problem, and then use a penalty function approach to reduce the number of constraints. Thus, we want to solve the following problem:

$$\begin{aligned} &\text{minimize} && -J(h) + 10,000 \times (\rho - \tilde{\rho})^2; \\ &\text{subject to} && H = (h_{i,j}) \in \mathcal{UDC}_3. \end{aligned} \tag{6}$$

Similar as in [36], we can rewrite the optimization problem (6) in terms of the seven vertices of  $\mathcal{UDC}_3$ . Any matrix  $H \in \mathcal{UDC}_3$  can be expressed as a convex combination of  $B_1, \dots, B_7$ , vertices of  $\mathcal{UDC}_3$  given by the following matrices:

$$B_1 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad B_2 = \begin{pmatrix} 0 & 1/2 & 1/2 \\ 0 & 1/2 & 1/2 \\ 1 & 0 & 0 \end{pmatrix}, \quad B_3 = \begin{pmatrix} 0 & 1/2 & 1/2 \\ 1/2 & 0 & 1/2 \\ 1/2 & 1/2 & 0 \end{pmatrix}, \quad B_4 = \begin{pmatrix} 0 & 0 & 1 \\ 1/2 & 1/2 & 0 \\ 1/2 & 1/2 & 0 \end{pmatrix},$$

**Table 1**The number of vertices of  $UDC_{p,q}$ ,  $CDQ_{p,q}$ ,  $DQ_{p,q}$ , and  $DC_{p,q}$  as computed using `polymake` [17].

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

$$B_5 = \begin{pmatrix} 1/3 & 1/3 & 1/3 \\ 1/3 & 1/3 & 1/3 \\ 1/3 & 1/3 & 1/3 \end{pmatrix}, \quad B_6 = \begin{pmatrix} 1/4 & 1/4 & 1/2 \\ 1/4 & 1/4 & 1/2 \\ 1/2 & 1/2 & 0 \end{pmatrix}, \quad B_7 = \begin{pmatrix} 0 & 1/2 & 1/2 \\ 1/2 & 1/4 & 1/4 \\ 1/2 & 1/4 & 1/4 \end{pmatrix}.$$

That is,  $H = \alpha_1 B_1 + \dots + \alpha_7 B_7$ , with  $\alpha_1 + \dots + \alpha_7 = 1$ , and  $\alpha_1, \dots, \alpha_7 \geq 0$ . Thus, the entropy function  $J(h)$  and the Spearman's  $\rho$  in (4) can be reformulated as functions of  $\alpha_1, \dots, \alpha_7$ . We denote by  $J(\alpha_1, \dots, \alpha_7)$  and  $\rho(\alpha_1, \dots, \alpha_7)$  the new reformulations of  $J(h)$  and  $\rho$ , and re-write the optimization problem in (6) as follows:

$$\begin{aligned} &\text{minimize} && -J(\alpha_1, \dots, \alpha_7) + 10,000\{\rho(\alpha_1, \dots, \alpha_7) - \tilde{\rho}\}^2 \\ &\text{subject to} && \alpha_1, \dots, \alpha_7 \geq 0, \quad \alpha_1 + \alpha_2 + \alpha_3 + \alpha_4 + \alpha_5 + \alpha_6 + \alpha_7 = 1. \end{aligned} \quad (7)$$

We use the MATLAB function `fmincon` to find the approximate solution  $\tilde{H}$  of the minimization problem (7). The result is

$$\tilde{H} = \begin{pmatrix} 0.0002 & 0.0998 & 0.9000 \\ 0.0998 & 0.8004 & 0.0998 \\ 0.9000 & 0.0998 & 0.0002 \end{pmatrix}.$$

The density  $\tilde{H}$  corresponds to the entropy value  $J(\tilde{h}) = -0.668$ , and Spearman's  $\rho$  equal to  $-0.799$ .

For low-dimensional examples, following the approach of [36] is a reasonable choice since there are less than  $pq$  vertices, and thus the optimization problem (7) solves for less variables than that in (6). At the same time, polytopes with efficiently sized minimal  $H$ -representations can have a super-exponential number of vertices, meaning that it may be difficult to obtain their complete  $V$ -representations. This paradigm appears to be the case for the polytopes  $UDC_{p,q}$  and  $CDQ_{p,q}$ , and  $\mathcal{UDC}_{p,q}$  and  $\mathcal{CDQ}_{p,q}$ , respectively, as suggested by the data in Table 1. These observations suggest that we should use  $H$ -representations when solving higher-dimensional instances of these optimization problems in practice, unlike the approach taken in [36]. On the other hand, future research may benefit from an understanding of the growth rate of the number of vertices of these polytopes and any statistical interpretations these vertices may admit. In the remainder of this section, we present some first results on the vertices of the polytopes  $UDC_{p,q}$  and  $CDQ_{p,q}$ , towards this general goal.

### 5.1. Some simple families of vertices

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  $C = (c_{i,j})_{i,j=0}^{p,q}$  whose entries are the values of  $C$ . Given this representation for  $C$ , we can consider its transpose  $C^\top$ . We then make the following observation, a proof of which can be derived using the definition of an extreme point and the fact that convex combinations are preserved under the transpose map.

