

CONSTRUCTION OF EXCEPTIONAL COPOSITIVE MATRICES

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ABSTRACT. An $n \times n$ symmetric matrix A is copositive if the quadratic form $x^T A x$ is nonnegative on the nonnegative orthant $\mathbb{R}_{\geq 0}^n$. 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 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. In this paper, we extend this result by establishing an analogous bound when the sections of the cones are unit balls in the Frobenius inner product.

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 [KP02, Bur09, RRW10, DR21]. In this article we streamline the proof of the main result of [KŠZ24], which compares the asymptotic volumes of these two cones of matrices. Moreover, we give an explicit construction of *exceptional matrices*, i.e., matrices that belong to the larger cone, but not to the 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 $\mathbb{S}_n = \{A \in M_n(\mathbb{R}) : A^T = A\}$ be its subspace of real symmetric matrices, where T stands for the usual transposition of matrices. Denote by $\mathbb{R}[\mathbf{x}]$ be the vector space of real polynomials in the variables $\mathbf{x} = (x_1, \dots, x_n)$

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

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

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

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

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

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

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 $p_A(\mathbf{x}) \geq 0$ for all $\mathbf{x} \in \mathbb{R}^n$ 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 $P \in \text{PSD}_n$ and $N \in \text{NN}_n$. We write $\text{SPN}_n := \text{PSD}_n + \text{NN}_n$ for the cone of all $n \times n$ SPN matrices.
- (5) **doubly nonnegative (DNN)** if it is PSD and NN. We use $\text{DNN}_n := \text{PSD}_n \cap \text{NN}_n$ for the cone of all $n \times n$ DNN matrices.
- (6) **completely positive (CP)**¹ 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., $A \in \text{DNN}_n \setminus \text{CP}_n$.
- (8) **exceptional copositive (e-COP)**² if it is copositive but not the sum of a positive semidefinite matrix and a nonnegative one, i.e., $A \in \text{COP}_n \setminus \text{SPN}_n$.

The presented matrices clearly form the following chain of inclusions:

$$(1.3) \quad \text{COP}_n \supseteq \text{SPN}_n \supseteq \text{PSD}_n \cup \text{NN}_n \supseteq \text{DNN}_n \supseteq \text{CP}_n.$$

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., $\langle A, B \rangle = \text{tr}(AB)$. It is well-known [BSM21] that CP matrices are dual to the COP matrices, meaning that $\text{CP}_n^\circ = \text{COP}_n$ and $\text{COP}_n^\circ = (\text{CP}_n^\circ)^\circ = \text{CP}_n$. In the same fashion, SPN matrices are dual to DNN matrices.

¹Despite the similar name, the CP matrices considered here are not related to the CP maps ubiquitous in operator algebra [Pau02].

²Note that this term appeared previously in [JR08].

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 [MK87] and NP-hard for CP_n [DG14]. For this reason, Parrilo [Par00] proposed an increasing hierarchy of cones $K_n^{(r)} := \{A \in \mathbb{S}_n : (\sum_{i=1}^n x_i^2)^r \cdot p_A(\mathbf{x}) \text{ is a sum of squares of forms}\}$, which give a tractable inner approximation of the cone COP_n based on semidefinite programming. Clearly,

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

and a result of Pólya [Pól28] gives a statement on the quality of the approximation, namely $\text{int}(\text{COP}_n) \subseteq \bigcup_{r \in \mathbb{N}_0} K_n^{(r)}$. It was shown in [Par00, p. 63–64] that $K_n^{(0)} = \text{SPN}_n$. Also, $\text{SPN}_n = \text{COP}_n$ for $n \leq 4$ by [MM62]. Whence, $K_n^{(0)} = \text{COP}_n$ and the inclusion in (1.4) is in fact equality for $n \leq 4$ (see also [Dia62]). 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 [HN63]

$$(1.5) \quad H = \begin{pmatrix} 1 & -1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 & 1 \end{pmatrix}$$

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

Further, $H \in K_5^{(1)}$ by [Par00], but $\text{COP}_5 \neq K_5^{(r)}$ for $r \in \mathbb{N}$ by [DDGH13]. Very recently it was shown in [LV22b, SV24] that for $n = 5$, the inclusion in (1.4) is also equality, while for $n \geq 6$, the inclusion becomes strict [LV22a]. The aim of this paper is first to find further testimonies of the gap between COP and CP matrices. Next, we imply that this construction cannot be randomized 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 [BSM21] and some open problems regarding COP and CP are presented in [BDSM15]. We also mention that the set COP_n is not a spectrahedral shadow for every $n \geq 5$ [BKT24, 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 [CHN17] 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

$$M_f g = fg$$

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

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

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 $P_{\mathcal{H}} : L^2[0, 1] \rightarrow \mathcal{H}$ the orthogonal projection onto \mathcal{H} . Then for any $f \in \mathcal{H}$, the operator $M_f^{\mathcal{H}} := P_{\mathcal{H}} M_f P_{\mathcal{H}}^T$ 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:

