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Construction of exceptional copositive matrices

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A B S T R A C T

An $n \times n$ symmetric matrix A is copositive if the quadratic form $x^T Ax$ is nonnegative on the nonnegative orthant $\mathbb{R}^n_{\geq 0}$. The cone of copositive matrices contains the cone of matrices which are the sum of a positive semidefinite matrix and a nonnegative one and the latter contains the cone of completely positive matrices. These are the matrices of the form BB^T for some $n \times r$ matrix B with nonnegative entries. The above inclusions are strict for $n \geq 5$. The first main result of this article is a free probability inspired construction of exceptional copositive matrices of all sizes ≥ 5, i.e., copositive matrices that are not the sum of a positive semidefinite matrix and a nonnegative one. The second contribution of this paper addresses the asymptotic ratio of the volume radii of compact sections of the cones of copositive and completely positive matrices. In a previous work by Klep and the authors, it was shown that, by identifying symmetric matrices naturally with quartic even forms, and equipping them with the L^2 inner product and the Lebesgue measure, the ratio of the volume radii of sections with a suitably chosen hyperplane is bounded below by a constant independent of n as n tends to infinity.

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In this paper, we complement this result by establishing an analogous bound when the sections of the cones are unit balls in the Frobenius inner product.

Contents

1. Introduction

Copositive and completely positive matrices have gained considerable attention in recent years. They appear in combinatorial analysis, computational mechanics, dynamical systems, control theory and especially in optimization. This is because many combinatorial and nonconvex quadratic optimization problems can be formulated as linear problems over the larger cone of copositive or the smaller cone of completely positive matrices [16,5,25,10]. In this article we expand on the main result of [15], which compares the asymptotic volumes of these two cones of matrices. Moreover, we give an explicit construction of two kinds of *exceptional matrices*, i.e., matrices that belong to a larger cone, but not to a smaller one.

1.1. Notation

Let $\mathbb{N}_0 = \mathbb{N} \cup \{0\}$ denote the set of non-negative integers. For $n \in \mathbb{N}$ denote by $M_n(\mathbb{R})$ the $n \times n$ real matrices and let $\mathbb{S}_n = \{A \in M_n(\mathbb{R}) \colon A^T = A\}$ be its subspace of real symmetric matrices, where ^{T} stands for the usual transposition of matrices. Denote by $\mathbb{R}[\mathtt{x}]$ be the vector space of real polynomials in the variables $\mathtt{x} = (x_1, \dots, x_n)$ and let

$\mathbb{R}[\mathtt{x}]_k$ be its subspace of **forms of degree** k, i.e., homogeneous polynomials from $\mathbb{R}[\mathtt{x}]$ of degree k. To any matrix $A = [a_{ij}]_{i,j=1}^n \in \mathbb{S}_n$ we associate the quadratic form

$$p_A(\mathtt{x}) := \mathtt{x}^T A\mathtt{x} = \sum_{i,j=1}^n a_{ij}x_ix_j \in \mathbb{R}[\mathtt{x}]_2. \tag{1.1}$$

1.2. Basic definitions and background

This article studies the inclusion properties of the cones of the following classes of matrices.

Definition 1.1. A matrix $A \in \mathbb{S}_n$ is:

(1) **copositive** if p_A is nonnegative on the nonnegative orthant

$$\mathbb{R}^n_{\geq 0} := \{(x_1, \dots, x_n) \colon x_i \geq 0,\ i = 1, \dots, n\},$$

i.e., $p_A(\mathtt{x}) \geq 0$ for every $\mathtt{x} \in \mathbb{R}^n_{\geq 0}$. Equivalently, A is copositive iff the quartic form

$$q_A(\mathtt{x}) := p_A(x_1^2, \dots, x_n^2) \in \mathbb{R}[\mathtt{x}]_4 \tag{1.2}$$

is nonnegative on $\mathbb{R}^n$. We write COP_n for the cone of all $n \times n$ copositive matrices.

(2) **positive semidefinite (PSD)** if all of its eigenvalues are nonnegative. Equivalently, A is PSD iff $p_A(\mathtt{x}) \geq 0$ for all $\mathtt{x} \in \mathbb{R}^n$ iff $A = BB^T$ for some matrix $B \in M_n(\mathbb{R})$. We write $A \succeq 0$ to denote that A is PSD and PSD_n stands for the cone of all $n \times n$ PSD matrices.

(3) **nonnegative (NN)** if all of its entries are nonnegative, i.e., $A = [a_{ij}]_{i,j=1}^n$ with $a_{ij} \geq 0$ for $i, j = 1, \dots, n$. We write NN_n for the cone of all $n \times n$ NN matrices.

(4) **SPN** (sum of a positive semidefinite matrix and a nonnegative one) if it is of the form $A = P + N$, where $P \in \mathrm{PSD}_n$ and $N \in \mathrm{NN}_n$. We write $\mathrm{SPN}_n := \mathrm{PSD}_n + \mathrm{NN}_n$ for the cone of all $n \times n$ SPN matrices.

(5) **doubly nonnegative (DNN)** if it is PSD and NN. We use $\mathrm{DNN}_n := \mathrm{PSD}_n \cap \mathrm{NN}_n$ for the cone of all $n \times n$ DNN matrices.

(6) **completely positive (CP)**[4] if $A = BB^T$ for some $r \in \mathbb{N}$ and $n \times r$ entrywise nonnegative matrix B. We write CP_n for the cone of all $n \times n$ CP matrices.

(7) **exceptional doubly nonnegative (e-DNN)** if it is doubly nonnegative but not completely positive, i.e., $A \in \mathrm{DNN}_n \setminus \mathrm{CP}_n$.

