EXTREME VALUES OF THE MASS DISTRIBUTION ASSOCIATED WITH d-QUASI-COPULAS VIA LINEAR PROGRAMMING

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Abstract. The recent survey [2] nicknamed "Hitchhiker's Guide" has raised the rating of quasi-copula problems in the dependence modeling community in spite of the lack of statistical interpretation of quasi-copulas. This paper concentrates on the Open Problem 5 of this list concerning bounds on the volume of a d–variate quasi-copula. We disprove a recent conjecture [23] on the lower bound of this volume. We also give evidence that the problem is much more difficult than suspected and give some hints towards its final solution.

1. Introduction

The role of copulas in dependence modeling is growing ever since Sklar [22] in 1959 observed their omnipotence. We can think of copula as a multivariate distribution with uniform margins, but when we insert into it arbitrary univariate distributions as margins, we get an arbitrary multivariate distribution and any distribution of a random vector can be acquired in this way. More details about copulas can be found in [8, 17]. Now, quasi-copulas have become their silent companions: they have no statistical interpretation because they may have negative volumes of certain boxes. While the upper Fréchet-Hoeffding bound M, the pointwise supremum of all d-variate copulas, is always a copula, the lower bound W, the pointwise infimum of all d-variate copulas, is in general a quasi-copula. In case $d = 2$ it is also a copula, but in case $d > 2$ it is not. Since 1993 when quasi-copulas were first introduced in [1] they have come a long way until the "hitchhiker's guide" of 2020 [2] with many references and a list of open problems.

Copula theory has been gaining in popularity perhaps due to a wide range of applications, from natural sciences and engineering through economics and finance and recently ecology and sustainable development. Their ability to describe a variety of different relationships among random variables has become indispensable. The applications of quasi-copulas mostly follow those of copulas, with some additional ones in fuzzy set theory and the theory of aggregation functions (e.g., [3, 4, 15]). This motivated further research on algebraic properties of quasi-copulas (e.g., [9, 10, 19–21]), in particular also the question of extreme values of volumes of rectangles [5, 19] which is the main topic of this work. We start with the usual algebraic definition of quasi-copulas.

Let $\mathcal{D} \subseteq [0, 1]^d$ be a set. We say that a function $Q : \mathcal{D} \to [0, 1]$ satisfies:

Date: October 26, 2024.

2020 *Mathematics Subject Classification.* Primary 62H05, 60A99; Secondary 60E05, 26B35.

Key words and phrases. mass distribution, d-quasi-copula, volume, Lipschitz condition, bounds.

[2]Supported by the ARIS (Slovenian Research and Innovation Agency) research core funding No. P1-0448.

[4]Supported by the ARIS (Slovenian Research and Innovation Agency) research core funding No. P1-0228 and grant No. J1-50002.

(BC) *Boundary condition:* If $\underline{u} := (u_1, \ldots, u_d) \in \mathcal{D}$ is of the form:

(a) $\underline{u} = (u_1, \ldots, u_{i-1}, 0, u_{i+1}, \ldots, u_d)$ for some i, then $Q(\underline{u}) = 0$.

(b) $\underline{u} = (1, \ldots, 1, u_i, 1, \ldots, 1)$ for some i, then $Q(\underline{u}) = u_i$.

(MC) *Monotonicity condition:* Q is nondecreasing in every variable, i.e., for each $i = 1, \ldots, d$ and each pair of d-tuples

$$\underline{u} := (u_1, \ldots, u_{i-1}, u_i, u_{i+1}, \ldots, u_d) \in \mathcal{D},$$
$$\underline{\widetilde{u}} := (u_1, \ldots, u_{i-1}, \widetilde{u}_i, u_{i+1}, \ldots, u_d) \in \mathcal{D},$$

such that $u_i \leq \widetilde{u}_i$, it follows that $Q(\underline{u}) \leq Q(\underline{\widetilde{u}})$.

(LC) *Lipschitz condition*: Given d–tuples $(u_1, \ldots, u_d)$ and $(v_1, \ldots, v_d)$ in $\mathcal{D}$ it holds that

$$|Q(u_1, \ldots, u_d) - Q(v_1, \ldots, v_d)| \leq \sum_{i=1}^{d} |u_i - v_i|.$$

If $\mathcal{D} = [0,1]^d$ and Q satisfies (BC), (MC), (LC), then Q is called a *d-variate quasi-copula* (or *d-quasi-copula*). We will omit the dimension d when it is clear from the context and write quasi-copula for short.

Let Q be a quasi-copula and $\mathcal{B} = \prod_{i=1}^{d}[a_i, b_i] \subseteq [0,1]$ a d-box with $a_i < b_i$ for each i. We will use multiindices of the form $\mathbb{I} := (i_1, i_2 \ldots i_d) \in \{0,1\}^d$ to index 2^d elements $\prod_{i=1}^{d}\{a_i, b_i\}$ of $\mathcal{B}$. We write

$$x_{\mathbb{I}} := ((x_{\mathbb{I}})_1, \ldots, (x_{\mathbb{I}})_d) \tag{1.1}$$

to denote the vertex with coordinates

$$(x_{\mathbb{I}})_k = \begin{cases} a_k, & \text{if } i_k = 0, \\ b_k, & \text{if } i_k = 1. \end{cases} \tag{1.2}$$

Let us denote the value of Q in the point $x_{\mathbb{I}}$ by

$$q_{\mathbb{I}} := Q(x_{\mathbb{I}}).$$

We write $\text{sign}(\mathbb{I}) := d - \sum_{j=1}^{d} i_j$ for the number of coordinates in the multiindex $\mathbb{I}$ equal to 0. The Q**-volume** of $\mathcal{B}$ is defined by:

$$V_Q(\mathcal{B}) = \sum_{\mathbb{I} \in \{0,1\}^d} (-1)^{\text{sign}(\mathbb{I})} q_{\mathbb{I}}. \tag{1.3}$$

In this paper we fix a dimension $d \geq 2$ and consider extreme values of the Q-volume $V_Q(\mathcal{B})$ over all quasi-copulas Q and all d-boxes $\mathcal{B}$. This is called Open Problem 5 on the list of the "hitchhiker's guide" [2]. It has recently been conjectured [23] that the minimal value is $-\frac{(d-1)^2}{2d-1}$, attained for some Q on $\mathcal{B} = \left[\frac{d-1}{2d-1}, \frac{2d-2}{2d-1}\right]^d$. This conjecture is based on the results for $d = 2$ [18], proved analytically, $d = 3$ [5] and $d = 4$ [23], proved via linear programming using software tool *Mathematica*. We were able to extend the linear programming approach to solve [2, Open Problem 5] up to $d = 9$ using *Mathematica* [25] and programming language *Julia* [6] up to $d = 16$. Our results disprove the conjecture of [23]. Indeed, based on the results for $d \leq 16$ the minimal and maximal values seem to follow the exponential function of the form $c2^d + d$ for suitable $c, d \in \mathbb{R}$. For the maximal value the boxes $\mathcal{B}$ are of the form $[a, 1]^d$, while for minimal values this is true for $d \geq 7$.

The organization of the paper is the following. In Section 2 we prove that it suffices to relax the problem of extremes of $V_Q(\mathcal{B})$ over all d-quasi-copulas to the problem of extremes of functions Q defined on a 2^d-element grid of the vertices of $\mathcal{B}$ or a 3^d–element grid obtained by allowing values 1 for the coordinates of points, such that three types of conditions coming from (BC), (MC), (LC) are satisfied (see Theorems 2.1 and 2.2). The proof of these results is constructive by extending the function from the grid to the whole d-box $[0,1]^d$. These results enable us to formulate the problem in terms of two linear programs in Section 3 (see (3.1) and (3.2)). Numerical results obtained are presented in Tables 1 (for the minimal values), 2 (for the maximal values) and graphically on Figure 1.

