**Mathematical Programming manuscript No.**
(will be inserted by the editor)

# Copositivity detection by difference-of-convex decomposition and $\omega$-subdivision

**Immanuel M. Bomze · Gabriele Eichfelder**

Received: date / Accepted: date

**Abstract** We present three new copositivity tests based upon difference-of-convex (d.c.) decompositions, and combine them to a branch-and-bound algorithm of $\omega$-subdivision type. The tests employ LP or convex QP techniques, but also can be used heuristically using appropriate test points. We also discuss the selection of efficient d.c. decompositions and propose some preprocessing ideas based on the spectral d.c. decomposition. We report on first numerical experience with this procedure which are very promising.

**Keywords** copositive programming

**Mathematics Subject Classification (2000)** 15A48 · 15A18 · 65F30 · 65K99 · 90C22

## 1 Preliminaries

### 1.1 Introduction

A symmetric $n \times n$ matrix is called $\mathbb{R}^n_+$-copositive (or shortly copositive), if it generates a quadratic form which takes no negative values on the nonnegative orthant $\mathbb{R}^n_+$. The problem of determining whether a matrix is not copositive is NP-complete [36]. Copositive optimization problems are particular conic programs: the task is to optimize linear forms over the copositive cone subject to linear (equality) constraints. Recently it has been shown [15] that every quadratic program with linear constraints can be formulated as a copositive program, even if some of the variables are binary. Hence, many combinatorial optimization problems can be cast into copositive programs. For further details we refer to the recent surveys [8, 16, 22] and to [13] for a clustered collection of references. These references also cover a multitude of procedures or conditions for copositivity detection, developed in the last 59 years since T.S. Motzkin coined this notion (apparently abbreviating "conditional positive-semidefinite") back in 1952. However, there are but a few implemented numerical algorithms

Immanuel M. Bomze
Department of Statistics and Operations Research, Universität Wien, A-1010 Wien, Austria
E-mail: immanuel.bomze@univie.ac.at

Gabriele Eichfelder
Institute of Mathematics, Ilmenau University of Technology, Weimarer Straße 25, 98693 Ilmenau, Germany
E-mail: Gabriele.Eichfelder@tu-ilmenau.de

which (a) apply to general symmetric matrices without any structural assumptions or dimensional restrictions; (b) are not merely recursive, i.e., do not rely on information taken from all principal submatrices, but rather focus on generating subproblems in a somehow data-driven way. Boundary cases, some possibly without implementation, are [1,3,17,33,37]. It seems that only the recent publication [14] satisfies criteria (a) and (b) to full extent.

In this paper we aim at both requirements. We present three easy-to-test, and apparently new, conditions which guarantee copositivity. This is of particular importance in view of the wide-spread belief in the community, that it is easier to detect violation of copositivity than to obtain a positive certificate for that property. Based on these ideas, we formulate a branch-and-bound algorithm of $\omega$-subdivision type, which we supplement by a series of preprocessing steps, some of them also apparently new. To be more specific, the paper is organized as follows: Section 2 introduces difference-of-convex (d.c.) based approaches to copositivity testing. These tests employ techniques of linear programming (LP; in Subsection 2.2) and convex quadratic programming (QP; in Subsection 2.3). Some of these can also be used heuristically using appropriate test points. We also give a first outline of our proposed algorithm. Section 3 deals with the question which d.c. decomposition should be chosen and may be skipped at first reading. We argue in Section 3 why the so-called spectral d.c. decomposition is preferable, and discuss in Section 4 some preprocessing steps, among them some based on spectral information. In Section 5 we describe a robustification step which may be of advantage both from a theoretical and practical point of view and combine these ingredients to a branch-and-bound algorithm. Section 6 reports very promising numerical experience, while the final Section 7 concludes.

## 1.2 Terminology and a motivation

Let us start introducing some notions and notations. For integers $i < k$, we abbreviate by $\{i : k\} := \{i, i+1, \dots, k\}$. Further denote by $\mathbf{e} = [1, \dots, 1]^\top = \sum_{i=1}^n \mathbf{e}_i \in \mathbb{R}^n$ (where $\mathbf{e}_i$ is the $i$-th column of the $n \times n$ identity matrix $I_n$) and by $E_n = \mathbf{e}\mathbf{e}^\top$ the $n \times n$ all-ones matrix. Then

$$\Delta^s := \{\mathbf{x} \in \mathbb{R}^n_+ : \mathbf{e}^\top \mathbf{x} = 1\}$$

is the *standard simplex* in $\mathbb{R}^n$. Closely related to copositivity testing are the so-called *Standard Quadratic optimization Problems* (StQPs) [5], to optimize a quadratic form over $\Delta^s$:

$$\alpha_Q := \min \left\{ \mathbf{x}^\top Q \mathbf{x} : \mathbf{x} \in \Delta^s \right\} , \tag{1.1}$$

where $Q \in \mathcal{S}^n$, the set of symmetric $n \times n$ matrices. Any feasible point $\mathbf{x}$ to (1.1) delivering a negative objective value is a certificate for non-copositivity of $Q$ (more generally, in the sequel we shall speak of a *violating vector* $\mathbf{v} \in \mathbb{R}^n_+$ if $\mathbf{v}^\top Q \mathbf{v} < 0$), while $\alpha_Q \geq 0$ means that $Q$ is copositive.

It will be convenient to use a more general copositivity notion w.r.t. a nonempty set $K \subset \mathbb{R}^n$: a matrix is called $K$-copositive ([23,24] call it $K$-semidefinite, [38] cone-positive), if the quadratic form takes no negative values on $K$ and thus [23, Thm. 2.19] on $\mathbb{R}_+ K := \{t\mathbf{x} : t \geq 0, \mathbf{x} \in K\}$, the cone generated by $K$ (e.g., $Q$ is $\Delta^s$-copositive if and only if $Q$ is ($\mathbb{R}^n_+$-)copositive). Therefore a matrix $Q$ is copositive if and only if $\Delta^s$ is contained in the *positivity cone* of $Q$, which we denote by

$$\mathrm{Pos}(Q) := \{\mathbf{x} \in \mathbb{R}^n : \mathbf{x}^\top Q \mathbf{x} \geq 0\} .$$

This cone is symmetric w.r.t. the origin $\mathbf{o}$, i.e., $-\mathrm{Pos}(Q) = \mathrm{Pos}(Q)$. The set of all violating vectors coincides with the cone $\mathbb{R}^n_+ \setminus \mathrm{Pos}(Q)$, which is empty if $Q$ is copositive, see Fig. 1.1.

A violating vector is not only useful as a negative certificate, it may even contain important information in a global optimization context. In fact, for general QPs of the form $\min \left\{ g(\mathbf{x}) = \mathbf{x}^\top Q \mathbf{x} + \mathbf{c}^\top \mathbf{x} : A\mathbf{x} \leq \mathbf{b} , \mathbf{x} \in \mathbb{R}^n \right\}$, where $Q$ may have negative eigenvalues, $A$ is an $m \times n$ matrix, and $\mathbf{c} \in \mathbb{R}^n$,

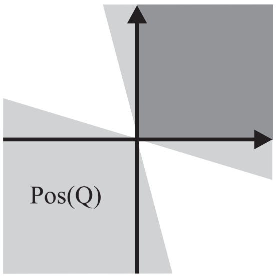


**Fig. 1.1** Positivity cone $\mathrm{Pos}(Q)$ for some $2 \times 2$-matrix $Q$, which is copositive since $\mathbb{R}^2_+ \subseteq \mathrm{Pos}(Q)$.

$\mathbf{b} \in \mathbb{R}^m$, we can characterize *global optimality* of a Karush-Kuhn-Tucker point $\bar{\mathbf{x}}$ by not more than $m$ copositivity conditions on suitable (indefinite) rank-two updates of $Q$, with respect to polyhedral cones derived from $\bar{\mathbf{x}}$ and the problem data with a worst-case complexity requirement of $\mathcal{O}(m+n)$; see [2,18]. If $\mathbf{v}$ is a vector violating one of these copositivity conditions, one can as easily construct a globally improving feasible point, and thus enable an escape from the inefficient (local) solution $\bar{\mathbf{x}}$; this means that $\mathbf{v}$ is a tunneling direction, i.e., $g(\bar{\mathbf{x}} + t\mathbf{v}) > g(\bar{\mathbf{x}})$ may happen for small $t > 0$. There is a direct application in case of specially structured feasible sets like $\Delta^s$, i.e., for Standard QPs; for details we refer to [4].

## 2 Copositivity detection via difference-of-convex approach

### 2.1 Basic ingredients and ideas

Given $Q \in \mathcal{S}^n$, we select two positive-semidefinite matrices $Q_+ \in \mathcal{S}^n$ and $Q_- \in \mathcal{S}^n$ such that

$$Q = Q_+ - Q_- \tag{2.1}$$

which means that we decompose the (possibly nonconvex) quadratic objective function $\mathbf{x}^\top Q \mathbf{x}$ of (1.1) into the difference of two convex quadratic functions $\mathbf{x}^\top Q_\pm \mathbf{x}$. Such a *difference-of-convex decomposition* (d.c.d.) of course always exists, and we will discuss selection of the $Q_\pm$ later in Section 3. Here let us only note that the most efficient d.c.d.s will necessary employ *singular* matrices $Q_\pm$ [11]. By this d.c.d., we can write the positivity cone as

$$\mathrm{Pos}(Q) = \{\mathbf{x} \in \mathbb{R}^n : \mathbf{x}^\top Q_+ \mathbf{x} \geq \mathbf{x}^\top Q_- \mathbf{x}\},$$

and this will be the starting point of our investigations. We immediately see that by construction, $Q$ is always $\ker Q_-$-copositive, hence any positive-semidefinite $Q$ (where $Q_- = O$ can be chosen) guarantees $\mathbb{R}^n_+$-copositivity of $Q$. Furthermore, any vector $\mathbf{v} \in \ker Q_+ \cap \mathbb{R}^n_+ \setminus \ker Q_-$ is violating. In particular, if $Q_+ = O$ but $Q_- \neq O$ (i.e, if $Q \neq O$ is negative-semidefinite), there is such a violating vector, as can be seen from the following lemma, which we will need to assess feasibility of auxiliary optimization problems for copositivity tests. Of course, a nonzero negative-semidefinite matrix cannot be copositive and hence no copositivity test has to be applied then. But beforehand let us notice that a violating vector $\mathbf{v} \in \ker Q_+ \cap \mathbb{R}^n_+ \setminus \ker Q_-$ can be found by LP methods, which will be detailed in Section 4 below.

**Lemma 2.1** *For $S \in \mathcal{S}^n$ define $C_S := \left\{\mathbf{x} \in \mathbb{R}^n_+ : \mathbf{x}^\top S \mathbf{x} = 1\right\}$. If $S$ is positive-semidefinite, we have*

$$C_S = \emptyset \quad \Longleftrightarrow \quad S = O\,.$$

*Proof* Only one implication is nontrivial. So suppose that $C_S = \emptyset$. Since $S$ is positive-semidefinite, we have by homogeneity that $C_S = \emptyset$ if and only if $\mathbb{R}^n_+ \subseteq \{\mathbf{x} \in \mathbb{R}^n : \mathbf{x}^\top S\mathbf{x} = 0\}$. Now, again by positive-semidefiniteness of $S$, any $\mathbf{x} \in \mathbb{R}^n$ with $\mathbf{x}^\top S\mathbf{x} = 0$ satisfies $\mathbf{x} \in \ker S$, which is a linear subspace. So we get $\mathbb{R}^n = \mathbb{R}^n_+ - \mathbb{R}^n_+ \subseteq \ker S$, which means $S = O$. □

Similar to the use of (1.1), we now may characterize copositivity by a program which has a convex quadratic objective:

**Proposition 2.2** *Given (2.1) with $Q_- \neq O$, consider the program*

$$\mu_{\mathrm{dcd}} := \inf\left\{\mathbf{x}^\top Q_+\mathbf{x} : \mathbf{x}^\top Q_-\mathbf{x} = 1\,,\ \mathbf{x} \in \mathbb{R}^n_+\right\} \geq 0\,. \tag{2.2}$$

*This program is always feasible and characterizes copositivity of $Q$ as follows:*

*(a) Any (2.2)-feasible $\bar{\mathbf{x}}$ with $\bar{\mathbf{x}}^\top Q_+\bar{\mathbf{x}} < 1$ is a violating vector.*
*(b) If $\mu_{\mathrm{dcd}} \geq 1$, then $Q$ is copositive.*

*Proof* The feasible set of (2.2) is $C_{Q_-} \neq \emptyset$ as argued in Lemma 2.1. Since $\ker Q_- \subseteq \mathrm{Pos}(Q)$ by construction, a violating vector must always lie in the cone $\mathbb{R}^n_+ \setminus \ker Q_- = \{\mathbf{x} \in \mathbb{R}^n_+ : \mathbf{x}^\top Q_-\mathbf{x} > 0\}$. Again, by homogeneity, we may restrict the search for a violating vector to $C_{Q_-}$, which implies both assertions, (a) and (b). □

Given a d.c.d. (2.1), we can also use a different quadratically constrained quadratic problem for the characterization of copositivity.

**Proposition 2.3** *Given (2.1) with $Q_+ \neq O$, consider the program*

$$\mu^+_{\mathrm{dcd}} := \sup\left\{\mathbf{x}^\top Q_-\mathbf{x} : \mathbf{x}^\top Q_+\mathbf{x} = 1\,,\ \mathbf{x} \in \mathbb{R}^n_+\right\} \geq 0\,. \tag{2.3}$$

*This program is always feasible and can be written as a convex quadratic maximization problem over a convex region as follows:*

$$\mu^+_{\mathrm{dcd}} = \sup\left\{\mathbf{x}^\top Q_-\mathbf{x} : \mathbf{x}^\top Q_+\mathbf{x} \leq 1\,,\ \mathbf{x} \in \mathbb{R}^n_+\right\} \geq 0\,. \tag{2.4}$$

*Further, both equivalent problems characterize copositivity of $Q$ as follows:*

*(a) Any (2.4)-feasible $\bar{\mathbf{x}}$ with $\bar{\mathbf{x}}^\top Q_-\bar{\mathbf{x}} > 1$ is a violating vector.*
*(b) If $\mu^+_{\mathrm{dcd}} \leq 1$, then $Q$ is copositive.*

*If both $Q_+ \neq O$ and $Q_- \neq O$, then we have $\mu^+_{\mathrm{dcd}} = [\mu_{\mathrm{dcd}}]^{-1}$, using the extension $0^{-1} = +\infty$ whenever necessary.*

*Proof* Feasibility is again clear from Lemma 2.1 which implies here $C_{Q_+} \neq \emptyset$. Further, homogeneity also implies that the optimal values of (2.3) and (2.4) coincide. Assertions (a) and (b) are proved as before, and the last assertion follows from standard arguments for switching constraint and objective on a cone-constrained problem. For the sake of completeness, we provide a proof: assume that $\mathbf{x}_k^\top Q_+\mathbf{x}_k \searrow \mu_{\mathrm{dcd}}$ where $\mathbf{x}_k \in C_{Q_-}$ with $\mathbf{x}_k^\top Q_+\mathbf{x}_k > 0$ for all $k$. Put $\mathbf{y}_k := \frac{1}{\sqrt{\mathbf{x}_k^\top Q_+\mathbf{x}_k}}\mathbf{x}_k \in C_{Q_+}$, then

$$\mu^+_{\mathrm{dcd}} \geq \mathbf{y}_k^\top Q_-\mathbf{y}_k = \frac{\mathbf{x}_k^\top Q_-\mathbf{x}_k}{\mathbf{x}_k^\top Q_+\mathbf{x}_k} = \frac{1}{\mathbf{x}_k^\top Q_+\mathbf{x}_k} \nearrow \frac{1}{\mu_{\mathrm{dcd}}}\,.$$

Now, if $\mu^+_{\rm dcd} = 0 \le \frac{1}{\mu_{\rm dcd}}$, there is nothing more to show. So finally suppose that $\mu^+_{\rm dcd} > 0$ and pick $\mathbf{u}_k \in C_{Q_+}$ such that $0 < \mathbf{u}_k^\top Q_- \mathbf{u}_k \nearrow \mu^+_{\rm dcd}$. Then $\mathbf{z}_k := \frac{1}{\sqrt{\mathbf{u}_k^\top Q_- \mathbf{u}_k}} \mathbf{u}_k \in C_{Q_-}$ and thus

$$\mu_{\rm dcd} \le \mathbf{z}_k^\top Q_+ \mathbf{z}_k = \frac{\mathbf{u}_k^\top Q_+ \mathbf{u}_k}{\mathbf{u}_k^\top Q_- \mathbf{u}_k} = \frac{1}{\mathbf{u}_k^\top Q_- \mathbf{u}_k} \searrow \frac{1}{\mu^+_{\rm dcd}} \,.$$

Hence $\mu^+_{\rm dcd} = [\mu_{\rm dcd}]^{-1}$. □

Note that there is no counterpart of (2.4) for (2.2), in the following sense: if we tried to modify the non-convex constraint from $\mathbf{x}^\top Q_- \mathbf{x} = 1$ into $\mathbf{x}^\top Q_- \mathbf{x} \le 1$, we would rather end up in triviality ($\mathbf{x} = \mathbf{o}$ is an optimal solution). However, one can consider the following optimization problem with a convex objective function and a reverse convex constraint [39]:

$$\mu_{\rm dcd} = \inf\left\{\mathbf{x}^\top Q_+ \mathbf{x} : \mathbf{x}^\top Q_- \mathbf{x} \ge 1\,,\, \mathbf{x} \in \mathbb{R}^n_+\right\} \ge 0\,. \tag{2.5}$$

Homogeneity again implies that the optimal values of (2.2) and of (2.5) coincide and thus the results of Proposition 2.2 also hold for the problem (2.5). Of course, any (2.5)-feasible $\bar{\mathbf{x}}$ with $\bar{\mathbf{x}}^\top Q_+ \bar{\mathbf{x}} < 1$ is a violating vector.