(8) **exceptional copositive (e-COP)**[5] if it is copositive but not the sum of a positive semidefinite matrix and a nonnegative one, i.e., $A \in \mathrm{COP}_n \setminus \mathrm{SPN}_n$.

[4] Despite the similar name, the CP matrices considered here are not related to the CP maps ubiquitous in operator algebra [23].

[5] Note that this term appeared previously in [13].

The presented matrices clearly form the following chain of inclusions:

$$\mathrm{COP}_n \supseteq \mathrm{SPN}_n \supseteq \mathrm{PSD}_n \cup \mathrm{NN}_n \supseteq \mathrm{DNN}_n \supseteq \mathrm{CP}_n\,. \tag{1.3}$$

Recall that for any cone $\mathcal{C} \subseteq \mathbb{S}_n$, its **dual cone** is

$$\mathcal{C}^\circ = \{A \in \mathbb{S}_n \mid \langle A, C\rangle \geq 0 \text{ for all } C \in \mathcal{C}\}.$$

Here $\langle \cdot, \cdot \rangle$ is the usual Frobenius inner product on symmetric matrices, i.e., $\langle A, B\rangle = \mathrm{tr}(AB)$. It is well-known [30] that CP matrices are dual to the COP matrices, meaning that $\mathrm{CP}_n^\circ = \mathrm{COP}_n$ and $\mathrm{COP}_n^\circ = \left(\mathrm{CP}_n^\circ\right)^\circ = \mathrm{CP}_n$. In the same fashion, SPN matrices are dual to DNN matrices.

After formulating a combinatorial problem as a conic linear problem over COP_n or CP_n, the complexity of the problem is reduced to the constraints of the respective cone. However, the membership problem for COP_n is co-NP-complete [21] and NP-hard for CP_n [9]. For this reason, Parrilo [22] proposed an increasing hierarchy of cones $K_n^{(r)} := \{A \in \mathbb{S}_n \colon (\sum_{i=1}^n x_i^2)^r \cdot p_A(\mathtt{x}) \text{ is a sum of squares of forms}\}$, which gives a tractable inner approximation of the cone COP_n based on semidefinite programming. Clearly,

$$\bigcup_{r \in \mathbb{N}_0} K_n^{(r)} \subseteq \mathrm{COP}_n, \tag{1.4}$$

and a result of Pólya [24] gives a statement on the quality of the approximation, namely $\mathrm{int}(\mathrm{COP}_n) \subseteq \bigcup_{r\in\mathbb{N}_0} K_n^{(r)}$. It was shown in [22, p. 63–64] that $K_n^{(0)} = \mathrm{SPN}_n$. Also, $\mathrm{SPN}_n = \mathrm{COP}_n$ for $n \leq 4$ by [20]. Whence, $K_n^{(0)} = \mathrm{COP}_n$ and the inclusion in (1.4) is in fact equality for $n \leq 4$ (see also [7]). However, for $n \geq 5$, the cone $K_n^{(0)}$ is strictly contained in COP_n. For $n = 5$, the strict inclusion is testified by the so-called Horn matrix [11]

$$H = \begin{pmatrix} 1 & -1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 & 1 \end{pmatrix} \tag{1.5}$$

giving a standard example of a copositive matrix that is not SPN.

Further, $H \in K_5^{(1)}$ by [22], but $\mathrm{COP}_5 \neq K_5^{(r)}$ for any $r \in \mathbb{N}$ by [8]. Very recently it was shown in [18,27] that for $n = 5$, the inclusion in (1.4) is also equality, while for $n \geq 6$, the inclusion becomes strict [17]. The aim of this paper is first to construct new families of exceptional matrices by identifying examples in the gaps between the DNN and CP cones, as well as the COP and SPN cones. Next, we show that the construction of such exceptional matrices cannot be easily randomized for the COP and CP case by showing that the asymptotic ratio of the volume radii of compact sections of the cones

COP and CP is strictly positive as n goes to infinity. A nice exposition on the classes of matrices defined above can be found in [30] and some open problems regarding COP and CP are presented in [1]. We also mention that the set COP_n is not a spectrahedral shadow for every $n \geq 5$ [4, Corollary 3.18].

1.3. Main results

The first main result is a bootstrap method to find exceptional doubly nonnegative (e-DNN) matrices, i.e., doubly nonnegative matrices that are not completely positive. We first find a seed e-DNN matrix of size 5×5, which then gives rise to a family of e-DNN matrices of arbitrary sizes ≥ 5.

The construction is inspired by the free probability construction in [6] of positive maps between matrix spaces that are not completely positive (in the operator theory sense). For each $f \in L^\infty[0,1]$ consider the corresponding multiplication operator M_f on $L^2[0,1]$; that is

$$M_f\, g = f g$$

for $g \in L^2[0,1]$. With respect to the standard orthonormal basis for $L^2[0,1]$ given by

$$\mathcal{B} := \{1\} \cup \{\sqrt{2}\cos(2k\pi x)\colon k \in \mathbb{N}\} \cup \{\sqrt{2}\sin(2k\pi x)\colon k \in \mathbb{N}\}, \tag{1.6}$$

each such multiplication operator can be represented by an infinite matrix. By abuse of notation, we use M_f to denote both the operator and the infinite matrix representing it with respect to the standard basis. For a closed subspace $\mathcal{H} \subseteq L^2[0,1]$ denote by $P_{\mathcal{H}} : L^2[0,1] \to \mathcal{H}$ the orthogonal projection onto $\mathcal{H}$. Then for any $f \in \mathcal{H}$, the operator $M_f^{\mathcal{H}} := P_{\mathcal{H}} M_f P_{\mathcal{H}}^{\mathrm{T}}$ is in fact a multiplication operator on $\mathcal{H}$ and can be as well represented by a (possibly infinite) matrix. Our idea is to find an infinite dimensional $\mathcal{H}$ and an $f \in \mathcal{H}$ such that $M_f^{\mathcal{H}}$ has all finite leading principal submatrices DNN but not CP.

