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Extreme mass distributions for quasi-copulas

Matjaž Omladič [a,1,*], Martin Vuk [b], Aljaž Zalar [c,2]

[a] Faculty of Mathematics and Physics, University of Ljubljana & Institute of Mathematics, Physics and Mechanics, Ljubljana, Slovenia
[b] Faculty of Computer and Information Science, University of Ljubljana, Slovenia
[c] Faculty of Computer and Information Science, University of Ljubljana & Faculty of Mathematics and Physics, University of Ljubljana & Institute of Mathematics, Physics and Mechanics, Ljubljana, Slovenia

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ABSTRACT

The recent survey [3] 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. In our previous work we addressed the question of extreme values of the mass distribution associated with a mutidimensional quasi–copulas. Using linear programming approach we were able to settle [3, Open Problem 5] up to $d = 17$ and disprove a recent conjecture from [14] on solution to that problem. In this note we use an analytical approach to provide a complete answer to the original question.

1. Introduction

Copula is simply a multivariate distribution with uniform margins, but when we insert arbitrary univariate distributions as margins into it, we can get any multivariate distribution. This seminal 1959 result of Sklar [12] has made them the most important tool of dependence modeling [6,8]. On the other hand, the statistical interpretation of quasi-copulas is problematic since they may have negative volumes locally. They come naturally as (pointwise) lower and upper bounds of sets of copulas. The lower Fréchet-Hoeffding bound W, say, the pointwise infimum of all d-variate copulas, $d \geq 2$, is in general a quasi-copula, unless $d = 2$, while the upper bound M, the pointwise supremum of all d-variate copulas, is always a copula. Quasi-copulas were first introduced in 1993 by Alsina, Nelsen, and Schweizer [1], but the dependence modeling community may have been somehow withheld from wider use of them perhaps due to their deficiency described above.

The new era for this notion starts in 2020 with the seminal paper [3] by Arias-García, Mesiar, and De Baets, listing the most important results and open problems in the area. Some vivid activity followed this paper. The six open problems listed there are sometimes nicknamed "hitchhiker's problems". The first one solved seems to have been hitchhiker's problem #6, Omladič and Stopar [10] in 2020; the second one was hitchhiker's problem #3, Omladič and Stopar [11] in 2022; the next solution appeared in 2023, it

* Corresponding author.
E-mail addresses: matjaz@omladic.net (M. Omladič), martin.vuk@fri.uni-lj.si (M. Vuk), aljaz.zalar@fri.uni-lj.si (A. Zalar).
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was hitchhiker's problem #2, Klement et al. [7]; and then, a possible solution for the bivariate case of hitchhiker's problem #4 was given by Stopar [13] in 2024. The hitchhiker's problem #5 appears to be more involved. It asks to find the maximal negative and positive mass over all boxes over all quasi-copulas as well as to characterize the type of boxes that have the maximal mass. We remark that the term *maximal negative* refers to the negative value with the largest absolute value. The problem started originally by Nelsen et al. in 2002 [9], where an analytical solution for the bivariate case is given. In 2007 de Baets et al. [4] propose a linear programming approach to give the trivariate case. In 2023 Úbeda-Flores [14] extends the linear programming approach up to dimension four and conjectures the growth for higher dimensions. In our very recent work [5] we extended this approach further, up to dimension 17 and disproved conjecture of [14]. In this paper we give the final solution of the problem for all dimensions. It turns out that there is no closed formula that applies simultaneously in all dimensions. However, there is an explicit formula for each dimension that requires performing a simple algorithm to determine the smallest positive integer that satisfies a particular inequality. This smallest integer then determines the maximal positive (resp. maximal negative) volume over all boxes over all quasi-copulas and also a realization of a box and a quasi-copula. The overall growth of the maximal volumes is exponential. For the maximal positive value, the boxes $\mathcal{B}$ are always of the form $[a,1]^d$, while for maximal negative values this applies to $d \geq 7$.

The paper is organized as follows. In Section 2 we state our main results, that solve [3, Open Problem 5] (see Theorems 1 and 2). Since there are no closed form solutions, we present a detailed numerical analysis of the solutions in Section 3. In Section 4 we formulate the maximal volume problems in terms of linear programs (see Proposition 2), simplify them (see Proposition 4) and derive the dual linear programs (see Proposition 5). In Section 5 we establish the basic technical result (see Proposition 6), which is then used in Sections 6 and 7 to solve the dual linear programs and thus prove Theorems 1 and 2. Finally, in Section 8, we solve the remaining cases of the maximal negative volume problem in the dimensions $d = 3,4,5,6$ analytically.

2. Statements of the main theorems

In this section we introduce the notation and state our main results that solve [3, Open Problem 5], i.e., Theorem 1 solves the maximal negative volume problem, while Theorem 2 solves the maximal positive volume problem. Concrete examples are also presented (see Examples 1 and 2).

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

1. *Boundary condition:* For any index $i = 1,\dots,d$ the following holds:
   (a) If $(u_1,\dots,u_{i-1},0,u_{i+1},\dots,u_d) \in \mathcal{D}$, then $Q(u_1,\dots,u_{i-1},0,u_{i+1},\dots,u_d) = 0$.
   (b) If $(1,\dots,1,u_i,1,\dots,1) \in \mathcal{D}$, then $Q(1,\dots,1,u_i,1,\dots,1) = u_i$.
2. *Monotonicity condition:* Q is nondecreasing in every variable, i.e., for each $i = 1,\dots,d$ and each pair of d-tuples
   $$\underline{u} := (u_1,\dots,u_{i-1},u_i,u_{i+1},\dots,u_d) \in \mathcal{D},$$
   $$\underline{\widetilde{u}} := (u_1,\dots,u_{i-1},\widetilde{u}_i,u_{i+1},\dots,u_d) \in \mathcal{D},$$
   such that $u_i \leq \widetilde{u}_i$, it follows that $Q(\underline{u}) \leq Q(\underline{\widetilde{u}})$.
3. *Lipschitz condition*: Given d–tuples $(u_1,\dots,u_d)$ and $(v_1,\dots,v_d)$ in $\mathcal{D}$ it holds that
   $$|Q(u_1,\dots,u_d) - Q(v_1,\dots,v_d)| \leq \sum_{i=1}^{d} |u_i - v_i|.$$

If $\mathcal{D} = [0,1]^d$ and Q satisfies (1), (2), (3), 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 multi-indices of the form $\mathbb{I} := (\mathbb{I}_1,\mathbb{I}_2,\dots,\mathbb{I}_d) \in \{0,1\}^d$ to index 2^d vertices $\prod_{i=1}^{d}\{a_i,b_i\}$ of $\mathcal{B}$. We write

$$x_{\mathbb{I}} := ((x_{\mathbb{I}})_1,\dots,(x_{\mathbb{I}})_d), \quad \text{where} \quad (x_{\mathbb{I}})_k = \begin{cases} a_k, & \text{if } \mathbb{I}_k = 0, \\ b_k, & \text{if } \mathbb{I}_k = 1. \end{cases}$$

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

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

Let $\|\mathbb{I}\|_1 := \sum_{i=1}^{d} \mathbb{I}_i$ be the 1-norm of the multi-index $\mathbb{I}$ and $\operatorname{sign}(\mathbb{I}) := (-1)^{d-\|\mathbb{I}\|_1}$ its sign. The **Q-volume** of $\mathcal{B}$ is defined by:

$$V_Q(\mathcal{B}) = \sum_{\mathbb{I}\in\{0,1\}^d} \operatorname{sign}(\mathbb{I}) q_{\mathbb{I}}. \tag{2.1}$$

The complete solution to [3, Open Problem 5] for the maximal negative volume, i.e., the largest in absolute value among negative ones, is the following.

Theorem 1. *Assume the notation above. Let $d \in \mathbb{N}$ and $d \geq 7$. Define*

$$(c_1, c_2, \dots, c_{\lfloor \frac{d}{2} \rfloor}) := \\ = \begin{cases} \left(\binom{d-1}{0}, \binom{d-1}{1}, \binom{d-1}{2}, \dots, \binom{d-1}{\frac{d}{2}-1}\right), & \text{if } d \text{ is even,} \\ \left(\binom{d-1}{1}, \binom{d-1}{1}, \binom{d-1}{3}, \binom{d-1}{3}, \dots, \binom{d-1}{\lfloor \frac{d}{2} \rfloor -1}, \binom{d-1}{\lfloor \frac{d}{2} \rfloor -1}\right), & \text{if } d \bmod 4 = 1, \\ \left(\binom{d-1}{1}, \binom{d-1}{1}, \binom{d-1}{3}, \binom{d-1}{3}, \dots, \binom{d-1}{\lfloor \frac{d}{2} \rfloor -2}, \binom{d-1}{\lfloor \frac{d}{2} \rfloor -2}, \binom{d-1}{\lfloor \frac{d}{2} \rfloor}\right), & \text{if } d \bmod 4 = 3. \end{cases}$$

Define $c_0 = 0$ and

$$w_{i,-} := \frac{1}{i+1}\left(\sum_{j=0}^{i-1} c_{\lfloor \frac{d}{2} \rfloor - j} - 1\right) \quad \text{for } i = 1, \dots, \lfloor \frac{d}{2} \rfloor.$$

Let i_0 be the smallest integer in $\{1, \dots, \lfloor \frac{d}{2} \rfloor\}$ such that

$$w_{i_0,-} \geq c_{\lfloor \frac{d}{2} \rfloor - i_0}. \tag{2.2}$$

Then:

1. *The maximal negative volume $V_Q(\mathcal{B})$ of some box $\mathcal{B}$ over all d-quasi-copulas Q is equal to $-w_{i_0,-}$.*
2. *One of the realizations of $\mathcal{B}$ and Q is*

$$\mathcal{B} = \left[\frac{i_0}{i_0+1}, 1\right]^d, \quad q_{(0,\dots,0)} = 0, \quad q_{\mathbb{I}} = \sum_{i=1}^{\|\mathbb{I}\|_1} \delta_i \quad \text{for all } \mathbb{I} \in \{0,1\}^d \setminus \{0\}^d,$$

where:

(a) If d is even, then for $j = 1, \dots, d$ we have

$$\delta_j = \begin{cases} \frac{1}{i_0+1}, & \text{if } j = d \text{ or } (j \text{ is odd and } \binom{d-1}{j-1} > c_{\frac{d}{2}-i_0}), \\ 0, & \text{otherwise.} \end{cases} \tag{2.3}$$

(b) If d is odd, then for $j = 1, \dots, d$ we have

$$\delta_j = \begin{cases} \frac{1}{i_0+1}, & \text{if } j = d \text{ or } (j \text{ is even and } \binom{d-1}{j-1} > c_{\lfloor \frac{d}{2} \rfloor - i_0}), \\ 0, & \text{otherwise.} \end{cases} \tag{2.4}$$

This realization of Q on $\left\{\frac{i_0}{i_0+1}, 1\right\}^d$ indeed extends to a quasi-copula $Q : [0,1]^d \to [0,1]$ by [5, Theorem 2.1].

Let us demonstrate the statement of Theorem 1 in the smallest dimension $d = 7$.

Example 1. Assume the notation from Theorem 1. Let $d = 7$. Define

$$(c_1, c_2, c_3) := \left(\binom{6}{1}, \binom{6}{1}, \binom{6}{3}\right) = (6, 6, 20)$$

and $c_0 = 0$. Let

$$w_{1,-} := \frac{1}{2}(c_3 - 1) = \frac{19}{2},$$
$$w_{2,-} := \frac{1}{3}(c_3 + c_2 - 1) = \frac{25}{3},$$
$$w_{3,-} := \frac{1}{4}(c_3 + c_2 + c_1 - 1) = \frac{31}{4}.$$

Note that the smallest $i \in \{1, 2, 3\}$ such that $w_{i,-} \geq c_{3-i}$, is $i_0 = 1$, i.e., $w_{1,-} \geq c_2$. By Theorem 1, the maximal negative volume of some box $\mathcal{B}$ over all 7-quasi-copulas Q is equal to

$$-w_{1,-} = -\frac{19}{2}.$$

Further on,

$$\delta_j = \begin{cases} \frac{1}{2}, & \text{if } j \in \{4, 7\}, \\ 0, & \text{if } j \in \{1, 2, 3, 5, 6\}. \end{cases}$$

Hence, one of the realizations of $\mathcal{B}$ and Q is

$$\mathcal{B} = \left[\frac{1}{2}, 1\right]^7, \quad q_{(0,\dots,0)} = 0, \quad q_{\mathbb{I}} = \begin{cases} 0, & \text{if } \|\mathbb{I}\|_1 \in \{0,1,2,3\}, \\ \frac{1}{2}, & \text{if } \|\mathbb{I}\|_1 \in \{4,5,6\}, \\ 1, & \text{if } \mathbb{I} = (1,\dots,1). \end{cases}$$

Note that this realization agrees with the one obtained by computer software approach in [5, Table 1].