**Proposition 2.** Suppose that  $C \in UDC_{p,q}$  ( $C \in CDQ_{p,q}$ ), then  $C^\top \in UDC_{q,p}$  ( $C^\top \in CDQ_{q,p}$ ). Moreover, if  $C$  is a vertex of  $UDC_{p,q}$  ( $CDQ_{p,q}$ ), then  $C^\top$  is a vertex of  $UDC_{q,p}$  ( $CDQ_{q,p}$ ).

Proposition 2 suggests that the most informative extremal discrete copulas of  $UDC_p$  are those  $\tilde{C} = (c_{i,j})$  such that  $c_{i,j}$  is not equal to  $c_{j,i}$ , 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.

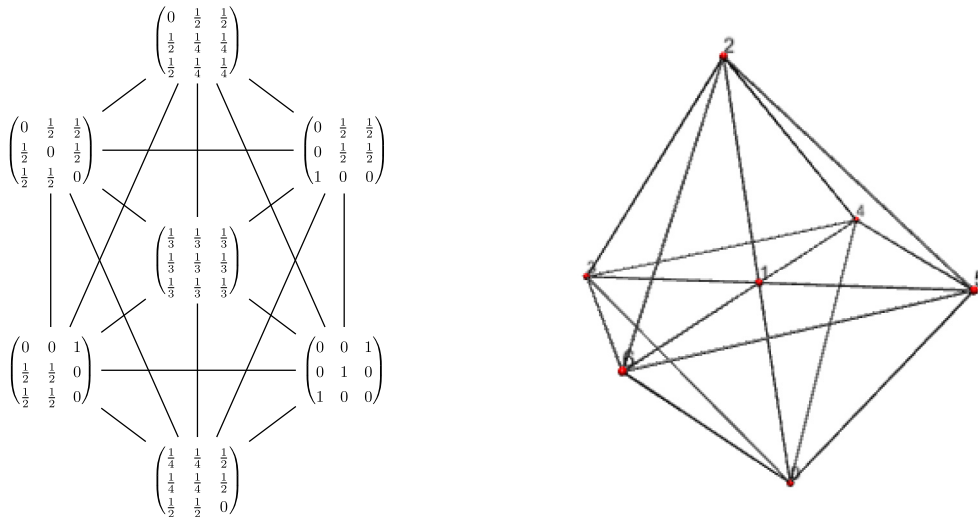
Next, recall from Proposition 1 that there is a linear map  $T : \mathbb{R}^{(p+1) \times (q+1)} \rightarrow \mathbb{R}^{p \times q}$  sending a discrete (quasi)-copula to a matrix in  $\mathcal{B}_{p,q}/(pq)$  (a matrix in  $\mathcal{ASM}_{p,q}/(pq)$ ). Further recall that  $\mathcal{UDC}_{p,q} = pqT(UDC_{p,q})$  and  $\mathcal{CDQ}_{p,q} = pqT(CDQ_{p,q})$ . 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

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

If we applied the transformation  $R : \mathbb{R}^{(p+s) \times (q+t)} \rightarrow \mathbb{R}^{(p+s) \times (q+t)}$  with  $e_{i,j} \mapsto e_{i(q+t-j+1)}$ , 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 of  $UDC_{p,q}$  and  $CDQ_{p,q}$ ).

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





**Fig. 2.** The edge-graph of the polytope  $UDC_3$ , with its seven vertices, is the edge graph of a triangulated octahedron.  $UDC_3$  is a four-dimensional polytope, with eight simplicial facets and one octahedral facet. On the right is a Schlegel diagram [44] of  $UDC_3$  as it appears when projected onto its three-dimensional, octahedral facet.

$CDQ_{p,q} \subset ASM_{p,q}$  admit a natural geometric generalization to subpolytopes  $UDC(u, v) \subset \mathcal{T}(u, v)$  and  $CDQ(u, v) \subset \mathcal{A}(u, v)$ . Namely, we let  $UDC(u, v)$  denote the subpolytope of  $\mathcal{T}(u, v)$  satisfying the additional inequalities (b3a) and (b3b), and we let  $CDQ(u, v)$  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  $\mathbf{m}_p = (m, \dots, m) \in \mathbb{R}^p$ , 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.

**Proposition 3.** 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 Proposition 3 can also be derived using the definition of extreme points; namely, by combining this with the fact that we assume that all entries in the matrices within  $UDC_{p,q}$  ( $CDQ_{p,q}$ ) are nonnegative. 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, Proposition 3 produces vertices of  $UDC_{p+s}$ . This observation yields the following corollary.

**Corollary 1.** 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  $UDC_{p+s}$  ( $CDQ_{p+s}$ ).

In the context of Corollary 1, the vertices  $B \oplus D$  admit the following statistical interpretation.

