Extreme Points of Polytopes of Discrete Copulas

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Abstract

Discrete copulas are useful tools in statistics to represent the joint distribution of discrete random vectors. Furthermore, they are fascinating mathematical objects that admit a representation as a convex polytope. In this work, we analyze the set of extreme points of convex polytopes of discrete copulas. We focus on the general class of discrete copulas defined on arbitrary grid domains of the unit square, thereby providing a complete characterization of extremal discrete copulas in the most general setting. To do so, we exploit well-known results on the extreme points of transportation polytopes. Finally, we show that the characterization presented here generalizes previous work on the topic.

Keywords: Discrete Copulas, Transportation Polytopes, Extreme points.

1 Introduction

Copulas are flexible mathematical tools to obtain marginal-free distributions of multivariate random vectors [8, 10, 17]. Key to the success of copulas in probability and statistics is *Sklar's Theorem*, which states that the joint distribution function $F_{\mathbf{X}}$ of any d-dimensional random vector $\mathbf{X} = (X_1, \ldots, X_d)$ can be expressed, for every $(x_1, \ldots, x_d) \in \mathbb{R}^d$, as

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

where the function $C : [0,1]^d \to [0,1]$ is a d-*dimensional copula* and $F_{X_1}, \ldots, F_{X_d}$ are univariate marginal distributions [25].

We note that the function C in Eq (1) is uniquely identified on the set $\text{Range}(F_{X_1}) \times \cdots \times \text{Range}(F_{X_d})$. As a consequence, if $F_{X_1}, \ldots, F_{X_d}$ are discrete probability distributions with finite support, Sklar's theorem identifies the so-called *discrete copulas*, which are restrictions of copulas on grid domains of the unit hyper-cube [12, 14, 15]. Discrete copulas can be easily extended to full-domain copulas by spreading the probability mass on each hyper-rectangle of their grid domain, but, in general, the extension is not unique [5]. In spite of that, discrete copulas are useful tools in many applied fields, where practitioners can take advantage of the mathematical properties of these functions alongside their probabilistic interpretation.

One of the most convenient mathematical features of discrete copulas is that they admit a representation as a convex polytope. A convex polytope is a bounded convex space consisting of all points satisfying a finite list of inequalities [27]. Convex polytopes naturally appear in many areas of applied mathematics, including statistics, probability, and operation research. Recent work in dependence modeling shows the several advantages of handling discrete copulas as convex polytopes. As an example, the polytopal representation of discrete copulas has been exploited in hydrology to obtain flexible copula models to generate syntetic data of rainfall totals [19, 20, 22]. Another work shows an application to copula selection in portfolio optimization [13]. In [18], the authors use tools from discrete geometry to define the polytopal representations of sub-families of discrete copulas with desirable stochastic properties. Such representations can be helpful to design a hypothesis test for a negative dependence property [7].

On the mathematical side, discrete copulas (and discrete quasi-copulas) have been extensively studied in terms of their matrix representations [1, 2, 9, 12, 14, 15, 16, 21]. In [18], the authors highlight that the space of discrete copulas with fixed marginal distributions of finite support of size p and q, respectively, corresponds to a polytope known as the generalized Birkhoff polytope [6]. A similar correspondence holds between the space of discrete quasi-copulas and a polytope known

as the alternating transportation polytope [11, 26]. The definition of discrete (quasi-) copulas is further generalized in [18] to the discrete (quasi-) copulas on arbitrary grid domains. There, the authors also show a connection between discrete (quasi-) copulas and other classes of (alternating) transportation polytopes.

Besides analyzing the matrix representation of discrete (quasi-) copulas, special attention has been given to the study of those points within the space of discrete (quasi-) copulas that cannot be expressed as a convex combination of other points. These points are the *extreme points* (or *vertices*) of the polytope, and they are also known as the *irreducible* discrete (quasi-) copulas. Notably, knowing the set of all extreme discrete (quasi-) copulas allows to describe any discrete copula as a convex combination of them. This latter aspect can be analogously expressed in the continuous case via Krein-Millman Theorem; see, e.g., [8].

