

# Matrix positivity preservers in fixed dimension

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## Abstract

A classical theorem of I.J. Schoenberg characterizes functions that preserve positivity when applied entrywise to positive semidefinite matrices of arbitrary size. Obtaining similar characterizations in fixed dimension is intricate. In this note, we provide a solution to this problem in the polynomial case. As consequences, we derive tight linear matrix inequalities for Hadamard powers of positive semidefinite matrices, and a sharp asymptotic bound for the matrix cube problem involving Hadamard powers.

## Résumé

**Sur les transformations positives des matrices d'une dimension donnée.** Un résultat classique de I.J. Schoenberg caractérise les fonctions préservant la positivité lorsque appliquées aux entrées des matrices semi-définies positives de dimension arbitraire. Le problème analogue lorsque la dimension est fixe est beaucoup plus complexe à résoudre. Dans cette note, nous résolvons ce problème dans le cas où la fonction est un polynôme. Nous dérivons de ce résultat des inégalités exactes pour les puissances d'Hadamard d'une matrice positive et pour le problème du cube matriciel.

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## 1. Introduction

During the last decade, the study of maps, linear or not, that preserve matrix structures with positivity constraints has had at least three different motivations: statistical mechanics, well illustrated in the highly original work of Borcea and Brändén on the Lee–Yang and Pólya–Schur programs [7,8]; global optimization algorithms based on the cone of hyperbolic or positive definite polynomials [4]; and the statistics of big data, having the correlation matrix of a large number of random variables as the central object of study [13,12,15]. Inspired by these works, our investigation evolves out of a classical result of Schoenberg [22], by imposing the challenging condition of dealing with matrices of a fixed size.

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Given a set  $K \subset \mathbb{C}$  and an integer  $N \geq 1$ , denote by  $\mathcal{P}_N(K)$  the cone of positive semidefinite  $N \times N$  matrices with entries in  $K$ . Also, let  $D(0, \rho) \subset \mathbb{C}$  denote the complex disc of radius  $\rho > 0$  centered at the origin. A function  $f : K \rightarrow \mathbb{C}$  acts naturally on  $\mathcal{P}_N(K)$  when applied entrywise:

$$f[A] := (f(a_{ij}))$$

for any  $A = (a_{ij}) \in \mathcal{P}_N(K)$ . Akin to the theory of positive definite functions, it is natural to seek characterizations of those functions  $f$  such that  $f[A]$  is positive semidefinite for all  $A \in \mathcal{P}_N(K)$ . This problem has been well studied in the literature. The following classical result of Schoenberg [22] classifies functions preserving positivity on matrices of arbitrary dimension. Recall that the *Gegenbauer* (or *ultraspherical*) polynomials  $C_n^{(\lambda)}(x)$  and the *Chebyshev polynomials of the first kind*  $C_n^{(0)}(x)$  are such that

$$(1 - 2xt + t^2)^{-\lambda} = \sum_{n=0}^{\infty} C_n^{(\lambda)}(x)t^n \quad (\lambda > 0), \quad (1 - xt)(1 - 2xt + t^2)^{-1} = \sum_{n=0}^{\infty} C_n^{(0)}(x)t^n.$$

**Theorem 1.1 (Schoenberg [22])** Fix an integer  $d \geq 2$  and a continuous function  $f : [-1, 1] \rightarrow \mathbb{R}$ .

(i)  $f(\cos \cdot)$  is positive definite on the unit sphere  $S^{d-1} \subset \mathbb{R}^d$  if and only if  $f$  can be written as a non-negative linear combination of the polynomials  $C_n^{(\lambda)}$ , where  $\lambda = (d - 2)/2$ :

$$f(x) = \sum_{n \geq 0} a_n C_n^{(\lambda)}(x) \quad (a_n \geq 0).$$

(ii)  $f[-] : \mathcal{P}_N([-1, 1]) \rightarrow \mathcal{P}_N(\mathbb{R})$  for all  $N \geq 1$  if and only if  $f$  is analytic on  $[-1, 1]$  and absolutely monotonic on  $[0, 1]$ , i.e.,  $f$  has a Taylor series with non-negative coefficients convergent on  $\overline{D}(0, 1)$ .

For more on absolutely monotonic functions, see the work [3] of Bernstein.