In the following subsections, we propose three new sufficient conditions for copositivity; the first starts with Problem (2.4) and relaxes the constraint, so it can be seen as an outer approximation. The second and the third both start from Problem (2.2) and shrink the feasible set $C_{Q_-}$ to a finite subset in two different ways, and then employ convex QPs to arrive at the copositivity conditions.

Note that there are many ways to use decompositions of $Q$ for estimating and/or bounding $\alpha_Q$ (remember the sign of this quantity is a copositivity certificate), among them underestimating techniques, (semi-) Lagrangian dual and other relaxation bounds, and those requiring Semidefinite Optimization, which – although enjoying polynomial-time worst case complexity – need much more effort than the subproblems studied here. For details, references, and a hierarchy of bounds we refer to [12].

## 2.2 An LP-based sufficient condition for copositivity

For convenience, we denote the feasible set of (2.4)

$$B_+ := \left\{\mathbf{x} \in \mathbb{R}^n_+ : \mathbf{x}^\top Q_+ \mathbf{x} \le 1\right\}\,.$$

This is a closed convex set with a boundary containing $C_{Q_+}$. If we enclose $B_+$ in a polytope with a few known vertices, we can relax (2.4) to a problem equivalent to maximization over a small finite set (the next result holds for any $N$ but for efficiency reasons we will restrict our attention to the minimal possible number $N = n$ and $\mathbf{y}_0 = \mathbf{o}$ below):

**Proposition 2.4** *Suppose* $P = \operatorname{conv}(\mathbf{y}_0, \ldots, \mathbf{y}_N)$ *is a polytope containing* $B_+$. *If*

$$\mathbf{y}_i^\top Q_- \mathbf{y}_i \le 1 \quad \text{for all } i \in \{0 : N\}\,, \tag{2.6}$$

*then* $Q$ *is copositive.*

*Proof* This follows immediately from convex maximization over $P \supset B_+$: indeed,

$$\mu^+_{\rm dcd} = \sup\left\{\mathbf{x}^\top Q_- \mathbf{x} : \mathbf{x} \in B_+\right\} \le \sup\left\{\mathbf{x}^\top Q_- \mathbf{x} : \mathbf{x} \in P\right\} = \max\left\{\mathbf{y}_i^\top Q_- \mathbf{y}_i : i \in \{0 : N\}\right\} \le 1$$

implies the assertion via Proposition 2.3(b). □

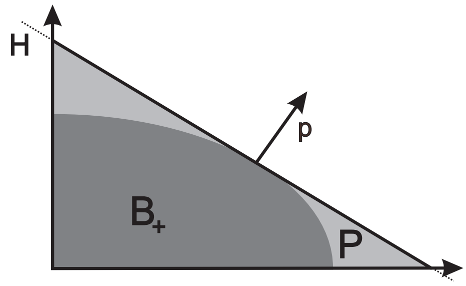


**Fig. 2.1** Feasible set $B_+$, the polytope $P$, the hyperplane $H$ with normal vector $\mathbf{p}$; see text.

Next we construct such a polytope $P$ by virtue of an affine hyperplane $H$ supporting $B_+$ at a boundary point, say $\mathbf{v}_0 := \frac{1}{\sqrt{\mathbf{x}^\top Q_+ \mathbf{x}}}\mathbf{x}$, of $B_+$, see Fig. 2.1. Here $\mathbf{x} \in \mathbb{R}^n_+$ such that $\mathbf{p} := Q_+\mathbf{x}$ has only positive coordinates (we will discuss existence of such a vector $\mathbf{x}$ later). Then $\mathbf{p}^\top \mathbf{v}_0 = \sqrt{\mathbf{x}^\top Q_+ \mathbf{x}}$ by construction, so that the hyperplane takes the form

$$H = \left\{ \mathbf{y} \in \mathbb{R}^n : \mathbf{p}^\top \mathbf{y} = \sqrt{\mathbf{x}^\top Q_+ \mathbf{x}} \right\} .$$

**Lemma 2.5** *Take any $\mathbf{x} \in \mathbb{R}^n_+$ such that $\mathbf{p} = Q_+\mathbf{x}$ has only positive coordinates, and define $\mathbf{y}_0 := \mathbf{o}$ as well as $\mathbf{y}_i := \frac{\sqrt{\mathbf{x}^\top Q_+ \mathbf{x}}}{p_i}\mathbf{e}_i$ for all $i \in \{1 : n\}$. Then the polytope*

$$P_{\mathbf{x}} := \operatorname{conv}(\mathbf{y}_0, \ldots, \mathbf{y}_n) = \operatorname{conv}\left(\mathbf{o}, \frac{\sqrt{\mathbf{x}^\top Q_+ \mathbf{x}}}{(Q_+\mathbf{x})_1}\mathbf{e}_1, \ldots, \frac{\sqrt{\mathbf{x}^\top Q_+ \mathbf{x}}}{(Q_+\mathbf{x})_n}\mathbf{e}_n\right) \tag{2.7}$$

*contains $B_+$.*

*Proof* The function $f(\mathbf{x}) = \frac{1}{2}\mathbf{x}^\top Q_+ \mathbf{x}$ is convex, and $\mathbf{p} = Q_+\mathbf{x} = \sqrt{\mathbf{x}^\top Q_+ \mathbf{x}}\nabla f(\mathbf{v}_0)$ supports the sublevel set $B_+$ of $f$ at the boundary point $\mathbf{v}_0 := \frac{1}{\sqrt{\mathbf{x}^\top Q_+ \mathbf{x}}}\mathbf{x} \in C_{Q_+}$ of $B_+$:

$$\mathbf{p}^\top(\mathbf{y} - \mathbf{v}_0) = \sqrt{\mathbf{x}^\top Q_+ \mathbf{x}}\,\nabla f(\mathbf{v}_0)^\top(\mathbf{y} - \mathbf{v}_0) \le \sqrt{\mathbf{x}^\top Q_+ \mathbf{x}}\,[f(\mathbf{y}) - f(\mathbf{v}_0)] \le 0\,,$$

if $f(\mathbf{y}) \le f(\mathbf{v}_0) = \frac{1}{2}$, i.e., if $\mathbf{y}^\top Q_+ \mathbf{y} \le 1$. This means that $B_+ \subseteq \left\{ \mathbf{y} \in \mathbb{R}^n : \mathbf{p}^\top \mathbf{y} \le \sqrt{\mathbf{x}^\top Q_+ \mathbf{x}} \right\}$, the half space generated by $H$. As $B_+ \subseteq \mathbb{R}^n_+$ by definition, we have

$$B_+ \subseteq P := \left\{ \mathbf{y} \in \mathbb{R}^n_+ : \mathbf{p}^\top \mathbf{y} \le \sqrt{\mathbf{x}^\top Q_+ \mathbf{x}} \right\} .$$

We now show that the polyhedron $P$ coincides with $P_{\mathbf{x}}$ given in (2.7). Indeed, since $\mathbf{y}_i$ satisfy by construction $\mathbf{p}^\top \mathbf{y}_i = \sqrt{\mathbf{x}^\top Q_+ \mathbf{x}}$ for $i \in \{1 : n\}$ while $\mathbf{p}^\top \mathbf{y}_0 = 0$, we immediately get $P_{\mathbf{x}} \subseteq P$. On the other hand, for any $\mathbf{y} \in P \subseteq \mathbb{R}^n_+$ we have the representation $\mathbf{y} = \sum_{i=1}^n \nu_i \mathbf{e}_i$ with $\nu_i \ge 0$ and of course $\sum_{i=1}^n \nu_i p_i = \mathbf{p}^\top \mathbf{y} \le \sqrt{\mathbf{x}^\top Q_+ \mathbf{x}}$, hence we arrive at the convex combination

$$\mathbf{y} = \left(1 - \frac{\sum_{i=1}^n \nu_i p_i}{\sqrt{\mathbf{x}^\top Q_+ \mathbf{x}}}\right)\mathbf{o} + \sum_{i=1}^n \frac{\nu_i p_i}{\sqrt{\mathbf{x}^\top Q_+ \mathbf{x}}}\mathbf{y}_i\,,$$

and $P \subseteq P_{\mathbf{x}}$ is established. □

**Theorem 2.6** *Given (2.1), take any $\mathbf{x} \in \mathbb{R}^n_+$ such that $\mathbf{p} = Q_+\mathbf{x}$ has only positive coordinates. If*

$$(\mathbf{x}^\top Q_+ \mathbf{x})(Q_-)_{ii} \le [(Q_+\mathbf{x})_i]^2 \quad \textit{for all } i \in \{1 : n\}\,, \tag{2.8}$$

*then $Q$ is copositive.*

*Proof* We use Lemma 2.5 and calculate $\mathbf{y}_i^\top Q_- \mathbf{y}_i = \frac{\mathbf{x}^\top Q_+ \mathbf{x}}{p_i^2} (Q_-)_{ii}$. Hence Proposition 2.4 yields (2.8) as a condition sufficient for copositivity of $Q$. □

The next step would be to determine an $\mathbf{x} \in \mathbb{R}^n_+$ such that $\mathbf{p} = Q_+\mathbf{x} \geq \mathbf{e} > \mathbf{o}$. Of course, this can be done by an LP, and it turns out that this LP is always feasible, given $\ker Q_+ \cap \Delta^s = \emptyset$:

**Proposition 2.7** *The condition* $\ker Q_+ \cap \Delta^s = \emptyset$ *is equivalent to* $\left\{\mathbf{x} \in \mathbb{R}^n_+ : Q_+\mathbf{x} \geq \mathbf{e}\right\} \neq \emptyset$.

*Proof* The condition $\left\{\mathbf{x} \in \mathbb{R}^n_+ : Q_+\mathbf{x} \geq \mathbf{e}\right\} \neq \emptyset$ is equivalent to saying that the LP

$$\inf\left\{\mathbf{f}^\top \mathbf{x} : Q_+\mathbf{x} \geq \mathbf{e}\,,\, \mathbf{x} \in \mathbb{R}^n_+\right\} \tag{2.9}$$

is feasible for any $\mathbf{f} \in \mathbb{R}^n$. The dual LP to (2.9) with $\mathbf{f} = \mathbf{o}$ is

$$\sup\left\{\mathbf{e}^\top \mathbf{z} : Q_+\mathbf{z} \leq \mathbf{o}\,,\, \mathbf{z} \in \mathbb{R}^n_+\right\}\,, \tag{2.10}$$

and this program (2.10) is always feasible (take $\mathbf{z} = \mathbf{o}$ for instance). So (2.9) is feasible if and only if (2.10) is bounded, which means that $\mathbf{e}^\top \mathbf{z} \leq 0$ whenever $\mathbf{z} \in \mathbb{R}^n_+$ and $Q_+\mathbf{z} \leq \mathbf{o}$. This means that $Q_+\mathbf{z} \leq \mathbf{o}$ and $\mathbf{z} \in \mathbb{R}^n_+$ imply $\mathbf{z} = \mathbf{o}$. In particular, any $\mathbf{z} \in \Delta^s \cap \ker Q_+$ would satisfy $\mathbf{z} = \mathbf{o}$, which is impossible. On the other hand, if indeed $\ker Q_+ \cap \Delta^s = \emptyset$, then $\ker Q_+ \cap \mathbb{R}^n_+ = \{\mathbf{o}\}$. $Q_+\mathbf{z} \leq \mathbf{o}$ and $\mathbf{z} \in \mathbb{R}^n_+$ imply

$$0 \leq \mathbf{z}^\top Q_+ \mathbf{z} \leq 0 \quad \text{or} \quad Q_+\mathbf{z} = \mathbf{o}\,,$$

since $Q_+$ is positive-semidefinite, so that $\mathbf{z} \in \ker Q_+ \cap \mathbb{R}^n_+$. Due to $\ker Q_+ \cap \mathbb{R}^n_+ = \{\mathbf{o}\}$ we conclude $\mathbf{z} = \mathbf{o}$, which means that (2.10) is bounded and therefore (2.9) is feasible. □

So to apply Theorem 2.6, we can solve one or several LPs of the form (2.9) with different $\mathbf{f}$, which means to solve a multiple cost-row problem allowing for warm-start techniques if $n$ is large. Reasonable choices are $\mathbf{f} = \mathbf{o}$ or $\mathbf{f} = \mathbf{e}$ or $\mathbf{f} = Q_+\mathbf{e}$. The latter choice is motivated by the following heuristics: to avoid a too large $P_\mathbf{x} = \operatorname{conv}(\mathbf{o}, \mathbf{y}_1, \ldots, \mathbf{y}_n)$, we should keep $\sqrt{\mathbf{x}^\top Q_+ \mathbf{x}}$ low (remember $\mathbf{y}_i := \frac{\sqrt{\mathbf{x}^\top Q_+ \mathbf{x}}}{p_i}\,\mathbf{e}_i$), and due to

$$\sqrt{\mathbf{x}^\top Q_+ \mathbf{x}} \geq \frac{\mathbf{e}^\top Q_+ \mathbf{x}}{\sqrt{\mathbf{e}^\top Q_+ \mathbf{e}}},$$

we could minimize $(Q_+\mathbf{e})^\top \mathbf{x} = \mathbf{e}^\top Q_+ \mathbf{x}$. Observe that a small $\mathbf{x}^\top Q_+ \mathbf{x}$ also increases chances that (2.8) is satisfied. Another, more numerical, argument would be that the choice of $\mathbf{f} = \mathbf{e}$ or $\mathbf{f} = Q_+\mathbf{e}$ would keep the optimal solutions to (2.9) reasonably bounded, due to the constraints $\mathbf{x} \geq \mathbf{o}$ and $Q_+\mathbf{x} \geq \mathbf{e}$.

For relatively small examples we refer to Subsection 2.4 below. On a larger scale, in a simulation study of 5000 randomly generated copositive $n \times n$ matrices of the form $P + N$ where $P$ is positive-semidefinite and $N$ has no negative entries (1000 matrices for each $n \in \{10, 20, 50, 100, 200\}$), only *one* (!) matrix failed to satisfy (2.8) with the choice $\mathbf{f} = Q_+\mathbf{e}$. With the choice of $\mathbf{f} = \mathbf{o}$, there were a total of 83 instances (fairly equi-distributed across $n$ in the above range) where (2.8) was violated.

The random $n \times n$ matrices above and in the remaining numerical simulations were created as follows: for an $n \times n$ matrix $C$ with entries independently drawn from a standard normal distribution, we obtain a random positive-semidefinite matrix $P = CC^\top$. A random nonnegative matrix $N$ is constructed by $N = B - b_{\min} I_n$ with $B = A + A^\top$ for a random matrix $A$ with entries uniformly distributed in $[0, 1]$ and $b_{\min}$ the minimal diagonal entry of $B$. By this construction we maintain nonnegativity of $N$ while increasing the chance that $P + N$ is indefinite, to avoid too easy instances.

Finally note that we can use condition (2.8) even without employing any LP techniques, if we are lucky enough to find a point $\mathbf{x} \in \mathbb{R}^n_+$ satisfying the assumption of Theorem 2.6. In another

| $n$ | $\min_i p_i > 0$ | $\mathbf{x} = \mathbf{e}$ fulfils (2.8) | psd |
|---|---|---|---|
| 10 | 852 | 714 | 165 |
| 20 | 672 | 466 | 32 |
| 50 | 302 | 94 | 0 |
| 100 | 94 | 6 | 0 |
| 200 | 10 | 0 | 0 |

**Table 2.1** Simulation results for $\mathbf{p} = Q_+\mathbf{e}$; 1000 matrices were generated for each $n$.

simulation, we counted how often this is the case for $\mathbf{x} = \mathbf{e}$, and how often this vector satisfies (2.8); see Table 2.1, where we also specified the number of generated matrices which are positive-semidefinite as a reference. It is remarkable how often this cheap check works in a range of low to medium dimensions (for $n \in \{10, 20, 50\}$ between 71,4% and 9,4%). Note that for this test only $n$ inequalities have to be evaluated, and no optimization problem has to be solved at all.

## 2.3 Two convex QP-based sufficient conditions for copositivity

Here we propose two variants of QP-based tests for copositivity, which in a natural way extend to subcones of the nonnegative cone $\mathbb{R}^n_+$.