**Remark 5.** Recall that given a copula  $C$ , a patchwork copula derived from  $C$  is any copula whose probability distribution coincides with that of  $C$  up to a finite number of rectangles  $R_i$  in  $[0, 1]^2$ ; see [10]. The vertices obtained via Corollary 1 correspond to a special class of patchwork (quasi-) copulas named W-ordinal sums; i.e., patchworks derived from the Fréchet–Hoeffding lower bound of copulas  $W(u, v) = \max(0, u + v - 1)$ ; see [31]. The (normalized) direct sum of two vertices  $B \in UDC_p$  ( $CDQ_p$ ) and  $D \in UDC_s$  ( $CDQ_s$ ) is a block matrix

$$B \oplus D = \frac{1}{p+s} \begin{pmatrix} \mathbf{0}_{p,s} & B \\ D & \mathbf{0}_{s,p} \end{pmatrix} \in \mathbb{R}^{(p+s) \times (p+s)}.$$

Any extension (quasi-)copula  $\tilde{C}$  on  $[0, 1]^2$ , whose associated mass is given by  $B \oplus D$ , satisfies  $\tilde{C}\{p/(p+s), s/(p+s)\} = 0$ . Furthermore, any (quasi-)copula  $C$  with  $C(u_0, 1 - u_0) = 0$  for  $u_0 \in (0, 1)$  can be written as a W-ordinal sum [8]. Thus, any such  $\tilde{C}$  associated to  $B \oplus D$  is a W-ordinal sum.

Corollary 1 produces vertices of  $UDC_p$  and  $CDQ_p$  from known, lower-dimensional vertices, but it is important to note that not all vertices of  $UDC_p$  and  $CDQ_p$  can be captured in this fashion. For example, as shown in Fig. 2,  $UDC_3$  has seven vertices, of which only three arise from this direct sum construction. However, as we discuss in the next subsection, Corollary 1 can be used to provide lower bounds on the number of vertices of these polytopes.

## 5.2. Discussion on generating functions for the number of vertices

In this section we consider the special case of the polytopes  $UDC_{p,q}$  and  $CDQ_{p,q}$  when  $p = q$ . For convenience, we only discuss the polytope  $UDC_p$ , but the results all hold analogously for  $CDQ_p$ . [Corollary 1](#) gives a convenient way by which to partition the collection of vertices  $\mathcal{V}(UDC_p)$  into two disjoint collections: we call a vertex of  $UDC_p$  decomposable if the corresponding vertex in  $\mathcal{UDC}_p$  admits a decomposition as a direct sum of two lower dimensional vertices as in [Corollary 1](#). 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

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

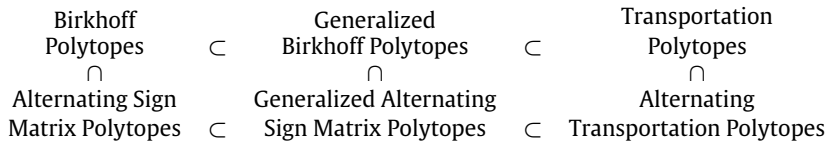
denote the generating functions for the values  $|\mathcal{V}(UDC_p)|$ ,  $|ID_p|$ , and  $|D_p|$ , respectively. As suggested by the data in [Table 1](#), the size of the set  $\mathcal{V}(UDC_p)$  appears to grow super-exponentially in  $p$ . The following observation, whose proof is given in the [Appendix](#), may be used to provide lower bounds supporting this observed growth rate.

**Proposition 4.** *The number of vertices of  $UDC_p$  is computable in terms of its number of decomposable vertices by the relationship  $V(x) = \{D(x)^2 + D(x) - 1\}/D(x)$ . Moreover, if  $M(x) \leq D(x)$ , is a lower-bound on the number of decomposable vertices of  $UDC_p$ , then  $V(x) \geq \{M(x)^2 + M(x) - 1\}/M(x)$ .*

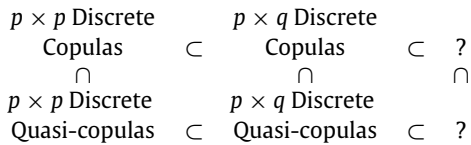
Since a lower bound on the number of decomposable vertices can be achieved by identifying a lower bound on the number of indecomposable vertices in lower dimensions, it is worthwhile to investigate large families of indecomposable extremal ultramodular discrete copulas. The identification of sufficiently 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 1](#).

## 6. Non-uniform discrete (quasi-) copulas and alternating transportation polytopes

We end this paper with a discussion aimed at completing the evolving parallel story between bivariate discrete copulas, Birkhoff polytopes and 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 discrete (quasi-) copulas defined on non-uniform discrete domains, which are restrictions of (quasi-) copulas on discrete domains different than  $I_p \times I_q$ .

We now consider two vectors  $\tilde{u} = (\tilde{u}_1, \dots, \tilde{u}_p) \in \mathbb{R}_{\geq 0}^p$  and  $\tilde{v} = (\tilde{v}_1, \dots, \tilde{v}_q) \in \mathbb{R}_{\geq 0}^q$  with  $\tilde{u}_p = \tilde{v}_q = pq$ , and  $u_i < u_{i+1}$ ,  $v_j < v_{j+1}$  for  $i \in [p-1]$  and  $j \in [q-1]$ , and define the two partitions of  $[0, 1]$ ,  $U_p = \{0, \tilde{u}_1/(pq), \dots, \tilde{u}_p/(pq)\}$ , and  $V_q = \{0, \tilde{v}_1/(pq), \dots, \tilde{v}_q/(pq)\}$ . Analogous to the case of discrete (quasi-) copulas on uniform grids  $I_p \times I_q$ , we can consider discrete (quasi-) copulas  $C_{U_p, V_q}$  on  $U_p \times V_q$  as discrete functions which satisfy the properties of a (quasi-) copula on  $U_p \times V_q$ .