The complete solution to [3, Open Problem 5] for the maximal positive volume is the following.

Theorem 2. *Assume the notation above. Let $d \in \mathbb{N}$ and $d \geq 2$. Define*

$$(c_1, c_2, \dots, c_{\lfloor \frac{d+1}{2} \rfloor - 1}) := \\ = \begin{cases} \left(\binom{d-1}{1}, \binom{d-1}{2}, \binom{d-1}{3}, \dots, \binom{d-1}{\frac{d}{2}-1}\right), & \text{if } d \text{ is even,} \\ \left(\binom{d-1}{0}, \binom{d-1}{2}, \binom{d-1}{2}, \binom{d-1}{4}, \binom{d-1}{4}, \dots, \binom{d-1}{\lfloor \frac{d}{2} \rfloor - 2}, \binom{d-1}{\lfloor \frac{d}{2} \rfloor - 2}, \binom{d-1}{\lfloor \frac{d}{2} \rfloor}\right), & \text{if } d \bmod 4 = 1, \\ \left(\binom{d-1}{0}, \binom{d-1}{2}, \binom{d-1}{2}, \binom{d-1}{4}, \binom{d-1}{4}, \dots, \binom{d-1}{\lfloor \frac{d}{2} \rfloor - 1}, \binom{d-1}{\lfloor \frac{d}{2} \rfloor - 1}\right), & \text{if } d \bmod 4 = 3. \end{cases}$$

Define $c_0 = 0$ and

$$w_{i,+} := \frac{1}{i+1}\left(\sum_{j=0}^{i-1} c_{\lfloor \frac{d+1}{2} \rfloor - 1 - j} + 1\right) \quad \text{for } i = 1, \dots, \lfloor \frac{d+1}{2} \rfloor - 1.$$

Let i_0 be the smallest integer in $\{1, \dots, \lfloor \frac{d+1}{2} \rfloor - 1\}$ such that

$$w_{i_0,+} \geq c_{\lfloor \frac{d+1}{2} \rfloor - 1 - i_0}. \tag{2.5}$$

Then:

1. *The maximal positive volume $V_Q(\mathcal{B})$ of some box $\mathcal{B}$ over all d-quasi-copulas Q is equal to $w_{i_0,+}$.*
2. *One of the realizations of $\mathcal{B}$ and Q is*

$$\mathcal{B} = \left[\frac{i_0}{i_0+1}, 1\right]^d, \quad q_{(0,\dots,0)} = 0, \quad q_{\mathbb{I}} = \sum_{i=1}^{\|\mathbb{I}\|_1} \delta_i \quad \text{for all } \mathbb{I} \in \{0,1\}^d \setminus \{0\}^d,$$

where:

(a) If d is even, then for $j = 1, \dots, d$ we have

$$\delta_j = \begin{cases} \frac{1}{i_0+1}, & \text{if } j = d \text{ or } (j \text{ is even and } \binom{d-1}{j-1} > c_{\frac{d}{2}-1-i_0}), \\ 0, & \text{otherwise.} \end{cases} \tag{2.6}$$

(b) If d is odd, then for $j = 1, \dots, d$ we have

$$\delta_j = \begin{cases} \frac{1}{i_0+1}, & \text{if } j = d \text{ or } (j \text{ is odd and } \binom{d-1}{j-1} > c_{\lfloor \frac{d+1}{2} \rfloor - 1 - i_0}), \\ 0, & \text{otherwise.} \end{cases} \tag{2.7}$$

This realization of Q on $\left\{\frac{i_0}{i_0+1}, 1\right\}^d$ indeed extends to a quasi-copula $Q : [0,1]^d \to [0,1]$ by [5, Theorem 2.1].

Let us demonstrate the statement of Theorem 1 in dimension $d = 8$.

Example 2. Assume the notation from Theorem 2. Let $d = 8$. Define

$$(c_1, c_2, c_3) := \left(\binom{7}{1}, \binom{7}{2}, \binom{7}{3}\right) = (7, 21, 35)$$

and $c_0 = 0$. Let

$$w_{1,+} := \frac{1}{2}(c_3 + 1) = 18,$$
$$w_{2,+} := \frac{1}{3}(c_3 + c_2 + 1) = 19,$$
$$w_{3,+} := \frac{1}{4}(c_3 + c_2 + c_1 + 1) = 16.$$

Note that the smallest $i \in \{1,2,3\}$ such that $w_{i,+} \geq c_{3-i}$ is $i_0 = 2$, i.e., $w_{2,+} \geq c_1$. By Theorem 2, the maximal positive volume of some box $\mathcal{B}$ over all 8-quasi-copulas Q is equal to

$$w_{2,+} = 19.$$

Further on,

$$\delta_j = \begin{cases} \frac{1}{3}, & \text{if } j \in \{4,6,8\}, \\ 0, & \text{if } j \in \{1,2,3,5,7\}. \end{cases}$$

Hence, one of the realizations of $\mathcal{B}$ and Q is

$$\mathcal{B} = \left[\frac{2}{3}, 1\right]^8, \quad q_{(0,\dots,0)} = 0, \quad q_{\mathbb{I}} = \begin{cases} 0, & \text{if } \|\mathbb{I}\|_1 \in \{0,1,2,3\}, \\ \frac{1}{3}, & \text{if } \|\mathbb{I}\|_1 \in \{4,5\}, \\ \frac{2}{3}, & \text{if } \|\mathbb{I}\|_1 \in \{6,7\}, \\ 1, & \text{if } \mathbb{I} = (1,\dots,1). \end{cases}$$

Note that this realization agrees with the one obtained by computer software approach in [5, Table 2].

In the next section we will give a detailed numerical aspects of Theorems 1 and 2. In the following remark we comment on the general connection between them.

Remark 1.

1. Let us first assume that d is even. Then the vectors of the coefficients c_i in Theorems 1 and 2 differ only in the fact that in the minimal volume case there is also a binomial symbol $\binom{d-1}{0}$ at the beginning. This difference arises because when dualising the primal linear program, which is the formulation of the problem we use, the important constraints that have a true influence on the solution in both cases are those with positive lower bounds. In our case, the bounds are signed binomial coefficients (i.e., coefficients appearing at variables in the primal objective function). In the case of minimal volume, the pattern of signed coefficients starts with + and alternates between signs, while in the case of maximal volume it starts with - and alternates. In the question for the maximal volume, the coefficient $\binom{d-1}{d-1} = \binom{d-1}{0}$ is missing, as we use its constraint to get rid of one of the variables. We prove that we must have equality in the optimal solution in this constraint.

   Let us now assume that d is odd. Then the coefficient vectors c_i in both theorems differ only in that in the minimal volume case all odd binomial symbols $\binom{d-1}{2i+1}$ occur, while in the maximal volume case all even binomial symbols $\binom{d-1}{2i}$ occur (with the exception of $\binom{d-1}{d-1}$, since we again use its constraint to get rid of one of the variables). This difference happens for exactly the same reason as for the even case explained in the first paragraph above, except that this time the sequences of the binomial symbols are also different. This is due to d being odd and therefore $\binom{d-1}{2i+1} = \binom{d-1}{d-2i}$, where $d - 2i$ is odd again.
2. Let us comment on the dimension constraint $d \geq 7$, which appears in Theorem 1, while it does not appear in Theorem 2. The reason for this difference is easiest to see in the feasibility regions of the dual linear programs (see (4.8) and (4.9)). In the case of the minimal volume, one of the constraints is $\ell_d - y_3 \geq -1$, while in the case of the maximal volume it is $\ell_d - y_3 \geq 1$. As all variables are nonnegative, in the case of the maximal volume the constraint $\ell_d \geq 1 + y_3$ is more restrictive than $\ell_d \geq 0$, while in the case of the minimal volume the constraint $\ell_d \geq 0$ could be more restrictive than the constraint $\ell_d \geq -1 + y_3$. When analysing both possibilities, it turns out that we actually obtain an optimal solution for $d \leq 6$ if we are on the hyperplane $\ell_d = 0$, in contrast to the cases $d \geq 7$, where none of the points with $\ell_d = 0$ lie in a feasibility region.
3. Let us comment on the realizations of the boxes $\mathcal{B}$ and the quasi-copula Q, given by Theorems 1 and 2. As already observed in [5, Remark 3.3], the realizations of the solution are not unique. In the case of a non-symmetric solution to (4.1) (i.e., $\|\mathbb{I}\|_1 = \|\mathbb{J}\|_1$ does not imply $q_{\mathbb{I}} = q_{\mathbb{J}}$ or a_i are not all equal or b_i are not all equal), many new solutions can be obtained by the action of the symmetric group (see the proof of Proposition 3). We can therefore form an equivalence relation $\sim$ on the set of all solutions. Two solutions are in relation if one can obtain the other by the action of an element of the symmetric group on the first (see (4.2) and (4.3)). If we take the average (see (4.4)) of all solutions in each equivalence class, we obtain the unique symmetric solution given in Theorems 1 and 2. In this sense, this unique symmetric solution is the canonical solution.

3. Numerical aspects of Theorems 1 and 2

In this section we present various numerical aspects of Theorems 1 and 2.[1] In Tables 1 and 2 we give maximal positive and negative volumes of the d-boxes over all d-quasi-copuas for dimensions up to 68. (This is not due to the limitations of the computer software but for paper space reasons.) We also state the numbers i_0 were the procedure in Theorems 1, 2 terminates. Figs. 1–3 demonstrate the growth of the number i_0 for the positive and the negative volume case, as well as their difference, respectively. Fig. 4 graphically represents the volumes of the solutions for both cases in the logarithmic scale with a base 2. We comment on the behaviour of the volumes in Remark 2 and on the behaviour of the difference in the values of i_0 in Remark 3. Proposition 1 states two possible regimes of the difference in even dimensions.

[1] The numerical analysis in arithmetic over $\mathbb{Q}$ was performed using the software tool *Mathematica* [15]. The source code is available at https://github.com/ZalarA/Quasi-copulas-extreme-volumes.

Table 1
Minimal values of $V_Q(\mathcal{B})$ over all d–variate quasi–copulas Q and all d–boxes $\mathcal{B} \subseteq [0,1]^d$. It turns out that for $d \geq 7$ the minimal box $B_{\min}$ is of the form $[\frac{i_0}{i_0+1}, 1]^d$. Dimensions $d < 7$ are treated separately in Section 8.

d	i_0	$V_Q([\frac{i_0}{i_0+1}, 1]^d)$
7	1	$-19/2$
8	2	$-55/3$
9	2	-37
10	2	$-209/3$
11	1	$-251/2$
12	2	$-791/3$
13	2	$-1583/3$
14	2	$-3002/3$
15	3	$-7435/4$
16	2	-3813
17	2	$-22879/3$
18	2	$-43757/3$
19	3	$-112267/4$
20	2	$-167959/3$
21	2	-111973
22	2	$-646645/3$
23	3	$-1700271/4$
24	2	$-2496143/3$
25	2	$-4992287/3$
26	3	$-12926459/4$
27	3	$-25852919/4$
d	i_0	$V_Q([\frac{i_0}{i_0+1}, 1]^d)$
28	3	$-25240027/2$
29	2	$-74884319/3$
30	3	$-197318609/4$
31	3	$-394637219/4$
32	3	$-385987897/2$
33	2	$-1131445439/3$
34	3	$-3022770629/4$
35	3	$-6045541259/4$
36	3	$-11845439759/4$
37	2	$-17194993199/3$
38	3	$-46453775279/4$
39	3	$-92907550559/4$
40	3	$-182303526209/4$
41	4	$-440029574399/5$
42	3	$-715904248019/4$
43	3	$-1431808496039/4$
44	3	$-2813088831929/4$
45	4	$-6842895760271/5$
46	3	$-11060241944075/4$
47	3	$-22120483888151/4$
48	3	$-43509459123197/4$
d	i_0	$V_Q([\frac{i_0}{i_0+1}, 1]^d)$
49	4	$-106543877604607/5$
50	3	$-171248556584475/4$
51	3	$-342497113168951/4$
52	3	$-674344248506151/4$
53	4	$-1660843019667103/5$
54	3	$-2656661186721807/4$
55	3	$-5313322373443615/4$
56	3	$-10470793684489291/4$
57	4	$-25918766458461183/5$
58	3	$-41285913247219255/4$
59	3	$-82571826494438511/4$
60	3	$-81426118154032613/2$
61	4	$-404908794653887719/5$
62	3	$-642608465005843433/4$
63	3	$-1285216930011686867/4$
64	3	$-1268300040500821345/2$
65	4	-1266363348322336051
66	4	-2504757439320041105
67	3	$-2003239721774933569 1/4$
68	4	$-4955296747013584098 3/5$

