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Novel shortcut strategies in copositivity detection: Decomposition for quicker positive certificates

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ABSTRACT

Copositivity is a property of symmetric matrices which is NP-hard to check. Nevertheless, it plays a crucial role in tight bounds for conic approaches of several hard optimization problems. In this paper, we present novel promising shortcut strategies to exploit favorable instances in a systematic way, using decomposition strategies based upon the idea to allow for overlapping, smaller blocks, profiting from a beneficial sign structure of the entries of the given matrix. The working hypothesis of this approach is the common empirical observation in the community that for detection of copositivity, a negative certificate is easier to obtain than a positive one. First empirical results on carefully orchestrated randomly generated instances seem to corroborate our approach.

1. Introduction

1.1. Motivation

Copositivity lies at the core of modern cone-based optimization methods to obtain tractable bounds of hard problems in both continuous (polynomial) and discrete domains (e.g., the maximum clique problem). Overviews of the various application fields can be found, e.g., in [1–3].

The property of copositivity of a symmetric matrix is well-studied, dating back to 1952 when it came up in [4]. From then on, numerous results have been achieved in this field [5], from general structural results in Linear Algebra to concrete algorithms in numerical implementations.

It has been shown that testing a matrix for copositivity is a co-NP-complete problem [6]. To find good algorithms for specific types of matrices (like for tridiagonal [7] or acyclic matrices [8]) is an active field of Operations Research.

Another branch of research is concerned with trying to find faster methods for the general case, exploiting favorable constellations of the problem data in an automated way. A most likely incomplete list of recent algorithmic attempts (either for solving the problem directly or else using approximation results on the cone of copositive matrices) is [9–14] and references therein; cf. [15].

For solving the decision problem whether or not a given matrix is copositive, i.e. whether or not the quadratic form it generates takes no negative values over the positive orthant, we need two types of certificates:

a **negative certificate**, i.e., a **violating vector** $\mathbf{x} \in \mathbb{R}^n_+$ such that $\mathbf{x}^\top \mathsf{A}\mathbf{x} < 0$ (here and in the sequel we denote transposition by $^\top$), or else a **positive certificate**, e.g. in form of a rigorous lower bound ℓ to the problem parameter

$$\gamma(\mathsf{A}) = \min\left\{\mathbf{x}^\top \mathsf{A}\mathbf{x} : \mathbf{x} \in \Delta^n\right\}$$

where $\Delta^n = \left\{\mathbf{x} \in \mathbb{R}^n_+ : \sum_i x_i = 1\right\}$ is the standard simplex. We can be sure that A is copositive if $\ell \geq 0$ due to $\ell \leq \gamma(\mathsf{A})$, by positive homogeneity of the quadratic form in $\mathbf{x}$. For the same reason, the search for a violating vector can also be restricted to Δ^n, or any intersection of a norm ball with the positive orthant.

Interestingly enough, it has been observed independently by many researchers (in almost all of above cited references) that empirically it seems to be easier to obtain negative certificates rather than positive ones; one reason might be that this can be achieved also by local descent search (and moderate multistart) for $\gamma(\mathsf{A})$. In practice, it seems that a violating vector (with negative feasible value) is more easily found than a non-negative rigorous lower bound ℓ for $\gamma(\mathsf{A})$, very much in line with adverse instances for branch-and-bound algorithms. In our case, there are of course exceptions: e.g., if $\mathsf{A} = [a_{ij}]_{ij}$ has no negative entries, then we can use obviously $\ell = \min_{ij} a_{ij} \geq 0$ as a positive certificate. Likewise, if A is positive-semidefinite, we can use $\ell = \frac{1}{n^2}\lambda_{\min}(\mathsf{A}) \geq 0$.

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1.2. Our contribution; organization of the paper and notation

Here we propose an innovative approach for decomposing a given matrix in a way that several but smaller matrices have to be checked on their copositivity. This way, we generate a hierarchy of smaller instances. Our aim here is to provide a powerful preprocessing tool which automatically detects easy cases at an early stage.

After introducing the principle of decomposition with overlaps for general matrices, we will focus on more benign scenarios when working with k-diagonal matrices. This matrix class allows a straightforward use of the proposed method, reducing computational effort tremendously and enabling insights into the procedure of proving copositivity. The special case of pentadiagonal matrices will be analyzed in more detail, along with a carefully designed experiment assessing the quality of this approach. A concluding section then summarizes and provides an outlook for potential future work.

Some notation:
$\mathcal{S}_n := \{\mathsf{A} \in \mathbb{R}^{n\times n} : \mathsf{A}^\top = \mathsf{A}\}$ the set of symmetric matrices of order n.
$\mathcal{P}_n := \{\mathsf{A} \in \mathcal{S}_n : \lambda_{\min}(\mathsf{A}) \geq 0\}$ the set of positive-semidefinite matrices.
$\mathcal{N}_n := \{\mathsf{A} \in \mathcal{S}_n : \min_{ij} a_{ij} \geq 0\}$ the set of symmetric nonnegative matrices.

The symbol O stands for a generic, possibly rectangular, matrix of zeroes of suitable size. In a similar fashion, $\mathbf{e}$ generically denotes the all-ones vector of suitable size. Finally, for $\mathsf{A} \in \mathcal{S}_n$ we denote by $\mathrm{Ddiag}(\mathsf{A}) \in \mathcal{S}_n$ a diagonal matrix with the same diagonal entries as A.

1.3. Some useful results on copositivity

Let us start by some helpful elementary properties of copositive matrices. First we observe that there is nothing special about the standard simplex (apart from being the simplest polytope), in that it can be replaced with any positive portion of a unit sphere: let $\|.\|$ denote any norm on $\mathbb{R}^n$ and define, for a symmetric $n \times n$ matrix A,

$$\mu(\mathsf{A}) := \min\left\{\mathbf{x}^\top \mathsf{A}\mathbf{x} : \|\mathbf{x}\| = 1\,,\ \mathbf{x} \in \mathbb{R}^n_+\right\}. \tag{1}$$

Then A is copositive if and only if $\mu(\mathsf{A}) \geq 0$.

The choice of ℓ^1-norm $\|\mathbf{x}\|_1 := \sum_i |x_i|$ would yield $\mu(\mathsf{A}) = \gamma(\mathsf{A})$ discussed above.

One of the essential properties is that copositivity is inherited by any principal submatrix (PSM) of a symmetric copositive matrix A. This result will be used repeatedly in later chapters and is, therefore, especially important.

Theorem 1.1 (*[5]*). *If A is a copositive, symmetric matrix, then also every PSM of A and every permutation similar matrix $\mathsf{P}^\top\mathsf{A}\mathsf{P}$ (with P a permutation matrix) is again copositive.*

Another useful result for simplification of later steps is concerned with rescaling of main diagonal elements.

Theorem 1.2 (*[16]*). *Let $\mathsf{A} \in \mathcal{S}_n$ have only positive diagonal elements and define $\mathsf{D} = [\mathrm{Ddiag}(\mathsf{A})]^{-1/2}$. Then A is a copositive matrix if and only if the rescaled matrix DAD, where all diagonal elements are 1, is copositive.*

While establishing copositivity of a matrix indeed becomes very hard for larger orders, there are closed-form solutions for matrices of small order [17–20].

Theorem 1.3. *A symmetric matrix $\mathsf{A} \in \mathcal{S}_2$ of order two is copositive if and only if*

$$a_{11} \geq 0 \quad \text{and} \quad a_{22} \geq 0$$

and

$$a_{12} + \sqrt{a_{11}a_{22}} \geq 0\,.$$

A symmetric matrix $\mathsf{A} \in \mathcal{S}_3$ of order three is copositive if and only if

$$a_{11} \geq 0\,,\ a_{22} \geq 0\,,\ a_{33} \geq 0\,,$$

$$\bar{a}_{12} = a_{12} + \sqrt{a_{11}a_{22}} \geq 0\,,$$

$$\bar{a}_{13} := a_{13} + \sqrt{a_{11}a_{33}} \geq 0\,,$$

$$\bar{a}_{23} := a_{23} + \sqrt{a_{22}a_{33}} \geq 0$$

and

$$\sqrt{a_{11}a_{22}a_{33}} + a_{12}\sqrt{a_{33}} + a_{13}\sqrt{a_{22}} + a_{23}\sqrt{a_{11}} + \sqrt{2\bar{a}_{12}\bar{a}_{13}\bar{a}_{23}} \geq 0\,. \tag{2}$$

In the special case where all diagonal entries are equal to one, and if there is a sign change in two rows off the diagonal (the only case where no row/column reduction is directly possible, see below), e.g., if $\min\{a_{13}, a_{23}\} \geq 0 > a_{12}$, these conditions reduce to

$$a_{12} \geq -1\,,$$

while for the opposite case $\max\{a_{13}, a_{23}\} < 0 \leq a_{12}$ they reduce to

$$\min\{a_{13}, a_{23}\} \geq -1 \quad \text{and} \quad 1 + a_{12} + \sqrt{2\bar{a}_{12}\bar{a}_{13}\bar{a}_{23}} \geq -(a_{13} + a_{23})\,.$$

Note that the original criterion in the case of order 3 in [19] is slightly different: while keeping the first 6 inequalities $a_{ii} \geq 0$ and $a_{ij} \geq -\sqrt{a_{ii}a_{jj}}$ above, condition (2) is replaced with the alternative condition

$$\det \mathsf{A} \geq 0 \quad \text{or} \quad \sqrt{a_{11}a_{22}a_{33}} + a_{12}\sqrt{a_{33}} + a_{13}\sqrt{a_{22}} + a_{23}\sqrt{a_{11}} \geq 0\,. \tag{3}$$

As claimed in [17], direct equivalence was proved by [18]. In the sequel we will employ either (2) or (3), whichever seems more convenient.

Similar closed-form conditions to determine copositivity of a matrix of order $n \leq 7$ can be found in [21] — beyond this order, to the best of the authors' knowledge, there are no algorithmic solutions to that do not either focus on an investigation on single rows/columns or require some recursive procedure. To this end, in the sequel we will focus on decomposition methods. For recursions, we only consider matrices of higher order ($n > 7$), as smaller ones can be solved directly.

1.4. Decomposition strategies for checking copositivity

In order to reduce the order of the matrix to be checked, the following theorem explains in which cases specific columns/rows can be omitted. Since every permuted version $\mathsf{P}^\top\mathsf{A}\mathsf{P}$ of A shares the same copositivity property with A, we can focus without loss of generality on the first row.