Characterizing the class of the extreme points of convex polytopes is a natural question in discrete geometry. In the context of discrete copulas, such a characterization is well-understood in special cases. For example, in [12], the authors show that the extreme points of the class of $(p \times p)-$discrete copulas are those of minimal range, i.e., the discrete copulas that only take values in the uniform partition of the unit square with step $1/p$. This is a beautiful result since, as explained in [15], the $(p \times p)-$discrete copulas of minimal range correspond to the so-called *empirical copulas*, which are the foundation of rank-based (non-parametric) copula approaches [23, 24]. The case of $(p \times q)$-discrete (quasi-) copulas is considered in [1, 2, 16]. There, a first characterization of the set of irreducible discrete copulas when $q = pk$ is also given. Again in this case, the irreducible discrete copulas correspond to the ones with minimal range. The general case $q \neq pk$ appears to be more complex. Recently, in [9], the authors shed more light on the set of irreducible discrete (quasi-) copulas when $q \neq pk$, providing negative answers to two open questions posed in [2].

Despite these results collectively cover many special cases, to the best of our knowledge, a complete characterization of the irreducible discrete copulas is not available in the copula literature. In this paper, we fill this gap and give a characterization of the extreme points of the polytopes of discrete copulas defined on arbitrary grid domains. In particular, we recall a well-known result in the transportation polytopes literature, thereby showing that the extremality of any discrete copula depends on the zero pattern of its associated transportation matrix.

The remainder of the paper is organized as follows. In Section 2, we introduce basic definitions and known re-

sults unifying the theory of discrete copulas and transportation polytopes. In Section 3, we give the characterization of the extreme points. In Section 4, we use such a characterization in several examples of discrete copulas that appear in [2] and [9]. In Section 5, we draw conclusions and briefly discuss the case of discrete quasi-copulas.

2 Discrete copulas and convex polytopes

We now present the definition of discrete copulas on non-uniform grid domains, originally introduced in [18], and the associated convex polytopes.

First, we clarify the notation, which is in line with [18]. For $p \in \mathbb{Z}_{>0}$, we denote $[p] = \{1, \ldots, p\}$, $\langle p \rangle = \{0, \ldots, p\}$, and $I_p = \{0, 1/p, \ldots, (p-1)/p, 1\}$. Assuming p and q both in $\mathbb{Z}_{>0}$, we consider two vectors $u = (u_1, \ldots, u_p) \in \mathbb{R}^p_{>0}$ and $v = (v_1, \ldots, v_q) \in \mathbb{R}^q_{>0}$ with the properties that $u_p = v_q = pq$, and $u_i < u_{i+1}, v_j < v_{j+1}$ for $i \in [p-1]$ and $j \in [q-1]$. The vectors u and v define two partitions of $[0,1]$, $U_p = \{0, u_1/(pq), \ldots, u_p/(pq)\}$, and $V_q = \{0, v_1/(pq), \ldots, v_q/(pq)\}$. As discussed in [18], we can consider discrete copulas C_{U_p, V_q} defined on $U_p \times V_q$ as functions which satisfy the properties of a copula on the domain $U_p \times V_q$.

In particular, the set of all discrete copulas $C_{U_p, V_q} : U_p \times V_q \to [0,1]$, denoted as $\mathrm{DC}(U_p, V_q)$, is composed of all matrices $(c_{i,j}) \in \mathbb{R}^{(p+1) \times (q+1)}$ with $c_{i,j} = C_{U_p, V_q}(u_i/(pq), v_j/(pq))$ satisfying the following conditions:

(p1) $c_{0,j} = 0, c_{i,0} = 0$ with $i \in \langle p \rangle, j \in \langle q \rangle$;

(p2) $c_{p,j} = v_j/(pq), c_{i,q} = u_i/(pq)$, with $i \in [p], j \in [q]$;

(p3) $c_{i,j} + c_{i-1,j-1} - c_{i-1,j} - c_{i,j-1} \geq 0$ for every $i \in [p], j \in [q]$.