Table 2
Maximal values of $V_Q(\mathcal{B})$ over all d–variate quasi–copulas Q and all d–boxes $\mathcal{B} \subseteq [0,1]^d$. It turns out that for $d \geq 3$ the maximal box $B_{\max}$ is of the form $[\frac{i_0}{i_0+1}, 1]^d$.

d	i_0	$V_Q\left([\frac{i_0}{i_0+1}, 1]^d\right)$
3	1	1
4	1	2
5	1	7/2
6	1	11/2
7	2	31/3
8	2	19
9	1	71/2
10	2	211/3
11	2	421/3
12	2	793/3
13	3	1915/4
14	2	3004/3
15	2	6007/3
16	2	11441/3
17	3	28887/4
18	2	43759/3
19	2	87517/3
20	2	55987
21	3	436697/4
22	2	215,549
23	2	1293293/3
24	2	2496145/3
d	i_0	$V_Q\left([\frac{i_0}{i_0+1}, 1]^d\right)$
25	3	6626669/4
26	3	12926461/4
27	2	6438467
28	3	12620014
29	3	100960111/4
30	3	197318611/4
31	2	290845351/3
32	3	192993949
33	3	1543951591/4
34	3	3022770631/4
35	2	4407922861/3
36	3	11845439761/4
37	3	23690879521/4
38	3	46453775281/4
39	2	67156001221/3
40	3	182303526211/4
41	3	364607052421/4
42	3	715904248021/4
43	4	1734977456941/5
44	3	2813088831931/4
45	3	5626177663861/4
46	3	11060241944077/4
d	i_0	$V_Q\left([\frac{i_0}{i_0+1}, 1]^d\right)$
47	4	26997208242193/5
48	3	43509459123199/4
49	3	87018918246397/4
50	3	171248556584477/4
51	4	420596950601801/5
52	3	674344248506153/4
53	3	1348688497012305/4
54	3	2656661186721809/4
55	4	6560130872627137/5
56	3	10470793684489293/4
57	3	20941587368978585/4
58	3	41285913247219257/4
59	4	102430771061474087/5
60	3	40713059077016307
61	3	325704472616130455/4
62	3	642608465005843435/4
63	4	1600998867547843289/5
64	3	634150020250410673
65	3	5073200162003285383/4
66	4	12523787196600205527/5
67	4	25047574393200411053/5
68	4	9910593494027168197

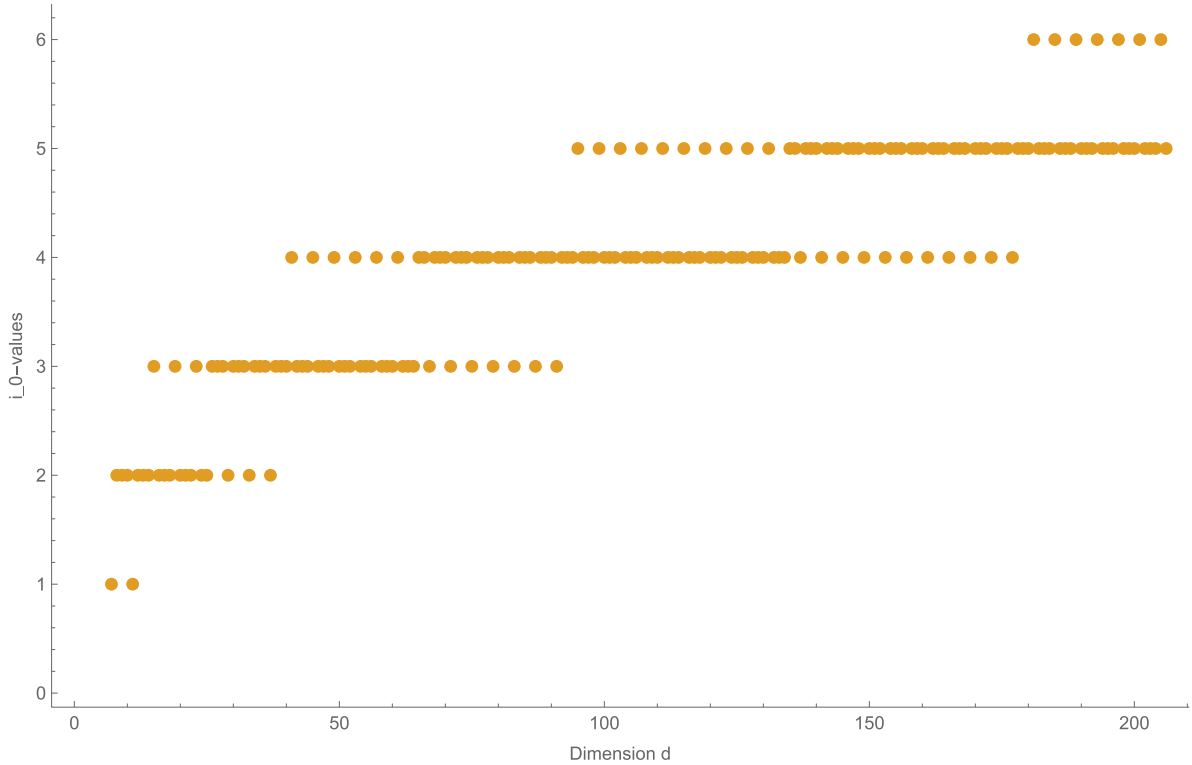

Fig. 1. Points represent the pairs (d, i_0) such that a d-box $\mathcal{B} = \left[\frac{i_0}{i_0+1}, 1\right]^d$, obtained by Theorem 1, is a maximal negative volume $V_Q(\mathcal{B})$ box in dimension d over all d-quasi-copulas and over all d-boxes.

Remark 2. Let us comment on the values of the solutions $w_{i_0,+}$ and $w_{i_0,-}$ in Theorems 1 and 2.

Assume that d is even. Then

$$w_{\frac{d}{2},-} = \frac{1}{\frac{d}{2}+1}\left[\sum_{j=0}^{\frac{d}{2}-1}\binom{d-1}{j} - 1\right] = \frac{1}{\frac{d}{2}+1}(2^{d-2}-1),$$

since the sum of binomial symbols in brackets is precisely half of the sum $(1+1)^{d-1} = \sum_{j=0}^{d-1}\binom{d-1}{j}$. Similarly, we have

$$w_{\frac{d}{2}-1,+} = \frac{1}{\frac{d}{2}}\left[\sum_{j=1}^{\frac{d}{2}-1}\binom{d-1}{j} + 1\right] = \frac{1}{d}2^{d-1}.$$

Assume now that d is odd. In $w_{\lfloor\frac{d}{2}\rfloor,-}$ the sum of all odd binomial coefficients $\binom{d-1}{2j+1}$ appears, which is equal to 2^{d-2}, and hence $w_{\lfloor\frac{d}{2}\rfloor,-} = \frac{1}{\lfloor\frac{d}{2}\rfloor+1}(2^{d-2}-1)$. In $w_{\lfloor\frac{d}{2}\rfloor,+}$ the sum of all even binomial coefficients $\binom{d-1}{2j}$ but $\binom{d-1}{d-1}$ appears, and hence $w_{\lfloor\frac{d}{2}\rfloor,+} = \frac{1}{\lfloor\frac{d+1}{2}\rfloor}2^{d-2}$.

So if the iterative procedures in Theorems 1 and 2 terminate after the maximal number of steps, the absolute volumes are as stated above. However, in practice the procedure terminates much earlier, since the sum of the binomial coefficients $\sum_{j=j_0}^{\frac{d}{2}-1}\binom{d-1}{j}$ is large in comparison to $\binom{d-1}{j_0-1}$ for relatively large j_0 and thus relatively small i_0. Observing Figs. 1 and 2 we see that i_0 is almost increasing function (with some exceptions) and its maximal value in dimensions up to $d = 200$ is 6. Experimentally, for a fixed d, we plot the function $w_{i,\pm}$, for $i = 1, \dots, \lfloor\frac{d}{2}\rfloor$, and the value $w_{\lfloor\frac{d}{2}\rfloor,\pm}$ was always the smallest. However, proving this rigorously would require involved analysis of the behaviour of binomial symbols and their sums. Moreover, this would not give actual behaviour of the extreme volume solutions, since we do not know how i_0 in Theorems 1 and 2 behaves. Based on Fig. 4, the actual volumes are of the form 2^{d-k} for some small k relative to d which is behaving similarly as i (i.e., growing with the dimension).

The next proposition states some relations among $i_0^{(\min)}$, $i_0^{(\max)}$, $w_{i_0^{(\min)},-}$ and $w_{i_0^{(\max)},+}$ from Theorems 1 and 2 in even dimensions.

Proposition 1. *Let $d \in 2\mathbb{N}$ with $d \geq 8$. Assume the notation from Theorems 1 and 2. Let $i_0^{(\min)}$ and $i_0^{(\max)}$ be the integers representing i_0 in Theorems 1 and 2, respectively. Then the following statements hold:*

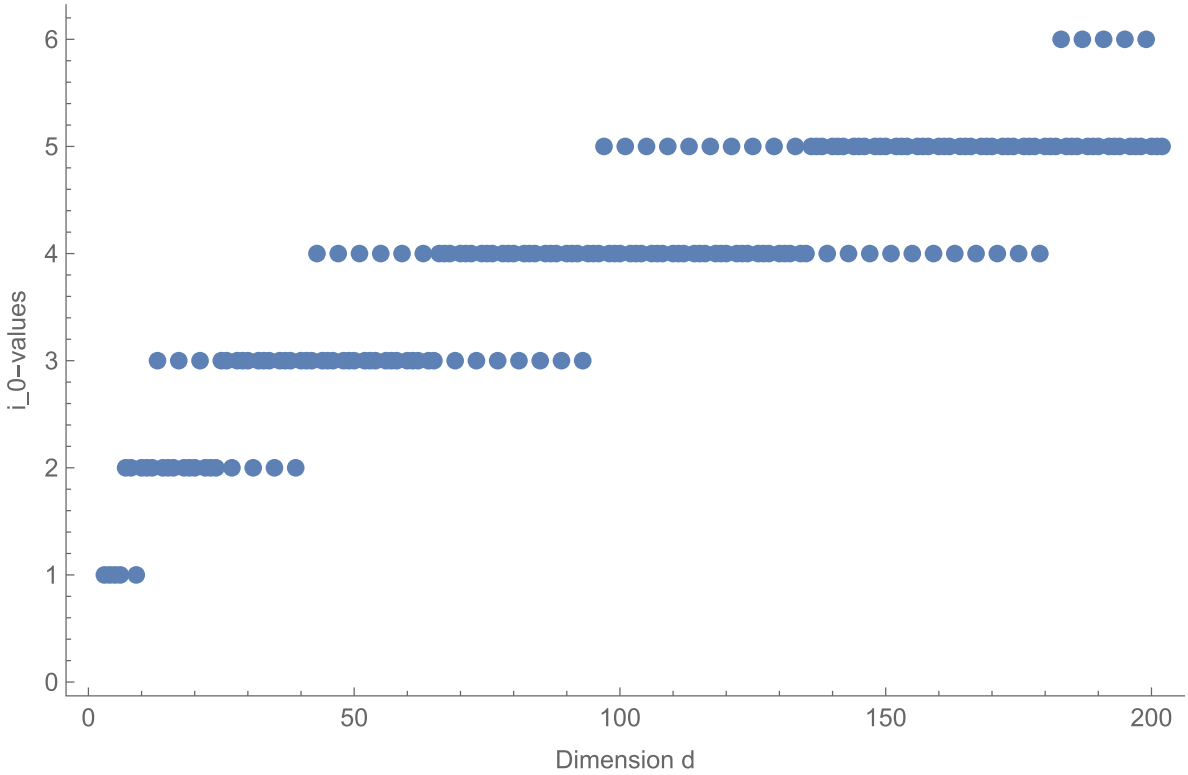

Fig. 2. Points represent the pairs (d, i_0) such that a d-box $\mathcal{B} = \left[\frac{i_0}{i_0+1}, 1\right]^d$, obtained by Theorem 2, is a maximal positive volume $V_Q(\mathcal{B})$ box in dimension d over all d-quasi-copulas and over all d-boxes.