Schoenberg's work has been extended in several directions; see, for example, [2,5,6,9,16,19,21,23]. However, when the dimension  $N$  is fixed, obtaining a useful characterization of entrywise functions preserving  $\mathcal{P}_N$  is difficult and remains out of reach as of today. A necessary condition on a continuous function  $f : (0, \infty) \rightarrow \mathbb{R}$  to preserve positivity comes from an inspired idea of Loewner, as developed by Horn in his doctoral dissertation; see [18]. The result was later extended in [12] to work with matrices of low rank. To state the result, let  $\mathbf{1}_{N \times N}$  denote the  $N \times N$  matrix with each entry equal to 1.

**Theorem 1.2 (Horn [18], Guillot–Khare–Rajaratnam [12])** Suppose  $f : I \rightarrow \mathbb{R}$ , where  $I := (0, \rho)$  and  $0 < \rho \leq \infty$ . Fix an integer  $N \geq 2$  and suppose that  $f[A] \in \mathcal{P}_N(\mathbb{R})$  for any matrix  $A = a\mathbf{1}_{N \times N} + \mathbf{u}\mathbf{u}^T$ , where  $a \in (0, \rho)$  and  $\mathbf{u} \in [0, \sqrt{\rho - a}]^N$ . Then  $f \in C^{N-3}(I)$ , with

$$f^{(k)}(x) \geq 0 \quad \forall x \in I, \quad 0 \leq k \leq N - 3,$$

and  $f^{(N-3)}$  is a convex non-decreasing function on  $I$ . Furthermore, if  $f \in C^{N-1}(I)$ , then  $f^{(k)}(x) \geq 0$  for all  $x \in I$  and  $0 \leq k \leq N - 1$ .

We note that Theorem 1.2 is sharp in the sense that there exist functions which preserve positivity on  $\mathcal{P}_N((0, \rho))$ , but not on  $\mathcal{P}_{N+1}((0, \rho))$ . For example,  $f(x) = x^\alpha$  with  $\alpha \in (N - 2, N - 1)$  is such a function; see [10,11,17] for more details. Note also that increasing the dimension  $N$  in Theorem 1.2 allows the recovery of a version of Schoenberg's Theorem 1.1(ii).

The study of functions that preserve positivity has recently received renewed attention, due to their application in high-dimensional probability and statistics. In practical applications, functions are often applied entrywise to covariance and correlation matrices, in order to improve their properties, such as better conditioning, or to induce a Markov random field structure; see [14,15]. Whether or not the resulting matrices are positive semidefinite is critical for the validity of these procedures. Allowing for arbitrary dimensions is unnecessarily restrictive, as the dimension of the problem is usually known. Motivated by such applications, characterizations of positivity preserving functions have recently been obtained in fixed dimensions, under further constraints that arise in practice; see, e.g., [13,12,15]. In this context, our note provides an effective criterion for verifying positivity preservation for polynomial maps.

## 2. Main result

We reconsider Schoenberg's original problem in fixed dimension for the case where  $f$  is a polynomial. Our main result characterizes the polynomials of degree  $N$  that preserve positivity on  $\mathcal{P}_N(\overline{D}(0, \rho))$ .

**Theorem 2.1** *Fix  $\rho > 0$  and integers  $M \geq N \geq 1$ , and let  $f(z) = \sum_{j=0}^{N-1} c_j z^j + c_M z^M$  be a polynomial with real coefficients. For any vector  $\mathbf{d} := (d_0, \dots, d_{N-1})$  with non-zero entries, define*

$$\mathfrak{C}(\mathbf{d}) = \mathfrak{C}(\mathbf{d}; z^M; N, \rho) := \sum_{j=0}^{N-1} \binom{M}{j}^2 \binom{M-j-1}{N-j-1}^2 \frac{\rho^{M-j}}{d_j}, \quad (1)$$

and let  $\mathbf{c} := (c_0, \dots, c_{N-1})$ . The following are equivalent.

(i)  $f[-]$  preserves positivity on  $\mathcal{P}_N(\overline{D}(0, \rho))$ .

(ii) The vector  $(c_0, \dots, c_{N-1}, c_M)$  belongs to the set

$$[0, \infty)^{N+1} \cup ((0, \infty)^N \times [-\mathfrak{C}(\mathbf{c})^{-1}, \infty)).$$

(iii)  $f[-]$  preserves positivity on  $\mathcal{P}_N^1((0, \rho))$ , the set of matrices in  $\mathcal{P}_N((0, \rho))$  having rank at most 1.