Remark 1. *We notice that the definition of discrete copulas on non-uniform grid domains includes the regular case of rectangular discrete copulas defined on $I_p \times I_q$. Indeed, for p and q in $\mathbb{Z}_{>0}$, we can obtain the uniform rectangular grid domain $I_p \times I_q$ by choosing $u = (q, 2q, \ldots, kq, \ldots, pq) \in \mathbb{R}^p$ and $v = (p, 2p, \ldots, kp, \ldots, qp) \in \mathbb{R}^q$.*

Given two vectors $\tilde{u} = (\tilde{u}_1, \ldots, \tilde{u}_p) \in \mathbb{R}^p_{>0}$ and $\tilde{v} = (\tilde{v}_1, \ldots, \tilde{v}_q) \in \mathbb{R}^q_{>0}$, we define the transportation polytope $\mathscr{T}(\tilde{u}, \tilde{v})$ as the convex polytope in the pq variables $x_{i,j}$ satisfying, for all $i \in [p]$ and $j \in [q]$, the following conditions

$$x_{i,j} \geq 0, \quad \sum_{h=1}^{q} x_{i,h} = \tilde{u}_i, \quad \sum_{\ell=1}^{p} x_{\ell,j} = \tilde{v}_j.$$

The vectors $\tilde{u}$ and $\tilde{v}$ are called the margins of $\mathscr{T}(\tilde{u},\tilde{v})$. In [18], the authors prove a correspondence between the discrete copulas C_{U_p,V_q} in $\mathrm{DC}(U_p,V_q)$ and the matrices within transportation polytopes $\mathscr{T}(\tilde{u},\tilde{v})$ with homogeneous marginals, i.e., $\sum_i \tilde{u}_i = \sum_j \tilde{v}_j = pq$. We report this result below for completeness.

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

(i) $C_{U_p,V_q} \in \mathrm{DC}(U_p,V_q)$.

(ii) *There is a $(p \times q)$ transportation matrix $(x_{i,j})$ in $\mathscr{T}(\tilde{u},\tilde{v})$, with $\sum_{h=1}^{q} \tilde{v}_h = \sum_{\ell=1}^{p} \tilde{u}_\ell = pq$, such that for every $i \in \langle p \rangle$, $j \in \langle q \rangle$*

$$c_{i,j} = C_{U_p,V_q}\left(u_i/(pq), v_j/(pq)\right) = \frac{1}{pq} \sum_{\ell=1}^{i} \sum_{h=1}^{j} x_{\ell,h}.$$

The linear map $T : \mathbb{R}^{(p+1)\times(q+1)} \longrightarrow \mathbb{R}^{p\times q}$ defined as $T(c_{i,j}) = c_{i,j} + c_{i-1,j-1} - c_{i,j-1} - c_{i-1,j}$ for all $i \in [p]$ and $j \in [q]$ brings any discrete copula of $\mathrm{DC}(U_p,V_q)$ into a transportation matrix in $\{1/(pq)\}\mathscr{T}(\tilde{u},\tilde{v})$, with margins given as follows:

$$\tilde{u} = (u_1, u_2 - u_1, \ldots, u_k - u_{k-1}, \ldots, u_p - u_{p-1})$$

$$\tilde{v} = (v_1, v_2 - v_1, \ldots, v_k - v_{k-1}, \ldots, v_q - v_{q-1}).$$

We notice that the scalar factor $1/(pq)$ does not change the geometric structure of the convex polytope nor its extreme points. Again in this more general case, the transportation matrix associated to a discrete copula represents, up to a scalar factor, the probability mass that lies in each rectangle of the grid domain.

We now give two simple numerical examples to illustrate our general theoretic framework in practice. In particular, the examples show how to move from the space of discrete copulas to the associated transportation polytope, and back.