1. $0 \le i_0^{(\min)} - i_0^{(\max)} \le 1$.
2. *If* $i_0^{(\min)} = i_0^{(\max)} =: I$, *then* $w_{i_0^{(\max)},+} = w_{i_0^{(\min)},-} + \frac{2}{I+1}$.

Proof. Observe that by definition of $w_{i,+}, w_{i,-}$, we have that $w_{i,+} = w_{i,-} + \frac{2}{i+1}$. In particular, this proves (1). Further, the lower bounds in the conditions (2.2) and (2.5) are the same, because d is even. Therefore if i satisfies (2.2), it also satisfies (2.5). This proves the left inequality in (1), i.e., $0 \le i_0^{(\min)} - i_0^{(\max)}$. It remains to prove $i_0^{(\min)} - i_0^{(\max)} \le 1$. Assume that $i_0^{(\min)} > i_0^{(\max)}$. This means that

$$w_{i_0^{(\min)},-} < \binom{d-1}{\frac{d}{2} - 1 - i_0^{(\max)}} \le w_{i_0^{(\max)},+}. \tag{3.1}$$

We have to prove that $i_0^{(\min)} = i_0^{(\max)} + 1$ or equivalently

$$\binom{d-1}{\frac{d}{2} - 2 - i_0^{(\max)}} \le w_{i_0^{(\max)}+1,-}. \tag{3.2}$$

Further, (3.2) is equivalent to

$$(i_0^{(\max)} + 2)\binom{d-1}{\frac{d}{2} - 2 - i_0^{(\max)}} + 1 \le \sum_{j=0}^{i_0^{(\max)}} \binom{d-1}{\frac{d}{2} - 1 - j}. \tag{3.3}$$

Note that the right inequality in (3.1) is equivalent to

$$(i_0^{(\max)} + 1)\binom{d-1}{\frac{d}{2} - 1 - i_0^{(\max)}} - 1 \le \sum_{j=0}^{i_0^{(\max)}-1} \binom{d-1}{\frac{d}{2} - 1 - j}. \tag{3.4}$$

Using (3.4) to bound below the right hand side of (3.3), (3.3) will follow if we prove that

$$(i_0^{(\max)} + 2)\binom{d-1}{\frac{d}{2} - 2 - i_0^{(\max)}} + 1 \le (i_0^{(\max)} + 1)\binom{d-1}{\frac{d}{2} - 1 - i_0^{(\max)}} - 1 + \binom{d-1}{\frac{d}{2} - 1 - i_0^{(\max)}} \tag{3.5}$$

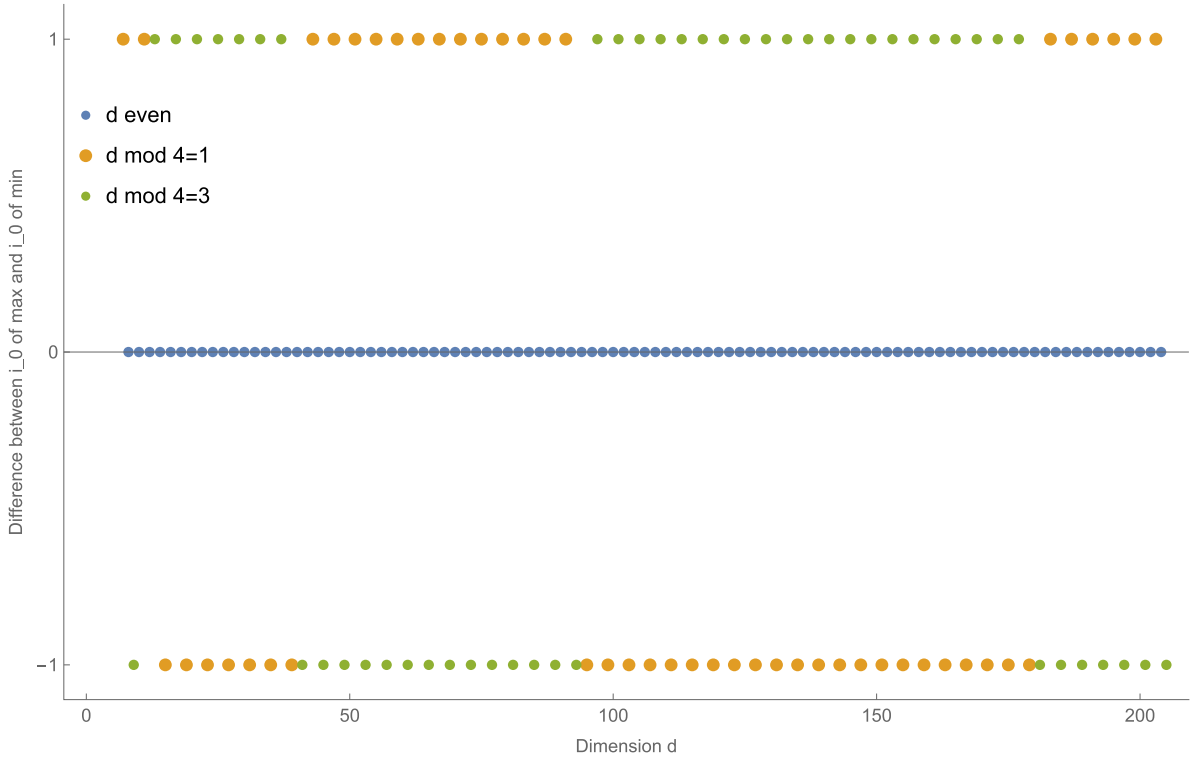

Fig. 3. Points represent the pairs (d, j), where d is the dimension and j is the difference $(i_0)_{\max} - (i_0)_{\min}$ such that a d-box $\mathcal{B}_{\max} = \left[\frac{(i_0)_{\max}}{(i_0)_{\max}+1}, 1\right]^d$, obtained by Theorem 1, (resp. $\mathcal{B}_{\min} = \left[\frac{(i_0)_{\min}}{(i_0)_{\min}+1}, 1\right]^d$, obtained by Theorem 2) is a maximal positive volume $V_Q(\mathcal{B}_{\max})$ (resp. a maximal negative volume $V_Q(\mathcal{B}_{\min})$) box in dimension d over all d-quasi-copulas and over all d-boxes.

or equivalently

$$2 \leq (i_0^{(\max)} + 2)\left[\binom{d-1}{\frac{d}{2} - 1 - i_0^{(\max)}} - \binom{d-1}{\frac{d}{2} - 2 - i_0^{(\max)}}\right] \tag{3.6}$$

But this inequality clearly holds, since both brackets are natural numbers larger that 1. □

Remark 3.

(1) Proposition 1 states that the solutions to the maximal positive and maximal negative volume box question in even dimension, given by iterative procedures in Theorems 1 and 2, are obtained after the same number of steps or after at most 1 more step for the maximal negative volume question. If both procedures end after the same number of steps I, then the maximal positive volume is larger for $\frac{2}{I+1}$ from the absolute value of the maximal negative volume. Moreover, the boxes realizing the solutions are then the same for both problems.

(2) For odd d the connection between the maximal volume box and the minimal volume box is more subtle. Observe that among all binomial symbols $\binom{d-1}{i}$, every symbol $\binom{d-1}{i}$ with odd i appears in the statement of Theorem 1, while every symbol $\binom{d-1}{i}$ with even i in the statement of Theorem 2. Hence, it is difficult to observe some clear connection between the solutions. However, we observe that (see Fig. 1) the difference between $i_0^{(\min)}$ and $i_0^{(\max)}$, which represent i_0 in Theorems 1 and 2, respectively, seems to always be either 1 or −1. The sign does not depend on i mod 4 but behaves somewhat randomly.

4. Towards the proof of Theorems 1 and 2

In this section we first recall the formulation of the maximal volume problems from [5] in terms of the linear programs (see Proposition 2). Then we simplify the linear programs by using symmetries in the variables (see Proposition 3 and Corollary 1). Next, the simplified linear programs are further reduced to smaller ones observing redundancy of some conditions (see Proposition 4). Finally, the dual linear programs, which need to be solved, are obtained (see Proposition 5). We use them to prove that the proposed solution is indeed optimal.

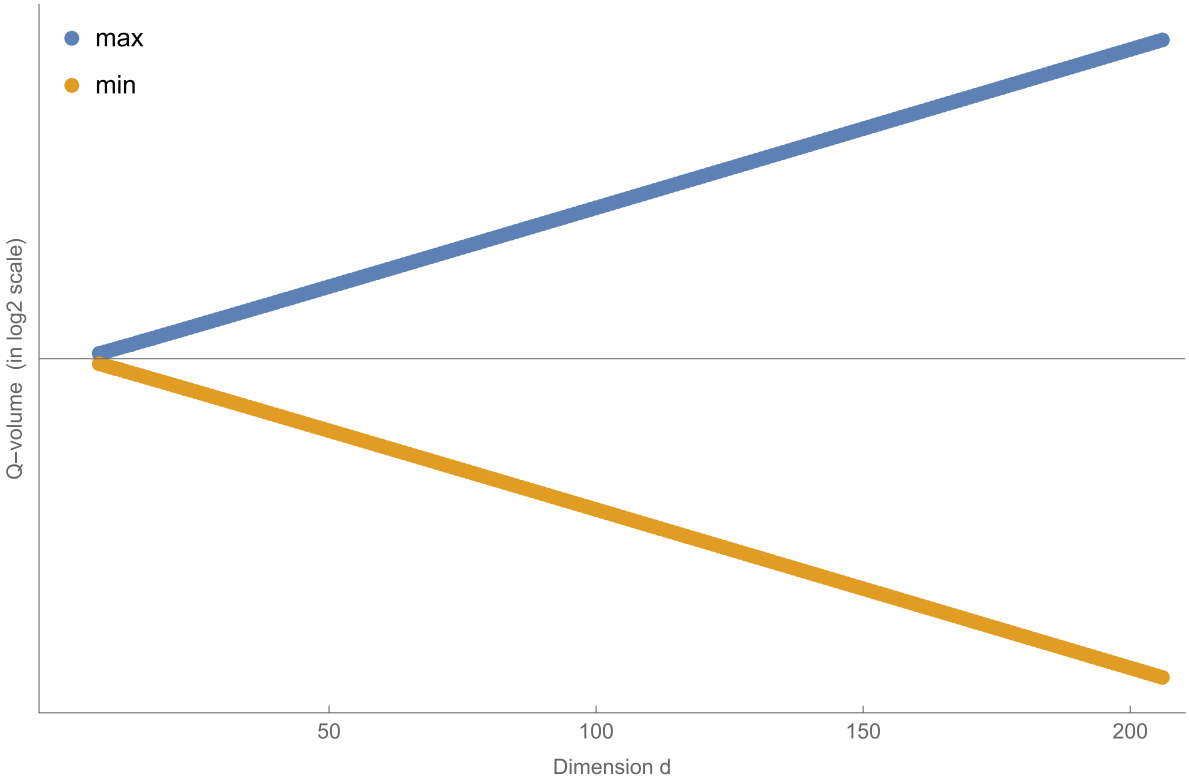

Fig. 4. Blue (and orange) points represent the volumes of boxes with maximal (and minimal) volume over all d-quasi-copulas and over all d-boxes. The x-axis represents the dimension d, while the y-axis represents the value of the volume in the logarithmic scale with base 2.

4.1. Notation and preliminaries

Fix $d \in \mathbb{N}$. For multi-indices

$$\mathbb{I} = (\mathbb{I}_1, \dots, \mathbb{I}_d) \in \{0,1\}^d \quad \text{and} \quad \mathbb{J} = (\mathbb{J}_1, \dots, \mathbb{J}_d) \in \{0,1\}^d$$

let

$$\mathbb{J} - \mathbb{I} = (\mathbb{J}_1 - \mathbb{I}_1, \dots, \mathbb{J}_d - \mathbb{I}_d) \in \{-1, 0, 1\}^d$$

stand for their usual coordinate-wise difference. Let $\mathbb{E}^{(\ell)}$ stand for the multi-index with the only non-zero coordinate the ℓ–th one, which is equal to 1. For each $\ell = 1, \dots, \ell$ we define a relation on $\{0,1\}^d$ by

$$\mathbb{I} \prec_\ell \mathbb{J} \quad \Leftrightarrow \quad \mathbb{J} - \mathbb{I} = \mathbb{E}^{(\ell)}.$$

For a point $\underline{x} = (x_1, \dots, x_d) \in \mathbb{R}^d$ we define the functions

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

In our previous work we proved the following proposition.