2. Relaxation of the problem

The first main results of this section, Theorem 2.1, states that every function Q defined on the vertices of a d-box $\prod_{i=1}^d [a_i, 1] \subseteq [0,1]^d$ satisfying certain conditions coming from the definition of a quasi-copula, extends to a quasi-copula. This enables us to formulate a relaxation of the problem of extremes of $V_Q(\mathcal{B})$ over all quasi-copulas Q and all d-boxes $\mathcal{B}$ as a linear program in Section 3.

The second main result, Theorem 2.2, is analogous to Theorem 2.1, where the 2^d-element grid $\prod_{i=1}^d \{a_i, 1\}$ is replaced by a 3^d-element grid $\prod_{i=1}^d \{a_i, b_i, 1\}$. We need this result in Section 3 to solve those cases, where the relaxation of the volume problem does not give grids of the form $\prod_{i=1}^d \{a_i, 1\}$ as a result. This happens for minima of $V_Q(\mathcal{B})$ in dimensions $d \le 6$.

Fix $d \in \mathbb{N}$. For $s \in \mathbb{N}$ we write

$$[s] := \{0, 1, \ldots, s\} \quad \text{and} \quad [-s; s] := \{-s, -s+1, \ldots, -1, 0, 1, \ldots, s\}.$$

For multiindices

$$\mathbb{I} = (i_1, \ldots, i_d) \in [s]^d \quad \text{and} \quad \mathbb{J} = (j_1, \ldots, j_d) \in [s]^d$$

let

$$\mathbb{J} - \mathbb{I} = (j_1 - i_1, \ldots, j_d - i_d) \in [-s; s]^d$$

stand for their usual coordinate-wise difference. Let $\mathbb{I}_\ell$ stand for the multiindex with the only non-zero coordinate the ℓ–th one, which is equal to 1.

For a tuple $\underline{x} = (x_1, \ldots, x_d)$ we define the functions

$$G_d : \mathbb{R}^d \to \mathbb{R}, \quad G_d(\underline{x}) := \sum_{i=1}^d x_i - d + 1,$$
$$H_d : \mathbb{R}^d \to \mathbb{R}, \quad H_d(\underline{x}) := \min\{x_1, x_2, \ldots, x_d\}.$$

Let $\mathcal{D} = \prod_{i=1}^d \{a_i, 1\}$ be a 2^d-element set with $0 \le a_i < 1$ for each i. For $\mathbb{I} \in [1]^d$ let $x_{\mathbb{I}} := ((x_{\mathbb{I}})_1, \ldots, (x_{\mathbb{I}})_d) \in \mathcal{D}$, where

$$(x_{\mathbb{I}})_k = \begin{cases} a_k, & \text{if } i_k = 0, \\ 1, & \text{if } i_k = 1. \end{cases} \tag{2.1}$$

The first main result of this section is the following.

Theorem 2.1. *Fix $d \in \mathbb{N}$. Given real numbers a_i, $i = 1, \dots, d$, points $x_{\mathbb{I}} \in \prod_{i=1}^{d}\{a_i, 1\}$ defined by (2.1) and real numbers $q_{\mathbb{I}}$ for each $\mathbb{I} \in [1]^d$, such that*

$$0 \le a_i < 1 \quad i = 1, \dots, d, \tag{2.2}$$

$$0 \le q_{\mathbb{J}} - q_{\mathbb{I}} \le 1 - a_\ell \quad \text{for all } \ell = 1, \dots, d \tag{2.3}$$
$$\text{and all } \mathbb{I}, \mathbb{J} \in [1]^d \text{ such that } \mathbb{J} - \mathbb{I} = \mathbb{I}_\ell,$$

$$\max\{0, G_d(x_{\mathbb{I}})\} \le q_{\mathbb{I}} \le H_d(x_{\mathbb{I}}) \quad \text{for each } \mathbb{I} \in \{0,1\}^d, \tag{2.4}$$

there exists a d-quasi-copula $Q_d : [0,1]^d \to \mathbb{R}$ satisfying

$$Q_d(x_{\mathbb{I}}) = q_{\mathbb{I}} \quad \text{for each } \mathbb{I} \in [1]^d.$$

Let now $\mathcal{D} = \prod_{i=1}^{d}\{a_i, b_i, 1\}$ be a 3^d-element set with $0 \le a_i < b_i < 1$ for each i. For $\mathbb{I} \in [2]^d$ let $x_{\mathbb{I}} := ((x_{\mathbb{I}})_1, \dots, (x_{\mathbb{I}})_d) \in \mathcal{D}$, where

$$(x_{\mathbb{I}})_k = \begin{cases} a_k, & \text{if } i_k = 0, \\ b_k, & \text{if } i_k = 1, \\ 1, & \text{if } i_k = 2. \end{cases} \tag{2.5}$$

The second main result of this section is the following.

Theorem 2.2. *Fix $d \in \mathbb{N}$. Given real numbers a_i, b_i, $i = 1, \dots, d$, points $x_{\mathbb{I}} \in \prod_{i=1}^{d}\{a_i, b_i, 1\}$ defined by (2.5) and $q_{\mathbb{I}}$ for each $\mathbb{I} \in [2]^d$, such that*

$$0 \le a_i < b_i < 1 \quad i = 1, \dots, d, \tag{2.6}$$

$$0 \le q_{\mathbb{J}} - q_{\mathbb{I}} \le b_\ell - a_\ell \quad \text{for all } \ell = 1, \dots, d \tag{2.7}$$
$$\text{and all } \mathbb{I}, \mathbb{J} \in [1]^d \text{ such that } \mathbb{J} - \mathbb{I} = \mathbb{I}_\ell,$$

$$0 \le q_{\mathbb{J}} - q_{\mathbb{I}} \le 1 - b_\ell \quad \text{for all } \ell = 1, \dots, d \tag{2.8}$$
$$\text{and all } \mathbb{I} \in [2]^d, \mathbb{J} \in [2]^d \setminus [1]^d \text{ such that } \mathbb{J} - \mathbb{I} = \mathbb{I}_\ell,$$

$$\max\{0, G_d(x_{\mathbb{I}})\} \le q_{\mathbb{I}} \le H_d(x_{\mathbb{I}}) \quad \text{for each } \mathbb{I} \in [2]^d, \tag{2.9}$$

there exists a d-quasi-copula $Q_d : [0,1]^d \to \mathbb{R}$ such that

$$Q_d(x_{\mathbb{I}}) = q_{\mathbb{I}} \quad \text{for each } \mathbb{I} \in [2]^d.$$

We will give constructive proofs of Theorems 2.1 and 2.2. First we establish some auxiliary results.

The next lemma shows that the Lipschitz condition is equivalent to the Lipschitz condition in each dimension.

Lemma 2.3. *Let $\delta_1, \dots, \delta_d$ be subsets of $[0,1]$ and $\mathcal{D} = \prod_{i=1}^{d}\delta_i \subseteq [0,1]^d$. Let $F : \mathcal{D} \to [0,1]$ be a function. The following statements are equivalent:*

(1) F satisfies the Lipschitz condition on $\mathcal{D}$.