Example 1. *We assume $p = 3$, $q = 4$, and we consider the two vectors $u = (2,7,12) \in \mathbb{R}^3$ and $v = (3,6,9,12) \in \mathbb{R}^4$. Thus, we are working on the grid domain $U_3 \times V_4 = \{0, 2/12, 7/12, 1\} \times \{0, 3/12, 6/12, 9/12, 1\}$ represented in Figure 1. The following matrix C_1 is an example of a discrete copula defined on $U_3 \times V_4$:*

$$C_1 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 2/12 & 2/12 & 2/12 & 2/12 \\ 0 & 3/12 & 6/12 & 7/12 & 7/12 \\ 0 & 3/12 & 6/12 & 9/12 & 1 \end{pmatrix}.$$

By applying the standard linear map T, we find the associated (3×4) transportation matrix below:

$$T_1 = \begin{pmatrix} 2 & 0 & 0 & 0 \\ 1 & 3 & 1 & 0 \\ 0 & 0 & 2 & 3 \end{pmatrix},$$
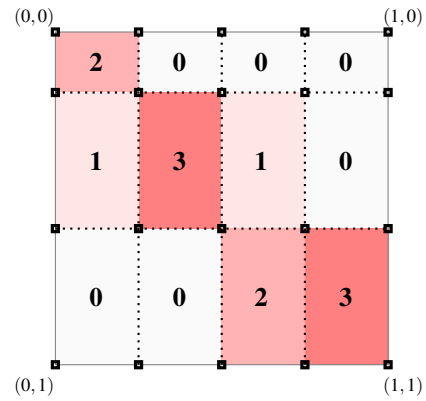

Figure 1: A graphical representation of the grid domain $U_3 \times V_4$ defined in Example 1 alongside the entries of the matrix T_1 in each corresponding rectangle.

which belongs to the transportation polytope $\mathscr{T}([2,5,5],[3,3,3,3])$, as expected.

Example 2. *In this example, we assume $p = q = 3$, and we consider the transportation polytope $\mathscr{T}(\tilde{u},\tilde{v})$, with $\tilde{u} = (1,5,3)$ and $\tilde{v} = (3,2,4)$. We notice that $\sum_i \tilde{u}_i = \sum_j \tilde{v}_j = pq = 9$. Thus, $\mathscr{T}(\tilde{u},\tilde{v})$ has homogeneous marginals. We now consider the matrix T_2 in $\mathscr{T}(\tilde{u},\tilde{v})$ defined as follows:*

$$T_2 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 1 & 3 \\ 2 & 0 & 1 \end{pmatrix},$$

and we obtain the corresponding discrete copula. To do so, we first find the grid domain $U_3 \times V_3$. By summing up the entries of $\tilde{u} = (1,5,3)$ and $\tilde{v} = (3,2,4)$, we obtain the two vectors $u = (1,6,9)$ and $v = (3,5,9)$. Hence, the grid domain of the discrete copula associated with T_2 is $U_3 \times V_3 = \{0, 1/9, 6/9, 1\} \times \{0, 3/9, 5/9, 1\}$, which is represented in Figure 2. From Proposition 1, we can derive the associated discrete copula C_2, which results in the following matrix:

$$C_2 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1/9 & 1/9 \\ 0 & 1/9 & 3/9 & 6/9 \\ 0 & 3/9 & 5/9 & 1 \end{pmatrix}.$$

We now recall a simple way to construct absolutely continuous copulas from discrete copulas.

Remark 2. *Any discrete copula can be used to construct an absolutely continuous copula $C : [0,1]^2 \to [0,1]$ with piecewise constant density on each rectangle of the partition of $[0,1]^2$ determined by $U_p \times V_q$. The density of a copula C derived by a discrete copula like the ones of Example 1 and Example 2 can be given by $x_{ij}(pq)/(\tilde{u}_i \tilde{v}_j)$, where x_{ij} is the entry of the corresponding transportation matrix for $i \in [p]$ and $j \in [q]$.*
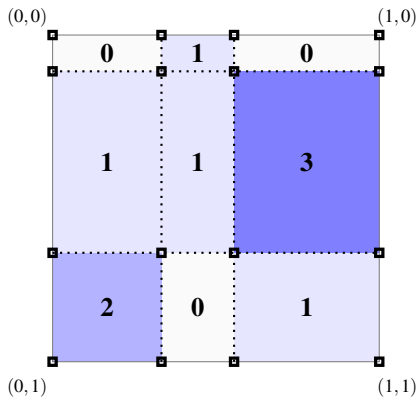
Figure 2: A representation of the grid domain $U_3 \times V_3$ defined in Example 2 alongside the entries of the matrix T_2 in each corresponding rectangle.