First note that the feasible set of (2.2), and likewise that of (2.5), may be non-convex (possibly even disconnected) and non-compact. So we avoid solving (2.2) or (2.5), and instead just try finitely many points for obtaining violating vectors. For instance, we can consider the $n$ vertices $\{\mathbf{w}_1, \ldots, \mathbf{w}_n\} \subset \Delta^s \setminus \ker Q_-$ of a subsimplex $\Delta = \operatorname{conv}(\mathbf{w}_1 \ldots, \mathbf{w}_n)$ of $\Delta^s$, and rescale them such that they are (2.2)-feasible: $\mathbf{v}_i^- := \frac{1}{\sqrt{\mathbf{w}_i^\top Q_- \mathbf{w}_i}} \mathbf{w}_i$, $i \in \{1 : n\}$, to see whether (a) in Proposition 2.2 holds. If this fails, we know

$$[\mathbf{v}_i^-]^\top Q_+ [\mathbf{v}_i^-] \geq 1 = [\mathbf{v}_i^-]^\top Q_- [\mathbf{v}_i^-] \quad \text{for all } i \in \{1 : n\} \ , \tag{2.11}$$

but still $\mathbf{v}^\top Q \mathbf{v} < 0$ may be possible for some $\mathbf{v} \in \Delta_{Q_-} = \operatorname{conv}(\mathbf{v}_1^-, \ldots, \mathbf{v}_n^-)$. The latter polytope is again a simplex, but not necessarily contained in $\Delta^s$. Its position depends on the subsimplex $\Delta \subseteq \Delta^s$, and also on the choice of the d.c.d. (2.1). On this simplex we can solve a convex quadratic program easily.

**Theorem 2.8** *Given a subsimplex $\Delta = \operatorname{conv}(\mathbf{w}_1 \ldots, \mathbf{w}_n)$ with vertices $\{\mathbf{w}_1, \ldots \mathbf{w}_n\} \subset \Delta^s \setminus \ker Q_-$, consider the simplex $\Delta_{Q_-} := \operatorname{conv}(\mathbf{v}_1^-, \ldots, \mathbf{v}_n^-)$ with $\mathbf{v}_i^- := \frac{1}{\sqrt{\mathbf{w}_i^\top Q_- \mathbf{w}_i}} \mathbf{w}_i$, and define*

$$r := \min \left\{ [\mathbf{v}_i^-]^\top Q_+ [\mathbf{v}_i^-] : i \in \{1 : n\} \right\} .$$

*If $r < 1$, then $\{\mathbf{w}_1, \ldots, \mathbf{w}_n\}$ contains a violating vector;*
*else ($r \geq 1$) consider the convex quadratic program on $\Delta_{Q_-}$*

$$\mu_\Delta^- := \min \left\{ \mathbf{v}^\top Q_+ \mathbf{v} : \mathbf{v} \in \Delta_{Q_-} \right\} , \tag{2.12}$$

*and denote by $\mathbf{v}_\Delta^-$ an optimal solution of (2.12). Then*

*($a_\Delta$) if $\mu_\Delta^- \geq 1$, then $Q$ is $\Delta$-copositive;*

*($b_\Delta$) if $\mu_\Delta^- < 1$, then $\mathbf{v}_\Delta^- \notin \left\{ \mathbf{v}_1^-, \ldots, \mathbf{v}_n^- \right\}$ (this is also true for $1 \leq \mu_\Delta^- < r$, but irrelevant).*

*Proof* ($\mathrm{a}_\Delta$) is a straightforward consequence of convexity of $\mathbf{x}^\top Q_-\mathbf{x}$ which entails

$$\mathbf{v}^\top Q_-\mathbf{v} \le \max\left\{[\mathbf{v}_i^-]^\top Q_-[\mathbf{v}_i^-] : i \in \{1:n\}\right\} = 1 \quad \text{for all } \mathbf{v} \in \Delta_{Q_-} = \operatorname{conv}(\mathbf{v}_1^-, \ldots, \mathbf{v}_n^-)$$

and therefore $\mathbf{v}^\top Q_+\mathbf{v} \ge \mu_\Delta^- \ge 1 \ge \mathbf{v}^\top Q_-\mathbf{v}$ which implies $\Delta_{Q_-}$-copositivity of $Q$. As we obtained $\Delta_{Q_-}$ from $\Delta$ by scaling the vertices, we have $\mathbb{R}_+\Delta_{Q_-} = \mathbb{R}_+\Delta$ and the result follows.
($\mathrm{b}_\Delta$) follows from $[\mathbf{v}_\Delta^-]^\top Q_+[\mathbf{v}_\Delta^-] = \mu_\Delta^- < r \le [\mathbf{v}_i^-]^\top Q_+[\mathbf{v}_i^-]$ for all $i \in \{1:n\}$. □

Note that, unless by chance a solution $\bar{\mathbf{v}}$ to (2.2) is among $\{\mathbf{v}_1, \ldots, \mathbf{v}_n\}$, in general we do not have $\mu_\Delta^- \le \mu_{\mathrm{dcd}}$, even for the case $\Delta = \Delta^s$, as $\Delta_{Q_-}$ is not contained in the feasible set $C_{Q_-}$ of (2.2).

An anonymous referee made us aware of another interpretation of Theorem 2.8: we rescale the simplex $\Delta$ to the simplex $\Delta_{Q_-}$ such that the concave function $\psi(\mathbf{v}) = -\mathbf{v}^\top Q_-\mathbf{v}$ takes the (constant) value $-1$ on all its vertices $\mathbf{v}_i^-$. The tightest convex underestimator $\overline{\psi}$ of $\psi$ over $\Delta_{Q_-}$ is therefore the constant function $\overline{\psi}(\mathbf{v}) \equiv -1$ (as $\overline{\psi}$ must always be an affine function with the same values at the vertices), and the condition $(a_\Delta)$ is nothing else than the requirement that $\mathbf{v}^\top Q_+\mathbf{v} + \overline{\psi}(\mathbf{v}) \ge 0$ for all $\mathbf{v} \in \Delta_{Q_-}$ which implies, by $\psi(\mathbf{v}) \ge \overline{\psi}(\mathbf{v})$, that $\mathbf{v}^\top Q\mathbf{v} = \mathbf{v}^\top Q_+\mathbf{v} + \psi(\mathbf{v}) \ge 0$, for all $\mathbf{v} \in \Delta_{Q_-}$, and hence $\Delta$-copositivity of $Q$.

We may also minimize $\mathbf{v}^\top Q_+\mathbf{v}$ over a simplex resulting from rescaling vertices in a different way. This gives another convex QP-based sufficient condition for copositivity.

**Theorem 2.9** *Given a subsimplex* $\Delta = \operatorname{conv}(\mathbf{w}_1 \ldots, \mathbf{w}_n)$ *with vertices* $\{\mathbf{w}_1, \ldots, \mathbf{w}_n\} \subset \Delta^s \setminus \ker Q_+$, *consider the simplex* $\Delta_{Q_+} := \operatorname{conv}(\mathbf{v}_1^+, \ldots, \mathbf{v}_n^+)$ *with* $\mathbf{v}_i^+ := \frac{1}{\sqrt{\mathbf{w}_i^\top Q_+\mathbf{w}_i}}\mathbf{w}_i$, *and define*

$$s := \max\left\{[\mathbf{v}_i^+]^\top Q_-[\mathbf{v}_i^+] : i \in \{1:n\}\right\} = r^{-1}\,.$$

*If* $s > 1$, *then* $\{\mathbf{w}_1, \ldots, \mathbf{w}_n\}$ *contains a violating vector*
*else* ($s \le 1$) *consider the convex quadratic program on* $\Delta_{Q_+}$

$$\mu_\Delta^+ := \min\left\{\mathbf{v}^\top Q_+\mathbf{v} : \mathbf{v} \in \Delta_{Q_+}\right\}\,. \tag{2.13}$$

*and denote by* $\mathbf{v}_\Delta^+$ *an optimal solution to (2.13). Then*

*($a_\Delta$) if* $\mu_\Delta^+ \ge s$, *then* $Q$ *is* $\Delta$*-copositive;*

*($b_\Delta$) if* $\mu_\Delta^+ < s$, *then* $\mathbf{v}_\Delta^+ \notin \left\{\mathbf{v}_1^+, \ldots, \mathbf{v}_n^+\right\}$ *(this is also true for* $s \le \mu_\Delta^+ < 1$, *but irrelevant).*

*Proof* The relation $s = r^{-1}$ is evident from the definitions. Again, assertion ($\mathrm{a}_\Delta$) is also a straightforward consequence of convexity of $\mathbf{x}^\top Q_+\mathbf{x}$ and $\mathbf{x}^\top Q_-\mathbf{x}$, which entails

$$\mathbf{v}^\top Q_-\mathbf{v} \le \max\left\{[\mathbf{v}_i^+]^\top Q_-[\mathbf{v}_i^+] : i \in \{1:n\}\right\} = s \quad \text{for all } \mathbf{v} \in \Delta_{Q_+} = \operatorname{conv}(\mathbf{v}_1^+, \ldots, \mathbf{v}_n^+)$$

and therefore $\mathbf{v}^\top Q_+\mathbf{v} \ge \mu_\Delta^+ \ge s \ge \mathbf{v}^\top Q_-\mathbf{v}$ which implies $\Delta_{Q_+}$-copositivity of $Q$. As we obtained $\Delta_{Q_+}$ from $\Delta$ by scaling the vertices, we have $\mathbb{R}_+\Delta_{Q_+} = \mathbb{R}_+\Delta$ and the result follows.
($\mathrm{b}_\Delta$) follows from $[\mathbf{v}_\Delta^+]^\top Q_+[\mathbf{v}_\Delta^+] = \mu_\Delta^+ < 1 = [\mathbf{v}_i^+]^\top Q_+[\mathbf{v}_i^+]$ for all $i \in \{1:n\}$. □

Now, in contrast to the situation in Theorem 2.8, we have $\Delta_{Q_+} \subseteq B_+$, but still cannot infer some relation between $\mu_\Delta^+$ and $\mu_{\mathrm{dcd}}^+$, because (2.4) is a maximization and (2.13) a minimization problem for different objective functions.

Very often in our simulations, the two QP-based tests deliver different violating vectors $\mathbf{v}_\Delta^-$ and $\mathbf{v}_\Delta^+$ if the matrix is not copositive, see for instance Example 2.12 below. For details we refer to Subsection 6.2.

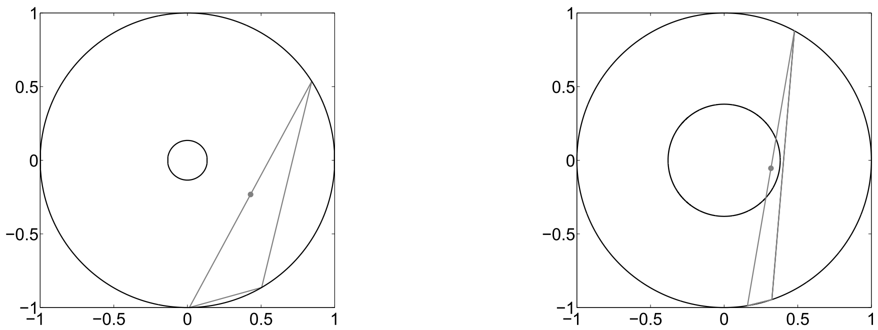


**Fig. 2.2** **(a)** on the left: illustration of Example 2.10. **(b)** on the right: illustration of Example 2.13.

## 2.4 Examples

*Example 2.10* We establish copositivity of the following matrix, a principal submatrix of the matrix from [33, Ex. 1]:

$$Q = \begin{bmatrix} 1 & 0.9 & -0.54 \\ 0.9 & 1 & -0.03 \\ -0.54 & -0.03 & 1 \end{bmatrix}.$$

A d.c.d. of $Q$ is given by

$$Q_+ = \begin{bmatrix} 1.019 & 0.884 & -0.531 \\ 0.884 & 1.014 & -0.038 \\ -0.531 & -0.038 & 1.005 \end{bmatrix} \quad \text{and} \quad Q_- = \begin{bmatrix} 0.019 & -0.016 & 0.009 \\ -0.016 & 0.014 & -0.008 \\ 0.009 & -0.008 & 0.005 \end{bmatrix}$$

(this is a rounded version of the so-called spectral d.c.d., see Section 3 below). This results for $\Delta = \Delta^s$ in the vectors

$$[\mathbf{v}_1^-, \mathbf{v}_2^-, \mathbf{v}_3^-] \approx \begin{bmatrix} 7.355 & 0 & 0 \\ 0 & 8.613 & 0 \\ 0 & 0 & 14.821 \end{bmatrix}$$

and the value $r \approx 55.097$, while $\mu_\Delta^- \approx 22.503$, and thus $Q$ is copositive according to Theorem 2.8. Theorem 2.9 yields $s = 1/r \approx 0.018$ as compared to $\mu_\Delta^+ \approx 0.238$, which also establishes copositivity. In Fig. 2.2(a) we plot a projection of the eigencoordinates $y_i$, ordered with increasing eigenvalues and scaled by the eigenvalues, such that $\mathbf{v}^\top Q_+ \mathbf{v} = y_2^2 + y_3^2$. The triangle represents $\Delta_{Q_+} = \operatorname{conv}(\mathbf{v}_1^+, \mathbf{v}_2^+, \mathbf{v}_3^+)$. The outer circle is the projection of the level set $\mathbf{v}^\top Q_+ \mathbf{v} = 1$ and contains $\{\mathbf{v}_1^+, \mathbf{v}_2^+, \mathbf{v}_3^+\}$, whereas the inner circle is the projection of the level set $\mathbf{v}^\top Q_+ \mathbf{v} = s$. As the triangle does not intersect the inner circle, the matrix is copositive. The solution $\mathbf{v}_\Delta^+$ of (2.13) at the boundary of the triangle is also indicated. Copositivity can also be shown using Theorem 2.6 with $\mathbf{x} \approx [0.5, 1.3, 1.3]^\top$ obtained by solving (2.9) for $\mathbf{f} = Q_+\mathbf{e}$, with $\mathbf{p} \approx [1, 1.8, 1]^\top$. Condition (2.8) is satisfied:

$$(\mathbf{x}^\top Q_+ \mathbf{x}) \operatorname{diag} Q_- \approx [0.08, 0.06, 0.02]^\top \le [1, 3.07, 1]^\top \approx [(Q_+\mathbf{x})_1^2, (Q_+\mathbf{x})_2^2, (Q_+\mathbf{x})_3^2]^\top.$$

*Example 2.11* The matrix

$$Q = \begin{bmatrix} 1 & 2 & -2 \\ 2 & 1 & -1 \\ -2 & -1 & 5 \end{bmatrix}$$

shows that the two QP-based tests are not completely symmetric. Again using the spectral d.c.d., we get $\mu^-_\Delta \approx 1.280 > 1$ for $\Delta = \Delta^s$, the matrix $Q$ is copositive according to Theorem 2.8. Indeed, $Q$ is the sum of a positive-semidefinite matrix and a nonnegative matrix:

$$Q = \begin{bmatrix} 1 & 0 & -2 \\ 0 & 1 & -1 \\ -2 & -1 & 5 \end{bmatrix} + \begin{bmatrix} 0 & 2 & 0 \\ 2 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} .$$

But $\mu^+_\Delta \approx 0.169 < 0.382 \approx s$, and hence the sufficient copositivity criterion of Theorem 2.9 is not satisfied. For this matrix also the sufficient LP-test with an $\mathbf{x}$ gained by solving (2.9) for $\mathbf{f} = Q_+\mathbf{e}$ fails.

*Example 2.12* Consider

$$Q = \begin{bmatrix} 1 & 1.63 & 1 & -0.77 & -0.67 \\ 1.63 & 1 & 0 & 0.32 & -0.82 \\ 1 & 0 & 1 & -0.26 & -0.67 \\ -0.77 & 0.32 & -0.26 & 1 & 0.77 \\ -0.67 & -0.82 & -0.67 & 0.77 & 1 \end{bmatrix} .$$

The QP-test of Theorem 2.8 delivers the optimal solution to (2.12)

$$\mathbf{v}^-_\Delta \approx [0.2, 0.18, 0.17, 0, 0.45]^\top \quad \text{with} \quad [\mathbf{v}^-_\Delta]^\top Q[\mathbf{v}^-_\Delta] \approx 0.13 > 0\,.$$

But Problem (2.13) of Theorem 2.9 gives a violating vector:

$$\mathbf{v}^+_\Delta = [0, 0.26, 0.3, 0, 0.44]^\top \quad \text{with} \quad [\mathbf{v}^+_\Delta]^\top Q[\mathbf{v}^+_\Delta] \approx -0.01 < 0\,.$$

Of course, the LP-based test failed before.

*Example 2.13* For the matrix

$$Q = \begin{bmatrix} 3 & 2 & -2 \\ 2 & 1 & -1 \\ -2 & -1 & 2 \end{bmatrix}$$

copositivity can be shown using the LP-based test (with $\mathbf{f} = Q_+\mathbf{e}$ delivering $\mathbf{x} \approx [0.94, 1.12, 2]^\top$) as well as the sufficient criterion of Theorem 2.8. The matrix is indeed copositive as it can be written as

$$Q = \begin{bmatrix} 3 & 1 & -2 \\ 1 & 1 & -1 \\ -2 & -1 & 2 \end{bmatrix} + \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} .$$

However evaluating the criterion in Theorem 2.9 for $\Delta = \Delta^s$ leads to $\mu^+_\Delta \approx 0.10 < 0.15 \approx s$, as illustrated in Fig. 2.2(b). The projected solution $\mathbf{v}^+_\Delta$ now lies inside the inner circle, and this sufficient criterion fails.