Proposition 2 ([5, Propositions 3.1 and 3.2]). *Define the following linear program*

$$\begin{aligned} \min_{\substack{a_1,\dots,a_d,\\ b_1,\dots,b_d,\\ q_{\mathbb{I}} \text{ for } \mathbb{I}\in\{0,1\}^d}} \quad & \sum_{\mathbb{I}\in\{0,1\}^d} \operatorname{sign}(\mathbb{I}) q_{\mathbb{I}}, \\ \textit{subject to} \quad & 0 \le a_i < b_i \le 1 \quad i = 1, \dots, d, \\ & 0 \le q_{\mathbb{J}} - q_{\mathbb{I}} \le b_\ell - a_\ell \quad \textit{for all } \ell = 1, \dots, d \textit{ and all } \mathbb{I} \prec_\ell \mathbb{J}, \\ & \max\{0, G_d(x_{\mathbb{I}})\} \le q_{\mathbb{I}} \le H_d(x_{\mathbb{I}}) \quad \textit{for all } \mathbb{I} \in \{0,1\}^d. \end{aligned} \tag{4.1}$$

Let $\mathbb{I}^{(1)}, \dots, \mathbb{I}^{(2^d)}$ be some order of all multi-indices $\mathbb{I} \in \{0,1\}^d$. If there exists an optimal solution $(a_1^*, \dots, a_d^*, b_1^*, \dots, b_d^*, q_{\mathbb{I}^{(1)}}, \dots, q_{\mathbb{I}^{(2^d)}})$ to (4.1), which satisfies $b_1^* = \dots = b_d^* = 1$, then the optimal value of (4.1) is the maximal negative volume of some box over all d-quasi-copulas.

Moreover, if there exists an optimal solution to (4.1) where min *is replaced with* max*, which satisfies $b_1^* = \dots = b_d^* = 1$, then the optimal value of (4.1) is the maximal positive volume of some box over all d-quasi-copulas.*

Remark 4. In [5, Section 3] we presented numerical solutions to (4.1) up to $d = 18$ for min and up to $d = 17$ for max. In the case of min and $7 \le d \le 18$ we obtained optimal solutions with $b_1^* = \dots = b_d^* = 1$ and so we solved the maximal negative volume problem. Cases $d < 7$ have to be considered separately by extending Proposition 2 from the 2^d-element grid $\prod_{i=1}^d \{a_i, b_i\}$ to the 3^d-element grid $\prod_{i=1}^d \{a_i, b_i, 1\}$. In the case of max and $2 \le d \le 17$ we obtained optimal solutions with $b_1^* = \dots = b_d^* = 1$ and so we solved the maximal positive volume problem. ■

4.2. Symmetrization of the linear program (4.1) and the dual

By the following proposition it suffices to consider symmetric solutions to the linear program (4.1).

Proposition 3. *Assume the notation from Proposition 2. There exists an optimal solution to the linear program (4.1) of the form*

$$\big(\underbrace{a^*, \dots, a^*}_{d}, \underbrace{b^*, \dots, b^*}_{d}, q^*_{\|\mathbb{I}^{(1)}\|_1}, \dots, q^*_{\|\mathbb{I}^{(2^d)}\|_1}\big)$$

for some $a, b, q_1, \dots, q_d \in [0,1]$.

Analogously, replacing min *with* max *in (4.1) above, the same statement holds.*

Proof. Let S_d be the set of all permutations of a d-element set $\{1, \dots, d\}$. For $\Phi \in S_d$ and $\mathbb{I}^{(j)} := (\mathbb{I}_1^{(j)}, \dots, \mathbb{I}_d^{(j)}) \in \{0,1\}^d$, let $\Phi(\mathbb{I}^{(j)}) := \big(\mathbb{I}^{(j)}_{\Phi(1)}, \dots, \mathbb{I}^{(j)}_{\Phi(d)}\big)$. If

$$\big(a_1^*, \dots, a_d^*, b_1^*, \dots, b_d^*, q^*_{\mathbb{I}^{(1)}}, \dots, q^*_{\mathbb{I}^{(2^d)}}\big) \tag{4.2}$$

is an optimal solution to (4.1), then

$$\big(a^*_{\Phi(1)}, \dots, a^*_{\Phi(d)}, b^*_{\Phi(1)}, \dots, b^*_{\Phi(d)}, q^*_{\Phi(\mathbb{I}^{(1)})}, \dots, q^*_{\Phi(\mathbb{I}^{(2^d)})}\big) \tag{4.3}$$

is also an optimal solution to (4.1). Hence, an optimal solution as stated in the proposition is equal to

$$\frac{1}{n!} \sum_{\Phi \in S_n} \big(a^*_{\Phi(1)}, \dots, a^*_{\Phi(d)}, b^*_{\Phi(1)}, \dots, b^*_{\Phi(d)}, q^*_{\Phi(\mathbb{I}^{(1)})}, \dots, q^*_{\Phi(\mathbb{I}^{(2^d)})}\big), \tag{4.4}$$

where the summation is the coordinate-wise one. The proof for max instead of min is the same. □

An immediate corollary to Proposition 3 is the following.

Corollary 1. *The optimal value of the linear program (4.1) is equal to the optimal value of the linear program*

$$\begin{aligned}
\min_{a,b,q_0,q_1,\dots,q_d} \quad & \sum_{i=0}^{d} (-1)^{d-i} \binom{d}{i} q_i, \\
\textit{subject to} \quad & 0 \le a < b \le 1, \\
& 0 \le q_i - q_{i-1} \le b - a \quad \textit{for } i = 1, \dots, d, \\
& \max\{0, (d-i)a + ib - d + 1\} \le q_i \le a \\
& \qquad\qquad \textit{for } i = 0, \dots, d-1, \\
& \max\{0, db - d + 1\} \le q_d \le b.
\end{aligned} \tag{4.5}$$

Analogously, replacing min *with* max *in (4.1) above, the same statement holds.*

It turns out that some of the constraints in (4.5) are redundant, while introducing new variables $\delta_i = q_i - q_{i-1}$ further decreases the number of constraints.

Proposition 4. *The optimal value of the linear program (4.5) is equal to the optimal value of the linear program*

$$\begin{aligned}
\min_{a,b,q_0,\delta_1,\dots,\delta_d} \quad & \sum_{j=1}^{d} (-1)^{d+j} \binom{d-1}{j-1} \delta_j, \\
\textit{subject to} \quad & b \le 1, \\
& \delta_i \le b - a \quad \textit{for } i = 1, \dots, d, \\
& q_0 + \sum_{i=1}^{d-1} \delta_i \le a, \\
& db - d + 1 \le q_0 + \sum_{i=1}^{d} \delta_i, \\
& a \ge 0,\ b \ge 0,\ q_0 \ge 0,\ \delta_i \ge 0 \quad \textit{for } i = 1, \dots, d.
\end{aligned} \tag{4.6}$$

Analogously, replacing min *with* max *in* (4.6) *above, the same statement holds.*

Proof. First let us prove that in (4.5) the conditions

$$\begin{aligned} &(d-i)a + ib - d + 1 \le q_i \quad \text{for } i = 0, \dots, d-1, \\ &q_i \le a \quad \text{for } i = 0, \dots, d-2, \\ &q_d \le b \end{aligned} \tag{4.7}$$

follow from the other conditions. We have that

$$q_{d-1} = q_d + (q_{d-1} - q_d) \ge db - d + 1 + a - b = a + (d-1)b - d + 1,$$

where we used the second and the fourth conditions from (4.5) for the inequality. This is the condition in the first line of (4.7) for $i = d-1$. Inductively, using

$$q_{d-j} = q_{d-j+1} + (q_{d-j} - q_{d+j+1}),$$

the conditions in the first line of (4.7) for $i = d-2, \dots, 1$ follow.

The conditions in the second line of (4.7) follow easily from

$$a \ge q_{d-1} \ge q_{d-2} \ge \dots \ge q_0.$$

Finally, the condition in the last line of (4.7) follows from

$$q_d = q_{d-1} + (q_d - q_{d-1}) \le a + (b - a) = b,$$

where we used the second and the third conditions from (4.5) for the inequality.

Now we introduce new variables $\delta_i = q_i - q_{i-1}$, $i = 1, \dots, d$ and the constraints of the reduced linear program (4.5), i.e., (4.5) without the constraints from (4.7), become as in (4.6). The only non-trivial thing to verify is the form of the objective function. But this follows by a simple computation:

$$\begin{aligned} \sum_{i=0}^{d} (-1)^{d-i} \binom{d}{i} q_i &= \sum_{i=0}^{d} (-1)^{d-i} \binom{d}{i} \Big(q_0 + \sum_{j=1}^{i} \delta_j \Big) \\ &= q_0 \underbrace{\sum_{k=0}^{d} (-1)^{d-i} \binom{d}{i}}_{0} + \sum_{j=1}^{d} \delta_j \underbrace{\Big(\sum_{k=j}^{d} (-1)^{d-k} \binom{d}{k} \Big)}_{(-1)^{d+j}\binom{d-1}{j-1}}, \end{aligned}$$

where we used $\sum_{k \le n} (-1)^k \binom{r}{k} = (-1)^n \binom{r-1}{n}$ in the last equality. □

4.3. *The dual linear program of* (4.6)

Recall that writing the linear program in the form $\max_x \{c^T x : \ Ax \le b, x \ge 0\}$ where $c \in \mathbb{R}^n$ and $b \in \mathbb{R}^m$ are real vectors, $A \in \mathbb{R}^{m \times n}$ is a matrix, x is a vector of variables and the inequalities are the coordinate-wise ones, its dual program is given by $\min_y \{b^T y : \ A^T y \ge c, y \ge 0\}$, where y is a vector of dual variables. Namely, for each constraint of the primal program, there is a variable for the dual program, while for each variable of the primal program, there is a constraint for the dual program.

Rewriting the objective function $\min_x c^T x$ of (4.6) in the form $-(\max_x (-c)^T x)$ the dual linear program of (4.6) is the following:

$$\begin{aligned} -\Big(\min_{y_1, l_1, \dots, l_d, y_2, y_3} \quad & y_1 + (d-1) y_3 \Big), \\ \text{subject to} \quad & \sum_{i=1}^{d} l_i - y_2 \ge 0, \\ & y_1 - \sum_{i=1}^{d} l_i + d y_3 \ge 0, \\ & y_2 - y_3 \ge 0, \\ & l_j + y_2 - y_3 \ge (-1)^{d+j+1} \binom{d-1}{j-1} \quad \text{for } j = 1, \dots, d-1, \\ & l_d - y_3 \ge -1, \\ & y_1 \ge 0, \ y_2 \ge 0, \ y_3 \ge 0, \ l_i \ge 0 \quad \text{for } i = 1, \dots, d. \end{aligned} \tag{4.8}$$

Analogously, the dual linear program of (4.6) with the objective function $\max_x c^T x$ is the following:

$$\begin{aligned}
\min_{y_1,l_1,\dots,l_d,y_2,y_3} \quad & y_1 + (d-1)y_3, \\
\text{subject to} \quad & \sum_{i=1}^{d} l_i - y_2 \geq 0, \\
& y_1 - \sum_{i=1}^{d} l_i + d y_3 \geq 0, \\
& y_2 - y_3 \geq 0, \\
& l_j + y_2 - y_3 \geq (-1)^{d+j}\binom{d-1}{j-1} \quad \text{for } j = 1,\dots,d-1, \\
& l_d - y_3 \geq 1, \\
& y_1 \geq 0,\ y_2 \geq 0,\ y_3 \geq 0,\ l_i \geq 0 \quad \text{for } i = 1,\dots,d.
\end{aligned} \tag{4.9}$$

It turns out that both linear programs can be simplified.