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

$\mathcal{H} \subseteq L^2[0, 1]$ 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

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

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

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

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.,

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

and

$$v^T = (1 \quad \cos(2\pi x) \quad \dots \quad \cos(2m'\pi x)) \quad \text{for some } m' \leq m.$$

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

$$(1.10) \quad \langle A^{(5)}, H \rangle < 0,$$

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 $A^{(n)} \notin \text{CP}_n$ for all n as we explain in Subsection 2.1.

Remark 1.2. In [Hil12], all exceptional copositive matrices generating the extreme rays of COP_5 are classified. In view of that, the Horn matrix H in (1.10) could be replaced by any of the other exceptional copositive matrix from [Hil12] to produce the 5×5 seed e-DNN matrix.

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

$$(1.11) \quad \begin{aligned} \text{tr}(A^{(5)} H) &= -\epsilon, \\ f &= v^T B v \quad \text{with } B \succeq 0, \\ a_i &\geq 0, \quad i = 1, \dots, 6, \end{aligned}$$

where $\epsilon > 0$ is predetermined (small enough). Solving (1.11) 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 1.11. 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

$$(1.12) \quad \begin{aligned} &\langle A^{(n)}, C \rangle < 0, \\ &\left(\sum_{i=1}^n x_i^2 \right)^k q_C \text{ is SOS for some } k \in \mathbb{N} \end{aligned}$$

with q_C as in (1.2). Searching for C satisfying (1.12) 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 $A^{(n)}$, the matrix $C = H \oplus 0_{n-5}$ is a trivial solution to the SDP (1.12), 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. The trivial solution $H \oplus 0$ is a rank-deficient matrix that lies on the boundary of the cone of positive semidefinite matrices. As such, it 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** [ST15a]

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

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

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

is equally informative (see also [KŠZ24, 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 w.r.t. the Frobenius inner product. 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

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

In particular,

$$\frac{1}{8\sqrt{2}} \leq \frac{\text{vrad}(K_n^{(B_n)})}{\text{vrad}(\text{COP}_n^{(B_n)})} \leq 1,$$

where $K \in \{\text{CP}, \text{DNN}, \text{PSD}, \text{NN}, \text{SPN}\}$.

Remark 1.4. (1) Deriving tight estimates for the ball-truncated volume $\text{btv}(K^{(B)})$ 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 on this problem one approach is to compare the cones when intersected with a suitably chosen half-space or equivalently, a hyperplane. For $x \in V$ let $H_x := \{u \in V : \langle x, u \rangle \leq 1\}$ be a closed halfspace and $\partial H_x := \{u \in V : \langle x, u \rangle = 1\}$ its boundary hyperplane.

- (a) A comparison of the sizes of the cones can be done in terms of their **least partial volumes** [ST15a, Definition 1.1]. The least partial volume of a cone K is the smallest volume of $K \cap H_x$, where x runs over the unit sphere in V .
- (b) When we want to compare the cones K_1, K_2 that are dual to each other in the inner product on V , i.e.,

$$K_2 = K_1^* = \{u \in V : \langle x, u \rangle \geq 0 \text{ for all } x \in K_1\},$$

a “fair” choice of x in H_x is the so-called **volumetric center** $\rho(K_1)$ of K_1 [ST15a, Definition 1.2]. This is because $\rho(K_1)$ is the centroid of $K_2 \cap \partial H_{\rho(K_1)}$ (see [ST15b, p. 2 and Lemma 5.2]), which is equivalent to the fact that $\rho(K_1)$ is the so-called Santaló point of $K_1 \cap \partial H_{\rho(K_1)}$, for which the Blaschke–Santaló inequality [MP90, p. 90] can be applied.

- (2) In our previous work [KŠZ24] 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 norm, i.e., $\langle f, g \rangle = \int_{S^{n-1}} fg \, d\sigma$, 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 an appropriate hyperplane H_x , where x is a multiple of $x_1^2 + \dots + x_n^2$, and then derived volume estimates for the intersections of all the cones with ∂H_x . For a detailed discussion on the choice of x see [KŠZ24, Section 2.2].
- (3) The proof of Theorem 1.3.3 is significantly less demanding than the proof of the corresponding result in [KŠZ24], namely Theorem 1.4. To establish the latter, we had to use two distinct inner products: in addition to the L^2 inner product, we also employed the so-called differential inner product on even quartics, which resembles the Frobenius inner product on matrices. The main observations for deriving the estimates relied on the differential inner product, while the connection between the volumes of the sets in both inner products, developed by Blekherman in [Ble04, Ble06], was crucial. Proving Theorem 1.3.3 closely follows the observations regarding the differential inner product from [KŠZ24].