Theorem 1.4 (*[7,22]*). *Let $\mathsf{A} \in \mathbb{R}^{n\times n}$ be a symmetric matrix with the following partitioning:*

$$\mathsf{A} = \begin{bmatrix} \alpha & \mathbf{b} \\ \mathbf{b}^\top & \mathsf{B} \end{bmatrix} \tag{4}$$

where B is an $(n-1)\times(n-1)$ (symmetric) matrix, $\alpha \in \mathbb{R}$ and $\mathbf{b} \in \mathbb{R}^{n-1}$. Then the following statements hold:

- *(a) If $\alpha < 0$ then A is not copositive.*
- *(b) If $\mathbf{b} \in \mathbb{R}^{n-1}_+$ and $\alpha \geq 0$ then A is copositive if and only if B is copositive.*
- *(c) If however $-\mathbf{b} \in \mathbb{R}^{n-1}_+$ and $\alpha > 0$ then A is copositive if and only if*

  $$\alpha\mathsf{B} - \mathbf{b}\mathbf{b}^\top\,,$$

  the Schur complement scaled by α, is copositive.
- *(d) If $\alpha = 0$ and at least one entry of $\mathbf{b}$ is negative, then A is not copositive.*

Generalizing above result (c) to more than one row, we obtain the following:

Theorem 1.5 ([23,24]). *Let $A \in \mathcal{S}_n$ with the decomposition*

$$A = \begin{bmatrix} B_{dec} & D_{dec} \\ D_{dec}^\top & C_{dec} \end{bmatrix} \tag{5}$$

where $B_{dec} \in \mathcal{S}_m$, $C_{dec} \in \mathcal{S}_l$ and $D_{dec} \in \mathbb{R}^{m\times l}$ with $m + l = n$. Let B_{dec} be positive-definite and assume that $B_{dec}^{-1} D_{dec}$ has no positive entry.

Then A is copositive if and only if $C_{dec} - D_{dec}^\top B_{dec}^{-1} D_{dec}$ is copositive.

Remark 1.6. If we assume B_{dec} only copositive instead, this result does not hold any longer — consider the following example:

$$A = \begin{bmatrix} 1 & 2 & -1 \\ 2 & 1 & -1 \\ -1 & -1 & 0.7 \end{bmatrix},\ B_{dec} = \begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix},\ D_{dec} = \begin{bmatrix} -1 \\ -1 \end{bmatrix},\ C_{dec} = \begin{bmatrix} 0.7 \end{bmatrix}$$

Then we have that

$$B_{dec}^{-1} D_{dec} = \begin{bmatrix} -\frac{1}{3} & \frac{2}{3} \\ \frac{2}{3} & -\frac{1}{3} \end{bmatrix} \begin{bmatrix} -1 \\ -1 \end{bmatrix} = \begin{bmatrix} -\frac{1}{3} \\ -\frac{1}{3} \end{bmatrix}$$

has no positive entry, and

$$C_{dec} - D_{dec}^\top B_{dec}^{-1} D_{dec} = 0.7 - \begin{bmatrix} -1 \\ -1 \end{bmatrix}^T \begin{bmatrix} -\frac{1}{3} & \frac{2}{3} \\ \frac{2}{3} & -\frac{1}{3} \end{bmatrix} \begin{bmatrix} -1 \\ -1 \end{bmatrix} = 0.1 > 0$$

is copositive. But the original matrix A is not copositive, as $\mathbf{x} = \begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix}$ with $\mathbf{x}^\top A \mathbf{x} = -0.3 < 0$ is a violating vector.

With the same decomposition, the following result uses different (sufficient) conditions.

Proposition 1.7. *Let $A \in \mathcal{S}_n$ with the decomposition*

$$A = \begin{bmatrix} B_{dec} & D_{dec} \\ D_{dec}^\top & C_{dec} \end{bmatrix} \tag{6}$$

where $B_{dec} \in \mathcal{S}_m$, $C_{dec} \in \mathcal{S}_l$ and $D_{dec} \in \mathbb{R}^{m\times l}$ with $m+l = n$, such that B_{dec} and C_{dec} are both copositive, and such that $D_{dec} \in \mathbb{R}_+^{m\times l}$ has no negative entry.

Then A is copositive.

Proof. It is trivial to see that the sum of copositive matrices is always copositive. In our case, A is the sum of three matrices

$$A = \begin{bmatrix} B_{dec} & O \\ O^\top & O \end{bmatrix} + \begin{bmatrix} O & D_{dec} \\ D_{dec}^\top & O \end{bmatrix} + \begin{bmatrix} O & O \\ O^\top & C_{dec} \end{bmatrix}, \tag{7}$$

each of which are copositive for different obvious reasons. □

This means that if a matrix is brought in a form where nonnegative values accumulate in the northeast (upper right) and southwest (lower left) corner, and hence forming 'rectangles' in the corners such that the decomposition in (6) can be applied, only B_{dec} and C_{dec} have to be checked for copositivity to verify the same for A. This is the main idea of the copositivity checking procedure explained in the sequel.

To ease formulation, let us introduce the undirected *negative sign-graph* $\mathcal{G}_-(A)$ of a given symmetric $n \times n$ matrix A: the vertex set is $V = \{1, \dots, n\}$ and every negative $a_{ij} < 0$ generates an edge $\{i, j\}$ in $\mathcal{G}_-(A)$, which then has adjacency matrix

$$A^\sigma := [H(-a_{ij})]_{\{i,j\}\in V\times V}\,.$$

with the Heaviside function $H(t) = \text{sign}(\max\{t, 0\})$, hence

$$H(t) = \begin{cases} 0 & \text{if } t \le 0\,, \\ 1 & \text{if } t > 0\,. \end{cases}$$

Obviously, if A is a symmetric matrix, then A^σ is also symmetric.

If $\mathcal{G}_-(A)$ has m connected components, Proposition 1.7 can be repeatedly applied:

Theorem 1.8. *If $A \in \mathbb{R}^{n\times n}$ is a symmetric matrix such that A^σ is a block diagonal matrix with off-diagonal zero blocks,*

$$A^\sigma = \begin{bmatrix} A_1^\sigma & O & \cdots & O \\ O & A_2^\sigma & \cdots & O \\ \vdots & \vdots & \ddots & \vdots \\ O & O & \cdots & A_m^\sigma \end{bmatrix}, \tag{8}$$

then A is copositive if and only if the respective matrices $A_1, \dots, A_m$ are copositive.

Proof. The assertion follows from Proposition 1.7 by induction on m and Theorem 1.1. □

2. Preprocessing, reordering and decomposition with overlaps

2.1. Matrix preprocessing

In the following sections we will assume that the given matrix A is preprocessed, meaning that the criteria of Theorem 1.4 are checked and applied repeatedly, until none of these criteria is met anymore. This means especially that rows/columns with only positive or negative values (apart from the main diagonal) are removed. Also, as a final step using Theorem 1.2 we ensure $A_{i,i} = 1$ for all positive main diagonal elements of A.

2.2. Fast reordering for decomposition

Both for visualization and easy implementation, the first step of our algorithm is to reorder A^σ such that connected components used in Theorem 1.8 can easily be identified. These components are then checked for copositivity.

To this end, the (reversed) Cuthill–McKee algorithm, as first mentioned in [25] is used to find an appropriate permutation of rows and columns; see [26]. A fast implementation in `Python` using the `'Scipy'` module [27] is available. Once the desired permutation of A^σ is reached, A gets permuted in the same way. This implicitly leads to non-negative values accumulating in the north-east and south-west (see Fig. 1).

The result is that starting from the lower right corner, connected points are kept together while separate components form their own clusters. If the graph has separated components, a clearly visible structure indicating the split point between the components will emerge.

An example is visualized and discussed in the appendix.

Proceeding for connected components (if necessary, for all), we finally have to deal with the connected case.

2.3. Case of connected $\mathcal{G}_-(A)$

Theorem 2.1. *Let $A \in \mathcal{S}_n$ be a matrix resulting from all preprocessing steps. After appropriate symmetric reordering of rows and columns, the following decomposition of A is always possible, generalizing (7):*

$$A = B + C + D - E \tag{9}$$

with

$$B = \begin{bmatrix} B_{dec} & O \\ O & O \end{bmatrix} \in \mathcal{S}_n \quad \textit{and} \quad B_{dec} \in \mathcal{S}_m\,,$$

$$C = \begin{bmatrix} O & O \\ O & C_{dec} \end{bmatrix} \in \mathcal{S}_n \quad \textit{and} \quad C_{dec} \in \mathcal{S}_l\,,$$

$$D = \begin{bmatrix} O & O & D_{dec} \\ O & O & O \\ D_{dec}^\top & O & O \end{bmatrix} \in \mathcal{N}_n \quad \textit{with} \quad D_{dec} \in \mathbb{R}_+^{k\times h}\,,$$

and

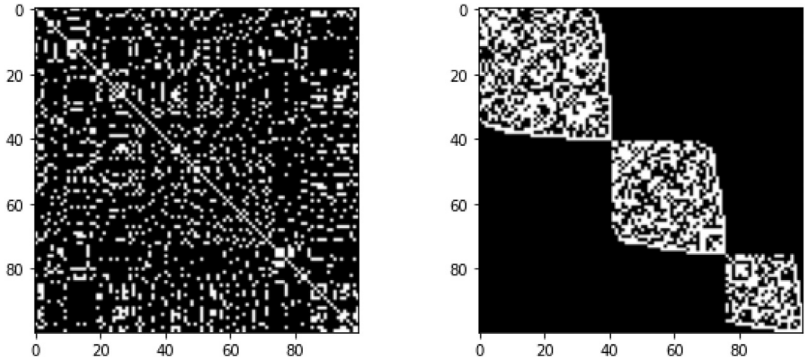

Fig. 1. left: unordered 'raw' adjacency matrix A^σ (black = 0, white = one or diagonal);right: the output of the reversed Cuthill–McKee algorithm.