Proposition 5. *The optimal solutions to (4.8) and (4.9) are equal to the optimal solutions to*

$$\begin{aligned}
-\Big(\min_{l_1,\dots,l_d,y_3} \quad & (d-1)y_3\Big), \\
\textit{subject to} \quad & -\sum_{i=1}^{d} l_i + d y_3 = 0, \\
& l_j + (d-1)y_3 \geq (-1)^{d+j+1}\binom{d-1}{j-1} \quad \textit{for } j = 1,\dots,d-1, \\
& l_d = \max(0, -1 + y_3), \\
& y_3 \geq 0,\ l_i \geq 0 \quad \textit{for } i = 1,\dots,d,
\end{aligned} \tag{4.10}$$

and

$$\begin{aligned}
\min_{l_1,\dots,l_d,y_3} \quad & (d-1)y_3, \\
\textit{subject to} \quad & -\sum_{i=1}^{d} l_i + d y_3 = 0, \\
& l_j + (d-1)y_3 \geq (-1)^{d+j}\binom{d-1}{j-1} \quad \textit{for } j = 1,\dots,d-1, \\
& l_d - y_3 = 1, \\
& y_3 \geq 0,\ l_i \geq 0 \quad \textit{for } i = 1,\dots,d,
\end{aligned} \tag{4.11}$$

respectively.

Proof. We will prove the proposition by first establishing a few claims.

Claim 1. Their exists an optimal solution $(y_1^*, l_1^*, \dots, l_d^*, y_2^*, y_3^*)$ to the linear program (4.8) (resp. (4.9)) which satisfies $y_2^* = y_1^* + d y_3^*$.

Proof of Claim 1. Let $(y_1^*, l_1^*, \dots, l_d^*, y_2^*, y_3^*)$ be an optimal solution to (4.8). From the first two constraints in (4.8) it follows that

$$y_1^* + d y_3^* \geq \sum_{i=1}^{d} l_i \geq y_2^*. \tag{4.12}$$

If the left inequality in (4.12) is strict and $y_1^* > 0$, then there exists $\epsilon > 0$ such that $(y_1^* - \epsilon, l_1^*, \dots, l_d^*, y_2^*, y_3^*)$ is a feasible solution to (4.8) such that

$$(y_1^* - \epsilon) + (d-1)y_3^* < y_1^* + (d-1)y_3^*.$$

But this contradicts to the optimality of $(y_1^*, l_1^*, \dots, l_d^*, y_2^*, y_3^*)$.

If the left inequality in (4.12) is strict, $y_1^* = 0$ and $y_3^* > 0$, then there exists $\epsilon > 0$ such that $(y_1^*, l_1^*, \dots, l_d^*, y_2^* - \epsilon, y_3^* - \epsilon)$ is a feasible solution to (4.8) such that

$$y_1^* + (d-1)(y_3^* - \epsilon) < y_1^* + (d-1)y_3^*.$$

But this contradicts to the optimality of $(y_1^*, l_1^*, \dots, l_d^*, y_2^*, y_3^*)$.

Hence, the left inequality in (4.12) is an equality. If the right inequality is strict, we just increase y_2^* to $\sum_{i=1}^{d} l_i$ and we get another optimal solution to (4.8). This proves the lemma for (4.8).

The proof for (4.9) is the same. ■

Using Claim 1, the linear programs (4.8) and (4.9) simplify to:

$$
\begin{aligned}
-\Big(\min_{y_1,l_1,\dots,l_d,y_3} \quad & y_1+(d-1)y_3\Big),\\
\text{subject to} \quad & y_1-\sum_{i=1}^{d} l_i + d y_3 = 0,\\
& y_1+(d-1)y_3 \ge 0,\\
& l_j + y_1 + (d-1)y_3 \ge (-1)^{d+j+1}\binom{d-1}{j-1}\\
& \qquad\qquad \text{for } j=1,\dots,d-1,\\
& l_d - y_3 \ge -1,\\
& y_1 \ge 0,\ \ y_3 \ge 0,\ l_i \ge 0 \quad \text{for } i=1,\dots,d,
\end{aligned}
\tag{4.13}
$$

and

$$
\begin{aligned}
\min_{y_1,l_1,\dots,l_d,y_3} \quad & y_1+(d-1)y_3,\\
\text{subject to} \quad & y_1-\sum_{i=1}^{d} l_i + d y_3 = 0,\\
& y_1+(d-1)y_3 \ge 0,\\
& l_j + y_1 + (d-1)y_3 \ge (-1)^{d+j}\binom{d-1}{j-1}\\
& \qquad\qquad \text{for } j=1,\dots,d-1,\\
& l_d - y_3 \ge 1,\\
& y_1 \ge 0,\ \ y_3 \ge 0,\ l_i \ge 0 \quad \text{for } i=1,\dots,d.
\end{aligned}
\tag{4.14}
$$

Observation 1. *Since $y_1 \ge 0, y_3 \ge 0$, the inequality $y_1+(d-1)y_3 \ge 0$ in (4.13) and (4.14) is redundant.*

Claim 2. There exists an optimal solution $(y_1^*, l_1^*, \dots, l_d^*, y_3^*)$ to the linear program (4.13) (resp. (4.14)) which satisfies $y_1^* = 0$.

Proof of Claim 2. Let $(y_1^*, l_1^*, \dots, l_d^*, y_2^*, y_3^*)$ be an optimal solution to (4.13). Assume that $y_1^* > 0$. Then $\big(0, l_1^*, \dots, l_{d-1}^*, l_d^* + \frac{y_1^*}{d-1}, y_3^* + \frac{y_1^*}{d-1}\big)$ is another optimal solution to (4.13).

The proof for (4.14) is the same. ■

Using Observation 1 and Claim 2, the linear programs (4.13) and (4.14) simplify to

$$
\begin{aligned}
-\Big(\min_{l_1,\dots,l_d,y_3} \quad & (d-1)y_3\Big),\\
\text{subject to} \quad & -\sum_{i=1}^{d} l_i + d y_3 = 0,\\
& l_j + (d-1)y_3 \ge (-1)^{d+j+1}\binom{d-1}{j-1} \quad \text{for } j=1,\dots,d-1,\\
& l_d - y_3 \ge -1,\\
& y_3 \ge 0,\ l_i \ge 0 \quad \text{for } i=1,\dots,d,
\end{aligned}
\tag{4.15}
$$

and

$$
\begin{aligned}
\min_{l_1,\dots,l_d,y_3} \quad & (d-1)y_3,\\
\text{subject to} \quad & -\sum_{i=1}^{d} l_i + d y_3 = 0,\\
& l_j + (d-1)y_3 \ge (-1)^{d+j}\binom{d-1}{j-1} \quad \text{for } j=1,\dots,d-1,\\
& l_d - y_3 \ge 1,\\
& y_3 \ge 0,\ l_i \ge 0 \quad \text{for } i=1,\dots,d,
\end{aligned}
\tag{4.16}
$$

respectively.

The following claim shows that in the optimal solution to the linear programs (4.15) and (4.16), one of constraints $l_d \ge 0$ and $l_d - y_3 \ge \pm 1$ is an equality.

Claim 3. If $(y_1^*, l_1^*, \dots, l_d^*, y_3^*)$ is an optimal solution to the linear program (4.15) (resp. (4.16)), then $l_d^* = \max(0, -1 + y_3^*)$ (resp. $l_d^* = 1 + y_3^*$).

Moreover, $l_d^* = 0$ can only occur for $d \le 6$.

Proof of Claim 3. Let $(y_1^*, l_1^*, \dots, l_d^*, y_3^*)$ be an optimal solution to (4.15). Assume that $c := l_d^* - \max(0, -1 + y_3^*) > 0$. Then there exists $\epsilon > 0$ such that

$$(y_1^*, l_1^* + (d-1)\epsilon, \dots, l_{d-1}^* + (d-1)\epsilon, l_d - (d^2 - d + 1)\epsilon, y_3^* - \epsilon)$$

is still a feasible solution to (4.15) with a smaller objective function, which is a contradiction to the optimality of $(y_1^*, l_1^*, \dots, l_d^*, y_3^*)$.

The proof for (4.16) is the same, using also that $l_d^* = \max(0, 1 + y_3^*) = 1 + y_3^*$.

Let us establish the moreover part. In this case $y_3^* \le 1$. Since every y_3 large enough extends to a feasible solution to (4.15) (e.g., $l_1 = \dots = l_{d-1} = 0$ and $l_d = dy_3$), convexity of the feasible region implies that there is a feasible solution with $y_3 = 1$. But then for this solution the first constraint in (4.15) implies that

$$\sum_{i=1}^{d} l_i = d. \tag{4.17}$$

We separate two cases according to the parity of d.

Case 1: $d = 2d'$ for some $d' \in \mathbb{N}$. Summing up the inequalities with positive right hand side in (4.15) we get

$$\sum_{\substack{j \text{ odd,}\\ j<d}} l_j + (d-1)\left(\frac{d}{2} - 1\right) \ge \sum_{\substack{j \text{ odd,}\\ j<d}} \binom{d-1}{j-1}. \tag{4.18}$$

Using (4.17) in (4.18), it follows that

$$d + (d-1)\left(\frac{d}{2} - 1\right) \ge \sum_{\substack{j \text{ odd,}\\ j<d}} \binom{d-1}{j-1} = \binom{d-1}{0} + \binom{d-1}{2} + \dots + \binom{d-1}{d-2}.$$

For $d \ge 8$ this is a contradiction.

Case 2: $d = 2d' - 1$ for some $d' \in \mathbb{N}$. Summing up the inequalities with positive right hand side in (4.15) above we get

$$\sum_{\substack{j \text{ even,}\\ j<d}} l_j + \frac{(d-1)^2}{2} \ge \sum_{\substack{j \text{ even,}\\ j<d}} \binom{d-1}{j-1}. \tag{4.19}$$

Using (4.17) in (4.19), it follows that

$$d + \frac{(d-1)^2}{2} \ge \sum_{\substack{j \text{ even,}\\ j<d}} \binom{d-1}{j-1} = \binom{d-1}{1} + \binom{d-1}{3} + \dots + \binom{d-1}{d-2}.$$

For $d \ge 7$ this is a contradiction.

This proves Claim 3. ■

Using Claim 3, the linear programs (4.15) and (4.16) simplify to the linear programs (4.10) and (4.11), respectively. □

5. Basic technical result

The following proposition is the basic result, which will be used to prove Theorems 1 and 2.

Proposition 6. *Let*

$$0 < c_1 \le c_2 \le \dots \le c_k$$

be given positive real numbers with $c_1 < c_k$,

$$e_1 < 0, \dots, e_r < 0$$

given negative real numbers, $\alpha \in \mathbb{R}$ *such that*

$$-c_k < \alpha \le c_k$$

and a linear program

$$\begin{aligned} &\min_{\substack{w, y_1, y_2, \dots, y_k,\\ z_1, z_2, \dots, z_r}} w \\ &\textit{subject to } y_1 + \dots + y_k + z_1 + \dots + z_r = w + \alpha, \\ &\qquad y_i + w \ge c_i \quad \textit{for } i = 1, \dots, k, \\ &\qquad z_i + w \ge e_i \quad \textit{for } i = 1, \dots, r, \\ &\qquad w \ge 0, \\ &\qquad y_i \ge 0 \quad \textit{for } i = 1, \dots, k, \\ &\qquad z_i \ge 0 \quad \textit{for } i = 1, \dots, r. \end{aligned} \tag{5.1}$$

Define

$$w_i := \frac{1}{i+1}\Big(\sum_{j=0}^{i-1} c_{k-j} - \alpha\Big) \quad \textit{for } i = 1, \dots, k.$$

and $c_0 := 0$. *Let*

$$i_0 \textit{ be the smallest integer in } \{1, \dots, k\} \textit{ such that } w_{i_0} \geq c_{k-i_0}. \tag{5.2}$$

Then the optimal solution $(w^*, y_1^*, \dots, y_k^*, z_1^*, \dots, z_r^*)$ *to* (5.1) *is*

$$(w^*, y_1^*, \dots, y_k^*, z_1^*, \dots, z_r^*) = (w_{i_0}, \underbrace{0, \dots, 0}_{k-i_0}, c_{k-i_0+1} - w_{i_0}, \dots, c_k - w_{i_0}, \underbrace{0, \dots, 0}_{r}).$$

Proof. First we establish two claims.