1.3.1. Construction of exceptional DNN matrices of all sizes ≥ 5

The setting in which we work is the following:

$$f \text{ is of the form } 1 + 2\sum_{k=1}^{m} a_k \cos(2k\pi x), \quad m \in \mathbb{N},\ a_1 \geq 0, \ldots, a_m \geq 0, \tag{1.7}$$

$$\mathcal{H} \subseteq L^2[0,1] \text{ is spanned by the functions } \cos(2k\pi x), k \in \mathbb{N}_0.$$

For $n \in \mathbb{N}$, let $\mathcal{H}_n$ be the finite-dimensional subspace of $\mathcal{H}$ spanned by the functions

$$1, \sqrt{2}\cos(2\pi x), \ldots, \sqrt{2}\cos(2(n-1)\pi x)$$

and let $P_n : \mathcal{H} \to \mathcal{H}_n$ the orthogonal projection onto $\mathcal{H}_n$. Clearly, all the matrices

$$A^{(n)} := P_n M_f^{\mathcal{H}} P_n^{\mathrm{T}}, \; n \in \mathbb{N} \tag{1.8}$$

are NN since f has nonnegative Fourier coefficients. To certify that they are PSD, we impose the condition that f is a sum of squares (SOS) of trigonometric polynomials, i.e.,

$$f = v^T B v, \quad \text{where} \quad B \in \mathrm{PSD}_{m'+1} \tag{1.9}$$

and

$$v^T = \begin{pmatrix} 1 & \cos(2\pi x) & \cdots & \cos(2m'\pi x) \end{pmatrix} \quad \text{for some } m' \leq m. \tag{1.10}$$

Finally, to achieve that $A^{(n)} \notin \mathrm{CP}_n$ for $n \geq 5$, we demand that

$$\langle A^{(5)}, H \rangle < 0, \tag{1.11}$$

where H is the Horn matrix of (1.5) and $\langle \cdot, \cdot \rangle$ is the Frobenius inner product on symmetric matrices. Since CP matrices are dual to the COP matrices w.r.t. the Frobenius inner product, this condition indeed certifies that $A^{(n)} \notin \mathrm{CP}_n$ for all n as we explain in Subsection 2.1.

Remark 1.2. In [12], all exceptional copositive matrices generating the extreme rays of COP_5 are classified. In view of that, the Horn matrix H in (1.11) could be replaced by any of the other exceptional copositive matrix from [12] to produce the 5×5 seed e-DNN matrix.

Now let $m = 6$. The above construction can be implemented via the following feasibility SDP

$$\begin{aligned} &\mathrm{tr}(A^{(5)} H) = -\epsilon, \\ &f = v^{\mathrm{T}} B v \quad \text{with} \quad B \succeq 0, \\ &a_i \geq 0, \quad i = 1, \ldots, 6, \end{aligned} \tag{1.12}$$

where $\epsilon > 0$ is predetermined (small enough). Solving (1.12) for different values of ϵ and $m' \leq 6$, Mathematica's semidefinite optimization solver gives an exceptional DNN matrix $A^{(5)}$ (see Subsection 2.3 for an explicit example). We remark that the idea is to search for an f as in (1.7) with the smallest m and m' as possible to reduce the complexity of the SDP (1.12). The choice of $m = 6$ and $m' = 3$ seemed optimal from our experiments.

1.3.2. Construction of exceptional copositive matrices of all sizes $n \geq 5$

To construct exceptional copositive matrices of arbitrary size we proceed as follows. For $n \geq 5$ let $A^{(n)}$ be a DNN matrix constructed by the above procedure. To obtain an exceptional copositive matrix C of size $n \times n$ we impose the conditions

$$\begin{aligned}&\langle A^{(n)}, C\rangle < 0,\\ &\Big(\sum_{i=1}^{n} x_i^2\Big)^k q_C \text{ is SOS for some } k \in \mathbb{N}\end{aligned} \tag{1.13}$$

with q_C as in (1.2). Searching for C satisfying (1.13) for fixed k can again be formulated as a feasibility SDP. For an explicit example obtained in this way see Subsection 2.3.

Remark 1.3. Note that given $A^{(n)}$ with $n > 5$, the matrix $C = H \oplus 0_{n-5}$ is a trivial solution to the SDP (1.13), where H is the Horn matrix. However, the numerical algorithms used to solve SDPs, typically interior-point methods, generate a sequence of iterates that traverse the interior of the feasible region. For $n > 5$, the trivial solution C is rank-deficient and lies on the boundary of COP_n. Its corresponding SOS form $(\sum_{i=1}^n x_i^2)^k q_C$ lies on the boundary of the cone of positive semidefinite matrices. Therefore C is an unlikely limit point for a standard interior-point solver.

1.3.3. Second main result

Let V be a finite-dimensional Hilbert space equipped with the pushforward measure of the Lebesgue measure μ on $\mathbb{R}^{\dim V}$. A natural way to compare the volumes of two cones K_1, K_2 in V is to compare the compact sections of both cones when intersected with some "fair" subset of V. A seemingly fair choice is the unit ball B of V. In this case the task is to derive an estimate for the so-called **ball-truncated volume of** K_i [28]

$$\mathrm{btv}(K_i) := \mathrm{Vol}(K_i \cap B),$$

where the volume Vol is computed with respect to μ. If one is interested only in the asymptotical behavior of the volume difference, then comparing **volume radii** $\mathrm{vrad}(K_i \cap B)$, defined by

$$\mathrm{vrad}(K_i \cap B) = \left(\frac{\mathrm{btv}(K_i \cap B)}{\mathrm{Vol}(B)}\right)^{1/\dim V},$$

is equally informative (see also [15, Remark 2.4] for a detailed discussion on the ratio of volumes versus the ratio of volume radii).