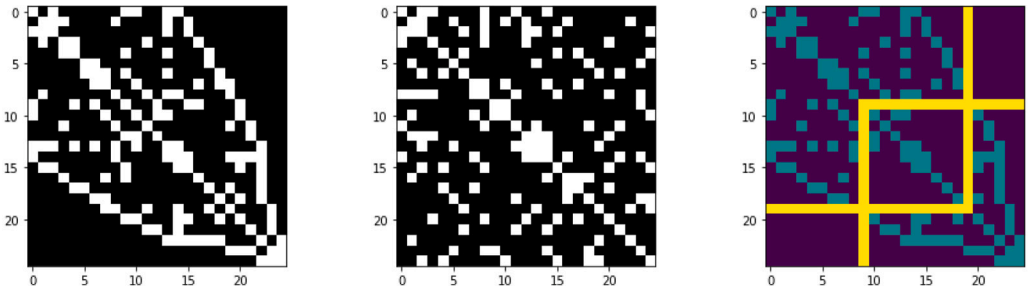

Fig. 2. Left: original matrix; center: reordered matrix; right: found decomposition with the matrices B_{dec}, C_{dec} and E_{dec} indicated by their yellow boundaries, defined by the matrix D_{dec} in the corners. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

$$E = \begin{bmatrix} O & O & O \\ O & E_{dec} & O \\ O & O & O \end{bmatrix} \in S_n \quad \textit{with} \quad E_{dec} \in S_u$$

such that E_{dec} *is the overlapping common part of the matrices* B_{dec} *and* C_{dec}. *This means that* $m + l - u = n$, $m + h = n$ *and* $l + k = n$.

Proof. Assume A to be a matrix as described. Then there must exist at least one non-negative entry in each row/column of the matrix (otherwise this row would have been deleted in the preprocessing steps of Theorem 1.4). Hence there always exists a permutation such that there is a non-negative entry in the upper right corner of the matrix. So D_{dec} can at least be set to only consist of this one entry and define the other matrices accordingly, which is a valid (but perhaps not very useful) decomposition according to the theorem. □

Based on Theorem 2.1, we note the equivalence of (9) to

$$A - D = (B - E) + (C - E) + E\,. \tag{10}$$

The matrix E represents the overlapping part between the matrices B and C, i.e. where their respective adjacency matrices B^σ and C^σ could have nonzero entries. In the case described in (6), E would be the empty matrix (of order 0). The matrix D consists of non-negative entries that accumulate in the northeast and southwest corners of the matrix A after reordering. See Fig. 2. The matrix D is by no means unique; in implementation it pays to pick the largest of available "dark rectangles" (by area).

Now we can derive some properties given the introduced decomposition:

Theorem 2.2. *Let* $A \in S_n$ *have the decomposition as discussed in Theorem 2.1.*

(a) If one of the matrices B, C *and* E *is not copositive, then* A *cannot be copositive. Constructing violating vectors for* A *using those of the other negative certificates is straightforward by augmentation.*

(b) All copositivity tests for above submatrices actually can be applied after dropping zero rows and columns, which may reduce order.

Proof. (a) The addressed matrices are all PSMs, so the result follows by Theorem 1.1. (b) is trivial. □

Now we introduce a sufficient condition for copositivity of A with connected $\mathcal{G}_-(A)$:

Theorem 2.3. *Let* $A \in S_n$ *be a real, symmetric matrix with connected* $\mathcal{G}_-(A)$, *decomposed as discussed in Theorem 2.1. Then* A *is copositive if there is a* $\lambda \in (0, 1)$ *such that*

$$B - (1 - \lambda)E = (B - E) + \lambda E \quad \textit{and} \quad C - \lambda E = (C - E) + (1 - \lambda)E$$

are both copositive.

Proof. If a λ exists such that both $B-(1-\lambda)E$ and $C-\lambda E$ are copositive, then by (10) we have

$$(A - D) = [(B - E) + \lambda E] + [(C - E) + (1 - \lambda)E]$$

which is copositive as the sum of copositive matrices is always copositive. Hence A is copositive. □

Remark 2.4. It is worth noting that

$$B - (1 - \lambda)E = (B - E) + \lambda E \quad \text{and} \quad C - \lambda E = (C - E) + (1 - \lambda)E$$

both copositive with $\lambda \in \{0, 1\}$ is not possible. If we assume $\lambda = 0$ we have

$$B - (1 - \lambda)E = B - E$$

which is equivalent to

$$\begin{bmatrix} B_1 & B_2 \\ B_2^\top & E_{\text{dec}} \end{bmatrix} - \begin{bmatrix} O & O \\ O & E_{\text{dec}} \end{bmatrix} = \begin{bmatrix} B_1 & B_2 \\ B_2^\top & O \end{bmatrix}.$$

Now, if any entry in B_2 were negative, the resulting matrix would not be copositive due to Theorem 1.4(d). But if there were indeed no negative

entries in B_2, $\mathcal{G}_-(\mathsf{A})$ would actually be disconnected, contradicting the assumption in Theorem 2.3.

For a positive certificate, the main task is now to find such a λ. In the following, some cases that can occur while searching for this are discussed. While looking for a suitable λ to prove copositivity, it is possible that only one of both resulting matrices is copositive while the other one is not. But such a mixed result yields no valuable insight since no conclusion about copositivity of A can be made. Hence, one has to keep looking for a 'decisive' λ – the following theorem ensures that this search will always terminate in either of the cases presented.

Theorem 2.5. *Let $\mathsf{A} \in S_n$ preprocessed and reordered with a decomposition as in Theorem 2.1 and assume B, C and E are copositive. Then there is always a $\lambda \in [0,1]$ such that either*

both $\mathsf{B}-(1-\lambda)\mathsf{E}$ and $\mathsf{C}-\lambda\mathsf{E}$ are copositive

or

both $\mathsf{B}-(1-\lambda)\mathsf{E}$ and $\mathsf{C}-\lambda\mathsf{E}$ are not copositive.

If there is a λ_1 such that both matrices are copositive, then there is no λ_2 such that both of them are not copositive and vice versa.

Proof. Define the functions

$$f(\lambda) = \min\{\mathbf{x}^\top(\mathsf{B}-(1-\lambda)\mathsf{E})\mathbf{x} : \mathbf{x} \in \mathbb{R}^n_+,\ \|\mathbf{x}\| = 1\}$$

and

$$g(\lambda) = \min\{\mathbf{x}^\top(\mathsf{C}-\lambda\mathsf{E})\mathbf{x} : \mathbf{x} \in \mathbb{R}^n_+,\ \|\mathbf{x}\| = 1\}$$

for some norm $\|.\|$. Obviously both functions are continuous in the variable λ. Also, since the matrix E is assumed to be copositive, both functions are monotone - f is monotonically increasing, g is monotonically decreasing.

If for some λ either f or g is negative, the respective matrix is not copositive - on the other hand, if the function takes a non-negative value, the respective matrix is copositive.

If for some λ both functions evaluate to a negative result case 2 is satisfied, and if both functions evaluate to a non-negative result, case 1 is satisfied. Now the focus lies on showing that either of both cases is always satisfied. Without loss of generality, we say that for $0 \le \lambda_1 < 1$ we have that $f(\lambda_1) < 0$ and $g(\lambda_1) \ge 0$ (e.g. we know that for $\lambda = 0$, $g(0) \ge 0$ since C is copositive, and if the negative sign graph $\mathcal{G}_-(\mathsf{A})$ is connected, $f(0) < 0$ as established in Remark 2.4).

Now, evaluate $f(1)$. If the result was negative, then B would be not copositive which contradicts the assumptions made on B.

By the intermediate value theorem, there must exist a $\lambda \in (\lambda_1, 1]$ such that $f(\lambda) = 0$. We therefore choose

$$\lambda_2 := \min\{\lambda \in (\lambda_1, 1] : f(\lambda) = 0\}\,.$$

Next, evaluate $g(\lambda_2)$; if the result is non-negative, both functions are non-negative with the same λ_2, and we are done since $f(\lambda_2) = 0$. If, on the other hand, $g(\lambda_2) < 0$, then (by continuity of f and g) there exists an $\epsilon > 0$ such that $g(\lambda_2 - \epsilon) < 0$ and $f(\lambda_2 - \epsilon) < 0$, which completes this part of the proof.

What is left to check is that there can never co-exist two $\lambda_1, \lambda_2 \in [0,1]$ with

$$g(\lambda_1) < 0 \text{ and } f(\lambda_1) < 0$$

and simultaneously

$$g(\lambda_2) \ge 0 \text{ and } f(\lambda_2) \ge 0\,.$$

Assume such λ_i existed. Then by monotonicity of f and g

$$g(\lambda_1) < 0 \le g(\lambda_2) \quad \Longrightarrow \quad \lambda_2 < \lambda_1$$

and at the same time

$$f(\lambda_1) < 0 \le f(\lambda_2) \quad \Longrightarrow \quad \lambda_2 > \lambda_1\,,$$

which are contradictory statements. □

Observe that the functions f and g are merely used for proof purposes, we need not know all values of them. One way of determining the correct λ in a concrete implementation would be to apply a bisection procedure, i.e., starting at $\lambda = 0.5$ and evaluating both matrices. If $f(\lambda)$ is positive and $g(\lambda)$ is negative, choose $\lambda = 0.25$ in the next step, if $f(\lambda)$ is negative and $g(\lambda)$ is positive continue with $\lambda = 0.75$ etc. until both matrices are copositive or both are not.

Even if it seems impossible to obtain a straightforward definitive statement on copositivity of A if $(\mathsf{A}-\mathsf{D})$ is not copositive in a general case, it is still worth investigating some properties that are connected to the described procedure.

Theorem 2.6. *If there is a λ such that both $\mathsf{B}-(1-\lambda)\mathsf{E}$ and $\mathsf{C}-\lambda\mathsf{E}$ are not copositive, then $(\mathsf{A}-\mathsf{D})$ is not copositive if the intersection of*

$$B_y^\lambda := \left\{ \mathbf{y} \in \mathbb{R}^u_+ : \begin{bmatrix}\mathbf{x}\\ \mathbf{y}\\ \mathbf{o}\end{bmatrix}^\top (\mathsf{B}-(1-\lambda)\mathsf{E}) \begin{bmatrix}\mathbf{x}\\ \mathbf{y}\\ \mathbf{o}\end{bmatrix} < 0 \text{ for some } \mathbf{x} \in \mathbb{R}^v_+ \right\}$$

and

$$C_{\mathbf{y}}^\lambda := \left\{ \mathbf{y} \in \mathbb{R}^u_+ : \begin{bmatrix}\mathbf{o}\\ \mathbf{y}\\ \mathbf{z}\end{bmatrix}^\top (\mathsf{C}-\lambda\mathsf{E}) \begin{bmatrix}\mathbf{o}\\ \mathbf{y}\\ \mathbf{z}\end{bmatrix} < 0 \text{ for some } \mathbf{z} \in \mathbb{R}^w_+ \right\}$$

is not empty, $B_y^\lambda \cap C_y^\lambda \neq \emptyset$. Here n is the order of the original matrix A and $u+v+w = n$.