Claim 1. There is at most one $i \in \{1, \dots, k\}$ such that $w_i \in [c_{k-i}, c_{k-i+1})$.
Proof of Claim 1. Let $\widetilde{i}$ be such that $w_{\widetilde{i}} \in [c_{k-\widetilde{i}}, c_{k-\widetilde{i}+1})$. Note that $w_{\widetilde{i}} \geq c_{k-\widetilde{i}}$ is equivalent to

$$\sum_{j=0}^{\widetilde{i}-1} c_{k-j} - \alpha \geq (\widetilde{i}+1)c_{k-\widetilde{i}}. \tag{5.3}$$

Hence,

$$w_{\widetilde{i}+1} = \frac{1}{\widetilde{i}+2}\Big(\sum_{j=0}^{\widetilde{i}} c_{k-j} - \alpha\Big) \underbrace{\geq}_{(5.3)} c_{k-\widetilde{i}},$$

which in particular implies that $w_{\widetilde{i}+1} \notin [c_{k-\widetilde{i}-1}, c_{k-\widetilde{i}})$. Inductively we can prove that $w_{\widetilde{i}+l} \geq c_{k-\widetilde{i}}$ for $l = 1, 2, \dots, k - \widetilde{i}$, whence $w_{\widetilde{i}+l} \notin [c_{k-\widetilde{i}-l}, c_{k-\widetilde{i}-l+1})$. This proves Claim 1. ■

Claim 2. Let i_0 be as in (5.2). Then $w_{i_0} \in [c_{k-i_0}, c_{k-i_0+1})$.

Proof of Claim 2. First note that i_0 is well-defined, since there exists $i \in \{1, \dots, k\}$ such that $w_i \geq c_{k-i}$, e.g., $i = k$ due to $w_k = \frac{1}{k}\big(\sum_{j=1}^{k} c_k - \alpha\big) \geq 0 = c_0$. Also note that $i = i_0$ is the unique candidate for the containment $w_i \in [c_{k-i}, c_{k-i+1})$. This follows from the following two observations:

- By definition of i_0, we have that $w_i < c_{k-i}$ for $i = 1, \dots, i_0 - 1$.
- As in the proof of Claim 1, $w_i \geq c_{k-i_0} \geq c_{k-i+1}$ for $i = i_0 + 1, \dots, k$.

So it only remains to prove that $w_{i_0} < c_{k-i_0+1}$. Assume on the contrary that $w_{i_0} \geq c_{k-i_0+1}$. First notice that in this case $i_0 \neq 1$, since $w_1 = \frac{1}{2}(c_k - \alpha) < \frac{1}{2}(c_k + c_k) = c_k$. Then

$$\sum_{j=0}^{i_0-1} c_{k-j} - \alpha \geq (i_0+1)c_{k-i_0+1},$$

which implies that

$$\sum_{j=0}^{i_0-2} c_{k-j} - \alpha \geq i_0 \cdot c_{k-i_0+1}.$$

Further on,

$$w_{i_0-1} = \frac{1}{i_0}\Big(\sum_{j=0}^{i_0-2} c_{k-j} - \alpha\Big) \geq c_{k-i_0+1}.$$

But this is a contradiction with the minimiality of i_0. ■

Let now $(w^*, y_1^*, \dots, y_k^*, z_1^*, \dots, z_r^*)$ be an optimal solution to (5.1).

Claim 3. $z_i^* = 0$ for $i = 1, \dots, r$.
Proof of Claim 3. If there is i such that $z_i > 0$, then there exists $\epsilon > 0$, such that

$$(w^* - \epsilon, y_1^* + \epsilon, \dots, y_k^* + \epsilon, z_1^*, \dots, z_{i-1}^*, z_i^* - (k+1)\epsilon, z_{i+1}^*, \dots, z_r^*) \tag{5.4}$$

is still a feasible solution to (5.1). This contradicts to the optimality of w^*. ■

Clearly $w = c_k$ extends to a feasible solution of (5.1), e.g., $y_1 = c_k + \alpha$, $y_i = 0$ for $i = 2, \dots, k$ and $z_i = 0$ for $i = 1, \dots, r$. So $w^* \le c_k$. We separate two cases for the value of w^*.

Case 1. $w^* = c_k$. Note that there is i such that $y_i > 0$. But then there exists $\epsilon > 0$, such that

$$(w^* - \epsilon, y_1^* + \epsilon, \dots, y_{i-1}^* + \epsilon, y_i^* - k\epsilon, y_{i+1}^* + \epsilon, \dots, y_k^* + \epsilon, \underbrace{0, \dots, 0}_{r}) \tag{5.5}$$

is still a feasible solution of (5.1), which contradicts to the optimality of w^*.

Case 2. $w^* < c_k$. Clearly $y_i^* \ge \max(c_i - w^*, 0)$. If there exists i such that $y_i^* > \max(c_i - w^*, 0)$, then there exists $\epsilon > 0$, such that (5.5) is still a feasible solution to (5.1). This contradicts to the optimality of w^*. So $y_i^* = \max(c_i - w^*, 0)$. Let $\widehat{i}_0$ be such that $w^* \in [c_{k-\widehat{i}_0}, c_{k-\widehat{i}_0+1})$. Then

$$y_1^* = \dots = y_{k-\widehat{i}_0}^* = 0 \quad \text{and} \quad y_i^* = c_i - w^* \text{ for } i > k - \widehat{i}_0.$$

Further on,

$$\sum_{i=1}^{k} y_i^* = \sum_{i=k-\widehat{i}_0+1}^{k} (c_i - w^*) = w^* + \alpha,$$

whence

$$w^* = \frac{1}{\widehat{i}_0 + 1}\Big(\sum_{i=k-\widehat{i}_0+1}^{k} c_i - \alpha\Big) = \frac{1}{\widehat{i}_0 + 1}\Big(\sum_{j=0}^{\widehat{i}_0-1} c_{k-j} - \alpha\Big) = w_{\widehat{i}_0}.$$

Since by Claims 1 and 2, the only i such that $w_i \in [c_{k-i_0}, c_{k-i_0+1})$ is i_0 defined by (5.2), it follows that $\widehat{i}_0 = i_0$ and the optimal solution to (5.1) is as stated in the proposition. □

6. Final step in the proof of Theorem 1

Assume the notation as in the statement of Theorem 1 and Section 4.2. In this section we will solve the linear programs (4.10) and (4.5), which by Proposition 2 also solves the maximal negative volume quasi-copula problem and proves Theorem 1.

Let $(l_1^*, \dots, l_d^*, y_3^*)$ be an optimal solution to (4.10). By the moreover part of Claim 3 in the proof of Proposition 5, under the assumption $d \ge 7$, we have that $l_d^* = -1 + y_3^*$. Writing $w := (d-1)y_3$, (4.10) becomes

$$\begin{aligned} &-\Big(\min_{l_1,\dots,l_{d-1},w} \quad w\Big), \\ &\text{subject to} \quad -\sum_{i=1}^{d-1} l_i + w + 1 = 0, \\ &\qquad l_j + w \ge (-1)^{d+j+1}\binom{d-1}{j-1} \quad \text{for } j = 1, \dots, d-1, \\ &\qquad w \ge 0,\ l_i \ge 0 \quad \text{for } i = 1, \dots, d-1. \end{aligned} \tag{6.1}$$

The solution to (6.1) will lean on the use of Proposition 6. Let c_i, $i = 1, \dots, \lfloor \frac{d}{2} \rfloor$ be as in Theorem 1. Let $r := d - 1 - \lfloor \frac{d}{2} \rfloor$ and let $e_1, \dots, e_r$ be the right hand sides $-\binom{d-1}{j-1}$ in (6.1) in some order. By Proposition 6 with $\alpha = 1$, the optimal solution to (6.1) is $w^* = w_{i_0,-}$ and:

1. If d is even, then

$$l_j^* = \begin{cases} \binom{d-1}{j-1} - w_{i_0,-}, & j \text{ is odd and } \binom{d-1}{j-1} > c_{\frac{d}{2}-i_0}, \\ 0, & \text{otherwise.} \end{cases} \tag{6.2}$$

2. If d is odd, then

$$l_j^* = \begin{cases} \binom{d-1}{j-1} - w_{i_0,-}, & j \text{ is even and } \binom{d-1}{j-1} > c_{\lfloor \frac{d}{2} \rfloor - i_0}, \\ 0, & \text{otherwise.} \end{cases} \tag{6.3}$$

Hence, in an optimal solution to (4.8) except (6.2) or (6.3), also the following hold: $y_1^* = 0$, $l_d^* = -1 + \frac{1}{d-1} w_{i_0,-}$, $y_2^* = \frac{d}{d-1} w_{i_0,-}$, $y_3^* = \frac{1}{d-1} w_{i_0,-}$. Using the complementary slackness, in an optimal solution to the dual (4.6) of (4.8), we have $a^* = \frac{i_0}{i_0+1}$, $b^* = 1$, $q_0^* = 0$ and δ_j^* are as in (2.3) if d is even, while δ_j^* are as in (2.4) if d is odd. This give the desired solution to (4.5) and proves Theorem 1.

7. Final step in the proof of Theorem 2

Assume the notation as in the statement of Theorem 2 and Section 4.2. In this section we will solve the linear program (4.11) and (4.5), where min is replaced by max, This solves the maximal positive volume quasi-copula problem and proves Theorem 2.

Let $(l_1^*, \dots, l_d^*, y_3^*)$ be an optimal solution to (4.11). By the moreover part of Claim 3 in the proof of Proposition 5, we have that $l_d^* = 1 + y_3^*$. Writing $w := (d-1)y_3$, (4.16) becomes

$$\begin{aligned} \min_{l_1,\dots,l_{d-1},w} \quad & w, \\ \text{subject to} \quad & -\sum_{i=1}^{d-1} l_i + w - 1 = 0, \\ & l_j + w \geq (-1)^{d+j}\binom{d-1}{j-1} \quad \text{for } j = 1, \dots, d-1, \\ & w \geq 0,\ l_i \geq 0 \quad \text{for } i = 1, \dots, d-1. \end{aligned} \tag{7.1}$$

The solution to (7.1) will lean on the use of Proposition 6. Let c_i, $i = 1, \dots, \lfloor \frac{d+1}{2} \rfloor - 1$ be as in Theorem 2. Let $r := d - \lfloor \frac{d+1}{2} \rfloor$ and let $e_1, \dots, e_r$ be the right hand sides $-\binom{d-1}{j-1}$ in (7.1) in some order. By Proposition 6 with $\alpha = -1$, the optimal solution to (7.1) is $w^* = w_{i_0,+}$ and:

1. If d is even, then

$$l_j^* = \begin{cases} \binom{d-1}{j-1} - w_{i_0,-}, & j \text{ is even and } \binom{d-1}{j-1} > c_{\frac{d}{2}-1-i_0}, \\ 0, & \text{otherwise.} \end{cases} \tag{7.2}$$

2. If d is odd, then

$$l_j^* = \begin{cases} \binom{d-1}{j-1} - w_{i_0,-}, & j \text{ is odd and } \binom{d-1}{j-1} > c_{\lfloor \frac{d+1}{2} \rfloor - 1 - i_0}, \\ 0, & \text{otherwise.} \end{cases} \tag{7.3}$$

Hence, in an optimal solution to (4.9) except (7.2) or (7.3), also the following hold: $y_1^* = 0$, $l_d^* = 1 + \frac{1}{d-1} w_{i_0,+}$, $y_2^* = \frac{d}{d-1} w_{i_0,+}$, $y_3^* = \frac{1}{d-1} w_{i_0,+}$. Using the complementary slackness, in an optimal solution to the dual (4.6), with max instead of min, of (4.9), we have $a^* = \frac{i_0}{i_0+1}$, $b^* = 1$, $q_0^* = 0$ and δ_j^* are as in (2.6) if d is even, while δ_j^* are as in (2.7) if d is odd. This give the desired solution to (4.5) with max instead of min, and proves Theorem 2.

8. Maximal negative volume problem in dimensions $d \leq 6$ analytically

The solutions to the maximal negative volume quasi-copula problem in dimensions $2 \leq d \leq 6$ are already known, i.e., see [9] for $d = 2$, [4] for $d = 3$, [14] for $d = 4$ and [5] for $d = 5, 6$. However, the solutions for $d \geq 3$ are numerical, based on the solution to the corresponding linear programs using computer software. In this section we will present analytical solutions.

Assume the notation as in Section 4.2. We will solve the linear program (4.10) and consequently (4.5) analytically for $3 \leq d \leq 6$.

Let $(l_1^*, \dots, l_d^*, y_3^*)$ be an optimal solution to (4.10). By the moreover part of Claim 3 in the proof of Proposition 5, we have to analyse the possibilities $l_d = 0$ for $d \leq 6$. If any of these gives a feasible solution, then there also exists an optimal solution with $l_d^* = 0$, as y_3 is at most 1 in this case. Below we derive the optimal solutions to these programs for $l_d = 0$. To complete the solution one needs to find a realization of the d-quasi-copula with such d-box but these are already given in the references from the first paragraph above.