Let $B_n \subseteq \mathbb{S}_n$ be the unit ball in the Frobenius inner product and μ the pushforward of the Lebesgue measure from $\mathbb{R}^{\dim \mathbb{S}_n}$ to $\mathbb{S}_n$ with respect to some unitary isomorphism. The same proof as for [14, Lemma 1.4] implies that μ does not depend on the unitary isomorphism chosen. Our second main result compares the sizes of the convex cones K from Definition 1.1 by comparing the volumes of their intersections with B_n, i.e., $K^{(B_n)} := K \cap B_n$.

Theorem 3.1. *We have that*

$$\frac{1}{8\sqrt{2}} \le \mathrm{vrad}(\mathrm{CP}_n^{(B_n)}) \le \mathrm{vrad}(\mathrm{NN}_n^{(B_n)}) = \frac{1}{2} \le \mathrm{vrad}(\mathrm{COP}_n^{(B_n)}) \le 1.$$

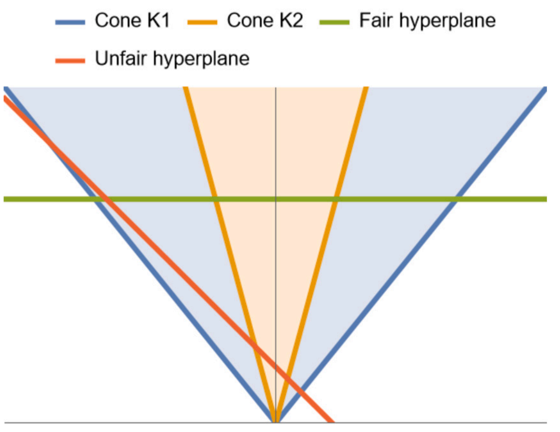

Fig. 1. Intersection of the cones with the unit ball in some metric.

In particular,

$$\frac{1}{8\sqrt{2}} \leq \frac{\operatorname{vrad}(K_n^{(B_n)})}{\operatorname{vrad}(\mathrm{COP}_n^{(B_n)})} \leq 1 \qquad \textit{and} \qquad \frac{1}{2} \leq \frac{\operatorname{vrad}(\widetilde{K}_n^{(B_n)})}{\operatorname{vrad}(\mathrm{COP}_n^{(B_n)})} \leq 1$$

where $K \in \{\mathrm{CP}, \mathrm{DNN}, \mathrm{PSD}\}$ *and* $\widetilde{K} \in \{\mathrm{NN}, \mathrm{SPN}\}$.

Remark 1.4.

(1) Deriving tight estimates for the ball-truncated volume $\operatorname{btv}(K^{(B)})$ of a cone K is very demanding and infeasible for most cones in dimensions beyond 3. This is due to the fact that the conditions defining the section $K^{(B)}$ are quadratic in the coordinates of $\mathbb{R}^{\dim V}$. To compensate for this problem one approach is to compare the cones when intersected with some half-space or equivalently, a hyperplane. However, the choice of the hyperplane is not arbitrary, since its position can have a large effect on the size difference of the intersections with the given cones K_1 and K_2 (see Fig. 1). For the results on the existence of the most fair hyperplane in case K_2 is the dual of K_1 in the inner product of V, i.e., $K_2 = K_1^* = \{u \in V : \langle x, u\rangle \geq 0 \text{ for all } x \in K_1\}$, we refer the reader to [28,29]; in particular to the notion of a *least partial volume* [28, Definition 1.1] and [29, Lemma 5.2].

(2) In our previous work [15] on estimating the quantitative gap between COP_n and CP_n we used the identification with quartic even forms (1.2) and then compared volumes of the corresponding cones in positive even quartics. The inner product is taken to be the L^2 one, i.e., $\langle f, g\rangle = \int_{S^{n-1}} fg \, \mathrm{d}\sigma$, where σ is the rotation invariant probability measure on the unit sphere $S^{n-1} \subset \mathbb{R}^n$. In this context, determining conclusive ball-truncated volumes is challenging. Therefore, we selected a fair hyperplane H, which has a multiple of the polynomial $x_1^2 + \ldots + x_n^2$ as a normal, and then derived volume

estimates for the intersections of all the cones with H. For a detailed discussion on the choice of H see [15, Section 2.2].

(3) The proof of Theorem 3.1 is much less demanding than the proof of its analog [15, Theorem 1.4], which relies on powerful techniques from real algebraic geometry, developed by Blekherman [2,3]. However, the statements of Theorem 3.1 and [15, Theorem 1.4] are not directly comparable, since the volume estimates are relative to the choice of the underlying distribution. Clearly, if we were to compare the volumes of the sets with respect to the Dirac measure at a selected point, then the volume ratio would be either 1 or 0, depending on whether the point belongs to both or only to the larger set. When identifying symmetric matrices with quartic forms, as described in (2) above, the most natural inner product is the L^p one for some $p \in \mathbb{N}$. How the L^2 inner product translates to matrices is described in [15, Remark 2.3]. It turns out that a pushforward of the Lebesgue measure from an Euclidean space via a unitary isomorphism depends on the inner product of the ambient vector space. So the volume estimates are relative to the choice of an inner product and different choices are not directly comparable. However, when studying matrices, the most natural choice of the inner product is the Frobenius one. The main contribution of Theorem 3.1 are volume ratio estimates for this choice of an inner product and the corresponding distribution. Moreover, the estimates are derived for the most natural choice of compact intersections, i.e., the ones with the unit ball in the Frobenius inner product. Surprisingly, the proof is not as involved as for the analogous result on the polynomial side.