Proof. Consider a vector $\bar{\mathbf{y}} \in B_y^\lambda \cap C_y^\lambda$. Also, based on the definition of both sets, there are vectors $\bar{\mathbf{x}} \in B_y^\lambda$, $\bar{\mathbf{z}} \in C_y^\lambda$ that satisfy

$$\bar{\mathbf{x}}^\top(\mathsf{B}-(1-\lambda)\mathsf{E})\bar{\mathbf{x}} < 0$$

and

$$\bar{\mathbf{z}}^\top(\mathsf{C}-\lambda\mathsf{E})\bar{\mathbf{z}} < 0$$

with

$$\bar{\mathbf{x}} = \begin{bmatrix}\mathbf{x}\\ \mathbf{y}\\ \mathbf{o}\end{bmatrix},\ \bar{\mathbf{y}} = \begin{bmatrix}\mathbf{o}\\ \mathbf{y}\\ \mathbf{o}\end{bmatrix},\ \bar{\mathbf{z}} = \begin{bmatrix}\mathbf{o}\\ \mathbf{y}\\ \mathbf{z}\end{bmatrix},\ \bar{\mathbf{x}}, \bar{\mathbf{y}}, \bar{\mathbf{z}} \in \mathbb{R}^n_+\,,$$

such that both contain the $\mathbf{y}$ vector. Then we have that

$$0 > \bar{\mathbf{x}}^\top(\mathsf{B}-(1-\lambda)\mathsf{E})\bar{\mathbf{x}} + \bar{\mathbf{z}}^\top(\mathsf{C}-\lambda\mathsf{E})\bar{\mathbf{z}} =$$

$$(\bar{\mathbf{x}}+\bar{\mathbf{z}}-\bar{\mathbf{y}})^\top(\mathsf{B}-(1-\lambda)\mathsf{E})(\bar{\mathbf{x}}+\bar{\mathbf{z}}-\bar{\mathbf{y}}) + (\bar{\mathbf{x}}+\bar{\mathbf{z}}-\bar{\mathbf{y}})^\top(\mathsf{C}-\lambda\mathsf{E})(\bar{\mathbf{x}}+\bar{\mathbf{z}}-\bar{\mathbf{y}}) =$$

$$(\bar{\mathbf{x}}+\bar{\mathbf{z}}-\bar{\mathbf{y}})^\top((\mathsf{B}-\mathsf{E})+(\mathsf{C}-\mathsf{E})+\mathsf{E})(\bar{\mathbf{x}}+\bar{\mathbf{z}}-\bar{\mathbf{y}}) = (\bar{\mathbf{x}}+\bar{\mathbf{z}}-\bar{\mathbf{y}})^\top(\mathsf{A}-\mathsf{D})(\bar{\mathbf{x}}+\bar{\mathbf{z}}-\bar{\mathbf{y}})^\top$$

and $\bar{\mathbf{x}}+\bar{\mathbf{z}}-\bar{\mathbf{y}} \in \mathbb{R}^n_+$ since the $\mathbf{y}$ part occurred in both vectors $\bar{\mathbf{x}}$ and $\bar{\mathbf{z}}$. The expansion of the vectors follows the structure of the matrices B, C, and E. □

In summary, the approach is the following:

Once the decomposition Theorem 2.1 has been applied, the following steps have to be taken:

1. Check if B, C and E are copositive matrices.
   - (1a) If they are copositive, continue;
   - (1b) else A is not copositive.
2. Find a λ for the matrices B and C as described in Theorem 2.5.
   - (2a) If both $\mathsf{B}-(1-\lambda)\mathsf{E}$ and $\mathsf{C}-\lambda\mathsf{E}$ are copositive. Then A is copositive;
   - (2b) If both $\mathsf{B}-(1-\lambda)\mathsf{E}$ and $\mathsf{C}-\lambda\mathsf{E}$ are not copositive. Then A is flagged 'not determined' - so no copositivity certificate on A can be issued at this stage.

Obviously, the algorithm can be applied recursively, splitting up very large matrices into smaller, easier-to-check parts.

3. Decomposition for k-diagonal matrices

Above decomposition strategy can be used on any arbitrary matrix in the quest to prove copositivity, but the computational cost may be growing exponentially with the order. However, for a special class of matrices this algorithm seems particularly appropriate:

Definition 3.1. Consider an odd $k \in \mathbb{N}$. A matrix $\mathsf{A} \in \mathcal{S}_n$ is called k-diagonal, if all its entries are 0, except for the main diagonal and the $(k-1)/2$ adjacent off-diagonals: $a_{ij} = 0$ if $|i-j| > k/2$.

Obviously, if the matrices B and C in the decomposition procedure are chosen properly, we are able to get $\mathsf{D} = \mathsf{O}$ (a zero matrix) rather easily with this specific type of matrices – namely when choosing B_{dec} and C_{dec} as 3×3 matrices. Then, starting from the upper left corner we can step by step check the individual block, i.e., the resulting matrices B, C and E, and try to find a λ such that the block becomes copositive. Hence, instead of ending up with a rapidly growing tree of possibilities for the best choice of λ-s, the search simplifies to a straightforward procedure.

This idea is demonstrated for the case $k = 5$, i.e., pentadiagonal matrices. But the exact same algorithm could be applied to arbitrary k - given that a sufficiently fast copositivity check for the intermediate matrices exists (following [21], one can imagine a comparably fast procedure for $k \le 13$).

Since every symmetric, pentadiagonal matrix can be processed such that the main diagonal only consists of ones (without having any effect on the property of copositivity), matrices considered in this section are of the form

$$\mathsf{A} = \begin{bmatrix} 1 & a_{12} & a_{13} & 0 & 0 & 0 \\ a_{21} & 1 & a_{23} & a_{24} & 0 & 0 \\ a_{31} & a_{32} & 1 & a_{34} & \ddots & 0 \\ 0 & a_{42} & a_{43} & 1 & \ddots & a_{n-2,n} \\ 0 & 0 & \ddots & \ddots & \ddots & a_{n-1,n} \\ 0 & 0 & 0 & a_{n,n-2} & a_{n,n-1} & 1 \end{bmatrix}$$

with $a_{ij} = a_{ji}$ and without loss of generality all entries in the range $[-1, 1]$; indeed, recall that $a_{ij} < -1$ renders the matrix not copositive, while $a_{ij} > 1$ can be truncated to one without changing the copositivity status of the matrix [22, Lemma 4.4].

3.1. Case $n = 4$

This is the smallest order where pentadiagonality has a meaning, namely $a_{14} = 0$. We will study this just to illustrate how this structure can simplify analysis. We will give only rough ideas and start with a case distinction according to sign patterns. Indeed, define k_- to be the number of negative entries above the diagonal, and assume that matrices of order three can be easily treated. Then obviously the cases $k_- \in \{0, 1\}$ are easy, because at least one row/column can be dropped. The next case $k_- = 2$ has essentially two patterns, one where again a non-negative row/column can be dropped. The other, not immediately reducible pattern looks like

$$\mathsf{A} = \begin{bmatrix} 1 & + & - & 0 \\ + & 1 & + & - \\ - & + & 1 & + \\ 0 & - & + & 1 \end{bmatrix}, \qquad \begin{array}{l} \text{with negative-sign graph } \mathcal{G}_-(\mathsf{A}) \\ \text{equal to two disjoint edges.} \end{array}$$

Proposition 3.2. *Suppose* A *follows above sign-pattern with all PSMs of order two positive-semidefinite. Then* A *is copositive.*

Proof. Exchanging rows/columns 2 and 3 by P, we are in the disjointly decomposable case

$$\mathsf{P}^\top \mathsf{A} \mathsf{P} = \begin{bmatrix} 1 & - & + & 0 \\ - & 1 & + & + \\ + & + & 1 & - \\ 0 & + & - & 1 \end{bmatrix}$$

where all PSMs of order 2 are copositive by hypothesis, therefore the whole A is as well, according to Proposition 1.7. □

We proceed to $k_- = 3$ and at first look at the sign pattern

$$\mathsf{A} = \begin{bmatrix} 1 & - & + & 0 \\ - & 1 & - & + \\ + & - & 1 & - \\ 0 & + & - & 1 \end{bmatrix}, \qquad \begin{array}{l} \text{with negative-sign graph} \\ \mathcal{G}_-(\mathsf{A}) = P_4 \text{ the path on 4 vertices.} \end{array}$$

This is not immediately reducible. The copositivity criteria are more complex than before, some may imply others, and they may be simplified a bit as well:

Proposition 3.3. *Suppose* A *follows above sign-pattern with all PSMs of order two positive-semidefinite. Then all PSMs of order three are copositive if and only if*

1. $a_{12}a_{23} \le a_{13}$ *or* $a_{12}^2 + a_{13}^2 + a_{23}^2 \le 1 + 2a_{12}a_{13}a_{23}$; *and*
2. $a_{23}a_{34} \le a_{24}$ *or* $a_{23}^2 + a_{24}^2 + a_{34}^2 \le 1 + 2a_{23}a_{24}a_{34}$.

Furthermore, in this case A *itself is copositive if the two following conditions are satisfied in addition:*

3. $a_{12}a_{13} + a_{24}a_{34} \le a_{23}$ *or* $(a_{12}a_{13} + a_{24}a_{34} - a_{23})^2 \le (1 - a_{12}^2 - a_{24}^2)(1 - a_{13}^2 - a_{34}^2)$; *and*
4. $\max\{a_{21}^2 + a_{24}^2, a_{31}^2 + a_{34}^2\} \le 1$.