## 2.5 Outline of the algorithm

Now let us reconsider the conditions in Subsection 2.3. First suppose we always obtain case $(\mathrm{a}_\Delta)$ in Theorems 2.8 or 2.9 for a collection of simplices $\Delta$ which together cover $\Delta^s$. Then we can infer copositivity of $Q$ because of the next observation (note that the assumption there is satisfied if $\Delta^s = \cup_{i\in I}\Delta_i$):

**Proposition 2.14** *Assume we have a family of nonempty $\varDelta_i$ (for $i$ from some index set $I$) with*

$$\mathbb{R}^n_+ = \bigcup_{i\in I} \mathbb{R}_+ \varDelta_i \ .$$

*Then $Q$ is copositive if and only if $Q$ is $\varDelta_i$-copositive for all $i \in I$.*

*Proof* follows from [23, Lemma 2.1]. □

If, however, we arrive at case ($b_\varDelta$) in both Theorems 2.8 and 2.9 for some $\varDelta$ in this collection, we may use both $\mathbf{v}^+_\varDelta$ and $\mathbf{v}^-_\varDelta$ as new trial points for violating vectors, i.e. check whether

$$\sigma_\varDelta := \min\left\{[\mathbf{v}^-_\varDelta]^\top Q[\mathbf{v}^-_\varDelta], [\mathbf{v}^+_\varDelta]^\top Q[\mathbf{v}^+_\varDelta]\right\} < 0\,. \tag{2.14}$$

If this is not the case, we have to continue our investigations with the help of the trial point with lower $\mathbf{v}^\top Q\mathbf{v}$, i.e., choose

$$\mathbf{v}_\varDelta \in \left\{\mathbf{v}^-_\varDelta, \mathbf{v}^+_\varDelta\right\} \quad \text{such that} \quad \mathbf{v}^\top_\varDelta Q\mathbf{v}_\varDelta = \sigma_\varDelta\,. \tag{2.15}$$

Suppose now that the LP-based test of Subsection 2.2 fails, and that the trial point $\mathbf{v}_\varDelta$ defined via (2.14) and (2.15) is not a violating vector, so that $\mathbf{v}^\top_\varDelta Q\mathbf{v}_\varDelta \geq 0$. As this vector still minimizes the positive part $\mathbf{v}^\top Q_+\mathbf{v}$ over $\varDelta_{Q_+}$ or $\varDelta_{Q_-}$, it seems reasonable to rescale it to a vector

$$\bar{\mathbf{w}} := \frac{1}{\mathbf{e}^\top\mathbf{v}_\varDelta}\,\mathbf{v}_\varDelta \in \varDelta^s\,. \tag{2.16}$$

This point will be used for subdivision of $\varDelta$. A very rough and inexact outline of our algorithm follows (most of the conditions will be made precise in the sequel, and also the algorithm will be presented in more detail in Section 5.2); the terminology "a test fails on $\varDelta$" is short for the situation where it neither delivers a certificate for $\varDelta$-copositivity nor a violating vector (in $\varDelta$).

**Sketch of algorithm**

Input: Matrix $Q$ with a d.c.d. $Q = Q_+ - Q_-$.

Output: Either a copositivity guarantee for $Q$ or a violating vector (a certificate for non-copositivity).

0.) Put $\varDelta = \varDelta^s = \operatorname{conv}(\mathbf{e}_1, \dots, \mathbf{e}_n)$, the columns of $I_n$.
1.) Run the tests on $\varDelta = \operatorname{conv}(\mathbf{w}_1, \dots, \mathbf{w}_n)$; if all tests fail on $\varDelta$ and $\sigma_\varDelta \geq 0$ (2.14), use the point $\bar{\mathbf{w}}$ defined in (2.16) for *$\omega$-subdivision* as follows:

$$\varDelta = \bigcup_{i=1}^n \varDelta_i \quad \text{with} \quad \varDelta_i = \operatorname{conv}\left(\{\bar{\mathbf{w}}\} \cup \{\mathbf{w}_j : j \neq i\}\right)\ ,\ i \in \{1:n\}\ ;$$

replace $\varDelta$ with all full-dimensional subsimplices $\varDelta_i$, and repeat from 1.) on all $\varDelta_i$.

*Example 2.15* We continue Example 2.13. Let us for presentational purposes assume we only use the sufficient criterion of Theorem 2.9, and hence copositivity of $Q$ is not yet established. In this case we may subdivide $\varDelta^s$ using

$$\bar{\mathbf{w}} := \frac{1}{\mathbf{e}^\top\mathbf{v}^+_\varDelta}\mathbf{v}^+_\varDelta \approx [0.45, 0, 0.55]^\top\ ,$$

which is the minimal solution $\mathbf{v}^+_\varDelta$ reprojected to the standard simplex. We get two full-dimensional successor simplices, $\varDelta_1 := \operatorname{conv}(\mathbf{e}_2, \mathbf{e}_3, \bar{\mathbf{w}})$ and $\varDelta_3 := \operatorname{conv}(\mathbf{e}_1, \mathbf{e}_2, \bar{\mathbf{w}})$, and a flat one, $\varDelta_2$, see Fig. 2.3(a). Solving Problem (2.13) we get $\mu^+_{\varDelta_1} \approx 0.162 > 0.145 \approx s$ so that $Q$ is $\varDelta_1$-copositive, and $\mu^+_{\varDelta_3} \approx 0.661 > 0.145 \approx s$ which entails $\varDelta_3$-copositivity of $Q$, see Fig. 2.4. We conclude that $Q$ is $\mathbb{R}^3_+$-copositive.


**Fig. 2.3** **(a)** on the left: subdivision for Example 2.15; **(b)** on the right: $\omega$-subdivision for Example 2.16.

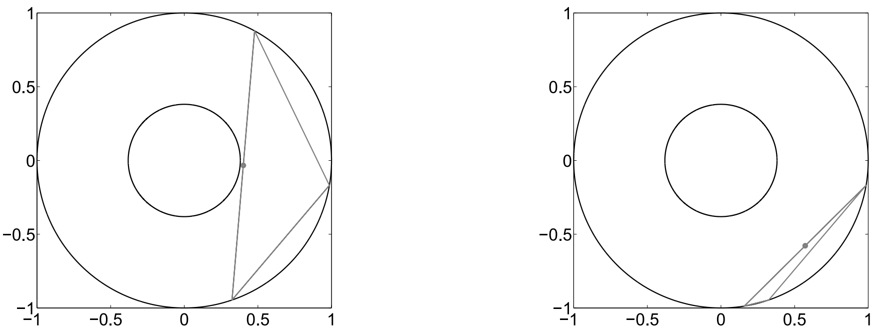


**Fig. 2.4** Subdivision for Example 2.15; **(a)** on the left: subsimplex $\Delta_1$; **(b)** on the right: subsimplex $\Delta_3$.

*Example 2.16* We investigate the matrix

$$Q = \begin{bmatrix} 2 & -3 & 5 \\ -3 & 1 & -2 \\ 5 & -2 & 2 \end{bmatrix} .$$

which is not copositive as $\mathbf{v} = [0, 0.6, 0.4]^\top \in \Delta^s$ is violating (see also Example 4.6 below). Indeed, the solution of (2.13) for $\Delta^s$ yields a point $\mathbf{v}_\Delta^+$ which results in $\bar{\mathbf{w}} = \frac{1}{\mathbf{e}^\top \mathbf{v}_\Delta^+} \mathbf{v}_\Delta^+ = [0.33, 0.61, 0.07]^\top$, see Fig. 2.3(b). This is a violating vector: $\bar{\mathbf{w}}^\top Q \bar{\mathbf{w}} \approx -0.55 < 0$.

The idea of partitioning is already used in [14] for a branch-and-bound copositivity test. There, the authors employ bisections (i.e. subdivision w.r.t. the mid-point of an edge) always on the longest edge between two vertices $\mathbf{w}_i$ and $\mathbf{w}_j$ for which $\mathbf{w}_i^\top Q \mathbf{w}_j < 0$ holds. They combine two subdivision strategies: the convergence-generating one is taking the midpoint on this edge (halving the edge), while the data-driven one is determined by the minimum of the function

$$\varphi(t) = [t\mathbf{w}_i + (1-t)\mathbf{w}_j]^\top Q \, [t\mathbf{w}_i + (1-t)\mathbf{w}_j] \ . \tag{2.17}$$

So all division points lie on the edges of subsimplices $\Delta$. In the method proposed here also subdivisions using an interior point of a subsimplex $\Delta$ are possible. Both methods have in common that they concentrate on interesting regions of the standard simplex $\Delta^s$ in a data-driven way. However, a problem is solved at the root by the method of [14] only if $Q$ has no negative entries. This is in contrast to our method, see, e.g. Subsection 2.4.

## 3 The choice of a d.c. decomposition

We shortly discuss the choice of the d.c.d. used in the preceding section. Recall that a d.c.d. $Q = Q_+ - Q_-$ is called *undominated* if there is no other d.c.d. $Q = Q'_+ - Q'_-$ such that $Q_\pm - Q'_\pm$ are positive-semidefinite. Undominated d.c.d.s for quadratic optimization problems were introduced, discussed and characterized in [11]. For instance, it is shown [11, Theorem 4] that if $Q$ is indefinite, there always exist infinitely many undominated d.c.d.s. Undominatedness favors the construction of tighter bounds for the StQP (1.1) on the standard simplex, so we expect that an undominated d.c.d. will be more efficient in copositivity detection. Here, we have implemented the most popular undominated d.c.d., the so-called *spectral d.c.d.* which is constructed as follows:

Take an orthonormal basis of eigenvectors $\mathbf{u}_i$ of $Q$ to the eigenvalues $\lambda_i$, $i \in \{1 : n\}$ (we may sort them in increasing order if needed). Define $\gamma_+ := \max\{0, \gamma\}$ for a number $\gamma$ and $\Lambda_+ := \mathrm{Diag}\,[(\lambda_i)_+]_i$, the $n \times n$ diagonal matrix containing the positive parts of the eigenvalues. Collect the columns $\mathbf{u}_i$ in an orthonormal $n \times n$ matrix $U$. Then $Q_+ := U\Lambda_+ U^\top$ and $Q_- := Q_+ - Q$ are both positive-semidefinite but singular if $Q$ is indefinite.

The spectral d.c.d. $Q = Q_+ - Q_-$ is undominated and dominates all other d.c.d.s which commute with $Q$ [11, Corollary 3]. One may wonder whether this choice of d.c.d. must be repeated on the subsimplices $\Delta_{Q_-}$ (or $\Delta_{Q_+}$ respectively). Indeed, we can rephrase for instance the program (2.12) as an StQP using the $n \times n$ matrix $V := [\mathbf{v}_1^-, \ldots, \mathbf{v}_n^-]$ as follows (note that if $\Delta$ is spanned by linearly independent $\mathbf{w}_1, \ldots, \mathbf{w}_n$, then $V$ is nonsingular): any $\mathbf{v} \in \Delta_{Q_-}$ can be written in barycentric coordinates w.r.t. $V$, i.e., $\mathbf{v} = V\mathbf{x}$ for some $\mathbf{x} \in \Delta^s$, so that

$$\mu_\Delta^- = \min\left\{\mathbf{x}^\top Q_+^\Delta \mathbf{x} : \mathbf{x} \in \Delta^s\right\} = \alpha_{Q_+^\Delta} \quad \text{with} \quad Q_\pm^\Delta := V^\top Q_\pm V\,. \tag{3.1}$$

Now compare the feasible sets of (2.2) and (2.12): the non-convex quadratic constraint $\mathbf{v}^\top Q_- \mathbf{v} = 1$ is replaced with the linear constraint $\mathbf{v} \in \Delta_{Q_-}$ in (2.12). Similarly (recall $\mathbf{x}^\top Q_-^\Delta \mathbf{x} = \mathbf{v}^\top Q_- \mathbf{v}$), the StQP (3.1) is used to approximate the problem

$$\mu_{\mathrm{dcd}}^\Delta := \inf\left\{\mathbf{x}^\top Q_+^\Delta \mathbf{x} : \mathbf{x}^\top Q_-^\Delta \mathbf{x} = 1\,,\ \mathbf{x} \in \mathbb{R}_+^n\right\}\,.$$

We now show that sandwiching transforms an undominated d.c.d. again into an undominated one, so that

$$Q^\Delta = V^\top Q V = V^\top Q_+ V - V^\top Q_- V = Q_+^\Delta - Q_-^\Delta \tag{3.2}$$

is undominated if $Q_\pm$ result by the spectral d.c.d. Unless $Q^\Delta Q_\pm^\Delta = Q_\pm^\Delta Q^\Delta$, the d.c.d (3.2) is *not* the spectral d.c.d. of $Q^\Delta$.

**Theorem 3.1** *Suppose that $V$ is a nonsingular $n \times n$ matrix. Then sandwiching an undominated d.c.d. $Q = Q_+ - Q_-$ by $V$ yields again an undominated d.c.d. $V^\top Q V = V^\top Q_+ V - V^\top Q_- V$.*

*Proof* First we note that for any $B \in \mathcal{S}^n$ we have $\ker V^\top B V = V^{-1}(\ker B)$. Next denote by

$$K_\pm = \ker Q_\pm \quad \text{and} \quad K_\pm^V = \ker(V^\top Q_\pm V) = V^{-1}(K_\pm)\,.$$

From [11, Theorem 1] we know that $K_+ + K_- = \mathbb{R}^n$, so that also

$$K_+^V + K_-^V = V^{-1}(K_+) + V^{-1}(K_-) = V^{-1}(K_+ + K_-) = V^{-1}(\mathbb{R}^n) = \mathbb{R}^n\,.$$

Hence, employing [11, Theorem 1] again, we deduce that $V^\top Q V = V^\top Q_+ V - V^\top Q_- V$ is an undominated d.c.d. $\square$

| | $\varepsilon=0$ | | $\varepsilon=0.001$ | | $\varepsilon=0.01$ | | $\varepsilon=0.1$ | |
|---|---|---|---|---|---|---|---|---|
| | $N$ | $\mathrm{cond}(Q_+^{\gamma,\varepsilon})$ | $N$ | $\mathrm{cond}(Q_+^{\gamma,\varepsilon})$ | $N$ | $\mathrm{cond}(Q_+^{\gamma,\varepsilon})$ | $N$ | $\mathrm{cond}(Q_+^{\gamma,\varepsilon})$ |
| $\gamma=\alpha$ | 14 | $73.88\cdot 10^{15}$ | 26 | $24.68\cdot 10^{3}$ | 43 | 2468.5 | 60 | 247.75 |
| $\gamma=2$ | 1061 | 57.83 | 1045 | 57.69 | 1059 | 56.53 | 1112 | 47.04 |
| $\gamma=4$ | 1316 | 57.83 | 1412 | 57.69 | 1429 | 56.53 | 1409 | 47.04 |
| $\gamma=6$ | 1661 | 83.01 | 1811 | 82.82 | 1926 | 81.13 | 2083 | 67.44 |
| $\gamma=8$ | 1657 | 112.05 | 1686 | 111.79 | 1978 | 109.50 | 2579 | 90.96 |
| $\gamma=10$ | 2552 | 141.08 | 2567 | 140.76 | 2620 | 137.88 | 3523 | 114.49 |

**Table 3.1** Results for different d.c.d.s of $Q$ from (3.3); see text.

There is only one obstacle in applying Theorems 3.1, 2.8 and 2.9: we need to assume that the vertices of $\varDelta$ are not contained in $\ker Q_-$ and $\ker Q_+$ respectively. Recall that $Q$ is $\varDelta$-copositive for sure if $\varDelta \subseteq \ker Q_-$, On the other hand, any vector in $\varDelta \cap \ker Q_+ \setminus \ker Q_-$ is a violating one. We treat a slightly more general case in Lemma 4.5 below.

Small values of $\mathbf{w}_i^\top Q_- \mathbf{w}_i$ suggest that $\mathbf{w}_i$ is not close to a violating vector. Numerically speaking, the scaling of vertices $\mathbf{w}_i$ even close to $\ker Q_-$ and $\ker Q_+$, so that $\mathbf{w}_i^\top Q_\pm \mathbf{w}_i < \varepsilon$, could be problematic for small $\varepsilon$. A robustification step avoiding this is discussed in Subsection 5.1 below. The experimental design in the following example resembles this on a macroscopic level with larger $\varepsilon$.