By way of the same linear transformation used in [Proposition 1](#), we now observe a correspondence between discrete (quasi-) copulas  $C_{U_p, V_q}$  on  $U_p \times V_q$  and the matrices within (alternating) transportation polytopes  $\mathcal{A}(u, v)$  with homogeneous marginals, i.e.,  $\sum_i u_i = \sum_j v_j = pq$ .

We denote as  $DC(U_p, V_q)$  the set of all discrete copulas  $C_{U_p, V_q}$  on  $U_p \times V_q$ . The set  $DC(U_p, V_q)$  is composed of all matrices  $(c_{i,j}) \in \mathbb{R}^{(p+1) \times (q+1)}$  with  $c_{i,j} = C_{U_p, V_q}(\tilde{u}_i/(pq), \tilde{v}_j/(pq))$  satisfying the following conditions:

- (NU1a)  $c_{0,j} = 0, c_{i,0} = 0$  with  $i \in \langle p \rangle, j \in \langle q \rangle$ ;
- (NU1b)  $c_{p,j} = \tilde{v}_j/(pq), c_{i,q} = \tilde{u}_i/(pq)$ , with  $i \in [p], j \in [q]$ ;
- (NU2a)  $c_{i,j} + c_{i-1,j-1} - c_{i-1,j} - c_{i,j-1} \geq 0$  for every  $i \in [p], j \in [q]$ .

The following proposition links the set  $DC(U_p, V_q)$  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 5.** For a function  $C_{U_p, V_q} : U_p \times V_q \rightarrow [0, 1]$ , the following statements are equivalent:

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

$$c_{i,j} = C_{U_p, V_q} \{ \tilde{u}_i / (pq), \tilde{v}_j / (pq) \} = \frac{1}{pq} \sum_{\ell=1}^i \sum_{h=1}^j x_{\ell,h}. \quad (8)$$

A similar construction offers a correspondence between discrete (quasi-) copulas on non-uniform domains  $U_p \times V_q$  and alternating transportation polytopes with homogeneous marginals. We denote as  $DQ(U_p, V_q)$  the set of all discrete quasi-copulas  $C_{U_p, V_q}$  on  $U_p \times V_q$ . The set  $DQ(U_p, V_q)$  is composed of all matrices  $(c_{i,j}) \in \mathbb{R}^{(p+1) \times (q+1)}$  where  $c_{i,j} = C_{U_p, V_q} \{ \tilde{u}_i / (pq), \tilde{v}_j / (pq) \}$  which satisfy conditions (NU1a), (NU1b), and

$$(NU2b) \quad c_{i_1, j_1} + c_{i_2, j_2} - c_{i_1, j_2} - c_{i_2, j_1} \geq 0 \text{ for all } i_1 \leq i_2 \in \langle p \rangle, j_1 \leq j_2 \in \langle q \rangle, \text{ and } i_1 = 0, \text{ or } i_2 = p, \text{ or } j_1 = 0, \text{ or } j_2 = q.$$

The next proposition shows the link between the set  $DQ(U_p, V_q)$  and an alternating transportation polytope  $\mathcal{A}(u, v)$ .

**Proposition 6.** For a function  $C_{U_p, V_q} : U_p \times V_q \rightarrow [0, 1]$ , the following statements are equivalent:

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

$$c_{i,j} = C_{U_p, V_q} \{ \tilde{u}_i / (pq), \tilde{v}_j / (pq) \} = \frac{1}{pq} \sum_{\ell=1}^i \sum_{h=1}^j x_{\ell,h}. \quad (9)$$

**Remark 6.** Propositions 5 and 6 together offer a natural completion for the question marks in our above hierarchy on discrete copulas that fits nicely within the current literature on copula functions. In particular, the points within the polytopes  $\mathcal{T}(u, v)$  and  $\mathcal{A}(u, v)$ , up to a multiplicative factor, are the transformation matrices, respectively the quasi-transformation matrices, originally introduced in [16] and [14] to construct copulas and quasi-copulas with fractal support. Although here we complete the picture of discrete (quasi-) copulas on arbitrary grid domains, we note that the correspondence described in Propositions 5 and 6 does not capture all  $p \times q$  (alternating) transportation polytopes, but only those with homogeneous marginals; i.e.,  $\sum_i u_i = \sum_j v_j = pq$ . For example, this generalized correspondence does not encompass the (alternating) transportation polytopes containing the polytopes considered in Proposition 3. To the best of the authors' knowledge, there does not yet exist a 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 hydrology and climatology [1,36,37,39] and shed light on well-known stochastic problems [12,15,27]. 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 furthered this connection by identifying the minimal  $H$ -representations of subfamilies of bivariate discrete copulas that appear in practice, and their generalizations. We showed that the families of  $p \times q$  ultramodular bivariate discrete copulas and of  $p \times q$  bivariate convex discrete quasi-copulas admit polyhedral representations 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. The size of each minimal  $H$ -representation presented within this paper is quadratic in  $p$  and  $q$ , which opens the door for selecting ultramodular bivariate copulas with maximum entropy useful in environmental applications. 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 discrete copulas and quasi-copulas defined on non-uniform grid domains 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 allow one 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 [36,37]. One interesting direction for future research is to build on our results to construct statistical tests for stochastic decreasingness of bivariate random vectors in the same fashion as symmetry tests [18,22]. Natural follow-ups to