In the next section, we finally present the general characterization of the extreme points of the polytopes of discrete copulas introduced above.

3 The extreme discrete copulas

The correspondence between transportation polytopes and discrete copulas allows us to shed light on the set of extreme discrete copulas. Before presenting the details of the characterization, we notice that a similar question, though not involving discrete copulas directly, has been considered in [3] thirty years ago. There, the authors analyze the extreme points of the set of all bivariate distributions with fixed marginals of finite support. In doing so, they draw connections to the transportation polytopes and collect well-known results in the field of discrete geometry, providing five ways of characterizing the (non-) extreme points of their set of distributions. In the following, we only report the statements of the characterization that are useful in our setting. The complete result is given in Theorem 2.9 of [3].

Theorem 1. *Let $T_{p,q}$ be any $(p \times q)$−matrix in the transportation polytope $\mathcal{T}(\tilde{u}, \tilde{v})$ with homogeneous marginals, i.e., $\sum_i \tilde{u}_i = \sum_j \tilde{v}_j = pq$. Then, the following statements are equivalent:*

1. *$T_{p,q}$ is not an extreme point of $\mathcal{T}(\tilde{u}, \tilde{v})$.*

2. *There exists a submatrix E of $T_{p,q}$ such that every row and column of E has at least two positive elements.*

3. *There exists a square submatrix D of $T_{p,q}$ such that every row and column of D contains at least two positive entries.*

4. *There exists a square submatrix F of $T_{p,q}$ of order $k \times k$ for some $k \geq 1$ such that the number of positive elements of F is at least $2k$.*

Theorem 1 provides a characterization of (non-) extreme points of transportation polytopes in terms of their zero pattern. A similar characterization for the extreme points of the generalized Birkhoff polytopes has been discussed in [4]. However, the characterization we give in Theorem 1 remains the most general one and the only one that covers the case of discrete copulas defined on arbitrary grid domains introduced in Section 2.

In the next section, we show how to use Theorem 1 to quickly check whether or not a discrete copula is an extreme point, i.e., it is irreducible.

4 Examples of extreme points

We now apply Theorem 1 to several examples of irreducible and non-irreducible discrete copulas defined on the uniform grid domain $I_p \times I_q$ that appear in the literature. We begin with Example 3 in [9], and we discuss the following (4×6) matrix A_1 (re-scaled according to our normalizing factor):

$$A_1 = \begin{pmatrix} 0 & 2 & 0 & 0 & 2 & 2 \\ 2 & 0 & 2 & 2 & 0 & 0 \\ 0 & 0 & 2 & 2 & 0 & 2 \\ 2 & 2 & 0 & 0 & 2 & 0 \end{pmatrix}.$$

Theorem 1 suggests to look at the distribution of the non-zero entries in the matrix. If we do so, we notice that there is indeed a square submatrix of A_1 of order $k = 2$ with four, i.e., $2k$, non-zero entries, namely

$$D = \begin{pmatrix} 2 & 2 \\ 2 & 2 \end{pmatrix}.$$

This is sufficient to conclude that A_1 is not irreducible, which is in line with [9]. Similarly, we can use Theorem 1 for Example 4 of [9]. Indeed, we consider the (4×6) matrix A_2 given as follows:

$$A_2 = \begin{pmatrix} 4 & 0 & 0 & 0 & 2 & 0 \\ 0 & 2 & 0 & 2 & 2 & 0 \\ 0 & 2 & 0 & 2 & 0 & 2 \\ 0 & 0 & 4 & 0 & 0 & 2 \end{pmatrix}.$$

We note that the (2×2) matrix D is also a submatrix of A_2. Thus, A_2 is not an extreme point, which is again in accordance with [9].