*Example 3.2* To examine the significance of choice of an undominated d.c.d., and also to corroborate the choice of the spectral d.c.d. among all undominated d.c.d.s, we run numerical tests with the copositive matrix $Q$ [41] given by

$$Q = \begin{bmatrix} 1 & -1 & 1 & 2 & -3 \\ -1 & 2 & -3 & -3 & 4 \\ 1 & -3 & 5 & 6 & -4 \\ 2 & -3 & 6 & 5 & -8 \\ -3 & 4 & -4 & -8 & 16 \end{bmatrix}. \tag{3.3}$$

Let $\lambda_1 < 0 < \lambda_2 \le \lambda_3 \le \lambda_4 \le \lambda_5$ denote the ordered eigenvalues of $Q$ and $U$ the orthonormal matrix of respective eigenvectors. Let $\alpha = \lambda_2 \approx 0.2828$ and $\beta = -\lambda_1 \approx 1.7520$. Then an infinite number of undominated d.c.d.s is given by [11, Theorem 4] $Q_+(\gamma) := UB(\gamma)U^\top$ and $Q_-(\gamma) := Q_+(\gamma) - Q$ for $\gamma \ge \alpha$, where $B(\gamma)$ is defined by

$$B(\gamma) := \begin{bmatrix} \frac{\beta}{\alpha}\gamma - \beta & \sqrt{\beta}\sqrt{\gamma^2/\alpha - \gamma} & 0 & 0 & 0 \\ \sqrt{\beta}\sqrt{\gamma^2/\alpha - \gamma} & \gamma & 0 & 0 & 0 \\ 0 & 0 & \lambda_3 & 0 & 0 \\ 0 & 0 & 0 & \lambda_4 & 0 \\ 0 & 0 & 0 & 0 & \lambda_5 \end{bmatrix}.$$

For $\gamma = \alpha$ we obtain the undominated spectral d.c.d. $Q_+(\alpha)$, $Q_-(\alpha)$. Dominated positive definite d.c.d.s are generated by a rank-one update: $Q_+(\gamma) + \varepsilon E_n$ and $Q_-(\gamma) + \varepsilon E_n$ for $\varepsilon > 0$. Table 3.1 shows the number $N$ of subsimplices which have to be considered in the procedure as presented in Subsection 2.5 and $\mathrm{cond}(Q_+^{\gamma,\varepsilon})$ gives the condition numbers of the matrices $Q_+^{\gamma,\varepsilon} := Q_+(\gamma) + \varepsilon E_n$.

In most cases, using dominated d.c.d.s significantly increases the number $N$ of used subsimplices. For other undominated d.c.d.s than the spectral d.c.d. also much more subsimplices have to be considered which supports our choice of the spectral d.c.d. This result is confirmed by repeating the above test with other, also noncopositive matrices. However, for the famous Horn matrix [25]

$$H = \begin{bmatrix} 1 & -1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 & 1 \end{bmatrix}, \tag{3.4}$$

| | $\varepsilon = 0$ | | $\varepsilon = 0.001$ | | $\varepsilon = 0.01$ | | $\varepsilon = 0.1$ | |
|---|---|---|---|---|---|---|---|---|
| | $N$ | $\mathrm{cond}(H_+^{\gamma,\varepsilon})$ | $N$ | $\mathrm{cond}(H_+^{\gamma,\varepsilon})$ | $N$ | $\mathrm{cond}(H_+^{\gamma,\varepsilon})$ | $N$ | $\mathrm{cond}(H_+^{\gamma,\varepsilon})$ |
| $\gamma = \alpha$ | 3711 | $268.76 \cdot 10^{15}$ | 5691 | 3237.1 | 5905 | 324.61 | 6179 | 33.36 |
| $\gamma = 2$ | 2737 | $358.04 \cdot 10^{14}$ | 2416 | 3237.1 | 2935 | 324.61 | 2805 | 33.36 |
| $\gamma = 4$ | 3342 | $412.57 \cdot 10^{15}$ | 3200 | 4001.0 | 3536 | 401.00 | 3516 | 41.00 |
| $\gamma = 6$ | 3101 | $504.45 \cdot 10^{14}$ | 2832 | 6181.3 | 3006 | 619.03 | 4652 | 62.80 |
| $\gamma = 8$ | 3923 | $894.25 \cdot 10^{13}$ | 4142 | 8653.5 | 4003 | 866.25 | 4715 | 87.52 |
| $\gamma = 10$ | 4759 | $373.18 \cdot 10^{14}$ | 4650 | 11125.6 | 4754 | 1113.46 | 4950 | 112.25 |

**Table 3.2** Results for different d.c.d.s of the Horn matrix $H$ from (3.4); see text.

other undominated d.c.d.s demanded less subsimplex evaluations, for the results see Table 3.2. Still, the results for the dominated d.c.d.s tend to be worse. The particular behavior of the Horn matrix is further discussed in Subsection 6.1.

## 4 Preprocessing for a copositivity test

### 4.1 Simple sign tests and diagonal normalization

We start with some simple sign tests, which we collect in a lemma for easy reference. Most of these are well known since long, see, e.g. [40].

**Lemma 4.1** *Let $Q = [q_{ij}] \in \mathcal{S}^n$ and choose an arbitrary $i \in \{1:n\}$.*

*(a) If $q_{ii} < 0$, then $\mathbf{v} = \mathbf{e}_i$ is a violating vector;*
*(b) if $q_{ii} = 0 > q_{ij}$ for some $j \in \{1:n\}$, then $\mathbf{v} = (q_{jj}+1)\mathbf{e}_i - q_{ij}\mathbf{e}_j$ is a violating vector;*
*(c) if $q_{ij} \geq 0$ for all $j \in \{1:n\}$, then*
*$Q$ is copositive if and only if $R := [q_{jk}]_{j\neq i, k\neq i} \in \mathcal{S}^{n-1}$ is copositive;*
*further, if $\mathbf{u} = [u_j]_{j\neq i} \in \mathbb{R}^{n-1}_+$ is a violating vector for $R$,*
*then $v_i = 0$ and $v_j = u_j$ for $j \neq i$ defines a violating vector $\mathbf{v} \in \mathbb{R}^n_+$ for $Q$.*

*Proof* is evident by straightforward calculation. □

Therefore, we can eliminate nonnegative rows and concentrate on the reduced matrix. However, as the example of the $2 \times 2$ permutation matrix $Q \neq I_2$ and its d.c.d. shows, deleting the first row and column of an undominated d.c.d. does not always yield an undominated d.c.d. of the smaller matrix. So one has to balance the advantage of dimension reduction with the additional effort of a new spectral decomposition and we decided here to use nonnegative row/column elimination only at the root of the branch-and-bound-algorithm.

If copositivity of the reduced matrix (which we for convenience of notation still denote by $Q \in \mathcal{S}^n$) is still unclear, $Q$ must have strictly positive diagonal entries and at least one negative off-diagonal entry in every row. The next test is a dominance test for these off-diagonal entries. Finally, we normalize $Q$ such that the diagonal is equal to $\mathbf{e}$ (see also [33] and Remark 1.1 and 1.2 in [42]).

**Lemma 4.2** *Let $Q = [q_{ij}] \in \mathcal{S}^n$ with strictly positive diagonal.*

*(a) $Q$ is copositive if and only if $DQD$ is copositive where $D \in \mathcal{S}^n$ is a positive-definite diagonal matrix; if $\mathbf{w} \in \mathbb{R}^n_+$ is a violating vector for $DQD$, then $\mathbf{v} = D\mathbf{w} \in \mathbb{R}^n_+$ is violating for $Q$.*

*(b) $Q$ is copositive if and only if*

$$Q' = \left[\frac{q_{ij}}{\sqrt{q_{ii}q_{jj}}}\right]$$

*is copositive. We have* $\operatorname{diag} Q' = \mathbf{e}$.

*(c) If $q_{ij} < -\sqrt{q_{ii}q_{jj}}$, then $\mathbf{v} = q_{ii}^{-1/2}\mathbf{e}_i + q_{jj}^{-1/2}\mathbf{e}_j$ is a violating vector.*

*Proof* (a) is straightforward to verify, noting that $D(\mathbb{R}^n_+) = \mathbb{R}^n_+$. (b) follows from (a) by putting $D = \operatorname{Diag}\,[q_{ii}^{-1/2}]_i$. To prove (c), we now may and do work with $Q'$ from (b) instead of $Q$. But $\mathbf{w} = D^{-1}\mathbf{v} = (\mathbf{e}_i + \mathbf{e}_j)$ is easily seen to be a violating vector for $Q'$. □

Again, Theorem 3.1 ensures that the spectral (or any undominated) d.c.d. $Q = Q_+ - Q_-$ gives an undominated d.c.d. $DQD = DQ_+D - DQ_-D$ which in general is *not* the spectral d.c.d. for $DQD$. Anyhow, we thus need not determine the spectral d.c.d. for the normalized $Q'$ anew. Although it has no immediate consequences for our implementation, it is instructive to see what happens on a subsimplex $\Delta = \operatorname{conv}(\mathbf{w}_1, \dots, \mathbf{w}_n)$ where $Q$ is replaced with $Q^\Delta$ (with strictly positive diagonal), and then $Q^\Delta$ is rescaled as above to $(Q^\Delta)'$ with $\operatorname{diag}\,(Q^\Delta)' = \mathbf{e}$. It turns out that in effect we rather rescale the original quadratic form and minimize the convex part on the subsimplex generated by $\mathbf{z}_i$ which are rescaled from the $\mathbf{w}_i$ by requiring $\mathbf{z}_i^\top Q\mathbf{z}_i = 1$.

**Proposition 4.3** *Let a subsimplex $\Delta = \operatorname{conv}(\mathbf{w}_1, \dots, \mathbf{w}_n)$ be given with linearly independent vertices $\{\mathbf{w}_1, \dots, \mathbf{w}_n\} \subset \Delta^s \setminus \ker Q_-$. Let $Q^\Delta = V^\top QV$ with $V = [\mathbf{v}_1^-, \dots, \mathbf{v}_n^-]$, $\mathbf{v}_i^- = \frac{1}{\sqrt{\mathbf{w}_i^\top Q_-\mathbf{w}_i}}\mathbf{w}_i$ and $(Q^\Delta)' = D^\top Q^\Delta D$ with $D = \operatorname{Diag}\,[(q_{ii}^\Delta)^{-1/2}]_i$. Suppose that $q_{ii}^\Delta = [\mathbf{v}_i^-]^\top Q[\mathbf{v}_i^-] > 0$ for all $i \in \{1:n\}$. Then Problem (2.12) for $(Q^\Delta)'$ yields the same value as*

$$\min\left\{\mathbf{z}^\top Q_+\mathbf{z} : \mathbf{z} \in \operatorname{conv}(\mathbf{z}_1, \dots, \mathbf{z}_n)\right\}, \tag{4.1}$$

*where $\mathbf{z}_i \in \mathbb{R}^n_+$ with $\mathbf{z}_i^\top Q\mathbf{z}_i = 1$ are scaled from $\mathbf{w}_i$ by $\mathbf{z}_i := \frac{1}{\sqrt{\mathbf{w}_i^\top Q\mathbf{w}_i}}\mathbf{w}_i$ for all $i \in \{1:n\}$.*

*Proof* First note that $0 < q_{ii}^\Delta = \frac{\mathbf{w}_i^\top Q\mathbf{w}_i}{\mathbf{w}_i^\top Q_-\mathbf{w}_i}$ by assumption so that $\mathbf{z}_i$ are well defined. We obtain the undominated d.c.d. (recall Theorem 3.1)

$$(Q^\Delta)' = D^\top V^\top QVD = D^\top V^\top Q_+VD - D^\top V^\top Q_-VD = (Q^\Delta)'_+ - (Q^\Delta)'_-\,,$$

so that the vertices for the feasible set of Problem (2.12) for $(Q^\Delta)'$ are $\mathbf{z}_i = (VD)\mathbf{e}_i$. Using the definitions of $D$ and $V$ as well as the definitions of $q_{ii}^\Delta$ (see above) and $\mathbf{v}_i^-$, we obtain

$$\mathbf{z}_i = (VD)\mathbf{e}_i = V\left(\frac{1}{\sqrt{q_{ii}^\Delta}}\,\mathbf{e}_i\right) = \frac{1}{\sqrt{q_{ii}^\Delta}}\,\mathbf{v}_i^- = \sqrt{\frac{\mathbf{w}_i^\top Q_-\mathbf{w}_i}{\mathbf{w}_i^\top Q\mathbf{w}_i}}\,\frac{1}{\sqrt{\mathbf{w}_i^\top Q_-\mathbf{w}_i}}\,\mathbf{w}_i = \frac{1}{\sqrt{\mathbf{w}_i^\top Q\mathbf{w}_i}}\,\mathbf{w}_i\,.$$

Hence the result. □

Note that we cannot easily transfer the proof of Theorem 2.8 to infer $\Delta$-copositivity of $Q$ from the fact that the optimal value in (4.1) is not exceeding one, since the quadratic function $\mathbf{z}^\top Q\mathbf{z}$ is non-convex, so we cannot control the condition $\mathbf{z}^\top Q\mathbf{z} \le 1$ as $\mathbf{z}$ ranges over $\operatorname{conv}(\mathbf{z}_1, \dots, \mathbf{z}_n)$.

4.2 Truncating positive off-diagonal entries

So, after these sign and dominance tests and after normalization we end up with a matrix (again denoted by $Q$ rather than $Q'$) with unity on the diagonal, all negative entries not smaller than $-1$, and at least one negative entry per row. In [28] it was shown that a matrix $Q$ with $\operatorname{diag} Q = \mathbf{e}$ remains copositive if each off-diagonal entry $q_{ij}$ is replaced by $\min\{q_{ij}, 1\}$. Collecting somehow scattered and implicit arguments in [28], we construct a violating vector in an explicit way here, apparently for the first time in literature.

**Lemma 4.4** *Let*

$$Q = \begin{bmatrix} 1 & \mathbf{b}^\top & q_{1n} \\ \mathbf{b} & A & \mathbf{c} \\ q_{1n} & \mathbf{c}^\top & 1 \end{bmatrix} \in \mathcal{S}^n$$

*with diagonal equal to* $\mathbf{e}$ *and off-diagonal entry* $q_{1n} > 1$*. Then the matrix*

$$M := \begin{bmatrix} 1 & \mathbf{b}^\top & 1 \\ \mathbf{b} & A & \mathbf{c} \\ 1 & \mathbf{c}^\top & 1 \end{bmatrix} \in \mathcal{S}^n$$

*is copositive if and only if* $Q$ *is copositive. If* $\mathbf{v} = [v_1, \mathbf{a}^\top, v_n]^\top \in \mathbb{R}^n_+$ *is a violating vector to* $M$*, then*

$$\mathbf{w} := \begin{cases} \left[\max\{0, -\mathbf{a}^\top \mathbf{b}\}, \mathbf{a}^\top, 0\right]^\top & \text{if } \mathbf{a}^\top \mathbf{b} \le \mathbf{a}^\top \mathbf{c}, \\ \left[0, \mathbf{a}^\top, \max\{0, -\mathbf{a}^\top \mathbf{c}\}\right]^\top & \text{if } \mathbf{a}^\top \mathbf{b} > \mathbf{a}^\top \mathbf{c} \end{cases}$$

*is a violating vector to* $Q$*.*

*Proof* Necessity is proved in [28, Theorem 1], while sufficiency is immediate noting that $Q$ is the sum of $M$ and a nonnegative matrix.

Let $\mathbf{v}$ be a violating vector to $M$, i.e.

$$0 > \mathbf{v}^\top M \mathbf{v} = v_1^2 + \mathbf{a}^\top A \mathbf{a} + v_n^2 + 2v_1 v_n + 2v_1 \mathbf{a}^\top \mathbf{b} + 2v_n \mathbf{a}^\top \mathbf{c} \ge [v_1 + v_n + \gamma_\mathbf{v}]^2 + \mathbf{a}^\top A \mathbf{a} - \gamma_\mathbf{v}^2$$

for $\gamma_\mathbf{v} := \min\{\mathbf{a}^\top \mathbf{b}, \mathbf{a}^\top \mathbf{c}\}$. We therefore obtain

$$\mathbf{a}^\top A \mathbf{a} - \gamma_\mathbf{v}^2 < 0\,. \tag{4.2}$$

In the case of $\gamma_\mathbf{v} \ge 0$, i.e., if $\mathbf{a}^\top \mathbf{b} \ge 0$ and $\mathbf{a}^\top \mathbf{c} \ge 0$, we also conclude

$$\mathbf{a}^\top A \mathbf{a} < -\left(v_1^2 + v_n^2 + 2v_1 v_n + 2v_1 \mathbf{a}^\top \mathbf{b} + 2v_n \mathbf{a}^\top \mathbf{c}\right) \le 0. \tag{4.3}$$

For $\mathbf{a}^\top \mathbf{b} \le \mathbf{a}^\top \mathbf{c}$ put $\mathbf{w} := \left[w_1, \mathbf{a}^\top, 0\right]^\top$ for some $w_1 \ge 0$, then

$$\mathbf{w}^\top Q \mathbf{w} = w_1^2 + \mathbf{a}^\top A \mathbf{a} + 2w_1 \mathbf{a}^\top \mathbf{b} = \left[\mathbf{a}^\top A \mathbf{a} - (\mathbf{a}^\top \mathbf{b})^2\right] + \left(w_1 + \mathbf{a}^\top \mathbf{b}\right)^2.$$

In the case of $\mathbf{a}^\top \mathbf{b} \ge 0$ set $w_1 = 0$ and then with (4.3) $\mathbf{w}^\top Q \mathbf{w} = \mathbf{a}^\top A \mathbf{a} < 0$. In the case of $\mathbf{a}^\top \mathbf{b} < 0$ set $w_1 = -\mathbf{a}^\top \mathbf{b}$ and get with (4.2) $\mathbf{w}^\top Q \mathbf{w} = \mathbf{a}^\top A \mathbf{a} - (\mathbf{a}^\top \mathbf{b})^2 < 0$. The remaining case $\mathbf{a}^\top \mathbf{c} < \mathbf{a}^\top \mathbf{b}$ can be dealt with by analogy. □

In Lemma 4.4, only for notational convenience we selected the corner entries $q_{1n}$ and $q_{n1}$ for truncation. Obviously, the same can be done for any positive off-diagonal entry. Hence, additionally to normalizing $Q$ to $Q'$ we can truncate all positive off-diagonal entries to 1 in a preprocessing step. Therefore we can even assume without loss of generality that all entries range between $-1$ and 1, and all diagonal entries equal one.