this research include defining the geometry of multivariate discrete copulas with the property of ultramodularity as well as considering other types of stochastic dependence such as multivariate total positivity of order two [7,33]. On the quasi-copula side, an interesting continuation of our work would be to analyze the properties of the full-domain component-wise convex quasi-copulas, and their relation to the ultramodular copulas.

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## Appendix A. Proofs for Section 3

This Appendix contains a proof of Theorems 1 and 2. The proof of Theorem 1 relies in part on the following auxiliary lemma.

**Lemma A.** Suppose that  $(c_{i,j}) \in \mathbb{R}^{(p+1) \times (q+1)}$  satisfies all of (d1), (d2), (d3a), and (d3b) as well as the equalities  $c_{0,k} = 0$ ,  $c_{p,k} = k/q$ ,  $c_{h,0} = 0$ ,  $c_{h,q} = h/p$  for all  $h \in \langle p \rangle$ ,  $k \in \langle q \rangle$ . Then  $(c_{i,j}) \in \text{UDC}_{p,q}$ .

**Proof.** To prove the result, we consider  $C = (c_{i,j}) \in \mathbb{R}^{(p+1) \times (q+1)}$  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 for  $C$ .

- (i)  $c_{1,1} + c_{2,2} - c_{1,2} - c_{2,1} \geq 0$ ;
- (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)  $c_{1,j+1} - c_{1,j} \geq 0$ , (b)  $c_{i+1,1} - c_{i,1} \geq 0$  for all  $i \in \langle p-1 \rangle$ ,  $j \in \langle q-1 \rangle$ ;
- (iv) (a)  $c_{p-1,j+1} - c_{p-1,j} \leq 1/q$ , (b)  $c_{i+1,q-1} - c_{i,q-1} \leq 1/p$  for all  $i \in \langle p-1 \rangle$ ,  $j \in \langle q-1 \rangle$ .

The matrix  $C$  satisfies conditions (d3a) and (d3b), respectively for  $(i,j) = (2,0)$  and  $(i,j) = (0,2)$ . Moreover,  $c_{1,1} \geq 0$ . Therefore, inequality (i) can be obtained from  $2(c_{1,1} + c_{2,2}) \geq 2c_{2,2} \geq 2(c_{1,2} + c_{2,1})$ .

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

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

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

$$c_{1,j+2} - c_{1,j+1} \geq^{(d3a)} c_{1,j+1} - c_{1,j} \geq \cdots \geq c_{1,2} + c_{1,1} \geq c_{1,1} \geq^{(d1)} 0.$$

Similarly, for (iv.a) we have that

$$1/q \geq^{(d1)} c_{p-1,q} - c_{q-1,q-1} \geq \cdots \geq c_{p-1,j+2} - c_{p-1,j+1} \geq^{(d3a)} c_{p-1,j+1} - c_{p-1,j}.$$

In an analogous manner one can derive (iii.b) and (iv.b), which completes the proof. We also note that the proof of the inequalities (i), (ii), (iii.a), and (iii.b) does not require any of the (d2) conditions.  $\square$

**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  $\text{UDC}_{p,q}$ . To do this, we identify  $(p \times q)$ -matrices  $M_{p,q}^{(i,j)} = (b_{i,j})$ , and  $H_{p,q}^{(i,j)} = (h_{i,j})$  for  $i \in [p]$  and  $j \in [q]$  such that

Case (b1). for every  $p$  and  $q$ ,  $M_{pq}^{(1,1)}$  satisfies all inequalities in the list (b1), (b2), (b3a), and (b3b) except for inequality of the type  $b_{1,1} \geq 0$ .

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

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

$$\sum_{h=1}^j b_{i+1,h} \geq \sum_{h=1}^j b_{i,h}.$$

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  $\text{UDC}_{p,q}$ . Indeed, let us assume  $M_{p,q}^{(i,j)} = (b_{i,j})$  to be a matrix

that satisfies (b1), (b2), (b3a), and (b3b), but for  $b_{i\hat{j}} \geq 0$  with  $\hat{i} \in \{2, \dots, \lfloor (p+1)/2 \rfloor\}$  and  $\hat{j} \in \{2, \dots, \lfloor (q+1)/2 \rfloor\}$ . Then, the matrix  $M_{p,q}^{(p-\hat{i}+1, q-\hat{j}+1)} = (b_{p-\hat{i}+1, q-\hat{j}+1})$  obtained by flipping the original matrix  $M_{p,q}^{(i,j)} = (b_{i,j})$  as follows

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

satisfies all of the constraints but for  $b_{p-\hat{i}+1, q-\hat{j}+1} \geq 0$ . We indicate this transformation with  $b_{i,j}^F$ .