(2) F satisfies the Lipschitz condition in each variable, i.e., if

$$\underline{x} := (a_1, \dots, a_{i-1}, x, a_{i+1}, \dots, a_d) \in \mathcal{D},$$
$$\underline{y} := (a_1, \dots, a_{i-1}, y, a_{i+1}, \dots, a_d) \in \mathcal{D},$$

then

$$|F(\underline{x}) - F(\underline{y})| \le |x - y|.$$

Proof. The nontrivial implication is (2) $\Rightarrow$ (1). Let $\underline{x} = (x_1, \dots, x_d) \in \mathcal{D}$ and $\underline{y} = (y_1, \dots, y_d) \in \mathcal{D}$. We have that

$$\begin{aligned}|F(\underline{x}) - F(\underline{y})| &= \big|F(x_1, x_2, \dots x_d) - F(y_1, x_2, \dots, x_d) + \\ &\qquad F(y_1, x_2, \dots, x_d) - F(y_1, y_2, x_3 \dots, x_d) + \dots + \\ &\qquad F(y_1, y_2, \dots, y_{d-1}, x_d) - F(y_1, y_2, \dots, y_d)\big| \\ &\le \big|F(x_1, x_2, \dots x_d) - F(y_1, x_2, \dots, x_d)\big| + \\ &\qquad \big|F(y_1, x_2, \dots, x_d) - F(y_1, y_2, x_3 \dots, x_d)\big| + \dots + \\ &\qquad \big|F(y_1, y_2, \dots, y_{d-1}, x_d) - F(y_1, y_2, \dots, y_d)\big| \\ &\le |x_1 - y_1| + |x_2 - y_2| + \dots + |x_d - y_d|,\end{aligned}$$

where we used the triangular inequality in the first inequality and the Lipschitz condition in each variable in the second inequality. □

The next lemma shows that for a function of a single variable the Lipschitz condition is equivalent to the piecewise Lipschitz condition.

Lemma 2.4. *Let $x_1 \le x_2 \le \dots \le x_n$ be points in $\mathbb{R}$ and $f : [x_1, x_n] \to \mathbb{R}$ a function. The following statements are equivalent:*

(1) f satisfies the Lipschitz condition on $[x_1, x_n]$.
(2) f satisfies the Lipschitz condition on $[x_i, x_{i+1}]$ for $i = 1, \dots, n-1$.

Proof. The nontrivial implication is (2) $\Rightarrow$ (1). Let $x < y$ with $x, y \in [x_1, x_n]$. Suppose that $x \in [x_{k-1}, x_k]$ and $y \in [x_\ell, x_{\ell+1}]$. We have that

$$\begin{aligned}|f(y) - f(x)| &= \big|f(x_k) - f(x) + f(x_{k+1}) - f(x_k) + \dots + \\ &\qquad f(x_\ell) - f(x_{\ell-1}) + f(y) - f(x_\ell)\big| \\ &\le \big|f(x_k) - f(x)\big| + \big|f(x_{k+1}) - f(x_k)\big| + \dots + \\ &\qquad \big|f(x_\ell) - f(x_{\ell-1})\big| + \big|f(y) - f(x_\ell)\big| \\ &\le (x_k - x) + (x_{k+1} - x_k) + \dots + (x_\ell - x_{\ell-1}) + (y - x_\ell) \\ &= y - x,\end{aligned}$$

where we used the triangular inequality in the first inequality and the piecewise Lipschitz condition from (2) in the second inequality. □

Recall that a multivariate function $F : \prod_{i=1}^d [a_i, b_i] \to \mathbb{R}$, where $\prod_{i=1}^d [a_i, b_i] \subseteq [0,1]^d$, is *multilinear* (resp. *piecewise multilinear*), if it is linear (resp. piecewise linear) separately in each variable, i.e., every restriction of F to a single variable by fixing values of all other variables is linear (resp. piecewise linear).

The next proposition states that for a multilinear function on a d-box the Lipschitz condition is equivalent to the Lipschitz condition of its restriction to the vertices of the box.

Proposition 2.5. *Let F be a multilinear function on a box $\mathcal{B} = \prod_{i=1}^d [a_i, b_i]$, where $0 \le a_i < b_i \le 1$ for each i. The following statements are equivalent:*

(1) F satisfies the Lipschitz condition.
(2) F satisfies the Lipschitz condition on the vertices, i.e.,

$$|F(u_1, u_2, \dots, u_d) - F(v_1, v_2, \dots, v_d)| \le \prod_{i=1}^d |u_i - v_i|$$

for every choice of $u_i, v_i \in \{a_i, b_i\}$.

Proof. The nontrivial implication is (2) $\Rightarrow$ (1). We will prove by induction on ℓ that F satisfies the Lipschitz condition on each ℓ-dimensional face of $\prod_{i=1}^d [a_i, b_i]$ for $\ell = 1, \ldots, d$. For $\ell = d$ we get the whole box $\mathcal{B}$. Note that all ℓ-dimensional faces are determined in the following way:

(1) Choose a set $\mathcal{I}_\ell = \{i_1, i_2, \ldots, i_\ell\}$ of ℓ coordinates $1 \le i_1 < i_2 < \ldots < i_\ell \le d$.
(2) Let $\mathcal{I}_\ell^c = \{j_1, \ldots, j_{d-\ell}\}$ be the remaining coordinates among the coordinates $1, \ldots, d$.
(3) Fix $c_j \in \{a_j, b_j\}$ for each $j \in \mathcal{I}_\ell^c$.
(4) The choices above determine a ℓ-dimensional face

$$\mathcal{F}_{\mathcal{I}_\ell, (c_{j_1}, \ldots, c_{j_{d-\ell}})} := \prod_{i=1}^d \delta_i,$$

where

$$\delta_i = \begin{cases} [a_i, b_i], & \text{if } i \in \mathcal{I}_\ell, \\ \{c_i\}, & \text{if } i \in \mathcal{I}_\ell^c. \end{cases}$$

To prove the base of induction let $\ell = 1$ and $\mathcal{I}_1$ be an arbitrary one-dimensional face of $\prod_{i=1}^d [a_i, b_i]$, i.e., an edge of $\prod_{i=1}^d [a_i, b_i]$. By symmetry we may assume without the loss of generality that $\mathcal{I}_1 = \{1\}$. So we need to prove that F satisfies the Lipschitz condition on each edge

$$\mathcal{F}_{\{1\}, \{c_2, \ldots, c_d\}} = \big\{(x, c_2, \ldots, c_d) \colon x \in [a_1, b_1]\big\},$$

where $c_i \in \{a_i, b_i\}$ for each i. Let $x, y \in [a_1, b_1]$ with $x \neq y$. Then

$$\begin{aligned} &\big|F(x, c_2, \ldots c_d) - F(y, c_2, \ldots, c_d)\big| = \\ =&\left|\frac{F(b_1, c_2, \ldots, c_d) - F(a_1, c_2, \ldots, c_d)}{b_1 - a_1}\right| |x - y| \\ \le&\frac{b_1 - a_1}{b_1 - a_1} |x - y| = |x - y|, \end{aligned}$$

where in the first equality we used linearity of F in the first variable and in the inequality we used the Lipschitz condition for a pair of vertices $(b_1, c_2, \ldots, c_d)$ and $(a_1, c_2, \ldots, c_d)$. This proves the base of induction.

Let us now assume F is Lipschitz on each of the ℓ-dimensional faces of $\prod_{i=1}^d [a_i, b_i]$ for $1 \le \ell \le \ell_0 - 1$ where $1 \le \ell_0 - 1 < d$, and prove F is Lipschitz on all ℓ_0-dimensional faces. By symmetry we may assume without the loss of generality that $\mathcal{I}_{\ell_0} = \{1, \ldots, \ell_0\}$. So we need to prove that F satisfies the Lipschitz condition on each face of the form

$$\mathcal{F} \equiv \mathcal{F}_{\mathcal{I}_{\ell_0}, \{c_{\ell_0+1}, \ldots, c_d\}} = \big\{(x_1, \ldots, x_{\ell_0}, c_{\ell_0+1}, \ldots, c_d) \colon x_i \in [a_i, b_i] \text{ for each } i\big\},$$

where $c_j \in \{a_j, b_j\}$ for each j. Using Lemma 2.3 with $\mathcal{D} = \mathcal{F}$ it suffices to prove the Lipschitz condition in each variable $i \in \mathcal{I}_{\ell_0}$. By symmetry we may assume without the loss of generality that $i = 1$. Let

$$\begin{aligned} (x, z_2, \ldots, z_{\ell_0}, c_{\ell_0+1}, \ldots, c_d) &\in \mathcal{F}, \\ (y, z_2, \ldots, z_{\ell_0}, c_{\ell_0+1}, \ldots, c_d) &\in \mathcal{F}. \end{aligned}$$