### 4.3 Spectral preprocessing

If we choose the spectral variant as an undominated d.c.d., we need to know the eigenpairs $(\lambda_i, \mathbf{u}_i)$ with $\mathbf{u}_i^\top \mathbf{u}_i = 1$. Note that $q_{ii} > 0$ for some $i$ already implies that $Q$ cannot be negative-definite, so there is a $k < n$ with $\lambda_k < 0 \leq \lambda_{k+1}$. Hence the next tests are almost for free. In the proof, we need the following notation: with $\gamma^+ = \max\{\gamma, 0\}$, for any vector $\mathbf{u} \in \mathbb{R}^n$ denote by $\mathbf{u}^+ = [(u_i)^+]_i \in \mathbb{R}^n_+$ and $\mathbf{u}^- = \mathbf{u}^+ - \mathbf{u} \in \mathbb{R}^n_+$ so that $\mathbf{u} = \mathbf{u}^+ - \mathbf{u}^-$ and $\mathbf{u}^\top \mathbf{u} = (\mathbf{u}^+)^\top(\mathbf{u}^+) + (\mathbf{u}^-)^\top(\mathbf{u}^-) = (\mathbf{u}^+ + \mathbf{u}^-)^\top(\mathbf{u}^+ + \mathbf{u}^-)$ because of $(\mathbf{u}^+)^\top(\mathbf{u}^-) = 0$ (one may define $\mathbf{u}^\pm$ also in terms of the spectral d.c.d. for Diag $\mathbf{u}$ = Diag $\mathbf{u}^+ -$ Diag $\mathbf{u}^-$).

**Lemma 4.5** *Denote by $\lambda_1 \leq \cdots \leq \lambda_k < 0 \leq \lambda_{k+1} \leq \cdots \leq \lambda_n$ the ordered eigenvalues of $Q$.*

*(a) If $\lambda_1 \geq 0$, then $Q$ is positive-semidefinite and hence copositive.*
*(b) If $\lambda_1 < -\lambda_n$, then at least one of the two vectors $\mathbf{u}_1^+$ or $\mathbf{u}_1^-$ is violating.*
*(c) If $\lambda_1 = -\lambda_n$ and if there is no eigenvector of $\lambda_n$ in $\mathbb{R}^n_+$ (e.g. if $\lambda_n$ is simple and $\mathbf{u}_n$ has entries with different signs), then at least one of the two vectors $\mathbf{u}_1^+$ or $\mathbf{u}_1^-$ is violating.*
*(d) Consider the polytope (possibly empty, may be checked by phase I in an LP):*

$$P_- = \left\{ \sum_{i=1}^k \mu_i \mathbf{u}_i : [\mu_i]_i \in \mathbb{R}^k \right\} \cap \Delta^s = \left\{ \mathbf{x} \in \Delta^s : \mathbf{u}_i^\top \mathbf{x} = 0 \ \text{ for all } i \in \{(k+1) : n\} \right\} .$$

*Then any $\mathbf{v} \in P_-$ is a violating vector.*

*Proof* (a) and (d) are immediate; (b) and its variant (c) are essentially shown in [27], cf. also [7]: let $\mathbf{y} = \mathbf{u}_1^+ + \mathbf{u}_1^- \in \mathbb{R}^n_+$ so that $\mathbf{y}^\top \mathbf{y} = \mathbf{u}_1^\top \mathbf{u}_1 = 1$. Then straightforward calculations yield

$$\mathbf{y}^\top Q \mathbf{y} + \mathbf{u}_1^\top Q \mathbf{u}_1 = 2 \left[ (\mathbf{u}_1^+)^\top Q (\mathbf{u}_1^+) + (\mathbf{u}_1^-)^\top Q (\mathbf{u}_1^-) \right] . \tag{4.4}$$

Under (b), we infer $\mathbf{y}^\top Q \mathbf{y} + \mathbf{u}_1^\top Q \mathbf{u}_1 \leq \lambda_n + \lambda_1 < 0$ while under (c), we know $\mathbf{y}^\top Q \mathbf{y} < \lambda_n$ and thus $\mathbf{y}^\top Q \mathbf{y} + \mathbf{u}_1^\top Q \mathbf{u}_1 < \lambda_n + \lambda_1 = 0$. In both cases, we arrive via (4.4) at $(\mathbf{u}_1^+)^\top Q (\mathbf{u}_1^+) + (\mathbf{u}_1^-)^\top Q (\mathbf{u}_1^-) < 0$, and the assertion follows. □

*Example 4.6* For $Q$ as in Example 2.16, the (rounded) vector $\mathbf{v} = [0, 0.6, 0.4]^\top \in \Delta^s$ is orthogonal to the eigenvector to the (unique) nonnegative eigenvalue 8.64 of $Q$, and hence violating.

Rather than checking multiplicity of $\lambda_n$, or the existence of a nonnegative eigenvector to this eigenvalue, it is much easier to check all the vectors $\mathbf{u}_i^\pm \in \mathbb{R}^n_+$ for $i \in \{1 : k\}$ whether they are violating.

## 5 An $\omega-$subdivision branch-and-bound approach

### 5.1 Subdivision and robustification

To begin with, let us recall the procedures in Section 2. If we always obtain case ($\mathrm{a}_\Delta$) in Theorems 2.8 or 2.9 for a collection of simplices $\Delta$ which together cover $\Delta^s$, then we know that $Q$ is copositive, due to Proposition 2.14.

If, however, we arrive at case ($\mathrm{b}_\Delta$) in both Theorems 2.8 and 2.9 for some $\Delta$ in this collection and if the trial point $\mathbf{v}_\Delta$ defined via (2.14) and (2.15) is not a violating vector, then $\mathbf{v}_\Delta^\top Q \mathbf{v}_\Delta \geq 0$. As indicated in Subsection 2.5, we rescale $\mathbf{v}_\Delta$ to a vector $\bar{\mathbf{w}} := \frac{1}{\mathbf{e}^\top \mathbf{v}_\Delta} \mathbf{v}_\Delta \in \Delta^s$, to use it for $\omega$-subdivision in further iterations.

**Lemma 5.1** *For linearly independent vertices* $\{\mathbf{w}_1, \ldots, \mathbf{w}_n\} \subset \Delta^s \setminus (\ker Q_- \cup \ker Q_+)$ *take* $\Delta = \operatorname{conv}(\mathbf{w}_1, \ldots, \mathbf{w}_n)$. *Assume that* $\mu_\Delta^- < 1 \le r = s^{-1} < [\mu_\Delta^+]^{-1}$. *Then* $\bar{\mathbf{w}} = \frac{1}{\mathbf{e}^\top \mathbf{v}_\Delta} \mathbf{v}_\Delta \in \Delta \setminus \{\mathbf{w}_1, \ldots, \mathbf{w}_n\}$, *and there is at least one* $\mathbf{w}_i$ *such that*

$$\{\bar{\mathbf{w}}\} \cup \{\mathbf{w}_j : j \neq i\} \quad \text{are linearly independent.}$$

*Proof* Let us treat the case $\mathbf{v}_\Delta = \mathbf{v}_\Delta^-$; the other case is completely symmetric. We know $\mathbf{v}_\Delta = V\mathbf{x}$ for some $\mathbf{x} \in \Delta^s$, so, recalling that $\mathbf{e}^\top \mathbf{w}_j = 1$ for all $j$, the coordinate sum amounts to

$$\mathbf{e}^\top \mathbf{v}_\Delta = \sum_{j=1}^n x_j \mathbf{e}^\top \mathbf{v}_j^- = \sum_{j=1}^n \frac{x_j}{\sqrt{\mathbf{w}_j^\top Q_- \mathbf{w}_j}} .$$

Hence

$$\bar{\mathbf{w}} = \sum_{i=1}^n \frac{x_i}{\mathbf{e}^\top \mathbf{v}_\Delta} \mathbf{v}_i = \frac{1}{\mathbf{e}^\top \mathbf{v}_\Delta} \sum_{i=1}^n \frac{x_i}{\sqrt{\mathbf{w}_i^\top Q_- \mathbf{w}_i}} \mathbf{w}_i \tag{5.1}$$

is a convex combination of all $\mathbf{w}_i$, since the coefficients of $\mathbf{w}_i$ are non-negative and sum up to one. Now assume $\bar{\mathbf{w}} = \mathbf{w}_i$ for some $i$. Since $\mathbf{w}_j$ are linearly independent, this means $x_i = 1$ while all other $x_j = 0$. But then $\mathbf{v}_\Delta = \mathbf{v}_i^-$, which contradicts Theorem 2.8 ($b_\Delta$). The assertion about linear independence follows from considering the union

$$\Delta = \operatorname{conv}(\mathbf{w}_1, \ldots, \mathbf{w}_n) = \bigcup_{i=1}^n \operatorname{conv}\left(\{\bar{\mathbf{w}}\} \cup \{\mathbf{w}_j : j \neq i\}\right) , \tag{5.2}$$

because by assumption $\Delta$ has full dimension. □

Numerically speaking, the scaling of vertices $\mathbf{w}_i$ as in (5.1) with $\mathbf{w}_i^\top Q_\pm \mathbf{w}_i < \varepsilon$ could be problematic for small $\varepsilon$. Therefore we decided to employ the following *robustification* step: once this case occurs, we deviate from the undominated d.c.d., by changing from $Q_\pm$ to a slightly dominated rank-one update, namely $Q_\pm^\varepsilon = Q_\pm + \varepsilon E_n$. This robustification resembles the usual regularization approach which perturbs $Q$ by adding $\varepsilon I_n$ rather than $\varepsilon E_n$.

However, unlike regularization, robustification just means an additive shift by a constant and thus does not affect curvature: $Q_\pm \mathbf{u} = Q_\pm^\varepsilon \mathbf{u}$ holds if $\mathbf{u}$ belongs to the $(n-1)$-dimensional subspace $\mathbf{e}^\perp$ parallel to $\Delta^s$. In addition, robustification guarantees $\mathbf{x}^\top Q_\pm^\varepsilon \mathbf{x} \ge \varepsilon > 0$ over $\Delta^s$. Hence this choice will in most cases still be quite efficient and the scaled vertices $\mathbf{v}_i$ always remain in a bounded region. Variants of this rank-one update approach could also be used for detecting strict copositivity (in (2.12) only replace $Q_-$ with $Q_-^\varepsilon$), or testing $\varepsilon$-copositivity, a relaxation of copositivity discussed in [14] (in (2.12) only replace $Q_+$ with $Q_+^\varepsilon$).

## 5.2 The algorithm

In the following algorithm we also accelerate detection by incorporating the LP-based method of Subsection 2.2, applied to $\Delta = \operatorname{conv}(\mathbf{w}_1, \ldots, \mathbf{w}_n)$ rather than to $\Delta^s$. Thus, if $W = [\mathbf{w}_1, \ldots, \mathbf{w}_n]$, replace $Q_\pm$ with $Q_\pm^W = W^\top Q_\pm W$ for an undominated d.c.d. of $Q^W = W^\top Q W$; if (2.8) is satisfied, we know that $Q^W$ is $\mathbb{R}_+^n$-copositive and hence that $Q$ is $\Delta$-copositive (recall that $Q^W$ and $Q_\pm^W$ differ from their counterparts $Q^\Delta = V^\top Q V$ and $Q_\pm^\Delta = V^\top Q_\pm V$; indeed, if $\Delta \neq \Delta^s$, then $\Delta$ must have been generated from subdividing its predecessor, say $\widehat{\Delta} = \operatorname{conv}(\widehat{\mathbf{w}}_1, \ldots, \widehat{\mathbf{w}}_n)$; if $\mathbf{v}_{\widehat{\Delta}} = \mathbf{v}_{\widehat{\Delta}}^-$, then $V = [\widehat{\mathbf{v}}_1^-, \ldots, \widehat{\mathbf{v}}_n^-]$, whereas if $\mathbf{v}_{\widehat{\Delta}} = \mathbf{v}_{\widehat{\Delta}}^+$, then $V = [\widehat{\mathbf{v}}_1^+, \ldots, \widehat{\mathbf{v}}_n^+]$, where, again, $\widehat{\mathbf{v}}_i^\pm = \frac{1}{\sqrt{\widehat{\mathbf{w}}_i^\top Q_\pm \widehat{\mathbf{w}}_i}} \widehat{\mathbf{w}}_i$

are the suitably scaled vertices of $\widehat{\Delta}$). In any case, the quantities $r$ and $s$ for the simplex $\Delta = W(\Delta^s)$ are given by

$$\frac{1}{r} = s = s_W := \max_i \frac{(Q_-^W)_{ii}}{(Q_+^W)_{ii}} = \max_i \frac{\mathbf{w}_i^\top Q_- \mathbf{w}_i}{\mathbf{w}_i^\top Q_+ \mathbf{w}_i} .$$

**Algorithm 1** Copositivity detection by d.c.d. and $\omega$-subdivision

**Require:** $\varepsilon \geq 0$ {*robustification parameter*}
**Require:** $Q, Q_+, Q_-$ {*(preprocessed) matrix* $Q$ *with spectral d.c.d.* $Q = Q_+ - Q_-$}
1: put $\Delta = \Delta^s = \mathrm{conv}(\mathbf{e}_1, \dots, \mathbf{e}_n)$, the columns of $I_n$
2: put $\mathcal{L} = \{\Delta\}$
3: put $\mathcal{L}^{\mathrm{new}} := \emptyset$
4: **while** $\mathcal{L} \neq \emptyset$ **do**
5: **for all** $\Delta = W(\Delta^s) = \mathrm{conv}(\mathbf{w}_1, \dots, \mathbf{w}_n) \in \mathcal{L}$ **do**
6: solve $\inf\left\{\mathbf{f}^\top \mathbf{x} : Q_+^W \mathbf{x} \geq \mathbf{e}\,,\ \mathbf{x} \in \mathbb{R}_+^n\right\}$ with, e.g., $\mathbf{f} = Q_+^W \mathbf{e}$, denote the solution by $\overline{\mathbf{x}}$ {*LP-based test*}
7: **if** $(\overline{\mathbf{x}}^\top Q_+^W \overline{\mathbf{x}})(Q_-^W)_{ii} > (Q_+^W \overline{\mathbf{x}})_i^2$ for any $i \in \{1:n\}$ **then**
8: robustify the current d.c.d. $Q^\Delta = Q_+^\Delta - Q_-^\Delta$, if necessary, to $Q^\Delta = [Q_+^\Delta]^\varepsilon - [Q_-^\Delta]^\varepsilon$
9: solve (2.12) and (2.13) {*QP-based tests*}
10: **if** $\mu_\Delta^- < 1$ **and** $\mu_\Delta^+ < s_W$ **then**
11: get $\mathbf{v}_\Delta$ from (2.15)
12: **if** $\mathbf{v}_\Delta^\top Q \mathbf{v}_\Delta < 0$ **then**
13: stop: $\mathbf{v}_\Delta$ ***is a violating vector***
14: **else**
15: use $\mathbf{v}_\Delta$ for $\omega$-subdivision of $\Delta$ as in Lemma 5.1 and put all full-dimensional subsimplices generated as in (5.2) on the list $\mathcal{L}^{\mathrm{new}}$
16: **end if**
17: **end if**
18: **end if**
19: **end for**
20: **if** $\mathcal{L}^{\mathrm{new}} = \emptyset$ **then**
21: stop: the matrix $Q$ ***is copositive***
22: **end if**
23: replace $\mathcal{L}$ by $\mathcal{L}^{\mathrm{new}}$ and re-initialize $\mathcal{L}^{\mathrm{new}} = \emptyset$
24: **end while**

Remember that preprocessing guarantees condition (2.11) at the root $\Delta = \Delta^s$, and that also all vertices $\mathbf{w}$ generated later are not violating, if the algorithm did not stop before. This explains why in the algorithmic description above, the case ($r < 1$ and) $s > 1$ treated in Theorems 2.8 and 2.9 does not occur.

Standard convergence results in branch-and-bound theory, see, e.g. [30, Theorem 3.8] are based on the assumption of *exhaustivity.* This means that any infinite nested sequence of simplices generated in the course of the algorithm is exhaustive, i.e. shrinks to a singleton. To ensure this with our subdivision strategy, we replace line 15. above in every $k$th iteration ($k$ to be chosen by the user) with a simple bisection step, halving the longest edge of $\Delta$. This remedy is related to Horst/Tuy's normal subdivision strategy [31] and also turned out to be beneficial from a numerical performance point of view. The above indicated variant of normal subdivision implies that the simplices shrink to singletons [32]. To be more precise: denote the list of subsimplices generated at the $l$th while loop by $\mathcal{L}_l$ and by

$$\delta(\mathcal{L}_l) = \max\left\{\mathrm{diam}\ (\Delta) : \Delta \in \mathcal{L}_l\right\} ,$$

with the Euclidean diameter diam $W(\Delta^s) = \max\left\{\|\mathbf{w}_i - \mathbf{w}_j\| : \{i, j\} \subseteq \{1:n\}\right\}$. Then under the above assumptions, $\delta(\mathcal{L}_l) \searrow 0$ as $l \to \infty$, if the algorithm does not stop. Now we are able to prove exactness of the algorithm for generic $Q$, as done in [14] for their bisection strategy.