In an analogous manner, one can obtain all of the remaining cases among inequalities (b3a). Moreover, matrices that satisfy all the inequalities of  $UDC_{p,q}$  except for one of the (b3b)-type can be obtained by transposing the ones of case (b3a) above.

The full list of matrices corresponding to cases (b1), (b2), and (b3) is given in a supplementary file made available online. When considered together with Lemma A, these subcases and their corresponding matrices complete the proof.  $\square$

**Proof of Theorem 2.** Every  $C \in UDC_{p,q}$  is a discrete copula on  $I_p \times I_q$ . Thus, according to Lemma 2.3.5 in [34], the bilinear extension  $\tilde{C}$  of  $C$  which is defined as

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

where  $i/p \leq u \leq (i+1)/p, j/q \leq v \leq (j+1)/q$ , and

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

is a copula on  $[0, 1]^2$ , whose restriction on  $I_p \times I_q$  is  $C$ . We now show that for any  $C \in UDC_{p,q}$ ,  $\tilde{C}$  is an ultramodular copula, i.e.,  $\tilde{C}$  has convex horizontal and vertical (coordinate-wise) 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. First,  $C_a$  is a  $p$ -piecewise continuous function. Therefore, to prove its convexity it is sufficient to show the Jensen convexity, i.e., for  $u_1, u_2 \in [0, 1]$

$$C_a(u_1/2 + u_2/2) \leq C_a(u_1)/2 + C_a(u_2)/2. \quad (A.1)$$

Without loss of generality, we assume  $j/q < a < (j+1)/q$  and define  $\mu_a = (a - j/q)q$ . We then proceed by induction on the number  $M$  of intervals that contain  $[u_1, u_2]$ . The thesis is trivial when  $M = 1$ . We thus focus on the following cases.

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

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

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

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

Thus, it follows that

$$\begin{aligned} C_a(u_1)/2 + C_a(u_2)/2 &\geq \{(1 - \mu_a)(1/2 - \lambda_1/2) - (1 - \mu_a)\lambda_2/2\}c_{i,j} + \{\mu_a(1/2 - \lambda_1/2) - \mu_a\lambda_2/2\}c_{i,j+1} \\ &\quad + \{(1 - \mu_a)\lambda_1/2 + (1 - \mu_a)/2 + (1 - \mu_a)\lambda_2/2\}c_{i+1,j} + \{\mu_a\lambda_1/2 + \mu_a/2 + \mu_a\lambda_2/2\}c_{i+1,j+1} \\ &= C_a(u_1/2 + u_2/2). \end{aligned}$$

Assuming  $(i+1)/p < u_3 < (i+2)/p$ . One has  $\lambda_3 = pu_1/2 + pu_2/2 - i = \lambda_1/2 + \lambda_2/2 - 1/2$ . Conditions (d3a) and (d3b) imply that for  $k \in \{j, j+1\}$ ,  $c_{i,k} \geq 2c_{i+1,k} - c_{i+2,k}$ . The result can therefore be derived as follows.

$$\begin{aligned} C_a(u_1)/2 + C_a(u_2)/2 &\geq \{(1 - \mu_a)(1 - \lambda_1 + \lambda_1/2 + 1/2 - \lambda_2/2)\}c_{i+2,j+1} + \{(1 - \mu_a)(-1/2 + \lambda_1/2 + \lambda_2/2)\}c_{i+2,j} \\ &\quad + \{\mu_a(1 - \lambda_1 + \lambda_1/2 + 1/2 - \lambda_2/2)\}c_{i+1,j+1} + \{\mu_a(-1/2 + \lambda_1/2 + \lambda_2/2)\}c_{i+2,j+1} \\ &= C_a(u_1/2 + u_2/2). \end{aligned}$$

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  $(N - 2)/p < u_1 < (N - 1)/p < u_2 < N/p$ . The thesis follows from case  $M = 2$ .  $\square$

## Appendix B. Proofs for Section 4

This Appendix presents a proof of [Theorems 3, 4, and 5](#). In particular, the proof of [Theorem 3](#) relies in part on [Lemma B](#), while [Theorem 3](#)'s proof relies on [Lemma C](#).

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

**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.  $\sum_{\ell=1}^p x_{\ell,j} = p$ ;  $\sum_{h=1}^q x_{i,h} = q$  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.  $0 \leq \sum_{h=1}^j x_{i,h} \leq q$  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)  $0 \leq \sum_{h=1}^j x_{i,h}$  for all  $i \in [p]$  and  $j \in [q]$ ; and
- 3(b)  $0 \leq \sum_{h=j+1}^q x_{i,h}$  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  $\sum_{\ell=1}^i x_{\ell,1} \geq 0$  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)  $0 \leq \sum_{h=1}^j x_{i,h}$  for all  $i \in \{2, \dots, p-1\}$  and  $j \in \{1, \dots, q-1\}$ ; and
- 3(b)  $0 \leq \sum_{h=j+1}^q x_{i,h}$  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)  $\sum_{h=1}^j x_{i,h} \geq 0$  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  $(b_{i,j}) \in \mathcal{ASM}_{p,q}$  then  $b_{i,j} \leq p$  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). So, if there existed some  $b_{i,j} > p$ , then since  $0 \leq \sum_{\ell=1}^i b_{\ell,j}$ , it would follow that  $\sum_{\ell=1}^i b_{\ell,j} > p$ , which contradicts the above inequalities defining  $\mathcal{ASM}_{p,q}$ .