We have that each z_j is of the form $z_j = t_j a_j + (1 - t_j) b_j$ for some $t_j \in [0, 1]$. Then by linearity of F in the ℓ_0-th variable we have that

$$\begin{aligned} &F(z_1, z_2, \ldots, z_{\ell_0}, c_{\ell_0+1}, \ldots, c_d) = \\ =&t_{\ell_0} F(z_1, z_2, \ldots, a_{\ell_0}, c_{\ell_0+1}, \ldots, c_d) + \\ &+ (1 - t_{\ell_0}) F(z_1, z_2, \ldots, b_{\ell_0}, c_{\ell_0+1}, \ldots, c_d). \end{aligned} \tag{2.10}$$

for each $z_1 \in [a_1, b_1]$. Hence,

$$\begin{aligned}
&\Big|F(x, z_2, \dots, z_{\ell_0}, c_{\ell_0+1}, \dots, c_d) - F(y, z_2, \dots, z_{\ell_0}, c_{\ell_0+1}, \dots, c_d)\Big| = \\
=&\Big|t_{\ell_0}\big(F(x, z_2, \dots, a_{\ell_0}, c_{\ell_0+1}, \dots, c_d) - F(y, z_2, \dots, a_{\ell_0}, c_{\ell_0+1}, \dots, c_d)\big) + \\
&+ (1-t_{\ell_0})\big(F(x, z_2, \dots, b_{\ell_0}, c_{\ell_0+1}, \dots, c_d) - F(y, z_2, \dots, b_{\ell_0}, c_{\ell_0+1}, \dots, c_d)\big)\Big| \le \\
\le& t_{\ell_0}\Big|F(x, z_2, \dots, a_{\ell_0}, c_{\ell_0+1}, \dots, c_d) - F(y, z_2, \dots, a_{\ell_0}, c_{\ell_0+1}, \dots, c_d)\Big| \\
&+ (1-t_{\ell_0})\Big|F(x, z_2, \dots, b_{\ell_0}, c_{\ell_0+1}, \dots, c_d) - F(y, z_2, \dots, b_{\ell_0}, c_{\ell_0+1}, \dots, c_d)\Big| \\
\le& t_{\ell_0}|x-y| + (1-t_{\ell_0})|x-y| = |x-y|,
\end{aligned}$$

where we used (2.10) in the first equality, the triangle inequality in the first inequality and the Lipschitz condition for the $(\ell_0 - 1)$-dimensional faces

$$\mathcal{F}_{\{1,\dots,\ell_0-1\},(a_{\ell_0},c_{\ell_0+1},\dots,c_d)} \quad \text{and} \quad \mathcal{F}_{\{1,\dots,\ell_0-1\},(b_{\ell_0},c_{\ell_0+1},\dots,c_d)},$$

respectively. This proves the induction step and concludes the proof of the proposition. □

The next proposition states that for a multilinear function on a d-box the monotonicity condition is equivalent to the monotonicity condition of its restriction to the vertices of the box.

Proposition 2.6. *Let Q be a multilinear function on a box $\mathcal{B} = \prod_{i=1}^{d}[a_i, b_i]$, where $0 \le a_i < b_i \le 1$ for each i. The following statements are equivalent:*

(1) Q satisfies the monotonocity condition in each variable.

(2) Q satisfies the monotonocity condition on the vertices, i.e.,

$$Q(u_1, u_2, \dots, u_d) \le Q(v_1, v_2, \dots, v_d),$$

where $u_i, v_i \in \{a_i, b_i\}$ and $u_i = v_i$ for all but at most one index j where $u_j \le v_j$.

Proof. The nontrivial implication is (2) ⇒ (1). By symmetry it suffices to prove monotonicity in the first variable. Let $\underline{x} = (x, z_2, \dots, z_d)$ and $\underline{y} = (y, z_2, \dots, z_d)$ with $a_1 \le x < y \le b_1$ and $z_j \in [a_j, b_j]$ for each j. We have to prove that

$$Q(a_1, z_2, \dots, z_d) \le Q(b_1, z_2, \dots, z_d). \tag{2.11}$$

We have that $x = t_x a_1 + (1-t_x)b_1$, $y = t_y a_1 + (1-t_y)b_1$ for some $0 \le t_y < t_x \le 1$ Each z_j is of the form $z_j = t_j a_j + (1-t_j)b_j$ for some $t_j \in [0,1]$. Then

$$\begin{aligned}
&Q(z_1, z_2, \dots, z_d) = \\
&= \sum_{(r_1,\dots,r_d)\in[1]^d} t_1^{r_1}(1-t_1)^{1-r_1} \cdots t_d^{r_d}(1-t_d)^{1-r_d} \cdot \\
&\qquad \cdot Q(r_1 a_1 + (1-r_1)b_1, r_2 a_2 + (1-r_2)b_2 \dots, r_d a_d + (1-r_d)b_d)
\end{aligned} \tag{2.12}$$

Using (2.12) for $z_1 = a_1$ and $z_1 = b_1$, it follows that (2.11) is equivalent to

$$\begin{aligned}
&\sum_{(r_2,\dots,r_d)\in[1]^{d-1}} (t_y - t_x) t_2^{r_2}(1-t_2)^{1-r_2} \cdots t_d^{r_d}(1-t_d)^{1-r_d} \cdot \\
&\qquad \cdot Q(b_1, r_2 a_2 + (1-r_2)b_2 \dots, r_d a_d + (1-r_d)b_d) \\
\le &\sum_{(r_2,\dots,r_d)\in[1]^{d-1}} (t_y - t_x) t_2^{r_2}(1-t_2)^{1-r_2} \cdots t_d^{r_d}(1-t_d)^{1-r_d} \cdot \\
&\qquad \cdot Q(a_1, r_2 a_2 + (1-r_2)b_2 \dots, r_d a_d + (1-r_d)b_d)
\end{aligned} \tag{2.13}$$

Since for each tuple $(r_2, \ldots, r_d) \in [1]^{d-1}$ we have

$$\begin{aligned} &Q(a_1, r_2a_2 + (1-r_2)b_2, \ldots, r_da_d + (1-r_d)b_d) \\ \leq &Q(b_1, r_2a_2 + (1-r_2)b_2, \ldots, r_da_d + (1-r_d)b_d) \end{aligned}$$

by assumption (2) and since $t_y - t_x < 0$, it follows that (2.13) holds. This proves the proposition. □

The next proposition is a first step toward establishing Theorems 2.1 and 2.2 by defining Q_d on $\mathcal{D}$ and all $(d-1)$–dimensional faces

$$\mathcal{L}_i = \{(x_1, \ldots, x_{i-1}, 0, x_{i+1}, \ldots, x_d) \colon x_i \in [0,1]\} \tag{2.14}$$

of $[0,1]^d$ containing $(0, \ldots, 0)$.

Proposition 2.7. *Let one of the following assumptions hold:*

(1) $s = 1$, *real numbers* a_i, $i = 1, \ldots, d,$, *points* $x_{\mathbb{I}} \in \prod_{i=1}^d \{a_i, 1\} =: \mathcal{D}$ *defined by* (2.1) *and real numbers* $q_{\mathbb{I}}$ *for each* $\mathbb{I} \in [1]^d$, *satisfy conditions* (2.2)–(2.4) *of Theorem 2.1.*

(2) $s = 2$, *real numbers* a_i, b_i, $i = 1, \ldots, d,$, *points* $x_{\mathbb{I}} \in \prod_{i=1}^d \{a_i, b_i, 1\} =: \mathcal{D}$ *defined by* (2.5) *and real numbers* $q_{\mathbb{I}}$ *for each* $\mathbb{I} \in [2]^d$, *satisfy conditions* (2.6)–(2.9) *of Theorem 2.1.*

Let

$$\mathcal{D}^{(\text{ext})} = \mathcal{D} \cup \Big(\cup_{i=1}^d \mathcal{L}_i \Big) \tag{2.15}$$

where $\mathcal{L}_i$ *are as in* (2.14). *Let*

$$Q : \mathcal{D}^{(\text{ext})} \to \mathbb{R}$$

be defined by

$$Q(x_1, \ldots, x_d) = \begin{cases} q_{\mathbb{I}}, & \text{if } (x_1, \ldots, x_d) = x_{\mathbb{I}} \text{ for some } \mathbb{I} \in [s]^d, \\ 0, & \text{if } (x_1, \ldots, x_d) \in \mathcal{L}_i \text{ for some } i \in \{1, \ldots, d\}, \end{cases} \tag{2.16}$$

Then Q is well-defined and satisfies (BC), (MC) and (LC).