**Theorem 5.2** *Suppose that* $\delta(\mathcal{L}_l) \searrow 0$ *as* $l \to \infty$*. If* $\alpha_Q \neq 0$*, then Algorithm 1 always stops after a finite number of while loops with the correct answer.*

*Proof* First we deal with the case $\alpha_Q < 0$ where $Q$ is not copositive and there is a violating vector $\mathbf{x} \in \Delta^s$ with $\mathbf{x}^\top Q\mathbf{x} = -\eta < 0$. We (very roughly) overestimate by $L_Q$ the Lipschitz constant for $\mathbf{w}^\top Q\mathbf{w}$ on $\Delta^s$ as follows:

$$\begin{aligned}\mathbf{y}^\top Q\mathbf{y} - \mathbf{w}^\top Q\mathbf{w} &= 2(\mathbf{y}-\mathbf{w})^\top Q\mathbf{w} + (\mathbf{y}-\mathbf{w})^\top Q(\mathbf{y}-\mathbf{w}) \\ &\geq -\|\mathbf{y}-\mathbf{w}\| \left(2\|Q\mathbf{w}\| + \|Q(\mathbf{y}-\mathbf{w})\|\right) \geq -L_Q\|\mathbf{y}-\mathbf{w}\|\,.\end{aligned} \tag{5.3}$$

Now diam $(\Delta^s) = \sqrt{2}$ and $\max\{\|\mathbf{w}\| : \mathbf{w} \in \Delta^s\} = 1 < \sqrt{2}$, so we get for $\mathbf{u} = \mathbf{w}$ or $\mathbf{u} = \mathbf{y} - \mathbf{w}$

$$\|Q\mathbf{u}\|^2 = \mathbf{u}^\top Q^2\mathbf{u} \leq \lambda_{\max}(Q^2)\|\mathbf{u}\|^2 \leq 2\lambda_{\max}(Q^2)$$

and we can choose

$$L_Q := 3\sqrt{2\lambda_{\max}(Q^2)} \tag{5.4}$$

in (5.3). Put $\delta_{\mathbf{x}} = \frac{\eta}{L_Q}$. Since for all $l$ we have

$$\mathbf{x} \in \Delta^s = \bigcup_{\Delta \in \mathcal{L}_l} \Delta\,,$$

there is a vertex $\mathbf{v}$ of a subsimplex $\Delta$ with $\|\mathbf{x}-\mathbf{v}\| \leq$ diam $(\Delta) \leq \delta(\mathcal{L}_l)$. If the algorithm did not stop before with a violating vector, then $\mathbf{v}$ cannot be violating, because $\Delta$ was generated by the algorithm. We deduce $\delta(\mathcal{L}_l) \geq \delta_{\mathbf{x}}$. Indeed, otherwise, we would arrive at the absurd chain of inequalities

$$\mathbf{v}^\top Q\mathbf{v} = \mathbf{v}^\top Q\mathbf{v} - \mathbf{x}^\top Q\mathbf{x} + \mathbf{x}^\top Q\mathbf{x} \leq L_Q\|\mathbf{v}-\mathbf{x}\| - \eta < L_Q\delta_{\mathbf{x}} - \eta = 0\,.$$

Hence the algorithm stops at some finite $l$ in this case.
Next, if $\eta = \alpha_Q > 0$, i.e., if $Q$ is strictly copositive, then the sequence $\delta(\mathcal{L}_l)$ can also not converge to zero, and the algorithm must stop with a copositivity guarantee: indeed, suppose that $\Delta = W(\Delta^s)$ has very small diameter and choose any $\mathbf{w} \in \Delta$. We show that then the LP-based test must establish $\Delta$-copositivity. If this holds true for all $\Delta \in \mathcal{L}_l$ because $\delta(\mathcal{L}_l)$ is small, we are done. Basically, $W \approx [\mathbf{w}, \ldots, \mathbf{w}]$ so that $Q^W \approx (\mathbf{w}^\top Q\mathbf{w})E_n$ and likewise $Q^W_\pm \approx (\mathbf{w}^\top Q_\pm\mathbf{w})E_n$, and $\mathbf{w}^\top Q_-\mathbf{w} + \eta \leq \mathbf{w}^\top Q_+\mathbf{w}$. Moreover, the LP is always feasible (for any $\mathbf{y} \in \Delta^s$, the point $\mathbf{x} = \frac{2}{\mathbf{w}^\top Q_+\mathbf{w}}\,\mathbf{y} \in \mathbb{R}^n_+$ satisfies $Q^W_+\mathbf{y} \approx 2\mathbf{e}$, thus for sure $Q^W_+\mathbf{y} \geq \mathbf{e}$), and likewise the solution $\bar{\mathbf{x}}$ for $\mathbf{f} = Q^W_+\mathbf{e} \approx n(\mathbf{w}^\top Q_+\mathbf{w})\mathbf{e}$ must satisfy $Q^W_+\bar{\mathbf{x}} \approx (\mathbf{w}^\top Q_+\mathbf{w})E_n\bar{\mathbf{x}} = \mathbf{e}$ (since the LP constraint also approximately is $\mathbf{e}^\top\mathbf{x} \geq \frac{1}{\mathbf{w}^\top Q_+\mathbf{w}}$) and hence $\bar{\mathbf{x}}^\top Q^W_+\bar{\mathbf{x}} \approx \frac{1}{\mathbf{w}^\top Q_+\mathbf{w}}$. Hence

$$(\bar{\mathbf{x}}^\top Q^W_+\bar{\mathbf{x}})(Q^W_-)_{ii} \approx \frac{\mathbf{w}^\top Q_-\mathbf{w}}{\mathbf{w}^\top Q_+\mathbf{w}} \leq \frac{\mathbf{w}^\top Q_+\mathbf{w} - \eta}{\mathbf{w}^\top Q_+\mathbf{w}} = 1 - \frac{\eta}{\mathbf{w}^\top Q_+\mathbf{w}} \approx (Q^W_+\bar{\mathbf{x}})_i^2 - \frac{\eta}{\mathbf{w}^\top Q_+\mathbf{w}} < (Q^W_+\bar{\mathbf{x}})_i^2$$

for all $i \in \{1:n\}$, and the LP test (2.8) works. ◻

Note that, like in [14], for the boundary case $\alpha_Q = 0$ where $Q$ is copositive but not strictly copositive, we cannot guarantee that the algorithm terminates after a finite number of steps. The next subsection provides a more detailed and quantitative analysis which is independent from the assumption $\delta(\mathcal{L}_l) \searrow 0$.

Mainly for concave minimization over a general polytope, there is an advanced convergence theory for $\omega$-subdivision without bisection steps [34,35], which does not need the exhaustivity assumption. A similar analysis for the above algorithm may constitute an interesting topic for future research.

### 5.3 Numerical flatness

In numerical practice, one has to decide on the threshold $\delta$ on the determinant of the $n \times n$ matrix $W_i$ with columns $\bar{\mathbf{w}}$ and $\mathbf{w}_j, j \neq i$, which determines if the successor $W_i(\Delta^s)$ is accepted in $\mathcal{L}$ or not (the latter if $|\det W_i| \leq \delta$). Counting the occurrence of the latter cases (say $r_\delta$) after the algorithm stopped, one may estimate the maximum volume (relative to $\mathbf{e}^\perp$) of $\Delta^s \setminus \mathrm{Pos}(Q)$, the set of violating vectors, by

$$\mathrm{vol}_{n-1}\,[\Delta^s \setminus \mathrm{Pos}(Q)] \leq \nu_\delta := \frac{\delta\, r_\delta}{(n-1)!}\,. \tag{5.5}$$

Also, tracking the longest edge of these "numerically flat" simplices $W_i(\Delta^s)$, one obtains a lower bound for the possibly negative values of $\mathbf{x}^\top Q\mathbf{x}$, which delivers a certificate of $\varepsilon$-copositivity [14]:

**Proposition 5.3** *Suppose the longest edge length* diam $W_i(\Delta^s)$ *of all numerically flat simplices (where $|\det W_i| \leq \delta$) does not exceed $\ell_\delta$. If the algorithm did not stop by delivering a violating vector, we have*

$$\mathbf{x}^\top Q\mathbf{x} \geq -\varepsilon_\delta \quad \textit{for all } \mathbf{x} \in \Delta^s \textit{ where } \varepsilon_\delta := 3\sqrt{2\lambda_{\max}(Q^2)}\,\ell_\delta\,. \tag{5.6}$$

*Proof* By assumption, we know that all vertices $\mathbf{w} \in \{\bar{\mathbf{w}}\} \cup \{\mathbf{w}_j : j \neq i\}$ of $W_i(\Delta^s)$ satisfy $\mathbf{w}^\top Q\mathbf{w} \geq 0$, because no violating vector was found, so that

$$\mathbf{x}^\top Q\mathbf{x} \geq \mathbf{w}^\top Q\mathbf{w} - L_Q\|\mathbf{x} - \mathbf{w}\| \geq 0 - L_Q\,\ell_\delta \quad \text{for all } \mathbf{x} \in W_i(\Delta^s)\,,$$

where $L_Q$ is the Lipschitz constant from (5.3). Hence the result follows from (5.4). □

So we may start with a relatively large $\delta$ and keep track of $\nu_\delta$ and $\varepsilon_\delta$. Once these bounds on volume (5.5) or on violation (5.6) exceed acceptable values, we can decrease $\delta$ (and even restart, resources permitting).

Based on the size of the (not numerically flat) subsimplices also a speedup of the proposed algorithm is possible, if one tries to find a violating vector as fast as possible. Since a violating vector can more probably be found in a larger subsimplex than in a smaller one, we suggest to sort the subsimplices with decreasing size (represented by the absolute value of the determinant of the matrix $W_i$ containing their vertices). Additionally, in each iteration (for-loop) one may only consider those submatrices $W_i$ for which

$$|\det W_i| \geq \frac{\sum_{j=1}^{\bar{s}} |\det W_j|}{\bar{s}} - t \cdot \left[\max_{j\in\{1:\bar{s}\}}\{|\det W_j|\} - \min_{j\in\{1:\bar{s}\}}\{|\det W_j|\}\right], i \in \{1 : \bar{s}\}\,, \tag{5.7}$$

for some value of $t$, e.g. $t = 0.1$. This means, that in the for-loop of the above algorithm, we consider $\Delta \in \mathcal{L}$ only if (5.7) is satisfied. The remaining $\Delta$ of the list $\mathcal{L}$ which do not satisfy (5.7) are directly moved to the new list $\mathcal{L}^{\mathrm{new}}$ for the next iteration and are considered in the next while-loop.

## 6 Empirical evidence

Besides the numerical examples already presented in the previous sections we apply the proposed algorithm to some test matrices which were already examined in the literature related to copositive matrices and copositivity tests. Most of these instances are known to be very difficult in some sense. In addition, we consider an application, the maximum clique problem.

## 6.1 Small but famous matrices

We choose the following parameters for the algorithm: at every fifth iteration we do a bisection step. A subsimplex $W_i$ is considered to be really flat if $|\det(W_i)| < 10^{-10}$ (and it will no longer be considered, not even for (5.5)) and numerically flat if $|\det(W_i)| \leq 10^{-6}$. For robustification we choose $\varepsilon = 10^{-6}$ and in each iteration we check all submatrices independently of their size.

For the matrix

$$Q = \begin{bmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{bmatrix}$$

the algorithm presented in [14] terminates after 7 iterations and needs 15 subsimplices. As we determine the eigenvalues in the preprocessing for the spectral d.c.d., this matrix is immediately detected as a positive-semidefinite matrix with eigenvalues $0, 3, 3$.

The following test matrices are considered in [33]:

$$K_1 = \begin{bmatrix} 1 & 0.9 & -0.54 & 0.21 \\ 0.9 & 1 & -0.03 & 0.78 \\ -0.54 & -0.03 & 1 & 0.52 \\ 0.21 & 0.78 & 0.52 & 1 \end{bmatrix}, \qquad K_2 = \begin{bmatrix} 1 & -0.72 & -0.59 & -0.6 \\ -0.72 & 1 & 0.21 & -0.46 \\ -0.59 & 0.21 & 1 & -0.6 \\ -0.6 & -0.46 & -0.6 & 1 \end{bmatrix}.$$

In the preprocessing step the last row/column in $K_1$ is deleted as it is nonnegative. Then the LP-based test recognizes the reduced matrix and thus $K_1$ to be copositive. The matrix $K_2$ is not copositive. Here the QP-based tests deliver in the first iteration the violating vector $\mathbf{v} \approx [0.3, 0.21, 0.21, 0.28]^\top$. In [33] also a copositive $10 \times 10$ matrix is specified. Our algorithm first reduces it to a $8 \times 8$ matrix by preprocessing, and then detects copositivity by the LP-based test at the root.

In [1] the following copositive matrix is given:

$$A = \begin{bmatrix} 2 & -2 & -1 & 2 \\ -2 & 3 & 2 & -3 \\ -1 & 2 & 1 & 1 \\ 2 & -3 & 1 & 4 \end{bmatrix}.$$

Without any preprocessing, copositivity is detected at the root, by an application of Theorem 2.8. However, by normalizing the diagonal and truncating this matrix as in Section 4, a partitioning of the standard simplex into two subsimplices is required. Then on each of these subsimplices the criterion of Theorem 2.8 applies and hence the matrix is recognized as copositive. This is an instance where preprocessing slightly complicates the process. To avoid this phenomenon, one could run the first one or two iterations without preprocessing, depending on some condition characteristic of the given matrix, and only then use it for numerical stabilization; or immediately try with the two undominated d.c.d.s at the root (recall the d.c.d.s most probably will be different). However, the next example exhibits a positive effect of preprocessing at the root.

According to [41] the matrix $Q$ from (3.3) is copositive but not strictly copositive, i.e. it holds $\mathbf{x}^\top Q\mathbf{x} = 0$ for some vector $\mathbf{x} \in \mathbb{R}^n_+ \setminus \{\mathbf{o}\}$, e.g., for $\mathbf{x} = [0, 4, 0, 4, 1]^\top$. For this matrix 16 subsimplices have to be considered. The LP-based sufficient criterion was never satisfied. The number of subsimplices can be reduced to 13 by doing no bisection steps, also not in any fifth iteration. If we apply a bisection in any second step, starting with a bisection — thus reduce the influence of the data-driven $\omega$-subdivisions — we need to consider 42 subsimplices. This was done without truncating positive entries. After preprocessing as in Subsection 4.2, these figures become smaller (14/11/27). Also the copositive $4 \times 4$ matrix $R$ obtained by dropping the last row and column of $Q$ is considered in the literature [3,6,40]. For $R$ copositivity is already shown at the root via the QP-test according to Theorem 2.8. Note that in [40] 10 tableaus have to be calculated for establishing copositivity.

Diananda [20] showed that every $3 \times 3$ or $4 \times 4$ copositive matrix is the sum of a positive-semidefinite and a nonnegative matrix. This does no longer hold for $n \times n$ matrices with $n \geq 5$. The Horn matrix $H$, see (3.4), is an example. The test in [14] for $H$ terminates after 19 simplices have been tested. Our algorithm needs 3 351 subsimplices, and stops after 17 iterations as only subsimplices are left which are numerically flat. The difficulty to detect copositivity of $H$ is due to its symmetry. To illustrate this phenomenon, we perturbed $H$ by adding a matrix of the form $P + N$ randomly generated as described above, scaled with entries in the interval $[-\frac{1}{100}, \frac{1}{100}]$. The number of subsimplices immediately dropped to an average below 871 (over 30 matrices), ranging between 644 and 1095. However, for the matrix $H^3$, our algorithm immediately delivers a violating vector with the help of the QP-tests already at the root. These are two instances prototypical for the widely reported phenomenon that non-copositive matrices are more easily detected than copositive ones, especially those at the boundary of the copositive cone (i.e., $Q$ with $\alpha_Q = 0$). Our approach softens this asymmetry of hardness a bit due to our preprocessing and the cheap sufficient tests.

A copositive matrix $Q$ is called *extreme*, see, e.g. [26], if $Q = Q_1 + Q_2$ with $Q_1, Q_2$ copositive, implies $Q_1 = \alpha Q$ and $Q_2 = (1 - \alpha)Q$ for some $\alpha \in [0, 1]$. Examples for extreme copositive matrices are $H$ above [26, p.273] and the Hoffman-Pereira matrix [29]:

$$P = \begin{bmatrix} 1 & -1 & 1 & 0 & 0 & 1 & -1 \\ -1 & 1 & -1 & 1 & 0 & 0 & 1 \\ 1 & -1 & 1 & -1 & 1 & 0 & 0 \\ 0 & 1 & -1 & 1 & -1 & 1 & 0 \\ 0 & 0 & 1 & -1 & 1 & -1 & 1 \\ 1 & 0 & 0 & 1 & -1 & 1 & -1 \\ -1 & 1 & 0 & 0 & 1 & -1 & 1 \end{bmatrix}.$$

For this matrix 20 001 subsimplices have to be considered. To break the symmetry, we employed, instead of $\omega$-subdivision, an asymmetric bisection (this means that the longest edge is divided in a ratio different from one; we used 1:4) right from the start and then at every tenth iteration; all other iterations were performed according to our previous description. Then the number of subsimplices is reduced to 12 129. This favorable reduction applied, at a more modest scale, also to the highly symmetric Horn matrix $H$. Apparently, the algorithm in [14] takes profit from this high degree of symmetry. Indeed, it is easy to see that for $Q = H$, the data-driven bisection by minimizing $\varphi$ from (2.17) coincides with the midpoint ($t = \frac{1}{2}$ at the root).