2. Construction of exceptional doubly nonnegative and exceptional copositive matrices

In this section we describe the details of the bootstrap method outlined in Subsection 1.3 to find exceptional doubly nonnegative (e-DNN) and exceptional copositive (e-COP) matrices. The idea is to find a seed e-DNN matrix of size 5×5 that is the compression of a multiplication operator M_f for a sum of squares cosine trigonometric polynomial f using a semidefinite optimization program (SDP). From the seed matrix we then read off the (finitely many) Fourier coefficients of f. Finally, we argue that all the larger finite compressions (leading principal submatrices) of M_f are e-DNN as well. Using the constructed e-DNN matrices we produce a corresponding family of exceptional copositive matrices.

2.1. Justification of the construction of a family of e-DNN matrices from a seed e-DNN matrix of size 5×5

Recall that the function f we are looking for is of the form

$$f(x) = 1 + 2\sum_{k=1}^{6} a_k \cos(2k\pi x) \tag{2.1}$$

with $a_1, \ldots, a_6 \geq 0$ (here we immediately set $m = 6$ as in (1.7)). Also, in (1.8), we defined $A^{(n)} = (A^{(n)}_{jk})_{j,k}$ to be the $n \times n$ leading principal submatrix of the infinite matrix pertaining to the multiplication operator $M_f^{\mathcal{H}}$ on $\mathcal{H}$. Here $\mathcal{H}$ is the closed subspace of $L^2[0,1]$ spanned by the $\cos(2k\pi x)$, $k \in \mathbb{N}_0$. The technical reasons why we restrict to $\mathcal{H}$ instead of considering the entire $L^2[0,1]$ are discussed in Remark 2.1. The restriction to matrices of size $n \geq 5$ is clear from the introduction since $\mathrm{DNN}_n = \mathrm{CP}_n$ for $n \leq 4$.

To find the general form of $A^{(n)}$ given arbitrary f note that

$$
\begin{aligned}
A^{(n)}_{11} &= \int_0^1 f(x)\,dx; \\
A^{(n)}_{1k} &= A^{(n)}_{k1} = \sqrt{2}\int_0^1 f(x)\cos(2(k-1)\pi x)\,dx \quad \text{for} \quad k = 2, \ldots, n; \\
A^{(n)}_{jk} &= 2\int_0^1 f(x)\cos(2(j-1)\pi x)\cos(2(k-1)\pi x)\,dx \quad \text{for} \quad j,k = 1, \ldots, n;
\end{aligned}
$$

where the integration is with respect to the Lebesgue measure on $[0,1]$. Using the well-known trigonometry formula involving the cosine product identity, the products of different cosine functions can be replaced with linear combinations of cosine functions with higher and lower frequency, i.e.,

$$
\cos(2j\pi x)\cos(2k\pi x) = \frac{1}{2}\Big(\cos\big(2(j-k)\pi x\big) + \cos\big(2(j+k)\pi x\big)\Big). \tag{2.2}
$$

From (2.2) it follows that

$$
\int_0^1 \cos(2j\pi x)\cos(2k\pi x)\cos(2\ell\pi x)dx = \begin{cases} \frac{1}{2}, & \text{if } j = \ell, k = 0, \\ \frac{1}{4}, & \text{if } k \neq 0 \text{ and } j \in \{\ell + k, \ell - k\}, \\ 0, & \text{otherwise.} \end{cases} \tag{2.3}
$$

Using (2.3) it is now easy to compute that for $A^{(5)}$ to be the 5×5 compression of $M_f^{\mathcal{H}}$, it must be of the form[6]

$$
A^{(5)} = \begin{pmatrix} 1 & \sqrt{2}a_1 & \sqrt{2}a_2 & \sqrt{2}a_3 & \sqrt{2}a_4 \\ \sqrt{2}a_1 & a_2 + 1 & a_1 + a_3 & a_2 + a_4 & a_3 + a_5 \\ \sqrt{2}a_2 & a_1 + a_3 & a_4 + 1 & a_1 + a_5 & a_2 + a_6 \\ \sqrt{2}a_3 & a_2 + a_4 & a_1 + a_5 & 1 + a_6 & a_1 \\ \sqrt{2}a_4 & a_3 + a_5 & a_2 + a_6 & a_1 & 1 \end{pmatrix}. \tag{2.4}
$$

[6] Note that given our choice of f, the matrix $A^{(n)}$ is 13-banded for $n \geq 8$. In general, if the 6 in (2.1) is replaced by $r \in \mathbb{N}$, then $A^{(n)}$ is $(2r+1)$-banded for $n \geq r + 2$.

Thus demanding that $a_i \geq 0$ for $i = 1, \dots, 6$ certifies that $A^{(5)}$ is NN. By the same reasoning $A^{(n)}$ is NN for every $n \geq 5$.

Further on, f being of the form (1.9) is equivalent to f being a sum of squares of trigonometric polynomials [19, Lemma 4.1.3]. This implies that all matrices $A^{(n)} = P_n M_f^{\mathcal{H}} P_n^{\mathrm{T}}$ as in (1.8) are PSD. Indeed, suppose

$$f = \sum_{i=0}^{k} \Big(\underbrace{\sum_{j=0}^{m'} h_{ij} \cos(2j\pi x)}_{h_i} \Big)^2$$

for some k and $h_{ij} \in \mathbb{R}$. Since f and the h_i are in $\mathcal{H}$, clearly $M_f^{\mathcal{H}}$ and the $M_{h_i}^{\mathcal{H}}$ are multiplication operators on $\mathcal{H}$ and

$$M_f^{\mathcal{H}} = \sum_{i=1}^{k} \big(M_{h_i}^{\mathcal{H}}\big)^2.$$

Here each $M_{h_i}^{\mathcal{H}}$ is self-adjoint, from which the claim follows.