Proof. First we prove well-definedness. We have to show that $x_{\mathbb{I}} \in \mathcal{L}_i$ implies that $q_{\mathbb{I}} = 0$. If $x_{\mathbb{I}} \in \mathcal{L}_i$, then $x_i = 0$ and by (2.4) we have that $0 \leq q_{\mathbb{I}} \leq H_d(x_{\mathbb{I}}) = 0$. Hence, $q_{\mathbb{I}} = 0$.

Q satisfies (BC) by definition of Q on $\mathcal{L}_i$ for each i.

By Lemma 2.3, it suffices to prove the Lipschitz condition separately for each variable. In what follows we will prove monotonicity and the Lipschitz condition for each variable simultaneously. By symmetry it suffices to prove them for the first variable. Let us take $\underline{x} := (x, a_2, \ldots, a_d)$ and $\underline{y} = (y, a_2, \ldots, a_d)$ with $0 \leq x < y$ such that $\underline{x}, \underline{y} \in \mathcal{D}^{(\text{ext})}$. We separate 3 cases:

Case 1: $\underline{x}, \underline{y} \in \mathcal{D}$. Then $0 \leq Q(\underline{y}) - Q(\underline{x}) \leq y - x$ by (2.3) or (2.7)-(2.8).

Case 2: $\underline{x} \in \mathcal{D}$ and $\underline{y} \in \mathcal{L}_i$ for some $i \in \{1, \ldots, d\}$. Then $i \neq 1$ (since $y > 0$). But then $a_i = 0$ and hence $\underline{x} \in \mathcal{L}_i$ as well. It follows that $Q(\underline{x}) = Q(\underline{y}) = 0$.

Case 3: $\underline{x} \in \mathcal{L}_i$ for some $i \in \{1, \ldots, d\}$.

First note that $0 = Q(\underline{x})$. We separate two subcases according to the value of i.

Assume that $i = 1$. If $\underline{y} \in \mathcal{D}$, then $Q(\underline{y}) \leq y$ by (2.4) or (2.9). If $\underline{y} \in \mathcal{L}_j$ for some j, then $Q(\underline{y}) = 0$. In all cases (MC) and (LC) are satisfied.

If $i > 1$, then $\underline{y} \in \mathcal{L}_i$ as well and $Q(\underline{y}) = 0$.

This concludes the proof of the proposition. □

Now we are ready to prove Theorems 2.1 and 2.2.

Proof of Theorem 2.1. Let $\mathcal{D}$, $\mathcal{D}^{(\text{ext})}$ and Q be as in Proposition 2.7 under assumption (1). We subdivide the box $[0,1]^d$ into 2^d smaller d-boxes

$$\mathcal{B}_{\mathbb{I}} = \prod_{j=1}^{d} \delta_j(\mathbb{I}) \tag{2.17}$$

for $\mathbb{I} = (i_1, \dots, i_d) \in \{0,1\}^d$, where

$$\delta_j(\mathbb{I}) = \begin{cases} [0, a_j], & \text{if } i_j = 0, \\ [a_j, 1], & \text{if } i_j = 1. \end{cases}$$

In particular,

$$\mathcal{B}_{(0,0\dots0)} = \prod_{k=1}^{d}[0,a_k], \quad \mathcal{B}_{(1,0\dots0)} = [a_1,1] \times \prod_{k=2}^{d}[0,a_k], \dots, \quad \mathcal{B}_{(1,1\dots1)} = \prod_{k=1}^{d}[a_k,1].$$

Note that the Q-volume $V_Q(\mathcal{B}_{\mathbb{I}})$ of each box $\mathcal{B}_{\mathbb{I}}$ is determined by the value of Q on the vertices of $\mathcal{B}_{\mathbb{I}}$. For each $\mathbb{I} \in \{0,1\}^d$ we define a constant function

$$\rho_{\mathbb{I}} : \mathcal{B}_{\mathbb{I}} \to \mathbb{R}, \quad \rho_{\mathbb{I}} := \frac{V_Q(\mathcal{B}_{\mathbb{I}})}{\prod_{j=1}^{d} \delta_j(\mathbb{I})}.$$

Let us define a piecewise constant function

$$\rho : [0,1]^d \to \mathbb{R}, \quad \rho(\underline{x}) := \begin{cases} \rho_{\mathbb{I}}, & \text{if } \underline{x} \in \operatorname{int}(\mathcal{B}_{\mathbb{I}}) \text{ for some } \mathbb{I} \in \{0,1\}^d, \\ 0, & \text{otherwise}, \end{cases}$$

where $\operatorname{int}(A)$ stands for the topological interior of the set A in the usual Euclidean topology. We will prove that a function $Q_d : [0,1]^d \to \mathbb{R}$, defined by

$$Q_d(x_1, x_2, \dots x_d) = \int_0^{x_1} \int_0^{x_2} \dots \int_0^{x_d} \rho(x_1, x_2, \dots x_d) \mathrm{d}x_1 \mathrm{d}x_2 \cdots \mathrm{d}x_d, \tag{2.18}$$

is a d-quasi-copula satisfying the statement of Theorem 2.1. Note that in case ρ is a density of a random vector, Q_d is by definition its cumulative distribution function.

First observe that Q_d is a piecewise multilinear function, which by construction extends Q and hence Q_d satisfies (BC).

Next we prove the Lipschitz condition. Let $\mathcal{B}_{\mathbb{I}}$ be as in (2.17). Since Q_d coincides with Q on $\mathcal{D}^{(\text{ext})}$, the values of Q_d at the vertices of any box $\mathcal{B}_{\mathbb{I}}$ coincide with the values of Q. By Proposition 2.7, Q satisfies the Lipschitz condition. Thus, Proposition 2.5 implies that Q satisfies the Lipschitz condition on each $B_{\mathbb{I}}$. It remains to prove that Q_d satisfies the Lipschitz condition on the whole box $[0,1]^d$. By Lemma 2.3, it suffices to prove the Lipschitz condition for each variable. By symmetry we may prove it only for the first variable. Let us fix $x_2, \dots, x_d \in [0,1]$ and let $f(x) := Q_d(x, x_2, \dots, x_d)$, $x \in [0,1]$, be a function. By construction of Q_d, f satisfies the Lipschitz condition on the intervals $[0,a_1]$, $[a_1,1]$, since the Lipschitz condition is satisfied on the boxes $\mathcal{B}_{\mathbb{I}}$. By Lemma 2.4, it follows that f satisfies the Lipschitz condition on the whole interval $[0,1]$. This concludes the proof of the Lipschitz condition of Q_d.