Proof. First we investigate copositivity of all PSMs of order three. For ease of notation let us decompose and denote in this proof

$$\mathsf{A} = \begin{bmatrix} 1 & \mathbf{a}^\top & 0 \\ \mathbf{a} & \mathsf{E} & \mathbf{b} \\ 0 & \mathbf{b}^\top & 1 \end{bmatrix} \quad \text{with} \quad \mathsf{E} = \begin{bmatrix} 1 & \sigma \\ \sigma & 1 \end{bmatrix},$$

where $\max\{a_1, b_2, \sigma\} < 0 \le \min\{a_2, b_1\}$. In the two PSMs of order three,

$$\begin{bmatrix} 1 & a_i & 0 \\ a_i & 1 & b_i \\ 0 & b_i & 1 \end{bmatrix}, \; i \in \{1, 2\},$$

dropping, respectively, row/column 1 if $i = 1$ and row/column 3 if $i = 2$ which both contain no negative entry. Thus they are copositive, as all PSMs of order two are by hypothesis.

By contrast, in both the remaining two PSMs $\begin{bmatrix} 1 & \mathbf{a}^\top \\ \mathbf{a} & \mathsf{E} \end{bmatrix}$ and in $\begin{bmatrix} \mathsf{E} & \mathbf{b}^\top \\ \mathbf{b} & 1 \end{bmatrix}$, the center row/columns contain only negative off-diagonals, so by Theorem 1.4(c) we have to check copositivity of the scaled Schur complements F_i, $i \in \{1, 2\}$, where

$$\mathsf{F}_1 = \begin{bmatrix} 1 - a_1^2 & a_2 - \sigma a_1 \\ a_2 - \sigma a_1 & 1 - \sigma^2 \end{bmatrix} \quad \text{and} \quad \mathsf{F}_2 = \begin{bmatrix} 1 - \sigma^2 & b_1 - \sigma b_2 \\ b_1 - \sigma b_2 & 1 - b_2^2 \end{bmatrix}.$$

As no diagonal elements of above 2×2 matrices F_i are negative, it is enough to check non-negativity of the off-diagonals, or else non-negativity of the determinants of F_i. Hence the result on the PSMs of order three.

Next define

$$\mathsf{F} := \mathsf{E} - \mathbf{a}\mathbf{a}^\top - \mathbf{b}\mathbf{b}^\top = \begin{bmatrix} 1 - a_1^2 - b_1^2 & \sigma - a_1a_2 - b_1b_2 \\ \sigma - a_1a_2 - b_1b_2 & 1 - a_2^2 - b_2^2 \end{bmatrix}.$$

If F is copositive, then so is

$$\mathsf{A} = \begin{bmatrix} 1 & \mathbf{a}^\top & 0 \\ \mathbf{a} & \mathbf{a}\mathbf{a}^\top & \mathbf{o} \\ 0 & \mathbf{o}^\top & 0 \end{bmatrix} + \begin{bmatrix} 0 & \mathbf{o}^\top & 0 \\ \mathbf{o} & \mathbf{b}\mathbf{b}^\top & \mathbf{b} \\ 0 & \mathbf{b}^\top & 1 \end{bmatrix} + \begin{bmatrix} 0 & \mathbf{o}^\top & 0 \\ \mathbf{o} & \mathsf{F} & \mathbf{o} \\ 0 & \mathbf{o}^\top & 0 \end{bmatrix}.$$

Here $\sigma < 0$, so positivity of the diagonal of F is not sufficient for its copositivity. We either need $\sigma - a_1a_2 - b_1b_2 \ge 0$ or else $\det \mathsf{F} \ge 0$, which

entails Condition 3. Condition 4 is the request that F has no negative diagonal entries. Hence the result. □

The next challenging sign pattern with $k_- = 3$ is

$$\mathsf{A} = \begin{bmatrix} 1 & + & - & 0 \\ + & 1 & - & - \\ - & - & 1 & + \\ 0 & - & + & 1 \end{bmatrix}, \quad \text{again with negative-sign graph } \mathcal{G}_-(\mathsf{A}) = P_4 \text{ the path on 4 vertices.}$$

However this is equivalent to the previous one up to a swap of row/column two with row/column three. As can be checked easily, all remaining patterns with $k_- \in \{3,4,5\}$ allow for immediate reduction in order, hence perhaps less interesting; nevertheless, similar conditions as in Propositions 3.2 and 3.3 can be derived explicitly with little additional effort.

3.2. Case $n > 4$: linear-time procedure

Given such a matrix, an attempt to prove copositivity in linear time can be made using the decomposition procedure introduced in Section 2.3.

For the first step, we choose

$$\mathsf{B}_{\text{dec}} = \begin{bmatrix} 1 & a_{12} & a_{13} \\ a_{21} & 1 & a_{23} \\ a_{31} & a_{32} & 1 \end{bmatrix} \text{ and } \mathsf{C}_{\text{dec}} = \begin{bmatrix} 1 & a_{23} & a_{24} & 0 & 0 \\ a_{32} & 1 & a_{34} & \ddots & 0 \\ a_{42} & a_{43} & 1 & \ddots & a_{n-2,n} \\ 0 & \ddots & \ddots & \ddots & a_{n-1,n} \\ 0 & 0 & a_{n,n-2} & a_{n,n-1} & 1 \end{bmatrix}$$

with $\mathsf{E}_{\text{dec}} = \begin{bmatrix} 1 & a_{23} \\ a_{32} & 1 \end{bmatrix}$. Then $\mathsf{D} = \mathsf{O}$ follows immediately from the fact that A is a pentadiagonal matrix. In this decomposition, we first check $\mathsf{E}_{\text{dec}} \in \mathcal{S}_2$ for copositivity by application of Theorem 1.3 (and omit the checks of B_{dec} and C_{dec}). Since the overlap between B and C is not empty, Theorem 2.3 is applicable, i.e., we have to find a λ such that both

$$\mathsf{B}-(1-\lambda)\mathsf{E} = (\mathsf{B}-\mathsf{E})+\lambda\mathsf{E} \quad \text{and} \quad \mathsf{C}-\lambda\mathsf{E} = (\mathsf{C}-\mathsf{E})+(1-\lambda)\mathsf{E} \quad \text{are copositive.}$$

While this would lead to a exponentially growing tree in a general case — as checking C_{dec} for copositivity would again require a decomposition and search for λ etc. - for pentadiagonal matrices it is quite the opposite. No tree forms at all, but instead one simply calculates the smallest λ such that

$$\mathsf{B} - (1-\lambda)\mathsf{E}$$

is copositive — which can be performed due to the small order of B in a very efficient manner. Given that E itself is copositive, if a λ can be found such that this condition is fulfilled, we can update the rest of the matrix by subtracting the already 'used up' part of E from C and continue the process from the beginning — treating C as a 'new' matrix 'A_k'.

Continuing this procedure, one of two cases will eventually arrive:

- No λ can be found such that $\mathsf{B} - (1-\lambda)\mathsf{E}$ is copositive.
- A λ can be found in every step until A_k itself is only a 3×3 matrix, which itself is copositive — in this case, the entire matrix A is copositive, and we obtain a positive certificate.

Therefore, for pentadiagonal instances, we have a polynomial-time heuristic procedure to determining copositivity which is complete unless it terminates prematurely which unfortunately may happen, see below and Appendix!

4. Algorithmic details for pentadiagonal matrices

The procedure iteratively reduces the order of a given pentadiagonal symmetric matrix A of order n until a decision is reached to backtrack for a certificate of the original matrix. Beforehand, preprocessing steps as introduced earlier are applied to the original matrix A.

First, we check the diagonal entries for positivity, removing rows/columns with no negative entries, and exiting with a negative certificate if $a_{ii} = 0 > a_{ij}$ for some $i \neq j$. Obviously, the result still is pentadiagonal (even more: if the second or third row/column is removed, there remains only one non-zero diagonal entry in the first row/column, and we can reduce it as above (if ≥ 0) or below, if negative; thus, order is even reduced by 2).

Next, following Theorem 1.4(b), we remove rows/columns where $a_{ii} \geq 0$ and $a_{ij} > 0$ for all $i \neq j$. This way, we arrive at a possibly smaller pentadiagonal matrix (which for convenience we again call A) with a strictly positive diagonal and a sign change in every row/column off the diagonal.

Following that, we scale A diagonally such that $\operatorname{diag} \mathsf{A} = \mathbf{e}$ and truncate entries $a_{ij} > 1$ to one, i.e., replace a_{ij} with $\max\{a_{ij}, 1\}$. This new matrix is copositive if and only if the original was, and negative certificates can be transferred easily [22, Lemma 4.4]. We obtain a matrix (again called A for easing notation) where all PSMs of order two are positive-semidefinite, or equivalently, where $|a_{ij}| \leq 1 = a_{ii}$ for all i, j. - as values smaller than -1 would immediately refute copositivity.

Now, initialize $\mathsf{A}_0 = \mathsf{A}$ (enjoying above property) and $n_0 = n$; the iterative step consists in processing $\mathsf{A}_k \in \mathcal{S}_{n_k}$ with $n_k \leq n - k$ until either (positive or negative) certificates of A_k are obtained, or else the stopping criterion $n_k \leq 4$ is met:

1. if possible, remove/reduce rows/columns (and update n_k), then scale A_k such that $\operatorname{diag} \mathsf{A}_k = \mathbf{e} \in \mathbb{R}^{n_k}$ and truncate; call the result again A_k;
2. decompose

   $$\mathsf{A}_k = \mathsf{B} + \mathsf{C} - \mathsf{E}$$

   as described in Theorem 2.1 with $\mathsf{B}_{\text{dec}} \in \mathcal{S}_3$, $\mathsf{E}_{\text{dec}} \in \mathcal{S}_2$ and $\mathsf{C}_{\text{dec}} \in \mathcal{S}_{n_k-1}$, so that $\mathsf{D}_{\text{dec}} = \mathsf{O} \in \mathbb{R}^{1\times(n_k-1)}$. Note that by truncation, $\mathsf{E}_{\text{dec}} \in \mathcal{S}_2$ is automatically copositive (because even positive-semidefinite);
3. aiming to profit from Theorem 2.3, we investigate a decomposition

   $$\mathsf{A}_k = [\mathsf{B} - (1-\lambda)\mathsf{E}] + [\mathsf{C} - \lambda\mathsf{E}],$$

   trying to match the sufficient condition there. As we already know $\mathsf{E} \in \mathcal{COP}_{n_k}$, the best chance will be to choose

   $$\underline{\lambda}(\alpha,\beta,\gamma) := \min\left\{\lambda \in [0,1] : \mathsf{B}_{\text{dec}}(\lambda) \in \mathcal{COP}_3\right\} \tag{11}$$

   with

   $$\mathsf{B}_{\text{dec}}(\lambda) = \mathsf{B}_{\text{dec}} - (1-\lambda)\begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & \gamma \\ 0 & \gamma & 1 \end{bmatrix} = \begin{bmatrix} 1 & \alpha & \beta \\ \alpha & \lambda & \lambda\gamma \\ \beta & \lambda\gamma & \lambda \end{bmatrix} \in \mathcal{S}_3\,. \tag{12}$$