Finally, we justify why (1.11) implies that $P_n M_f^{\mathcal{H}} P_n^{\mathrm{T}}$ is not CP for any $n \geq 5$. Since CP matrices are dual to copositive matrices in the usual Frobenius inner product, (1.11) certifies that $A^{(5)}$ is not CP. Now if Q is the orthogonal projection of $\mathcal{H}_n$ onto $\mathcal{H}_5$, then the equality

$$A^{(5)} = Q(P_n M_f^{\mathcal{H}} P_n^{\mathrm{T}})Q^{\mathrm{T}} = QA^{(n)}Q^{\mathrm{T}} \tag{2.5}$$

for any $n \geq 5$, implies that $A^{(n)}$ is not CP for any $n \geq 5$. Indeed, suppose that $A^{(n)} = BB^{\mathrm{T}}$ for some $n \geq 5$ and (not necessarily square) matrix B with nonnegative entries. By (2.5), $A^{(5)} = QB(QB)^{\mathrm{T}}$ and since Q only has $0, 1$ entries, this contradicts $A^{(5)}$ not being CP.

2.2. Justification of the construction of exceptional COP matrices from exceptional DNN matrices

It remains to justify our procedure for constructing an exceptional copositive matrix C of size $n \times n$ for any $n \geq 5$ from the obtained e-DNN matrix $A^{(n)}$. Since SPN matrices are dual to the DNN matrices in the Frobenius inner product, the first condition in (1.13),

$$\langle A^{(n)}, C \rangle < 0,$$

implies that C is not SPN. On the other hand, the second condition in (1.13),

$$\Big(\sum_{i=1}^{n} x_i^2\Big)^k q_C \text{ is SOS for some } k \in \mathbb{N},$$

is a relaxation of the copositivity of C and it clearly implies that q_C is nonnegative on $\mathbb{R}^n$. Whence, C is COP (see Subsection 2.3.2 for a 5×5 example). We remark that in practice, it suffices to consider only $k = 1$ or $k = 2$.

Remark 2.1. We explain the reason for restricting M_f to the closed subspace $\mathcal{H}$ of $L^2[0,1]$ generated by the cosine functions. As in Subsection 1.3.1, with respect to the standard orthonormal basis for $L^2[0,1]$ given by

$$1, \ \sqrt{2}\cos\big(2k\pi x\big), \ \sqrt{2}\sin\big(2k\pi x\big) \tag{2.6}$$

for $k \in \mathbb{N}$, each multiplication operator M_f for $f \in L^\infty[0,1]$ can be represented by an infinite matrix.

It seems natural to start by considering the entire space $L^2[0,1]$ and compressions $\widetilde{P}_n M_f (\widetilde{P}_n)^{\mathrm{T}}$ of M_f for some trigonometric polynomial f and $n \geq 2$, onto the $(2n+1)$-dimensional span $\widetilde{\mathcal{H}}_n$ of the functions in (2.6) for $k = 1, \ldots, n$. Here $\widetilde{P}_n : L^2[0,1] \to \widetilde{\mathcal{H}}_n$ are orthogonal projections.

Suppose that A is the 5×5 compression of M_f and is given with respect to the ordered (orthonormal) basis consisting of the functions

$$1, \sqrt{2}\cos(2\pi x), \sqrt{2}\cos(4\pi x), \sqrt{2}\sin(2\pi x), \sqrt{2}\sin(4\pi x).$$

Moreover, assume that the corresponding function f has finite Fourier series

$$f(x) = 1 + 2\sum_{k=1}^{m} a_k \cos(2k\pi x) + 2\sum_{k=1}^{m} b_k \sin(2k\pi x) \tag{2.7}$$

for some $m \in \mathbb{N}$ and real numbers a_k, b_k with $k = 1, \ldots, m$. Again, using well-known trigonometry formulas involving product identities, i.e.,

$$\begin{aligned} \sin(2j\pi x)\sin(2k\pi x) &= \frac{1}{2}\Big(\cos\big(2(j-k)\pi x\big) - \cos\big(2(j+k)\pi x\big)\Big), \\ \cos(2j\pi x)\sin(2k\pi x) &= \frac{1}{2}\Big(\sin\big(2(k-j)\pi x\big) + \sin\big(2(j+k)\pi x\big)\Big) \end{aligned} \tag{2.8}$$

in addition to (2.2), it is easy to compute that for A to be the 5×5 compression of a multiplication operator M_f for f as in (2.7) with $m \geq 4$, it must be of the form

$$A = \begin{pmatrix} 1 & \sqrt{2}a_1 & \sqrt{2}a_2 & \sqrt{2}b_1 & \sqrt{2}b_2 \\ \sqrt{2}a_1 & a_2+1 & a_1+a_3 & b_2 & b_1+b_3 \\ \sqrt{2}a_2 & a_1+a_3 & a_4+1 & b_3-b_1 & b_4 \\ \sqrt{2}b_1 & b_2 & b_3-b_1 & 1-a_2 & a_1-a_3 \\ \sqrt{2}b_2 & b_1+b_3 & b_4 & a_1-a_3 & 1-a_4 \end{pmatrix}.$$