It remains to prove the monotonicity of Q_d. Note that it is sufficient to prove that Q_d is monotone on each box $\mathcal{B}_{\mathbb{I}}$. Since on each of these boxes the function Q_d is multilinear and for the vertices of the box the condition of monotonicity holds, monotonicity on the whole boxes follows by Proposition 2.6. □

Proof of Theorem 2.2. The proof is analogous to the proof of Theorem 2.1 only that the definitions of $\mathcal{D}$, $\mathcal{D}^{(\text{ext})}$ and Q are replaced by the ones under the assumption

(2) of Proposition 2.7 and the box $[0,1]^d$ is subdivided into 3^d smaller d-boxes $\mathcal{B}_{\mathbb{I}} = \prod_{j=1}^{d} \delta_j(\mathbb{I})$ for $\mathbb{I} = (i_1, \ldots, i_d) \in \{0,1,2\}^d$, where

$$\delta_j(\mathbb{I}) = \begin{cases} [0, a_j], & \text{if } i_j = 0, \\ [a_j, b_j], & \text{if } i_j = 1, \\ [b_j, 1], & \text{if } i_j = 2. \end{cases}$$

The construction of Q_d and the arguments are then the same as in the proof of Theorem 2.1. □

3. Numerical results

Assume the notation as in Sections 1 and 2. By Theorem 2.1, the following linear program relaxes the problem of determining a d-quasi-copula Q, such that the volume $V_Q(\mathcal{B})$ is minimal among all d-quasi-copulas and all boxes $\mathcal{B} \subseteq [0,1]^d$:

$$\begin{aligned} &\min_{\substack{a_1,\ldots,a_d,\\ b_1,\ldots,b_d,\\ q_{\mathbb{I}} \text{ for } \mathbb{I}\in[1]^d}} && \sum_{\mathbb{I}\in[1]^d} (-1)^{\operatorname{sign}(\mathbb{I})} q_{\mathbb{I}}, \\ &\text{subject to} && \text{(I)} \quad 0 \le a_i < b_i \le 1 \quad i = 1, \ldots, d, \\ & && \text{(II)} \quad 0 \le q_{\mathbb{J}} - q_{\mathbb{I}} \le b_\ell - a_\ell \quad \text{for all } \ell = 1, \ldots, d \\ & && \qquad \text{and all } \mathbb{I}, \mathbb{J} \in [1]^d \text{ such that } \mathbb{J} - \mathbb{I} = \mathbb{I}_\ell, \\ & && \text{(III)} \quad \max\{0, G_d(x_{\mathbb{I}})\} \le q_{\mathbb{I}} \le H_d(x_{\mathbb{I}}) \quad \text{for } \mathbb{I} \in [1]^d. \end{aligned} \tag{3.1}$$

Remark 3.1. (1) The relaxation refers to the fact, that a solution to (3.1) gives an upper bound for the most negative volume of some box over all quasi-copulas. Moreover, if in the solution to (3.1) we have that $b_1 = \ldots = b_d = 1$, then this bound is exact. This follows by Theorem 2.1, because the solution indeed extends to a quasi-copula.

(2) Note that to obtain a relaxation of the problem of finding a d-quasi-copula Q and a box $\mathcal{B}$ with a maximal Q-volume among all d-quasi-copulas and all d-boxes, we only need to replace min with max in (3.1) above or equivalently just multiply the objective function with -1. Again, if in the solution $b_1 = \ldots = b_d = 1$, then the bound is exact. ■

If in the solution to (3.1), we do not have $b_1 = \ldots = b_d = 1$, then the solution might not extend to a quasi-copula. In this case, by Theorem 2.2, one has to solve the following extension of (3.1):

$$\begin{aligned} &\min_{\substack{a_1,\ldots,a_d,\\ b_1,\ldots,b_d,\\ q_{\mathbb{I}} \text{ for } \mathbb{I}\in[2]^d}} && \sum_{\mathbb{I}\in[1]^d} (-1)^{\operatorname{sign}(\mathbb{I})} q_{\mathbb{I}}, \\ &\text{subject to} && \text{(I)} \quad 0 \le a_i < b_i < 1 \quad i = 1, \ldots, d, \\ & && \text{(II)} \quad 0 \le q_{\mathbb{J}} - q_{\mathbb{I}} \le b_\ell - a_\ell \quad \text{for all } \ell = 1, \ldots, d \\ & && \qquad \text{and all } \mathbb{I}, \mathbb{J} \in [1]^d \text{ such that } \mathbb{J} - \mathbb{I} = \mathbb{I}_\ell, \\ & && \text{(II)} \quad 0 \le q_{\mathbb{J}} - q_{\mathbb{I}} \le 1 - b_\ell \quad \text{for all } \ell = 1, \ldots, d \\ & && \qquad \text{and all } \mathbb{I} \in [2]^d, \mathbb{J} \in [2]^d \setminus [1]^d \text{ such that } \mathbb{J} - \mathbb{I} = \mathbb{I}_\ell, \\ & && \text{(IV)} \quad \max\{0, G_d(x_{\mathbb{I}})\} \le q_{\mathbb{I}} \le H_d(x_{\mathbb{I}}) \quad \text{for } \mathbb{I} \in [2]^d. \end{aligned} \tag{3.2}$$

We wrote a function, which generates the linear program (3.1) given dimension d, using software tools *Mathematica* [25] and the modeling language *JuMP* [16] implemented in *Julia* [6]. Then we used the simplex method in *Mathematica* and a combination of the simplex and the interior point method using *Julia* bindings [14] to *HiGHS* solver [12, 13] to solve it. The advantage of *Mathematica* is that it does exact computations with rational numbers, while *HiGHS* in *Julia* uses floating point arithmetic. However, *Mathematica* could compute the results up to dimension $d = 9$ before running out of memory, while *Julia* computed the results up to $d = 16$ in reasonable time. In Tables 1 and 2 below we list the results for the minimal and maximal Q-volumes, respectively. For dimension $d > 9$ the results are rounded to a rational number with absolute error lower than 10^{-6}, while for $d \leq 9$ the results are exact from *Mathematica*. The code and the results are publicly available in the Gitlab repository [24].

Table 1. Minimal values of $V_Q(B)$ over all d–variate quasi–copulas Q and all d–boxes $B \subseteq [0,1]^d$. It turns out that the minimal box $B_{\min}$ is of the form $[a,b]^d$ and that the values $q_{\mathbb{I}}$, $\mathbb{I} = (i_1, \ldots, i_d) \in \{0,1\}^d$, depend only on the sum $|\mathbb{I}| := \sum_{j=1}^d i_j$. We denote $q_{|\mathbb{I}|} := q_{\mathbb{I}}$.