8.1. Case $d = 3$

The linear program (4.10) for $d = 3$ is

$$\begin{aligned} -\Big(\min_{l_1,l_2,y_3} \quad & 2y_3\Big), \\ \text{subject to} \quad & 3y_3 = l_1 + l_2, \\ & l_1 + 2y_3 \geq -\binom{2}{0} = -1 \\ & l_2 + 2y_3 \geq \binom{2}{1} = 2 \\ & 1 \geq y_3 \geq 0,\ l_1 \geq 0,\ l_2 \geq 0. \end{aligned}$$

Repeating the arguments from the proof of Proposition 6, in the optimal solution (l_1^*, l_2^*, y_3^*) we have that $l_1^* = 0$ and $l_2^* + 2y_3^* = 2$. Using this in $3y_3^* = l_1^* + l_2^*$ we get $y_3^* = \frac{2}{5}$. So the minimal volume box of some 3-quasi-copula has value $-\frac{4}{5}$. Hence, an optimal solution $(y_1^*, l_1^*, l_2^*, l_3^*, y_2^*, y_3^*)$ to (4.8) for $d = 3$ is $\left(0, 0, \frac{2}{5}, 0, \frac{6}{5}, \frac{2}{5}\right)$. Using the complementary slackness, an optimal solution $(a^*, b^*, q_0^*, \delta_1^*, \delta_2^*, \delta_3^*)$ to its dual (4.6) is equal to $\left(\frac{2}{5}, \frac{4}{5}, 0, 0, \frac{2}{5}, 0\right)$. Finally, an optimal solution to (4.5) is

$$(a^*, b^*, q_0^*, q_1^*, q_2^*, q_3^*) = \left(\frac{2}{5}, \frac{4}{5}, 0, 0, \frac{2}{5}, \frac{2}{5}\right).$$

8.2. Case $d = 4$

The linear program (4.10) for $d = 4$ is

$$\begin{aligned}
-\Big(\min_{l_1,l_2,l_3,y_3} \quad & 3y_3\Big), \\
\text{subject to} \quad & 4y_3 = l_1 + l_2 + l_3, \\
& l_1 + 3y_3 \geq \binom{3}{0} = 1 \\
& l_2 + 3y_3 \geq -\binom{3}{1} = -3 \\
& l_3 + 3y_3 \geq \binom{3}{2} = 3 \\
& 1 \geq y_3 \geq 0,\ l_1 \geq 0,\ l_2 \geq 0,\ l_3 \geq 0.
\end{aligned}$$

Repeating the arguments from the proof of Proposition 6, in the optimal solution (l_1^*, l_2^*, y_3^*) we have that $l_2^* = 0$ and one of the cases:

- $l_1^* + 3y_3^* = 1$ and $l_3^* + 3y_3^* = 3$, or
- $l_1^* = 0$ and $l_3^* + 3y_3^* = 3$,

Using these in $4y_3^* = l_1^* + l_2^*$ we get $y_3^* = \frac{2}{5}$ in the first case and $y_3^* = \frac{3}{7}$ in the second case. In the first case $l_1^* = -\frac{1}{5} < 0$, which is not in the feasible region. So the second case applies and the minimal volume box of some 4-quasi-copula has value $-\frac{9}{7}$. Hence, an optimal solution $(y_1^*, l_1^*, l_2^*, l_3^*, y_2^*, y_3^*)$ to (4.8) for $d = 4$ is $\left(0, 0, 0, \frac{12}{7}, \frac{12}{7}, \frac{3}{7}\right)$. Using the complementary slackness, an optimal solution $(a^*, b^*, q_0^*, \delta_1^*, \delta_2^*, \delta_3^*, \delta_4^*)$ to its dual (4.6) is equal to $\left(\frac{3}{7}, \frac{6}{7}, 0, 0, 0, \frac{3}{7}, 0\right)$. Finally, an optimal solution to (4.5) is

$$(a^*, b^*, q_0^*, q_1^*, q_2^*, q_3^*, q_4^*) = \left(\frac{3}{7}, \frac{6}{7}, 0, 0, 0, \frac{3}{7}, \frac{3}{7}\right).$$

8.3. Case $d = 5$

The linear program (4.10) for $d = 5$ is

$$\begin{aligned}
-\Big(\min_{l_1,l_2,l_3,l_4,y_3} \quad & 4y_3\Big), \\
\text{subject to} \quad & 5y_3 = l_1 + l_2 + l_3 + l_4, \\
& l_1 + 4y_3 \geq -\binom{4}{0} = -1 \\
& l_2 + 4y_3 \geq \binom{4}{1} = 4 \\
& l_3 + 4y_3 \geq -\binom{4}{2} = -6 \\
& l_4 + 4y_3 \geq \binom{4}{3} = 4 \\
& 1 \geq y_3 \geq 0,\ l_1 \geq 0,\ l_2 \geq 0,\ l_3 \geq 0,\ l_4 \geq 0.
\end{aligned}$$

Repeating the arguments from the proof of Proposition 6, in the optimal solution $(l_1^*, l_2^*, l_3^*, l_4^*, y_3^*)$ we have that $l_1^* = l_3^* = 0$ and $l_2^* + 4y_3^* = l_4^* + 4y_3^* = 4$. Using these in $5y_3^* = l_2^* + l_4^*$ we get $y_3^* = \frac{8}{13}$ So the minimal volume box of some 5-quasi-copula has value $-\frac{32}{13}$. Hence, an optimal solution $(y_1^*, l_1^*, l_2^*, l_3^*, l_4^*.y_2^*, y_3^*)$ to (4.8) for $d = 5$ is $\left(0, 0, \frac{20}{13}, 0, \frac{20}{13}, \frac{30}{13}, \frac{8}{13}\right)$. Using the complementary slackness, an optimal solution $(a^*, b^*, q_0^*, \delta_1^*, \delta_2^*, \delta_3^*, \delta_4^*, \delta_5^*)$ to its dual (4.6) is equal to $\left(\frac{8}{13}, \frac{12}{13}, 0, 0, \frac{4}{13}, 0, \frac{4}{13}, 0\right)$. Finally, an optimal solution to (4.5) is

$$(a^*, b^*, q_0^*, q_1^*, q_2^*, q_3^*, q_4^*, q_5^*) = \left(\frac{8}{13}, \frac{12}{13}, 0, 0, \frac{4}{13}, \frac{4}{13}, \frac{8}{13}, \frac{8}{13}\right).$$

8.4. Case $d = 6$

The linear program (4.10) for $d = 6$ is

$$
\begin{aligned}
-\Big(\min_{l_1,l_2,l_3,l_4,l_5,y_3} \quad & 5y_3\Big),\\
\text{subject to} \quad & 6y_3 = l_1 + l_2 + l_3 + l_4 + l_5 + l_6,\\
& l_1 + 5y_3 \geq \binom{5}{0} = 1\\
& l_2 + 5y_3 \geq -\binom{5}{1} = -5\\
& l_3 + 5y_3 \geq \binom{5}{2} = 10\\
& l_4 + 5y_3 \geq -\binom{5}{3} = -10\\
& l_5 + 5y_3 \geq \binom{5}{4} = 5\\
& 1 \geq y_3 \geq 0,\ l_1 \geq 0,\ l_2 \geq 0,\ l_3 \geq 0,\ l_4 \geq 0,\ l_5 \geq 0.
\end{aligned}
$$

Repeating the arguments from the proof of Proposition 6, in the optimal solution $(l_1^*, l_2^*, l_3^*, l_4^*, l_5^*, y_3^*)$ we have that $l_2^* = l_4^* = 0$ and and one of the cases:

- $l_1^* + 5y_3^* = 1$, $l_3^* + 5y_3^* = 10$ and $l_5^* + 5y_3^* = 5$, or
- $l_1^* = 0$, $l_3^* + 5y_3^* = 10$ and $l_5^* + 5y_3^* = 5$, or
- $l_1^* = 0$, $l_3^* + 5y_3^* = 10$ and $l_5^* = 0$.

Using these in $6y_3^* = l_1^* + l_3^* + l_5^*$ we get $y_3^* = \frac{16}{21}$ in the first case, $y_3^* = \frac{15}{16}$ in the second case and $y_3^* = \frac{10}{11}$ in the third case. In the smallest candidate for the solution, i.e., $\frac{16}{21}$, we have that $l_1^* = -\frac{59}{21} < 0$, which is not in the feasible region. The second smallest candidate for the solution, i.e., $\frac{15}{16}$ indeed comes from the feasible (and hence optimal) solution, i.e., $(l_1^*, l_2^*, l_3^*, l_4^*, l_5^*, y_3^*) = \big(0, 0, \frac{85}{16}, 0, \frac{5}{16}, \frac{15}{16}\big)$. So the minimal volume box of some 6-quasi-copula has value $-\frac{75}{16}$. Hence, an optimal solution $(y_1^*, l_1^*, l_2^*, l_3^*, l_4^*, l_5^*, l_6^*, y_2^*, y_3^*)$ to (4.8) for $d = 6$ is $\big(0, 0, 0, \frac{85}{16}, 0, \frac{5}{16}, 0, \frac{90}{16}, \frac{15}{16}\big)$. Using the complementary slackness, an optimal solution $(a^*, b^*, q_0^*, \delta_1^*, \delta_2^*, \delta_3^*, \delta_4^*, \delta_5^*, \delta_6^*)$ to its dual (4.6) is equal to $\big(\frac{5}{8}, \frac{15}{16}, 0, 0, 0, \frac{5}{16}, 0, \frac{5}{16}, 0\big)$. Finally, an optimal solution to (4.5) is

$$(a^*, b^*, q_0^*, q_1^*, q_2^*, q_3^*, q_4^*, q_5^*, q_6^*) = \Big(\frac{5}{8}, \frac{15}{16}, 0, 0, 0, \frac{5}{16}, \frac{5}{16}, \frac{5}{8}, \frac{5}{8}\Big).$$

9. Concluding remarks and future research

In this paper, we addressed the problem of extreme values of the mass distribution associated with a multidimensional quasi-copula, following the approach of reformulating the problem in the linear programming language introduced in [4] for the three-dimensional case. As shown in our previous work [5], solving the linear program using computer software becomes infeasible already at relatively low dimensions (less than 20). However, the symmetry of the solutions suggested that this symmetry could also be preserved in a general dimension. This was a crucial observation that allowed us to simplify the problem by symmetrizing the linear program (see (4.5) and (4.6)) and then solving it explicitly via the corresponding dual linear program (see (4.10) and (4.11)). Moreover, with this approach we can also explain why dimensions up to six are special for the maximal negative volume question (see Remark 1.(2)). However, it turns out that a closed form solution for the extreme values does not exist, which is also supported by the numerical analysis of the solutions in Section 3.

Finally, we give some directions for future research. To explain the difference in extreme volumes between quasi-copulas and copulas, it would be interesting to study a larger class of aggregation functions (see [6, Chapter 8], [2,3]) such as (Lipschitz-continuous or continuous) semi-copulas on the one hand and intermediate classes of k-dimensional increasing d-quasi-copulas for $k \in \{2, \dots, d-1\}$ on the other hand. Note that $k = 1$ and $k = d$ are exactly quasi-copulas and copulas, respectively. Understanding the behaviour of the extreme volumes for these classes would show how important is the size of k relative to d and thus explain why copulas are so much more restrictive than quasi-copulas in terms of volumes.

It would be also interesting to characterize extreme points and faces of the convex set of all d-quasi-copulas, since by Krein-Milman theorem every quasi-copula is a convex combinations of extreme points of the set of quasi-copulas. Clearly, extreme points form a subset of the extreme volume points, but the other inclusion does not necessarily hold. The symmetric quasi-copulas from Theorems 1 and 2 are examples of extreme volume solutions which are not necessarily extreme points, since they are obtained as convex combinations of non-symmetric extreme volume solutions (see (4.4)).

CRediT authorship contribution statement

Matjaž Omladič : Writing – review & editing, Validation, Supervision, Project administration, Methodology, Investigation, Formal analysis, Conceptualization; **Martin Vuk:** Writing – review & editing, Software, Formal analysis, Data curation; **Aljaž Zalar:** Writing – original draft, Validation, Supervision, Methodology, Investigation, Formal analysis.

Data availability

No data was used for the research described in the article.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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