Note that since we want all the finite-dimensional compressions of M_f to be NN, f needs to have an infinite Fourier series. Indeed, suppose f has finite Fourier series as in (2.7) for some $m \in \mathbb{N}$. Then for all j, k with $k < j \leq m$ and $m < j + k$, the $(j+1, k+m+1)$-entry of the compression $\widetilde{P}_m M_f (\widetilde{P}_m)^{\mathrm{T}}$,

$$\int_0^1 f(x)\,\sqrt{2}\cos(2j\pi x)\,\sqrt{2}\sin(2k\pi x)\,dx =$$

$$\int_0^1 f(x)\sin\big(2(k-j)\pi x\big)\,dx \;+\; \int_0^1 f(x)\sin\big(2(j+k)\pi x\big)\,dx,$$

equals $-a_{j-k}$. Furthermore, we see from (2.8) that the Fourier sine coefficients of f must satisfy

$$b_{j+k} \geq b_{j-k}$$

for all k, j. But then the containment $f \in L^2[0,1]$ implies that $b_k = 0$ for all k. Hence, f has a Fourier cosine series. To avoid technical difficulties, we thus restrict our attention to $\mathcal{H}$.

2.3. *Examples*

2.3.1. *A seed e-DNN 5×5 matrix*

Let $\epsilon = 1/20$. After solving the SDP[7] (1.12) with this parameter and rounding the appearing rational numbers (i.e., the coefficients of f) to fewer decimal digits (while making sure the matrix still solves the SDP), we obtain the 5×5 compression

$$A^{(5)} = \begin{pmatrix} 1 & \frac{16\sqrt{2}}{27} & \frac{\sqrt{2}}{123} & \frac{1}{147\sqrt{2}} & \frac{5\sqrt{2}}{21} \\ \frac{16\sqrt{2}}{27} & \frac{124}{123} & \frac{1577}{2646} & \frac{212}{861} & \frac{1205}{8526} \\ \frac{\sqrt{2}}{123} & \frac{1577}{2646} & \frac{26}{21} & \frac{572}{783} & \frac{1777340\sqrt{2}-2413803}{3254580} \\ \frac{1}{147\sqrt{2}} & \frac{212}{861} & \frac{572}{783} & \frac{1777340\sqrt{2}+814317}{3254580} & \frac{16}{27} \\ \frac{5\sqrt{2}}{21} & \frac{1205}{8526} & \frac{1777340\sqrt{2}-2413803}{3254580} & \frac{16}{27} & 1 \end{pmatrix}. \tag{2.9}$$

By comparing the above $A^{(5)}$ with the general form (2.4) we read off the Fourier coefficients of the corresponding function f as in (1.9), i.e.,

[7] The used tool for generating examples was Mathematica's SDP solver. The source code for the two examples is available at https://github.com/ZalarA/Exceptional-Copositive-Matrices.

$$\begin{aligned} f(x) = 1 &+ \frac{32}{27}\cos(2\pi x) + \frac{2}{123}\cos(4\pi x) + \frac{1}{147}\cos(6\pi x) \\ &+ \frac{10}{21}\cos(8\pi x) + \frac{8}{29}\cos(10\pi x) \\ &+ \frac{-2440263 + 1777340\sqrt{2}}{1627290}\cos(12\pi x). \end{aligned}$$

This function is indeed SOS, since we have $f = v^{\mathrm{T}} B v$ for v as in (1.10) with $m' = 3$ and

$$B = \begin{pmatrix} \frac{9}{22} & \frac{7}{37} & -\frac{3}{22} & -\frac{206923}{5678316} \\ \frac{7}{37} & \frac{336929}{243540} - \frac{88867\sqrt{2}}{162729} & \frac{2210}{28971} & \frac{88867}{162729\sqrt{2}} - \frac{200129}{487080} \\ -\frac{3}{22} & \frac{2210}{28971} & \frac{46466763-19550740\sqrt{2}}{35800380} & \frac{4}{29} \\ -\frac{206923}{5678316} & \frac{88867}{162729\sqrt{2}} - \frac{200129}{487080} & \frac{4}{29} & \frac{1777340\sqrt{2}-2440263}{1627290} \end{pmatrix} \succeq 0.$$

2.3.2. Exceptional copositive matrix from a DNN matrix

Now let $\epsilon' = 1/10$ and $k = 1$. From the matrix $A^{(5)}$ in (2.9) we construct an exceptional copositive matrix C as described in Subsection 1.3.1 by solving the feasibility SDP

$$\begin{aligned} &\operatorname{tr}(CA^{(5)}) = -\epsilon', \\ &\Big(\sum_{i=1}^{n} x_i^2\Big)\, q_C = w^{\mathrm{T}} B w \quad \text{with} \quad B \succeq 0, \end{aligned}$$

where w is the vector with all the degree at most 3 words in the variables $x_1, \ldots, x_n$. Again, after a suitable rationalization, we get an exceptional copositive matrix

$$C = \begin{pmatrix} 17 & -\frac{91}{5} & \frac{33}{2} & \frac{38}{3} & -\frac{36}{5} \\ -\frac{91}{5} & \frac{59}{3} & -\frac{53}{4} & 8 & \frac{33}{4} \\ \frac{33}{2} & -\frac{53}{4} & \frac{39}{4} & -\frac{13}{2} & 8 \\ \frac{38}{3} & 8 & -\frac{13}{2} & \frac{16}{3} & -\frac{13}{3} \\ -\frac{36}{5} & \frac{33}{4} & 8 & -\frac{13}{3} & \frac{1373628701}{353935575} \end{pmatrix}.$$

3. Quantifying the gap between COP_n and CP_n

In this section we prove our second main result (Theorem 3.1) on the estimates of volume radii of the cones from Definition 1.1:

Theorem 3.1. *We have that*

$$\frac{1}{8\sqrt{2}} \le \operatorname{vrad}(\mathrm{CP}_n^{(B_n)}) \le \operatorname{vrad}(\mathrm{NN}_n^{(B_n)}) = \frac{1}{2} \le \operatorname{vrad}(\mathrm{COP}_n^{(B_n)}) \le 1.$$

In particular,

$$\frac{1}{8\sqrt{2}} \le \frac{\operatorname{vrad}(K_n^{(B_n)})}{\operatorname{vrad}(\mathrm{COP}_n^{(B_n)})} \le 1 \qquad \textit{and} \qquad \frac{1}{2} \le \frac{\operatorname{vrad}(\widetilde{K}_n^{(B_n)})}{\operatorname{vrad}(\mathrm{COP}_n^{(B_n)})} \le 1$$

where $K \in \{\mathrm{CP}, \mathrm{DNN}, \mathrm{PSD}\}$ *and* $\widetilde{K} \in \{\mathrm{NN}, \mathrm{SPN}\}$.