### 6.2 Randomly generated instances

In [42] the following empirical test is proposed: 1000 symmetric $n \times n$ matrices with unit diagonal and with off-diagonal entries in the interval $[-1, 1]$ are randomly generated for different dimensions $n$. The copositivity test is performed and then the number of matrices which are copositive, not copositive, or undetermined are counted. For $n \leq 7$ according to [42] with their test no matrix was undetermined, for $n = 8$, eight matrices, for $n = 9$, six and for $n = 10$, two matrices were undetermined. With the algorithm proposed here, the copositivity status of *all* matrices was correctly detected for each $n = 1, \ldots, 10$ as well as for larger dimensions $n = 20, 40, 60, 80, 100, 120, 140, 200$. For $n \geq 20$ all randomly generated matrices were recognized as not copositive without any partitioning. For $n = 200$, we only generated 100 random matrices. In each of these instances, both QP-tests generated different violating vectors, rescaled to lie in $\Delta^s$, with a distance exceeding $10^{-5}$ (the average exceeds 0.01).

We also repeated the simulation study proposed for the LP-test (see end of Subsection 2.2) with 3000 randomly generated copositive $n \times n$ matrices of the form $P + N$ where $P$ is positive-semidefinite and $N$ has no negative entries (1000 matrices for each $n \in \{20, 40, 60\}$). All matrices were detected as copositive already by preprocessing, or after performing the LP-test or the QP-test on $\Delta^s$. In some

| instance | nodes | $\omega(\mathcal{G})$ | l.b. (d.c.d.) | l.b. in [14] | l.b. in [43] |
|---|---|---|---|---|---|
| Brock200_4 | 200 | 17 | 7 | — | 13 |
| Hamming6-2 | 64 | 32 | 32 | 28 | 32 |
| Hamming8-2 | 256 | 128 | 128 | — | 128 |
| Hamming8-4 | 256 | 16 | 16 | 12 | 16 |
| Johnson8-2-4 | 28 | 4 | 4 | 4 | 4 |
| Johnson8-4-4 | 70 | 14 | 14 | 14 | 14 |
| Johnson16-2-4 | 120 | 8 | 8 | 8 | 8 |
| Keller4 | 171 | 11 | 6 | 9 | 8 |

**Table 6.1** Instances from 2nd DIMACS Challenge (selection by [14,43] and us).

cases a robustification was necessary (in 146 cases for $n = 20$, in 54 cases for $n = 40$, and in 21 cases for $n = 60$ without truncating positive entries, slightly less with truncation as in Subsection 4.2). For monitoring purposes solely, we repeated the run with the same matrices but only using the QP-based tests and achieved the same results. Note that the LP-test demands less numerical effort than the QP-test, and therefore we always start with the LP-test; sometimes this saves time as the slightly more expensive QP-tests no longer have to be applied.

## 6.3 Application: maximum clique problem

Like in [14] we tested our procedure for checking copositivity also on the well known maximum clique problem: given a simple (i.e. loopless and undirected) graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ with node set $\mathcal{V} = \{1 : n\}$ and edge set $\mathcal{E}$, a *clique* $\mathcal{C}$ is a subset of $\mathcal{V}$ such that every pair of nodes in $\mathcal{C}$ is connected by an edge in $\mathcal{E}$. A clique $\mathcal{C}$ is said to be a *maximum clique* if it contains the most elements among all cliques, and its size $\omega(\mathcal{G})$ is called the *(maximum) clique number*. For a survey of this problem which was shown very early to be NP-complete, we refer to [9]. The maximum clique problem can be reformulated as a copositive optimization problem [10,19]:

$$\omega(\mathcal{G}) = \min\{\lambda \in \mathbb{N} \mid \lambda(E_n - A_{\mathcal{G}}) - E_n \text{ is copositive}\} \tag{6.1}$$

with $E_n$ the $n \times n$ all-ones matrix and $A_{\mathcal{G}} = [a_{ij}]_{i,j}$ the adjacency matrix of the graph $\mathcal{G}$, i.e. $a_{ij} = 1$ if $\{i, j\} \in \mathcal{E}$, and $a_{ij} = 0$ else, $i, j \in \{1 : n\}$.

In Table 6.1 the results for some instances of the Second DIMACS Challenge [21] are listed, which are known to be very hard instances for copositive programming because of their inherent symmetry. In view of the aforementioned asymmetry of hardness ($\alpha_Q < 0$ is easier detected than $\alpha_Q \geq 0$). we focus on lower bounds, as done also in [14]. For instance, the lower bound for Hamming8-2, i.e. the non-copositivity for $\lambda = 127$, was shown by the algorithm proposed here in about a second in the preprocessing step (Lemma 4.5 applied). For all instances, we chose the parameters as in Subsection 6.1 and we put $t = 0.1$ in (5.7).

In [43] it is proposed to consider in addition smaller maximum clique test problems. For these, we report in Table 6.2 the lower bound $\lambda$, and the number $N$ of tested subsimplices ($N = 0$ represents a successful result already in the preprocessing; otherwise we chose $t = 0$ in (5.7) here). For several test instances also the copositivity of $\lambda(E_n - A_{\mathcal{G}}) - E_n$ for $\lambda = \omega(\mathcal{G})$ could be shown, but frequently we had to stop the procedure (after more than 10 minutes) before obtaining any result. In [43] for many more instances copositivity was shown but with much larger computational time (quite often around 40 minutes, in one case even more than 400 minutes).

For Hamming4-4 (16 nodes) copositivity for $\lambda = \omega(\mathcal{G}) = 2$ was established after one subsimplex-test (as compared to 511 in [43]). The procedure also successfully determined $\lambda = \omega(\mathcal{G})$ for sanchis20 (20 nodes) after 8 139 subsimplices (as compared to 25 204 809 in [43]) and for sanchis22 (22 nodes) after 5 921 subsimplices (57 308 615 in [43]). But for showing copositivity for $\lambda = \omega(\mathcal{G}) = 6$ in the Jagota14 instance (14 nodes), 30 777 (as compared to 323 621 in [43]) subsimplices had to be tested.

| instance | nodes | $\omega(\mathcal{G})$ | $\lambda$ | $N$ (d.c.d.) | $N$ in [43] |
|---|---|---|---|---|---|
| c-fat14-1 | 14 | 6 | 5 | 0 | 5 |
| Brock14 | 14 | 5 | 4 | 3 | 13 |
| Brock16 | 16 | 5 | 4 | 1 | 24 848 |
| Brock18 | 18 | 5 | 4 | 3 | 7 |
| Brock20 | 20 | 5 | 4 | 22 | 7 |
| Morgen14 | 14 | 5 | 4 | 1 | 4 |
| Morgen16 | 16 | 5 | 4 | 1 | 12 |
| Morgen18 | 18 | 5 | 4 | 1 | 5 |
| Morgen20 | 20 | 5 | 4 | 59 | 9 |
| Morgen22 | 22 | 5 | 4 | 181 | 11 |
| Johnson6-2-4 | 15 | 3 | 2 | 1 | 2 |
| Johnson6-4-4 | 15 | 3 | 2 | 1 | 2 |
| Johnson7-2-4 | 21 | 3 | 2 | 1 | 2 |
| Jagota14 | 14 | 6 | 5 | 5 | 58 105 |
| Jagota16 | 16 | 8 | 7 | 5 | 20 968 165 |
| Jagota18 | 18 | 10 | 9 | 11 141 | — |
| sanchis14 | 14 | 5 | 4 | 143 | 4 |
| sanchis16 | 16 | 5 | 4 | 6 | 11 |
| sanchis18 | 18 | 5 | 4 | 1 | 4 |
| sanchis20 | 20 | 5 | 4 | 1 | 4 |
| sanchis22 | 22 | 5 | 4 | 1 | 6 |

**Table 6.2** Smaller maximum clique problems from [43]: $N$ subsimplices generated when testing $\lambda(E_n - A_{\mathcal{G}}) - E_n$.

## 7 Conclusions and outlook

Based upon a difference-of-convex decomposition of a given symmetric matrix $Q$, we propose an algorithm to detect copositivity of $Q$ which combines LP and/or convex QP technology with spectral information. Three apparently new copositivity tests are presented, and we show by example that all three tests are *a priori* needed. The resulting algorithm either provides a guarantee for copositivity, or delivers a violating vector as a certificate for non-copositivity. To exploit the present algorithm in context of general (mixed-binary) QPs, and likewise of general copositive programs, to escape from inefficient solutions, remains as a topic for future research.

Empirical evidence suggests that our algorithm is remarkably powerful in detecting violating vectors, or copositivity, as long as there is not too much symmetry. The simulation results make us believe that almost all matrices $Q = P + N$, where $P$ is positive-semidefinite, and $N$ has no negative entries, will be detected quickly (sometimes without invoking any optimization procedure) as copositive, with an effort which is by far exceeded by that of using SDP solvers, which would be the current technology to deal with such matrices. We also saw that breaking symmetries or perturbing may reduce the number of subproblems generated. Last but not least, aiming at numerical stability, we have provided a concise collection of different preprocessing steps, most of them scattered in the literature, but so far without a focus on constructing violating vectors.

**Acknowledgement.** The authors are indebted to the handling MPA co-editor, Adrian Lewis, as well as to two anonymous referees and an anonymous handling editor for their careful reading. Their comments on previous versions of the paper significantly helped to improve presentation.

## References

1. Andersson, L.E., Chang, G., Elfving, T.: Criteria for copositive matrices using simplices and barycentric coordinates. *Linear Algebra Appl.* **220**, 9–30 (1995).
2. Bomze, I.M.: Copositivity conditions for global optimality in indefinite quadratic programming problems. *Czechoslovak J. Operations Research* **1**, 7–19 (1992).
3. Bomze, I.M.: Block pivoting and shortcut strategies for detecting copositivity. *Linear Algebra Appl.* **248**, 161–184 (1996).

4. Bomze, I.M.: Global escape strategies for maximizing quadratic forms over a simplex. *J. Global Optim.* **11**, 325–338 (1997).
5. Bomze, I.M.: On standard quadratic optimization problems. *J. Global Optim.* **13**, 369-387 (1998).
6. Bomze, I.M.: Linear-time copositivity detection for tridiagonal matrices and extension to block-tridiagonality. *SIAM J. Matrix Anal. Appl.* **21**, 840–848 (2000).
7. Bomze, I.M.: Perron-Frobenius property of copositive matrices, and a block copositivity criterion. *Linear Algebra Appl.* **429**, 68–71 (2008).
8. Bomze, I.M.: Copositive optimization – recent developments and applications. *Europ. J. Oper. Research* **216**, 509–520 (2012).
9. Bomze, I.M., Budinich, M., Pardalos, P., Pelillo, M.: The maximum clique problem. In: D.-Z. Du, P.M. Pardalos (eds.), *Handbook of Combinatorial Optimization* (supp. Vol. A), 1–74. Kluwer, Dordrecht (1999).
10. Bomze, I.M., Dür, M., de Klerk, E., Roos, C., Quist, A.J., Terlaky, T.: On copositive programming and standard quadratic optimization problems. *J. Global Optim.* **13**, 369–387 (1998).
11. Bomze, I.M., Locatelli, M.: Undominated d.c. decompositions of quadratic functions and applications to branch-and-bound approaches. *Computational Optimization Appl.* **28**, 227–245 (2004).
12. Bomze, I.M., Locatelli, M., Tardella, F.: New and old bounds for standard quadratic optimization: dominance, equivalence and incomparability. *Math. Programming* **115**, 31–64 (2008).
13. Bomze, I.M., Schachinger, W., Uchida, G.: Think co(mpletely )positive! Matrix properties, examples and a clustered bibliography on copositive optimization. *J. Global Optim.* **52**, 423–445 (2012).
14. Bundfuss, S., Dür, M.: Algorithmic copositivity detection by simplicial partition. *Linear Algebra Appl.* **428**, 1511–1523 (2008).
15. Burer, S.: On the copositive representation of binary and continuous nonconvex quadratic programs. *Math. Programming* **120**, 479–495 (2009).
16. Burer, S.: Copositive programming. In: M.F. Anjos, J.-B. Lasserre (eds.), *Handbook of Semidefinite, Cone and Polynomial Optimization: Theory, Algorithms, Software and Applications*, 201—218. Springer, New York (2012).
17. Danninger, G.: A recursive algorithm for determining (strict) copositivity of a symmetric matrix. In: U. Rieder et al. (eds.), *Methods OR* **62**, 45–52. Hain, Meisenheim (1990).
18. Danninger, G., Bomze, I.M.: Using copositivity for global optimality criteria in concave quadratic programming problems. *Math. Programming* **62**, 575–580 (1993).
19. de Klerk, E., Pasechnik, D.V.: Approximation of the stability number of a graph via copositive programming. *SIAM J. Optim.* **12**, 875–892 (2002).
20. Diananda, P.H.: On non-negative forms in real variables some or all of which are non-negative. *Proc. Cambridge Philos. Soc.* **58**, 17–25 (1962).
21. DIMACS: Second DIMACS Challenge. Test instances available at http://dimacs.rutgers.edu/challenges, last accessed 13 Jan. 2010.
22. Dür, M.: Copositive Programming – a survey. In: M. Diehl, F. Glineur, E. Jarlebring, W. Michiels (eds.), *Recent Advances in Optimization and its Applications in Engineering*, 3–20. Springer, New York (2010).
23. Eichfelder, G., Jahn, J.: Set-semidefinite optimization. *J. Convex Anal.* **15**, 767–801 (2008).
24. Eichfelder, G., Jahn, J.: Foundations of set-semidefinite optimization. In: P. Pardalos, Th.M. Rassias and A.A. Khan (eds.), *Nonlinear Analysis and Variational Problems*, pp. 259–284. Springer, New York (2009).
25. Hall, M.Jr., Newman, M.: Copositive and completely positive quadratic forms. *Proc. Cambridge Philos. Soc.* **59**, 329–339 (1963).
26. Hall, M.Jr.: *Combinatorial Theory.* Blaisdell, Waltham, Mass. (1967).
27. Haynsworth, E., Hoffman, A.J.: Two remarks on copositive matrices. *Linear Algebra Appl.* **2**, 387–392 (1969).
28. Hogben, L., Johnson, C.R., Reams, R.: The copositive completion problem. *Linear Algebra Appl.* **408**, 207–211 (2005).
29. Hoffman, A.J., Pereira, F.: On copositive matrices with -1,0,1 entries. *Journal of Combinatorial Theory* (A) **14**, 302–309 (1973).
30. Horst, R., Pardalos, P., Thoai, N.: *Introduction to Global Optimization.* Kluwer, Dordrecht (1995).
31. Horst, R., Tuy, H.: *Global optimization – deterministic approaches, 3rd ed.* Springer, Berlin (1996).
32. Horst, R.: On generalized bisection of $n$-simplices. *Math. Comput.* **218**, 691–698 (1997).
33. Kaplan, W.: A copositivity probe. *Linear Algebra Appl.* **337**, 237–251 (2001).
34. Locatelli, M., Raber, U.: On the convergence of the simplicial branch-and-bound algorithm based on $\omega$-subdivisions. *J. Optim. Theo. Appl.* **107**, 69–79 (2000).
35. Locatelli, M., Raber, U.: A finiteness result for the simplicial branch-and bound algorithm based on $\omega$-subdivisions. *J. Optim. Theo. Appl.* **107**, 81–88 (2000).
36. Murty, K.G., Kabadi, S.N.: Some NP-complete problems in quadratic and linear programming. *Math. Programming* **39**, 117–129 (1987).
37. Parrilo, P.A.: Semidefinite programming based test for matrix copositivity. *Proceedings of the 39th IEEE Conference on Decision and Control* 5 (2000), 4624–4629.
38. Quist, A.J., de Klerk, E., Roos, C., Terlaky, T.: Copositive relaxation for general quadratic programming. *Optim. Methods Softw.* **9**, 185–209 (1998).
39. Tuy, H.: Convex programs with an additional reverse convex constraint. *J. Optim. Theo. Appl.* **52**, 463–486 (1987).
40. Väliaho, H.: Criteria for copositive matrices. *Linear Algebra Appl.* **81**, 19–34 (1986).
41. Väliaho, H.: Quadratic-programming criteria for copositive matrices. *Linear Algebra Appl.* **119**, 163–182 (1989).
42. Yang, S., Li, X.: Algorithms for determining the copositivity of a given symmetric matrix. *Linear Algebra Appl.* **430**, 609–618 (2009).
43. Žilinskas, J., Dür, M.: Depth-first simplicial partition for copositivity detection, with an application to Maxclique. *Optim. Meth. Software* **26**, 499-510 (2011).