d	a	b	$\vec{q} = (q_{\lvert\mathbb{I}\rvert})_{\lvert\mathbb{I}\rvert=0}^d$	$V_Q([a,b]^d)$
2	$\frac{1}{3}$	$\frac{2}{3}$	$\left(0, \frac{1}{3}, \frac{1}{3}\right)$	$-\frac{1}{3}$
3	$\frac{2}{5}$	$\frac{4}{5}$	$\left(0, 0, \frac{2}{3}, \frac{2}{3}\right)$	$-\frac{4}{5}$
4	$\frac{3}{7}$	$\frac{6}{7}$	$\left(0, 0, 0, \frac{3}{7}, \frac{3}{7}\right)$	$-1\frac{2}{7}$
5	$\frac{8}{13}$	$\frac{12}{13}$	$\left(0, 0, \frac{4}{13}, \frac{4}{13}, \frac{8}{13}, \frac{8}{13}\right)$	$-2\frac{6}{13}$
6	$\frac{5}{8}$	$\frac{15}{16}$	$\left(0, 0, 0, \frac{5}{16}, \frac{5}{16}, \frac{5}{8}, \frac{5}{8}\right)$	$-4\frac{11}{16}$
7	$\frac{1}{2}$	1	$\left(0, 0, 0, 0, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, 1\right)$	$-9\frac{1}{2}$
8	$\frac{2}{3}$	1	$\left(0, 0, 0, \frac{1}{3}, \frac{1}{3}, \frac{2}{3}, \frac{2}{3}, \frac{2}{3}, 1\right)$	$-18\frac{1}{3}$
9	$\frac{2}{3}$	1	$\left(0, 0, 0, 0, \frac{1}{3}, \frac{1}{3}, \frac{2}{3}, \frac{2}{3}, \frac{2}{3}, 1\right)$	-37
10	$\frac{2}{3}$	1	$\left(0, 0, 0, 0, 0, \frac{1}{3}, \frac{1}{3}, \frac{2}{3}, \frac{2}{3}, \frac{2}{3}, 1\right)$	$-69\frac{2}{3}$
11	$\frac{1}{2}$	1	$\left(0, 0, 0, 0, 0, 0, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, 1\right)$	$-125\frac{1}{2}$
12	$\frac{2}{3}$	1	$\left(0, 0, 0, 0, 0, \frac{1}{3}, \frac{1}{3}, \frac{2}{3}, \frac{2}{3}, \frac{2}{3}, \frac{2}{3}, \frac{2}{3}, 1\right)$	$-263\frac{2}{3}$
13	$\frac{2}{3}$	1	$\left(0, 0, 0, 0, 0, 0, \frac{1}{3}, \frac{1}{3}, \frac{2}{3}, \frac{2}{3}, \frac{2}{3}, \frac{2}{3}, \frac{2}{3}, 1\right)$	$-527\frac{2}{3}$
14	$\frac{2}{3}$	1	$\left(0, 0, 0, 0, 0, 0, 0, \frac{1}{3}, \frac{1}{3}, \frac{2}{3}, \frac{2}{3}, \frac{2}{3}, \frac{2}{3}, \frac{2}{3}, 1\right)$	$-1000\frac{2}{3}$
15	$\frac{3}{4}$	1	$\left(0, 0, 0, 0, 0, 0, \frac{1}{4}, \frac{1}{4}, \frac{1}{2}, \frac{1}{2}, \frac{3}{4}, \frac{3}{4}, \frac{3}{4}, \frac{3}{4}, \frac{3}{4}, 1\right)$	$-1858\frac{3}{4}$
16	$\frac{2}{3}$	1	$\left(0, 0, 0, 0, 0, 0, 0, \frac{1}{3}, \frac{1}{3}, \frac{2}{3}, \frac{2}{3}, \frac{2}{3}, \frac{2}{3}, \frac{2}{3}, \frac{2}{3}, \frac{2}{3}, 1\right)$	-3813

Note that for $d \geq 7$ the solutions to (3.1) are attained for $b_1 = \ldots = b_d = 1$ and hence by Remark 3.1.(1), they solve the problem of minimal volumes of $V_Q(B)$. For dimensions $d \leq 6$ we needed to confirm the solutions extend to some feasible points of the linear program (3.2). We implemented this in the software tool *Mathematica.* It turned out that for $d = 5$ and $d = 6$ these extensions are not unique but we strived for the most symmetric extension, i.e., the value of Q is invariant with respect to the permutation of coordinates. As stated in §1, the realizations of Q for $d \leq 4$ are already known [5, 18, 23], while here we state the realizations for $d = 5$ (Example 3.2) and $d = 6$ (Example 3.3).

To state the realizations of Q with boxes of minimal negative volume for $d \in \{5, 6\}$ we need some notation. Let $\mathcal{D} = \prod\{a_i, b_i, 1\}$ with $0 < a_i < b_i < 1$. We will use multiindices of the form $\mathbb{I} := (i_1, i_2 \dots i_d) \in \{0, 1, d+1\}^d$ to index 3^d elements of $\mathcal{D}$. We write $\mathbf{x}_\mathbb{I} := ((x_\mathbb{I})_1, \dots, (x_\mathbb{I})_d)$ to denote the vertex with coordinates

$$(x_\mathbb{I})_k = \begin{cases} a_k, & \text{if } i_k = 0, \\ b_k, & \text{if } i_k = 1, \\ 1, & \text{if } i_k = d+1. \end{cases}$$

The sum of coordinates of $\mathbb{I}$ is denoted by $|\mathbb{I}| := \sum_{j=1}^d i_j$. Note that $|\mathbb{I}|$ is an integer between 0 and $d(d+1)$. The value of $Q : \mathcal{D} \to [0, 1]$ in the point $x_\mathbb{I}$ is $q_\mathbb{I} := Q(\mathbf{x}_\mathbb{I})$.

Example 3.2. *Let $d = 5$ and $\mathcal{D} = \prod_{i=1}^5 \{\frac{8}{13}, \frac{12}{13}, 1\}$. We define*

$$q_i = \begin{cases} \frac{1}{13}, & \textit{if } i = 6, \\ \frac{4}{13}, & \textit{if } i \in \{2, 3, 7, 8\}, \\ \frac{5}{13}, & \textit{if } i \in \{12, 13\}, \\ \frac{6}{13}, & \textit{if } i = 18, \\ \frac{8}{13}, & \textit{if } i \in \{4, 5, 9, 14, 19, 24\}, \\ \frac{9}{13}, & \textit{if } i = 10, \\ \frac{10}{13}, & \textit{if } i = 15, \\ \frac{11}{13}, & \textit{if } i = 20, \\ \frac{12}{13}, & \textit{if } i = 25, \\ 1, & \textit{if } i = 30, \\ 0, & \textit{for other } 0 \leq i \leq 30. \end{cases} \tag{3.3}$$

Then $q_\mathbb{I} := q_{|\mathbb{I}|}$ extends the function from Table 1 defined on $\prod_{i=1}^5 \{\frac{8}{13}, \frac{12}{13}\}$ to $\mathcal{D}$, and is a solution to (3.2) *with $a_1 = \ldots = a_5 = \frac{8}{13}$ and $b_1 = \ldots = b_5 = \frac{12}{13}$. By Theorem 2.2 this function in turn extends to a 5-quasi-copula. Note that the values i in the right column of* (3.3) *correspond to elements $(c_1, c_2, c_3, c_4, c_5)$ of $\mathcal{D}$ in the* *following way:*

i	$\#coordinates\ \frac{8}{13}$	$\#coordinates\ \frac{12}{13}$	$\#coordinates\ 1$
2	3	2	0
3	2	3	0
4	1	4	0
5	0	5	0
6	4	0	1
7	3	1	1
8	2	2	1
9	1	3	1
10	0	4	1
12	3	0	2
13	2	1	2
14	1	2	2
15	0	3	2
18	2	0	3
19	2	1	3
20	0	2	3
24	1	0	4
25	0	1	4
30	0	0	5

Example 3.3. *Let $d = 6$ and $\mathcal{D} = \prod_{i=1}^{5}\{\frac{5}{8}, \frac{15}{16}, 1\}$. We define*

$$q_i = \begin{cases} \frac{1}{16}, & \text{if } i = 8, \\ \frac{1}{8}, & \text{if } i = 14, \\ \frac{5}{16}, & \text{if } i \in \{3, 4, 9, 15, 21\}, \\ \frac{3}{8}, & \text{if } i = 10, \\ \frac{7}{16}, & \text{if } i = 16, \\ \frac{1}{2}, & \text{if } i \in \{22, 28\}, \\ \frac{5}{8}, & \text{if } i \in \{5, 11, 17, 23, 29\}, \\ \frac{11}{16}, & \text{if } i = 12, \\ \frac{3}{4}, & \text{if } i = 18, \\ \frac{13}{16}, & \text{if } i = 24, \\ \frac{7}{8}, & \text{if } i = 30, \\ \frac{15}{16}, & \text{if } i = 36, \\ 1, & \text{if } i = 42, \\ 0, & \text{otherwise.} \end{cases} \tag{3.4}$$

Then $q_{\mathbb{I}} := q_{|\mathbb{I}|}$ extends the function from Table 1 defined on $\prod_{i=1}^{6}\{\frac{5}{8}, \frac{15}{16}\}$ to $\mathcal{D}$, and is a solution to (3.2) with $a_1 = \ldots = a_6 = \frac{5}{8}$ and $b_1 = \ldots = b_6 = \frac{15}{16}$. By Theorem 2.2 this function in turn extends to a 6-quasi-copula. Note that the values i in the right column of (3.4) correspond to elements $(c_1, c_2, c_3, c_4, c_5, c_6)$ of $\mathcal{D}$ in *the following way:*