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

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

with $a_1, \dots, a_6 \geq 0$ (here we immediately set $m = 6$ as in (1.7)). Also, in (1.8), we defined $A^{(n)} = (A_{jk}^{(n)})_{j,k}$ 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 $\text{DNN}_n = \text{CP}_n$ for $n \leq 4$.

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

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

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.,

$$(2.2) \quad \cos(2j\pi x) \cos(2k\pi x) = \frac{1}{2} \left(\cos(2(j-k)\pi x) + \cos(2(j+k)\pi x) \right).$$

From (2.2) it follows that

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

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 form³

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

³Note 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 [Mar08, Lemma 4.1.3]. This implies that all matrices $A^{(n)} = P_n M_f^{\mathcal{H}} P_n^T$ as in (1.8) are PSD. Indeed, suppose

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

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

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

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

Finally, we justify why (1.10) implies that $P_n M_f^{\mathcal{H}} P_n^T$ is not CP for any $n \geq 5$. Since CP matrices are dual to copositive matrices in the usual Frobenius inner product, (1.10) 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

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

for any $n \geq 5$, implies that $A^{(n)}$ is not CP for any $n \geq 5$. Indeed, suppose that $A^{(n)} = B B^T$ for some $n \geq 5$ and (not necessarily square) matrix B with nonnegative entries. By (2.5), $A^{(5)} = Q B (Q B)^T$ 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 (1.12),

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

implies that C is not SPN. On the other hand, the second condition in (1.12),

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

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

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

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 $\tilde{P}_n M_f (\tilde{P}_n)^\top$ of M_f for some trigonometric polynomial f and $n \geq 2$, onto the $(2n + 1)$ -dimensional span $\tilde{\mathcal{H}}_n$ of the functions in (2.6) for $k = 1, \dots, n$. Here $\tilde{P}_n : L^2[0, 1] \rightarrow \tilde{\mathcal{H}}_n$ 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

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

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

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

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 $\tilde{P}_m M_f (\tilde{P}_m)^\top$,

$$\begin{aligned} \int_0^1 f(x) \sqrt{2} \cos(2j\pi x) \sqrt{2} \sin(2k\pi x) dx &= \\ \int_0^1 f(x) \sin(2(k-j)\pi x) dx &+ \int_0^1 f(x) \sin(2(j+k)\pi x) dx, \end{aligned}$$

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 SDP⁴ (1.11) 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

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

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.,

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

This function is indeed SOS, since we have $f = v^T B v$ for v as in (1.3.1) 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

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

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

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

⁴The 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>.

3. QUANTIFYING THE GAP BETWEEN COP_n AND CP_n

In this section we prove our second main result (Theorem 1.3.3) on the estimates of volume radii of the cones from Definition 1.1:

Theorem 3.1. *We have that*

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

In particular,

$$\frac{1}{8\sqrt{2}} \leq \frac{\text{vrad}(K_n^{(B_n)})}{\text{vrad}(\text{COP}_n^{(B_n)})} \leq 1,$$

where $K \in \{\text{CP}, \text{DNN}, \text{PSD}, \text{NN}, \text{SPN}\}$.

Proof. First we establish two claims.

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

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

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

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, $\text{Vol}(\mathcal{S}) = 0$ and $\text{Vol } S_A = \text{Vol } \text{NN}_n^{(B_n)}$ for every $A \in \{0, 1\}^{n \times n} \cap \mathbb{S}_n$. Hence

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

which immediately proves Claim 1. □

Next, denote by

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

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

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

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

extreme points of $\text{NN}_n^{(B_n)}$ are of two types:

$$(3.1) \quad E_{ii} \quad \text{for some } i = 1, \dots, n,$$

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

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 $\text{CP}_n^{(B_n)} \subseteq \text{Diff}(\text{CP}_n^{(B_n)})$. It remains to study the extreme points of the form (3.2). Note that

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

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

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

which concludes the proof of Claim 2. \square

By the Rogers-Shepard inequality [RS57, Theorem 1] we have that

$$(3.3) \quad \text{vrad}(\text{Diff}(\text{CP}_n^{(B_n)})) \leq 4 \text{vrad}(\text{CP}_n^{(B_n)}).$$

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

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

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

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