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

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

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

**Proof of Theorem 3.** By [Lemma B](#), 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  $(b_{i,j}) \in \mathbb{R}^{p \times q}$  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  $P$

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



can be seen to satisfy all inequalities among (a1), (a2), and (a3) except for  $x_{1,1} \geq 0$ . 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  $\sum_{h=1}^j x_{2,h} \geq 0$  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

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

Here, permuting the rows and flipping the matrix along its vertical axis produces the remaining desired matrices. Collectively, these matrices combined with [Lemma B](#) complete the proof.  $\square$

**Lemma C.** Suppose that  $(c_{i,j}) \in \mathbb{R}^{(p+1) \times (q+1)}$  satisfies all of (v1), (v3a), and (v3b), as well as, for all  $h \in \langle p \rangle$  and  $k \in \langle q \rangle$ , the equalities

$$c_{0,k} = 0, \quad c_{p,k} = k/q, \quad c_{h,q} = h/p, \quad c_{h,0} = 0.$$

Then  $(c_{i,j}) \in CDQ_{p,q}$ .

**Proof.** Let us consider  $C = (c_{i,j}) \in \mathbb{R}^{(p+1) \times (q+1)}$  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 A](#) also shows that  $C$  meets the following requirements for  $i \in \langle p-1 \rangle$  and  $j \in \langle q-1 \rangle$ .

- (a) (1)  $c_{1,j+1} - c_{1,j} \geq 0$ ; (2)  $c_{i+1,1} - c_{i,j} \geq 0$ ;
- (b) (1)  $c_{p-1,j+1} - c_{p-1,j} \leq 1/q$ ; (2)  $c_{i+1,q-1} - c_{i+1,q-1} \leq 1/p$ .

Conditions (iv.a) and (iv.b) of [Lemma A](#) 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 A](#), we deduce the following chain of inequalities:

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

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

$$1/q \geq^{(v1)} c_{p-1,q} - c_{p-1,q-1} \geq^{iv.(b)} c_{i,q} - c_{i,q-1} \geq^{(v3b)} c_{i,j+1} - c_{i,j} \geq c_{i,j} - c_{i,j-1} \geq^{(v1)} 0,$$

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

**Proof of Theorem 4.** By [Lemma C](#), we know that the minimal  $H$ -representation of  $CDQ_{p,q}$  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  $CDQ_{p,q}$ . In particular, we identify  $(p \times q)$ -matrices  $M_{p,q}^{(i,j)} = (b_{i,j})$ , and  $H_{p,q}^{(i,j)} = (h_{i,j})$  for  $i \in [p]$  and  $j \in [q]$  such that

Case (a1): For every  $p$  and  $q$ ,  $M_{p,q}^{(1,1)}$  satisfies all inequalities in the list (a1), (a3a), and (a3b) except for inequality of the type  $b_{1,1} \geq 0$ .

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

As shown in the proof of [Theorem 1](#), the matrices we shall identify suffice to prove the thesis as the other inequalities of (a1), (a3a), and (a3b) can be obtained from  $M_{p,q}^{(1,1)}$  and  $H_{p,q}^{(i,j)}$  via suitable transformations.

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

**Proof of Theorem 5.** Lemma C shows each  $C \in \mathcal{CDQ}_{p,q}$  to be a discrete quasi-copula. According to Theorem 2.3 in [38], the bilinear extension  $\tilde{C}$  of  $C$  defined as

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

where  $i/p \leq u \leq (i+1)/p$ ,  $j/q \leq v \leq (j+1)/q$ , and

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

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. Proof of Proposition 4

To prove this proposition, we first recall that a (weak) composition of a positive integer  $p \in \mathbb{Z}_{>0}$  with  $k$  parts is a sum  $c_1 + \dots + c_k = p$ , 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  $c_1 + \dots + c_k = p$  such that there are indecomposable matrices  $C_1 \in \mathcal{ID}_{c_1}, \dots, C_k \in \mathcal{ID}_{c_k}$  such that  $C = C_1 \oplus \dots \oplus C_k$ . It then follows that

$$D(x) = \sum_{k \geq 0} \left( \sum_{\ell \geq 0} |\mathcal{ID}_\ell| x^\ell \right)^k = \sum_{k \geq 0} \{\mathcal{ID}(x)\}^k = \sum_{k \geq 0} \{V(x) - D(x)\}^k = \frac{1}{1 + D(x) - V(x)}.$$

In the above, the first equality says that to construct a  $p \times p$  decomposable vertex we pick a composition  $c_1 + \dots + c_k = p$  of  $p$  length  $k$  and for each part  $c_i$  we pick an  $c_i \times c_i$  indecomposable vertex. Note that all possible composition  $c_1 + \dots + c_k = p$  for all possible  $k \geq 0$  arise as the exponents of the summation on the right-hand-side when it is expanded. By the correspondence between compositions of  $p$  and decompositions of decomposable vertices into their indecomposable parts outlined above, the first equality follows. Based on the final line of the equality, it is quick to conclude that  $V(x) = \{D(x)^2 + D(x) - 1\}/D(x)$ . In a similar fashion, the inequality follows.