   Lemma 4.1 below gives a closed-form expression for this $\underline{\lambda}(\alpha,\beta,\gamma)$ which will be the updated λ_k. Alternatively, this value could be found by line search in conjunction with (frequently) checking the conditions in Theorem 1.3 for $\mathsf{B}_{\text{dec}}(\lambda)$.
4. The corresponding block in $\mathsf{C} - \lambda_k\mathsf{E}$ has the form

   $$\mathsf{C}_{\text{dec}}(\lambda_k) = \begin{bmatrix} (1-\lambda_k)\mathsf{E}_{\text{dec}} & \mathsf{R}^\top \\ \mathsf{R} & \mathsf{S} \end{bmatrix} \in \mathcal{S}_{n_k-1} \tag{13}$$

   and we will take the preprocessed version of it (row/columns removed or reduced, rescaled and truncated) as the update $\mathsf{A}_{k+1} \in \mathcal{S}_{n_{k+1}}$. Should preprocessing already provide certificates, we exit (either with a positive certificate of A_k and therefore, by construction, certifying copositivity of A, or else with a negative certificate, which leads to premature termination and allows no immediate conclusion about whether A is copositive or not). This case is also reached if $\lambda_k = 1$ as $\mathsf{C}_{\text{dec}}(\lambda_k)$ would not be copositive by the same argument as in Remark 2.4 and the fact that (due to the preprocessing) $\mathsf{R} \not\geq \mathsf{O}$; else we increment k by one and repeat.

Next we will present a closed-form expression for $\underline{\lambda}(\alpha,\beta,\gamma)$ defined in (11):

Lemma 4.1. *(a) Consider the case $\gamma=-1$; then the matrix $\mathsf{B}_{\rm dec}=\mathsf{B}_{\rm dec}(1)$ defined in (12) is copositive if and only if $\max\{|\alpha|,|\beta|\}\le 1$ and $\alpha+\beta\ge 0$. (b) Consider the case $\gamma>-1$, the matrix $\mathsf{B}_{\rm dec}(\lambda)\in\mathcal{S}_3$ defined in (12) and $\underline{\lambda}(\alpha,\beta,\gamma)$ as defined in (11) with $\max\{|\alpha|,|\beta|,|\gamma|\}\le 1$ and $\alpha\beta<0$, as well as $\mathsf{B}_{\rm dec}(1)\in\mathcal{COP}_3$. Then we have*

$$\underline{\lambda}(\alpha,\beta,\gamma)=\begin{cases}\max\{\alpha^2,\beta^2\}, & \text{if}\quad \alpha+\beta\ge 0 \text{ or } \gamma=1,\\ \max\{\alpha^2,\beta^2,\mu(\alpha,\beta,\gamma)\}, & \text{if}\quad \alpha+\beta<0 \text{ and } |\gamma|<1,\end{cases}$$

where

$$\mu(\alpha,\beta,\gamma)=\min\left\{\left(\tfrac{\alpha+\beta}{1+\gamma}\right)^2,\tfrac{\alpha^2+\beta^2-2\alpha\beta\gamma}{1-\gamma^2}\right\}\quad \text{if}\quad |\gamma|<1\,.$$

Proof. For both (a) and (b), we use the copositivity conditions on $\mathsf{B}_{\rm dec}(\lambda)\in\mathcal{S}_3$ (in (a) for $\lambda=-\gamma=1$) provided by Theorem 1.3. The psd conditions on the PSM of order two reduce to $\lambda\ge\alpha^2$, $\lambda\ge\beta^2$ and the automatically satisfied $\lambda(1-\gamma^2)\ge 0$. So it only remains to investigate (3) or (2), which we will use alternatively, distinguishing cases.

In case $\alpha+\beta\ge 0$, (2) reduces to

$$(1+\gamma)\lambda+(\alpha+\beta)\sqrt{\lambda}+\sqrt{2\lambda(1+\gamma)(\alpha+\sqrt{\lambda})(\beta+\sqrt{\lambda})}\ge 0\,,$$

which does not restrict $\lambda\ge 0$ at all, due to $\gamma\ge -1$. In case $\gamma=-1$, this reduces to $(\alpha+\beta)\sqrt{\lambda}\ge 0$ which shows (a) as well, as (considering $\mathsf{B}_{\rm dec}(\lambda=1)=\mathsf{B}_{\rm dec}$) it in turn enforces $\alpha+\beta\ge 0$. Summarizing above, we arrive at

$$\underline{\lambda}(\alpha,\beta,\gamma)=\max\{\alpha^2,\beta^2\}\quad\text{if } \alpha+\beta\ge 0\,,$$

and $\gamma=-1$ with $\mathsf{B}_{\rm dec}\in\mathcal{COP}_3$ implies $\alpha+\beta\ge 0$. Next to the case $\gamma=1$ but $\alpha+\beta<0$: here we always have

$$\det\mathsf{B}_{\rm dec}(\lambda)=-\lambda(\alpha-\beta)^2<0$$

due to $\lambda>0$ and $\alpha\ne\beta$, so employing (3), we focus on the other condition which reduces to $\lambda\ge\left(\frac{\alpha+\beta}{2}\right)^2$, which is implied by

$$\lambda\ge\max\{\alpha^2,\beta^2\}>\tfrac{\alpha^2+2\alpha\beta+\beta^2}{2}>\left(\tfrac{\alpha+\beta}{2}\right)^2,$$

using $\alpha\beta<0$. So also

$$\underline{\lambda}(\alpha,\beta,+1)=\max\{\alpha^2,\beta^2\}\,.$$

Finally we deal with the case $\alpha+\beta<0$ and $|\gamma|<1$. Again using (3), $\lambda\ge\max\{\alpha^2,\beta^2\}$ has to satisfy at least one of the conditions

$$(\alpha+\beta)\sqrt{\lambda}+(1+\gamma)\lambda\ge 0\quad\text{or}\quad \lambda^2(1-\gamma^2)-\lambda(\alpha^2+\beta^2-2\alpha\beta\gamma)=\det\mathsf{B}_{\rm dec}(\lambda)\ge 0\,,$$

which is equivalent to $\lambda\ge\mu(\alpha,\beta,\gamma)$ as defined above. Hence the result. □

Remark 4.2. As can be easily shown, we have (if $\alpha\beta<0$)

$$\mu(\alpha,\beta,\gamma)=\begin{cases}\left(\tfrac{\alpha+\beta}{1+\gamma}\right)^2, & \text{if}\quad \tfrac{\alpha\beta}{\alpha^2+\beta^2}\le\tfrac{\gamma}{1+\gamma^2},\\ \tfrac{\alpha^2+\beta^2-2\alpha\beta\gamma}{1-\gamma^2}, & \text{else.}\end{cases}$$

5. Experiments

In order to prove effectiveness of the proposed method, an experiment was carried out on randomly generated pentadiagonal matrices. The method to generate the matrices allows to influence the likelihood of a matrix to be copositive or not and is explained in the following:

First, a positive definite, symmetric 3 × 3-matrix (the first block) with unit entries on the diagonal is generated as the Gram matrix of randomly chosen unit vectors, with a sign pattern conforming that of Proposition 3.3. We fix the value of a single parameter ρ with $0<\rho<1$ which shall serve to control the likelihood that the generated matrix is copositive in the following way.

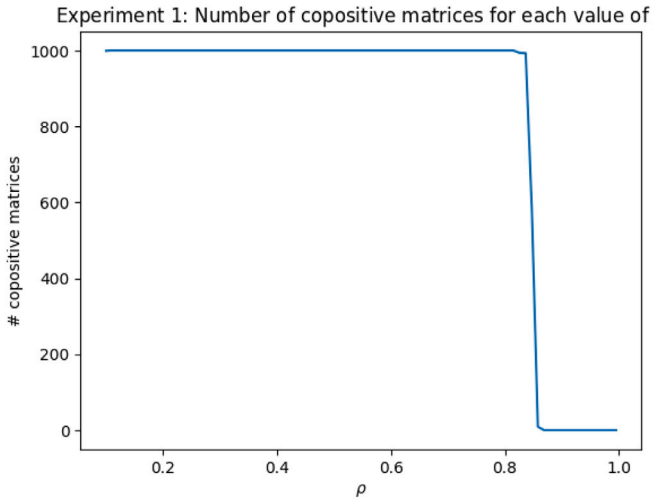

Fig. 3. For $\rho<0.81$ (almost) all matrices could be proved to be copositive, for values $0.81<\rho<0.87$ we can observe a rapid drop in success rate of proving copositivity — until eventually for $0.87<\rho$ no matrix is proved to be copositive anymore.

Iteratively, 3 × 3 blocks — which have a 2 × 2 overlap with the previous block (call it W) – are computed by augmenting a row $[0,\rho v_1,\rho v_2,1]$ and its transpose as the last column, using the parameter ρ to scale the newly added part. Thereby we obtain a 4 × 4 matrix, choosing $v_1>0>v_2$ but randomly otherwise, scaling such that $\mathbf{v}^\top\mathsf{W}\mathbf{v}=1$, which ensures that the new 3 × 3 block (the south-east part of the 4 × 4 block) is positive-definite (as $\rho<1$). This procedure ensures that the first off-diagonal only contains negative entries, while the second off-diagonal only contains positive entries. Points 3 and 4 in Proposition 3.3 with $a_{i4}\to 0$ imply that a small value for ρ guarantees copositivity of the new 4 × 4 block, suggesting a higher likelihood for the entire matrix to be copositive.

For the first experiment, all the generated matrices were of order 1000. For ρ, we sampled 100 values randomly from the interval $[0.1,0.9999]$ and took their square root to increase density in the upper (more interesting) region of values. For each value of ρ, a total of 1000 matrices were generated. Upon generation, the decomposition algorithm was applied — if the matrix was proved to be copositive, the result was counted as a 1, in case it failed at some point to find a suitable λ (cf. Lemma 4.1 and Remark 4.2) to continue the chain, the result was counted as 0.