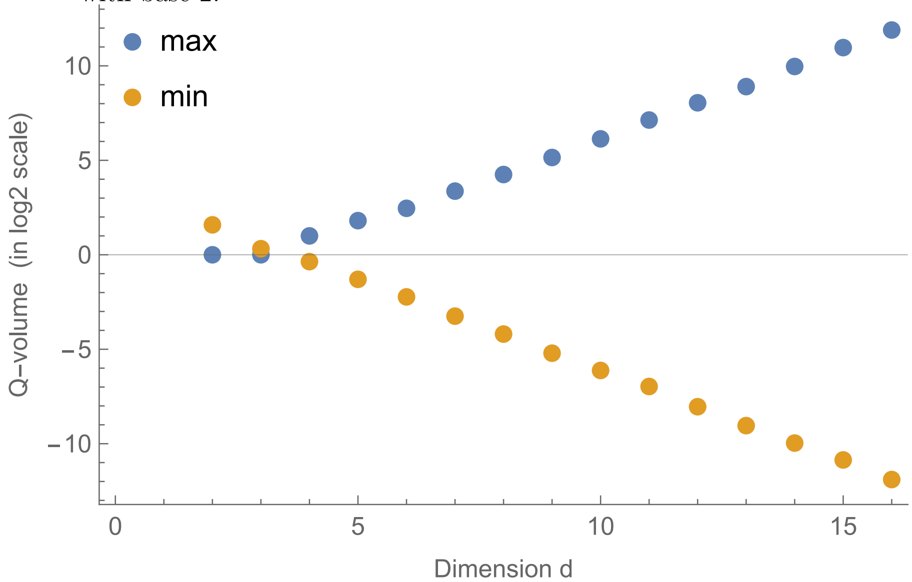
i	$\#coordinates\ \frac{5}{8}$	$\#coordinates\ \frac{15}{16}$	$\#coordinates\ 1$
3	3	3	0
4	2	4	0
5	1	5	0
7	6	0	1
8	5	1	1
9	3	2	1
10	2	3	1
11	1	4	1
12	0	5	1
14	5	0	2
15	3	1	2
16	2	2	2
17	1	3	2
18	0	4	2
21	3	0	3
22	1	3	2
23	1	2	3
24	0	3	3
28	2	0	4
29	1	1	4
30	0	2	4
36	0	1	5
42	0	0	6

TABLE 2. Maximal values of $V_Q(B)$ over all d–variate quasi–copulas Q and all d–boxes $B \subseteq [0,1]^d$. It turns out that the maximal box $B_{\max}$ is of the form $[a,b]^d$ and that the values $q_{\mathbb{I}}$, $\mathbb{I} = (i_1, \ldots, i_d) \in \{0,1\}^d$, depend only on the sum $|\mathbb{I}| := \sum_{j=1}^d i_j$. We denote $q_{|\mathbb{I}|} := q_{\mathbb{I}}$.

d	a	b	$\vec{q} = (q_{\lvert\mathbb{I}\rvert})_{\lvert\mathbb{I}\rvert=0}^d$	$V_Q([a,b]^d)$
2	0	1	$(0,0,1)$	1
3	0	1	$(0,0,0,1)$	1
4	$\frac{1}{2}$	1	$\left(0,0,\frac{1}{2},\frac{1}{2},1\right)$	2
5	$\frac{1}{2}$	1	$\left(0,0,0,\frac{1}{2},\frac{1}{2},1\right)$	$3\frac{1}{2}$
6	$\frac{1}{2}$	1	$\left(0,0,0,0,\frac{1}{2},\frac{1}{2},1\right)$	$5\frac{1}{2}$
7	$\frac{2}{3}$	1	$\left(0,0,0,\frac{1}{3},\frac{1}{3},\frac{2}{3},\frac{2}{3},1\right)$	$10\frac{1}{3}$
8	$\frac{2}{3}$	1	$\left(0,0,0,0,\frac{1}{3},\frac{1}{3},\frac{2}{3},\frac{2}{3},1\right)$	19
9	$\frac{1}{2}$	1	$\left(0,0,0,0,0,\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2},1\right)$	$35\frac{1}{2}$
10	$\frac{2}{3}$	1	$\left(0,0,0,0,\frac{1}{3},\frac{1}{3},\frac{2}{3},\frac{2}{3},\frac{2}{3},\frac{2}{3},1\right)$	$70\frac{1}{3}$
11	$\frac{2}{3}$	1	$\left(0,0,0,0,0,\frac{1}{3},\frac{1}{3},\frac{2}{3},\frac{2}{3},\frac{2}{3},\frac{2}{3},1\right)$	$140\frac{1}{3}$
12	$\frac{2}{3}$	1	$\left(0,0,0,0,0,0,\frac{1}{3},\frac{1}{3},\frac{2}{3},\frac{2}{3},\frac{2}{3},\frac{2}{3},1\right)$	$264\frac{1}{3}$
13	$\frac{3}{4}$	1	$\left(0,0,0,0,0,\frac{1}{4},\frac{1}{4},\frac{1}{2},\frac{1}{2},\frac{3}{4},\frac{3}{4},\frac{3}{4},\frac{3}{4},1\right)$	$478\frac{3}{4}$
14	$\frac{2}{3}$	1	$\left(0,0,0,0,0,0,\frac{1}{3},\frac{1}{3},\frac{2}{3},\frac{2}{3},\frac{2}{3},\frac{2}{3},\frac{2}{3},\frac{2}{3},1\right)$	$1001\frac{1}{3}$
15	$\frac{2}{3}$	1	$\left(0,0,0,0,0,0,0,\frac{1}{3},\frac{1}{3},\frac{2}{3},\frac{2}{3},\frac{2}{3},\frac{2}{3},\frac{2}{3},\frac{2}{3},1\right)$	$2002\frac{1}{3}$
16	$\frac{2}{3}$	1	$\left(0,0,0,0,0,0,0,0,\frac{1}{3},\frac{1}{3},\frac{2}{3},\frac{2}{3},\frac{2}{3},\frac{2}{3},\frac{2}{3},\frac{2}{3},1\right)$	$3813\frac{2}{3}$

Note that for all $d \geq 2$ the solutions to (3.1) with min replaced by max are attained for $b_1 = \ldots = b_d = 1$ and hence, by Remark 3.1.(2), they solve the problem of maximal volumes of $V_Q(B)$.

Figure 1. Blue (and orange) points represent the volumes of boxes with maximal (and minimal) volume over all d-quasi-copulas and all d-boxes. The x-axis represents the dimension d, while the y-axis represents the value of the volume in thee logarithmic scale with base 2.



Tables 1 and 2 solve [2, Open Problem 5] up to $d = 16$. Our results agree with [18] for $d = 2$, with [5] for $d = 3$ and with [23] for $d = 4$. We disprove the conjecture from [23], which states that the minimal value of $V_Q(\mathcal{B})$ in dimension d is $-\frac{(d-1)^2}{2d-1}$, attained for some Q on $\mathcal{B} = \left[\frac{d-1}{2d-1}, \frac{2d-2}{2d-1}\right]^d$. Our results show that the growth is exponential of the form $c2^d + d$ for suitable $c, d \in \mathbb{R}$, while boxes are of the form $[a, 1]^d$, $a \in (0, 1)$, for $d \geq 7$.

The approach via linear programming to obtain results for d larger than 16 does not seem to be feasible due to computer memory limits. However, we believe that the true behaviour of the extremes of the Q-volume is already captured in dimensions $d \leq 16$. In future, our perspective is to determine the formulas for extreme values in terms of the dimension d.

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