Proof. First we establish two claims.

Claim 1. $\operatorname{vrad}(\mathrm{NN}_n^{(B_n)}) = \frac{1}{2}$.

Proof of Claim 1. We first show that B_n is a disjoint union of $2^{\dim \mathbb{S}_n}$ copies of $\mathrm{NN}_n^{(B_n)}$ and a set of volume zero. Hence

$$\operatorname{Vol}(\mathrm{NN}_n^{(B_n)}) = 2^{-\dim \mathbb{S}_n} \cdot \operatorname{Vol}(B_n).$$

Indeed, for $A = [a_{ij}]_{ij} \in \{0,1\}^{n\times n} \cap \mathbb{S}_n$ let $S_A := B_n \cap H_A$, where

$$H_A = \{[b_{ij}]_{ij} \in \mathbb{S}_n : (-1)^{a_{ij}+1} \cdot b_{ij} > 0 \text{ for all } i,j\}.$$

The ones (zeros resp.) in the matrix A thus determine the entries b_{ij} that have positive (negative resp.) sign. Note that

$$B_n = \mathcal{S} \ \cup \bigsqcup_{A\in\{0,1\}^{n\times n}\cap\mathbb{S}_n} S_A,$$

where $\mathcal{S}$ consists of all matrices in B_n with at least one zero. Clearly, $\operatorname{Vol}(\mathcal{S}) = 0$ and $\operatorname{Vol} S_A = \operatorname{Vol}\mathrm{NN}_n^{(B_n)}$ for every $A \in \{0,1\}^{n\times n} \cap \mathbb{S}_n$. Hence

$$\operatorname{Vol} B_n = \sum_{A\in\{0,1\}^{n\times n}\cap\mathbb{S}_n} \operatorname{Vol} S_A = 2^{\dim \mathbb{S}_n} \operatorname{Vol}(\mathrm{NN}_n^{(B_n)}),$$

which immediately proves Claim 1. □

Next, denote by

$$\operatorname{Diff}(\mathrm{CP}_n^{(B_n)}) := \mathrm{CP}_n^{(B_n)} - \mathrm{CP}_n^{(B_n)} = \{U - V : U, V \in \mathrm{CP}_n^{(B_n)}\}$$

the difference body of $\mathrm{CP}_n^{(B_n)}$.

Claim 2. $\mathrm{CP}_n^{(B_n)} \subseteq \mathrm{NN}_n^{(B_n)} \subseteq \sqrt{2}\operatorname{Diff}(\mathrm{CP}_n^{(B_n)})$.

Proof of Claim 2. The left inclusion is clear. To prove the right inclusion it suffices to prove that every extreme point of $\mathrm{NN}_n^{(B_n)}$ is contained in $\operatorname{Diff}(\mathrm{CP}_n^{(B_n)})$. Note that the extreme points of $\mathrm{NN}_n^{(B_n)}$ are of two types:

$$E_{ii} \qquad \text{for some } i = 1, \ldots, n, \tag{3.1}$$

$$\frac{1}{\sqrt{2}}(E_{ij} + E_{ji}) \qquad \text{for some } i, j = 1, \ldots, n, \ i \neq j, \tag{3.2}$$

where E_{ij} are the standard matrix basis, i.e., the only nonzero entry of E_{ij} is 1 at position (i, j). The extreme points of the form (3.1) clearly belong to $\mathrm{CP}_n^{(B_n)} \subseteq \mathrm{Diff}(\mathrm{CP}_n^{(B_n)})$. It remains to study the extreme points of the form (3.2). Note that

$$F := E_{ij} + E_{ji} + E_{ii} + E_{jj} = xx^{\mathrm{T}} \in 2\,\mathrm{CP}_n^{(B_n)},$$

where $x \in \mathbb{R}^n$ is a vector with zeros except at positions i and j, where it has ones. Hence

$$\frac{1}{\sqrt{2}}(E_{ij} + E_{ji}) = \frac{1}{\sqrt{2}}F - \frac{1}{\sqrt{2}}(E_{ii} + E_{jj}) \in \sqrt{2}\,\mathrm{Diff}(\mathrm{CP}_n^{(B_n)}),$$

which concludes the proof of Claim 2. $\square$

By the Rogers-Shepard inequality [26, Theorem 1] we have that

$$\mathrm{vrad}(\mathrm{Diff}(\mathrm{CP}_n^{(B_n)})) \leq 4\,\mathrm{vrad}(\mathrm{CP}_n^{(B_n)}). \tag{3.3}$$

By (3.3) and Claims 1 and 2, it follows that

$$\frac{1}{8\sqrt{2}} \leq \mathrm{vrad}(\mathrm{CP}_n^{(B_n)}) \leq \frac{1}{2}. \tag{3.4}$$

The statements in Theorem 3.1 now follow from Claim 1 and (3.4). $\square$

Declaration of competing interest

There is no competing interest.

Data availability

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

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