In the second experiment, additional to the copositivity check, if the algorithm was not successful on proving copositivity, the largest 'connected' copositive submatrix was recorded. To achieve this, the same method was used — if a matrix was not found to be copositive, the first row/column was removed and the procedure was repeated. Due to computational limitations, the interval for values of ρ was shrunk to $[0.80,0.9999]$, and the matrix order was decreased to 200.

The goal of the second experiment was to understand whether there is an abrupt transition between different values of ρ that produce copositive and non-copositive matrices, or whether the size of copositive submatrices steadily decreases. Naturally, with higher order of the matrix in question, likelihood of it being copositive decreases. Hence, the second experiment allows a better insight in whether it is likely that the generated matrices which could not be proved copositive are indeed not copositive.

The result matches the expected outcome — the very drastic drop starting at $\rho\approx 0.81$ in Fig. 3 is surprising though. Of course, with higher probability for smaller (sub)matrices to be not copositive, it becomes very unlikely that the entire matrix of order 1000 is still copositive

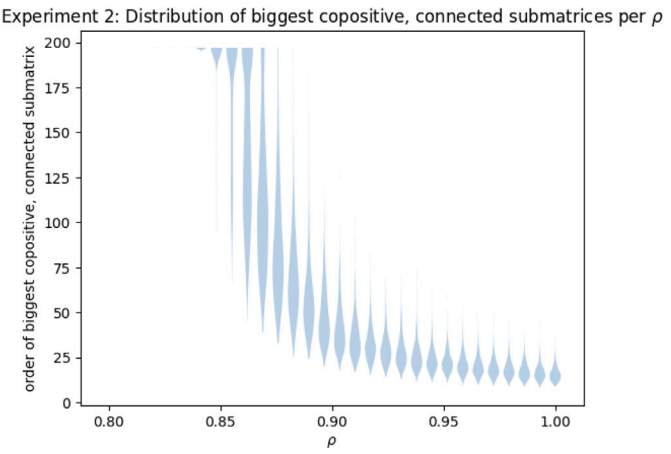

Fig. 4. Distribution of order of largest connected submatrices.

— the second experiment tried to uncover how a growing value for ρ influences the size of the largest connected copositive submatrix.

In Fig. 4 it becomes visible that with increasing ρ and around the "critical" value of $\rho \approx 0.85$ with the sharp drop in Fig. 3, the distribution of order of largest connected submatrices decreases rapidly as well, eventually reaching its mean at around 13 for $\rho = 0.9999$. But one can still see that even for higher values of ρ, big portions of a matrix can be identified as copositive. E.g., only for $\rho > 0.9$ no copositive submatrix with order ≥ 100 could be identified.

The outcome of the second experiment suggests that it is indeed extremely unlikely that the generated matrices are copositive for large values of ρ - for values larger than 0.9 one would not expect to find a copositive matrix anymore. In general, the algorithm was able to efficiently prove $\approx 82\%$ of all generated matrices of order 1000 to be copositive — with $\approx 11.7\%$ matrices almost certainly being indeed not copositive.

6. Conclusion and outlook

In this paper, a novel decomposition strategy for copositivity detection was introduced that is applicable to arbitrary matrices and leads to a linear-time proving procedure for k-diagonal matrices. The main downside of the procedure is the case where the procedure fails: a negative certificate along the procedure leads to premature termination with no definitive conclusion on the copositivity status of the instance. However, even in this case we obtain some information by occurrence of negative certificate (in what iteration/what part of the matrix). This information could be used to reduce the search space for finding violating vectors for the given instance, or in some restricted areas of it. In the experiments with fast search methods in [28], in many situations this improves success quite significantly.

Furthermore, options for re-evaluation of blocks that yield negative certificates, e.g., by reverting the 'proof direction' (i.e., starting from south-east rather than north-west) came up that might hold potential to overcome some currently present hurdles and to identify critical parts in a matrix (which should be examined closer to prove or refute copositivity). All these potential directions of future research may be particularly well suited for k-diagonal matrices. The results of the numerical experiments using pentadiagonal matrices prove effectiveness of the proposed algorithm by efficiently retrieving a proof for copositivity – if successful – within less than a second, even for large matrices, illustrating the big potential of the method.

CRediT authorship contribution statement

Johannes Zischg: Writing – review & editing, Writing – original draft, Visualization, Validation, Software, Project administration, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Immanuel Bomze:** Writing – review & editing, Writing – original draft, Validation, Supervision, Project administration, Methodology, Investigation, Formal analysis, Data curation, Conceptualization.

Declaration of competing interest

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

Appendix A. Example of disconnected $\mathcal{G}_{-}(\mathsf{A})$

First, we introduce the original matrix, which is 11×11 in this case (see Figs. A.5 and A.6).

Obviously, the algorithm's main step is the reordering step.

From this, the other matrices can be derived already. As can be seen in Fig. A.7, there will be 3 parts in the end — of orders 4, 4, and 3. The corresponding matrices read

$$\begin{bmatrix} 1.00 & -0.32 & -0.54 & 0.58 \\ -0.32 & 1.00 & -0.89 & 0.59 \\ -0.54 & -0.89 & 1.00 & -0.57 \\ 0.58 & 0.59 & -0.57 & 1.00 \end{bmatrix}, \quad \begin{bmatrix} 1.00 & -0.63 & -0.18 & 0.69 \\ -0.63 & 1.00 & -0.97 & 0.06 \\ -0.18 & -0.97 & 1.00 & -0.73 \\ 0.69 & 0.06 & -0.73 & 1.00 \end{bmatrix},$$

and

$$\begin{bmatrix} 1.00 & -0.79 & 0.20 \\ -0.79 & 1.00 & -0.01 \\ 0.20 & -0.01 & 1.00 \end{bmatrix}.$$

Now, to verify or refute copositivity, only these three matrices have to be checked, which is significantly easier than checking the original matrix. Let us continue by investigating the first one. According to Theorem 1.4(c), the third column can be removed since it contains no positive off-diagonal values, and corresponding adjustment yields the 3×3 matrix

$$\begin{bmatrix} 1.00 & -2.09 & 0.39 \\ -2.09 & 1.00 & 0.22 \\ 0.39 & 0.22 & 1.00 \end{bmatrix}.$$

In turn, this matrix has a non-negative last row and column which can be dropped, according to Theorem 1.4(b); the resulting 2×2 matrix is obviously not copositive; a violating vector is, for example, $[1, 1]^\top$, hence the original 11×11 matrix A is not copositive. Since the first matrix investigated already refuted copositivity of A, there is no need to check any further matrices. If, on the other hand, this was copositive, we would have continued with the second and the third matrix in the same way until either all of them are proved copositive, or we find at least one matrix which is not.

Appendix B. Pentadiagonal example with premature termination

As already mentioned, in case the procedure breaks (i.e., when encountering a negative certificate at any point), the result is that neither copositivity can be proved nor can it be refuted with the aforementioned method. This section displays such a scenario.

Let us have a look at the matrix

$$\mathsf{A} = \begin{bmatrix} 1.0 & -0.5 & 0.4 & 0.0 & 0.0 \\ -0.5 & 1.0 & -0.9 & -0.7 & 0.0 \\ 0.4 & -0.9 & 10. & 0.9 & 0.3 \\ 0.0 & -0.7 & 0.9 & 1.0 & -0.9 \\ 0.0 & 0.0 & 0.3 & -0.9 & 1.0 \end{bmatrix}$$

which is clearly pentadiagonal. We can also visualize this in similar fashion as previously — the result can be seen in Fig. B.8.

$$\begin{bmatrix}
1.00 & 0.28 & 0.79 & 0.4 & 0.3 & -0.54 & 0.55 & -0.89 & 0.48 & 0.56 & -0.57 \\
0.28 & 1.00 & 0.08 & 0.5 & 0.99 & 0.66 & 0.20 & 0.83 & -0.79 & 0.83 & 0.58 \\
0.79 & 0.08 & 1.00 & -0.18 & -0.73 & 0.13 & 0.58 & 0.16 & 0.06 & -0.97 & 0.06 \\
0.4 & 0.5 & -0.18 & 1.00 & 0.69 & 0.89 & 0.07 & 0.54 & 0.73 & -0.63 & 0.95 \\
0.3 & 0.99 & -0.73 & 0.69 & 1.00 & 0.72 & 0.13 & 0.57 & 0.22 & 0.06 & 0.04 \\
-0.54 & 0.66 & 0.13 & 0.89 & 0.72 & 1.00 & 0.8 & -0.32 & 0.96 & 0.74 & 0.58 \\
0.55 & 0.20 & 0.58 & 0.07 & 0.13 & 0.8 & 1.00 & 0.72 & -0.01 & 0.98 & 0.79 \\
-0.89 & 0.83 & 0.16 & 0.54 & 0.57 & -0.32 & 0.72 & 1.00 & 0.20 & 0.08 & 0.59 \\
0.48 & -0.79 & 0.06 & 0.73 & 0.22 & 0.96 & -0.01 & 0.20 & 1.00 & 0.25 & 0.64 \\
0.56 & 0.83 & -0.97 & -0.63 & 0.06 & 0.74 & 0.98 & 0.08 & 0.25 & 1.00 & 0.36 \\
-0.57 & 0.58 & 0.06 & 0.95 & 0.04 & 0.58 & 0.79 & 0.59 & 0.64 & 0.36 & 1.0
\end{bmatrix}$$

Fig. A.5. 11×11 matrix A.

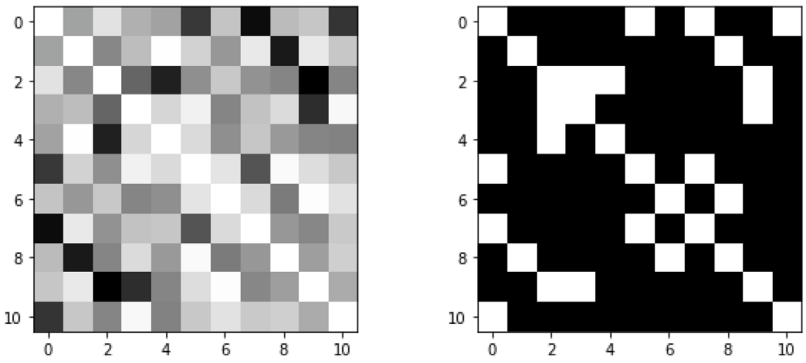

Fig. A.6. left: grey-scale visualization of A (darker=more negative);right: respective matrix A^{σ}.