### Appendix D. Proofs for Section 6

**Proof of Proposition 5.** (i)  $\Rightarrow$  (ii): We consider  $C_{U_p, V_q} \in \mathcal{DC}(U_p, V_q)$ . For every  $i \in \langle p \rangle, j \in \langle q \rangle$ , we can take  $C_{U_p, V_q}$  to a  $(p \times q)$  matrix  $(x_{i,j})$  through the following linear transformation

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

We here show that the new constructed matrix  $(x_{i,j})$  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 (NU2a) implies that  $x_{i,j} \geq 0$  for every  $i \in \langle p \rangle, j \in \langle q \rangle$ . By construction, one has that  $\sum_{h=1}^q x_{i,h} = pq(c_{i,q} - c_{i-1,q}) = \tilde{u}_i - \tilde{u}_{i-1} = u_i$ . Similarly, it follows that  $\sum_{\ell=1}^p x_{\ell,j} = v_j$ . Hence, the thesis.

(i)  $\Leftarrow$  (ii): We here verify that every  $C_{U_p, V_q}$  defined as in Eq. (8) belongs to the set  $\mathcal{DC}(U_p, V_q)$ , with vectors  $\tilde{u} \in \mathbb{R}^p$  and  $\tilde{v} \in \mathbb{R}^q$  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  $C_{U_p, V_q}$  satisfies condition (NU2a). Since the empty sum equals zero by convention, (NU1a) holds as well. It remains to show the validity of (NU1b). From Eq. (8), one has that

$$c_{p,j} = \frac{1}{pq} \sum_{\ell=1}^p \sum_{h=1}^j x_{\ell,h} = \frac{1}{pq} \sum_{h=1}^j v_h = \frac{\tilde{v}_j}{pq}, \quad c_{i,q} = \frac{1}{pq} \sum_{\ell=1}^i \sum_{h=1}^q x_{\ell,h} = \frac{1}{pq} \sum_{\ell=1}^i u_\ell = \frac{\tilde{u}_i}{pq},$$

which completes the proof.  $\square$

**Proof of Proposition 6.** (i)  $\Rightarrow$  (ii): We consider  $C_{U_p, V_q} \in \mathcal{DQ}(U_p, V_q)$ . For every  $i \in \langle p \rangle, j \in \langle q \rangle$ , we can take  $C_{U_p, V_q}$  to a  $(p \times q)$  matrix  $(x_{i,j})$  through the following linear transformation

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

The new constructed matrix  $(x_{i,j})$  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 the proof of Proposition 5, one can derive the marginal constraints of  $(x_{i,j})$  from (NU1a) and (NU1b).

It remains to check that  $0 \leq \sum_{\ell=1}^i x_{\ell,j} \leq v_j$ , and  $0 \leq \sum_{h=1}^j x_{i,h} \leq u_i$ , for every  $i \in \langle p \rangle, j \in \langle q \rangle$ . It is useful to observe that

$$\sum_{\ell=1}^i x_{\ell,j} = pq \sum_{\ell=1}^i (c_{\ell,j} + c_{\ell-1,j-1} - c_{\ell-1,j} - c_{\ell,j-1}) = pq(c_{i,j} - c_{i,j-1}).$$

We now notice that for every  $i \in \langle p \rangle$  and  $j \in \langle q \rangle$ , one has  $(c_{i,j} - c_{i,j-1} - c_{0,j} + c_{0,j-1}) \geq 0$ , from (NU2b) and (NU1a). Hence  $\sum_{\ell=1}^i x_{\ell,j} \geq 0$ . Moreover, from (NU2b) and (NU1b), one has  $(c_{i,j-1} - c_{i,j} - c_{p,j-1} + c_{p,j}) \geq 0$ . Thus,  $c_{i,j} - c_{i,j-1} \leq c_{p,j} - c_{p,j-1}$  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  $C_{U_p, V_q}$  defined as in Eq. (9) belongs to the set  $DC(U_p, V_q)$ , with vectors  $\tilde{u} \in \mathbb{R}^p$  and  $\tilde{v} \in \mathbb{R}^q$  given by  $\tilde{u}_i = \sum_{\ell=1}^i u_\ell$ , for  $i \in [p]$ , and  $\tilde{v}_j = \sum_{h=1}^j v_h$ , for  $j \in [q]$ . Conditions (NU1a) and (NU1b) can be derived according to Proposition 5'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  $\sum_{\ell=i_1+1}^{i_2} (x_{\ell,j_1+1} + \dots + x_{\ell,j_2})$ , if  $i_2 = p$ . In either case, the sums are nonnegative. In similar way, one can derive the cases  $j_2 = q$  and  $j_1 = 0$ .  $\square$

## Appendix E. Supplementary data

A supplementary file containing the full list of matrices that complete the proof of Theorem 1 can be found online at <https://doi.org/10.1016/j.jmva.2019.01.014>.

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