We can use the same argument to conclude that the transportation matrix T_2 of Example 2 is not an extreme

point. Indeed, there exists a (2×2) submatrix of T_2 with four positive entries, that is the following matrix:

$$F = \begin{pmatrix} 1 & 3 \\ 2 & 2 \end{pmatrix}.$$

We now discuss some cases of irreducible discrete-copulas. Again, we start with an example originally presented in [9]. Namely, we look at the (3×8) matrix given as follows:

$$A_3 = \begin{pmatrix} 3 & 3 & 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 1 & 3 & 3 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 & 3 & 3 \end{pmatrix}.$$

If we analyze the matrix A_3, we notice that there are no submatrices of A_3 with the property that every row and column contains at least two positive entries. Therefore, A_3 is irreducible. From a similar argument we deduce that the matrix T_1 introduced in Example 1 is also an extreme point. In fact, the discrete copula associated with the matrix T_1 of Example 1 comes from the co-monotonic copula $M = \min\{u, v\}$.

Our last example for this section is a (3×8) matrix A_4 taken from [2] and defined as follows:

$$A_4 = \begin{pmatrix} 3 & 3 & 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 3 & 3 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 & 3 & 3 \end{pmatrix}.$$

As discussed in [2], the matrix A_4 is irreducible. Moreover, it is an example of an irreducible matrix that cannot be constructed extending a (3×6) extreme point of the corresponding generalized Birkhoff polytope. Therefore, it shows that the construction given in [16] fails to capture all the irreducible discrete copulas. We now have a closer look at the matrix A_4 by analyzing the first (3×6) matrix block:

$$B_4 = \begin{pmatrix} 3 & 3 & 2 & 0 & 0 & 0 \\ 0 & 0 & 1 & 3 & 3 & 1 \\ 0 & 0 & 0 & 0 & 0 & 2 \end{pmatrix}.$$

We notice that B_4 cannot be associated to a discrete copula defined on $I_3 \times I_6$ because its row sums are not uniform. Though, B_4 belongs to the transportation polytope $\mathscr{T}(\tilde{u}, \tilde{v}) = \mathscr{T}([8,8,2], [3,3,3,3,3,3])$, which contains all transportation matrices corresponding to discrete copulas defined on the grid domain $U_3 \times V_6 = \{0, 1/6, 1/3, 1\} \times \{0, 1/6, 1/3, 1/2, 2/3, 5/6, 1\}$. By means of Theorem 1, we derive that B_4 is an extreme point of $\mathscr{T}(\tilde{u}, \tilde{v})$. This suggests that the construction of irreducible discrete copulas given in [16] might work, in principle, if boundary cases like the one of matrix A_4 could also be included. However, alternative ways of constructing irreducible transportation matrices with uniform marginals can be found in [4].

5 Conclusion

In this paper, we provide a simple characterization of the (non-) extreme points of the space of arbitrary discrete copulas in terms of the zero patterns of their associated transportation matrices. We consider several examples and demonstrate how the presented characterization can be used to quickly check if a discrete copula is irreducible.

Although the focus of this work is on discrete copulas, a natural question arises whether or not similar characterizations can be obtained for discrete quasi-copulas. To the best of the authors' knowledge, there are no similar results for the alternating transportation polytopes, i.e., the convex polytopes that correspond to the space of discrete quasi-copulas. We know that the alternating transportation polytopes are much more complex than the transportation polytopes, and a generalization of the characterization of Theorem 1 is not obvious. Though, the alternating transportation polytopes appeared in the discrete geometry literature recently [11], and many properties of these polytopes have not been studied yet. For example, the complete description in terms of minimal bounding hyperplanes of the alternating transportation polytopes with uniform margins has been given in [18]. Still, there are many open questions regarding these polytopes which all correspond to interesting questions for the discrete quasi-copulas introduced in [18]. Such research questions deserve the attention of our research community and will be the focus of future work.

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