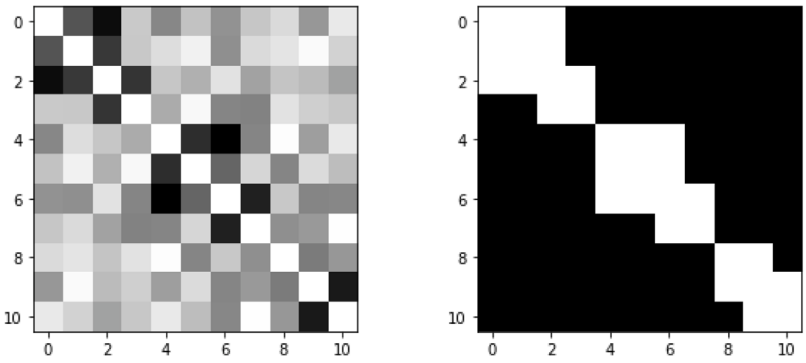

Fig. A.7. left: reordered matrix A; right: respective matrix A^{σ}.

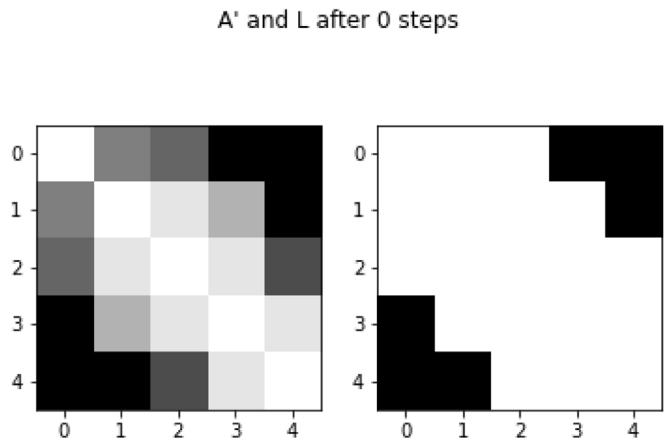

Fig. B.8. The starting matrix A.

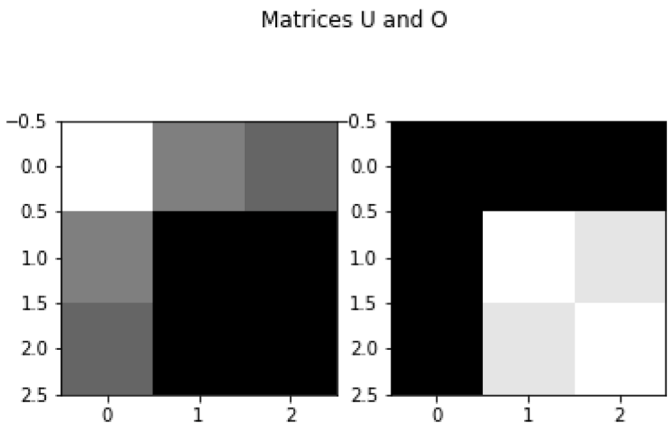

Fig. B.9. Left: The matrix $B_{dec} - E_{dec}$; right: matrix E_{dec}.

All blocks (submatrices) of order 2 and 3 are themselves copositive. Still, this procedure cannot prove copositivity of the overall matrix as we will see in the next calculation steps. In the first iteration we focus on the 3×3 block in the upper-left corner, i.e., we look at the matrices B_{dec} and E_{dec} depicted in Fig. B.9. Now we have to find the smallest λ_1 such that $B_{dec} - (1 - \lambda_1)E_{dec}$ is still copositive (if such a λ_1 exists

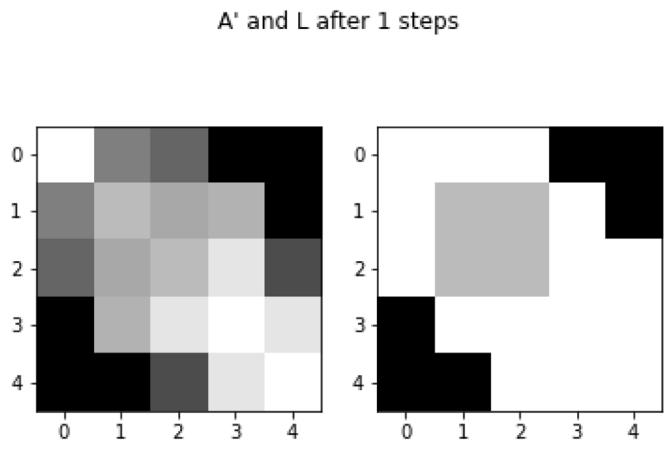

Fig. B.10. The matrix A' after the first iteration.

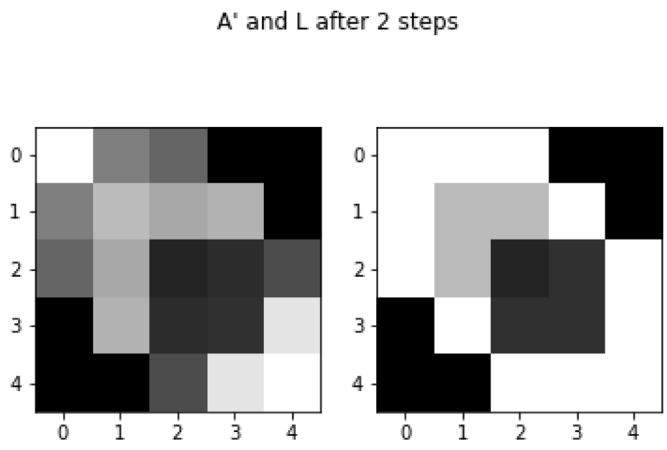

Fig. B.12. Updated matrix A'' after the second iteration.

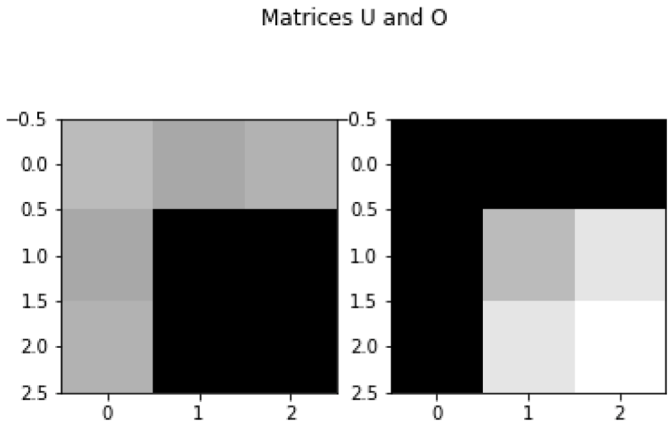

Fig. B.11. Left: the current matrix $\mathsf{B}_{dec} - \mathsf{E}_{dec}$; right: E_{dec}.

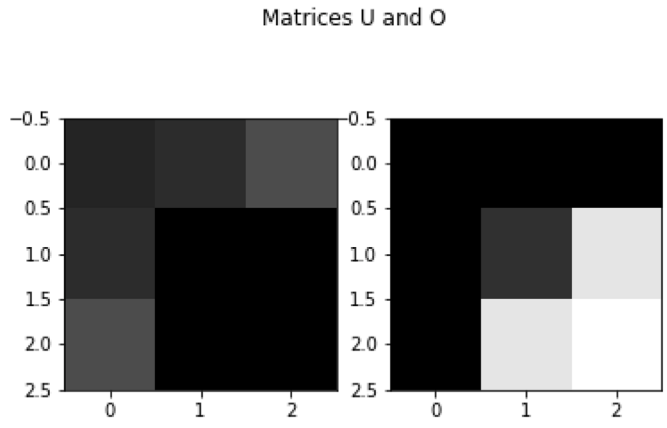

Fig. B.13. Left: the current matrix $\mathsf{B}_{dec} - \mathsf{E}_{dec}$; right: E_{dec}.

at all, which is the case in this example). The smallest λ_1 found that way is $\lambda_1 \approx 0.2631$. Since λ_1 was found, we can proceed with dropping the first row/column of matrix A, subtract the "used up" part of E_{dec} from the 2×2 block in the top-left corner and rescale the remaining matrix to have only ones along the main diagonal, as described in Theorem 1.2. This results in the following matrix $\mathsf{A}' \in \mathcal{S}_4$, visualized in Fig. B.10 (note that for better readability values were rounded to 4 decimal places, suppressing trailing zeroes).

$$\mathsf{A}' = \begin{bmatrix} 1 & -0.9 & -0.8155 & 0 \\ -0.9 & 1 & 1.0485 & 0.3495 \\ -0.8155 & 1.0485 & 1 & -0.9 \\ 0 & 0.3495 & -0.9 & 1 \end{bmatrix}$$

The same procedure is repeated again, starting with picking the matrices B_{dec} and E_{dec} (Fig. B.11). Again, we want to find a suitable λ_2, but have to settle with the already very large $\lambda_2 = 0.81$. This means that only a 'small portion' of E_{dec} will be available for the last step. This can be seen in the remaining updated 3×3 matrix A'' visualized in Fig. B.12.

$$\mathsf{A}'' = \begin{bmatrix} 1 & 1.0485 & 0.8019 \\ 1.0485 & 1 & -2.0651 \\ 0.8019 & -2.0651 & 1 \end{bmatrix}$$

Now we come to the last iteration, where B_{dec} and E_{dec} together make up A''. As we can see, E_{dec} has very small entries and is far from being copositive (see Fig. B.13). Also, there is no λ_3 to make $\mathsf{B}_{dec} - (1-\lambda_3)\mathsf{E}_{dec}$ copositive. Hence the procedure terminates.

But we still cannot make any assumption about the overall (non) copositiveness of the original matrix A just based on this result (A is actually not copositive, a violating vector is $\mathbf{v} = [0.175, 0.35, 0, 0.75, 0.75]^\top$ with $\mathbf{v}^\top \mathsf{A} \mathbf{v} = -0.1631$).

Data availability

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

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