The necessity of having  $c_0, \dots, c_{N-1} \geq 0$  when  $f[-]$  preserves positivity follows from Theorem 1.2.

The constant  $\mathfrak{C}(\mathbf{c}) = \mathfrak{C}(\mathbf{c}; z^M; N, \rho)$  provides a threshold for polynomials that preserve positivity on  $\mathcal{P}_N$ . Our result thus provides a quantitative version in fixed dimension of Schoenberg's result, Theorem 1.1(ii), as well as of Horn's result, Theorem 1.2. Surprisingly, preserving positivity on  $\mathcal{P}_N(\overline{D}(0, \rho))$  is equivalent to preserving positivity on the much smaller set of real rank-one matrices.

The proof of Theorem 2.1 relies on a careful analysis of the polynomial

$$p_t[A] := \det(t(c_0 \mathbf{1}_{N \times N} + c_1 A + \dots + c_{N-1} A^{\circ(N-1)}) - A^{\circ M})$$

for rank-one matrices  $A \in \mathcal{P}_N^1(\overline{D}(0, \rho))$ . Recall that given a non-increasing  $N$ -tuple of non-negative integers,  $n_N \geq \dots \geq n_1$ , the corresponding *Schur polynomial* over a field  $\mathbb{F}$  is the unique polynomial extension to  $\mathbb{F}^N$  of

$$s_{(n_N, \dots, n_1)}(x_1, \dots, x_N) := \frac{\det(x_i^{n_j+j-1})}{\det(x_i^{j-1})} \quad (2)$$

for pairwise distinct  $x_i \in \mathbb{F}$ . Note that the denominator is precisely the Vandermonde determinant  $\Delta_N(x_1, \dots, x_N) := \det(x_i^{j-1}) = \prod_{1 \leq i < j \leq N} (x_j - x_i)$ .

**Theorem 2.2** *Let  $c_0, \dots, c_{N-1} \in \mathbb{F}^\times$  be non-zero scalars, where  $N \geq 1$ , and let the polynomial*

$$p_t(x) := t(c_0 + \dots + c_{N-1} x^{N-1}) - x^M,$$

where  $t$  is a variable and  $M \geq N$  are integers. Let the partition  $\lambda(M, N, j) := (M-N+1, 1, \dots, 1, 0, \dots, 0)$ , with  $N-j-1$  entries after the first equal to 1 and the remaining  $j$  entries equal to 0. The following identity holds for all  $\mathbf{u} = (u_1, \dots, u_N)$ ,  $\mathbf{v} := (v_1, \dots, v_N) \in \mathbb{F}^N$ :

$$\det p_t[\mathbf{u}\mathbf{v}^T] = t^{N-1} \Delta_N(\mathbf{u}) \Delta_N(\mathbf{v}) \prod_{j=1}^N c_{j-1} \left( t - \sum_{j=0}^{N-1} \frac{s_{\lambda(M, N, j)}(\mathbf{u}) s_{\lambda(M, N, j)}(\mathbf{v})}{c_j} \right). \quad (3)$$

Moreover,

$$s_{\lambda(M, N, j)}(1, \dots, 1) = \binom{M}{j} \binom{M-j-1}{N-j-1} \quad (0 \leq j \leq N-1). \quad (4)$$

We now explain how Theorem 2.2 is used to prove (iii)  $\Rightarrow$  (ii) in Theorem 2.1. Suppose  $f[-]$  preserves positivity on  $\mathcal{P}_N^1((0, \rho))$ ; using Theorem 1.2, it is not hard to show that the coefficients  $c_0, \dots, c_{N-1}$  are non-negative, and are strictly positive if  $c_M < 0$ . Now suppose  $c_0, \dots, c_{N-1} > 0 > c_M$ . With  $p_t(x)$  as in

Theorem 2.2 and  $t := |c_M|^{-1}$ , the function  $|c_M|^{-1}f(x) = p_t(x)$  preserves positivity on rank-one matrices  $A = \mathbf{u}\mathbf{u}^T$ , for any  $\mathbf{u} \in (0, \sqrt{\rho})^n$ . Hence, by Equation (3),

$$0 \leq \det p_t[\mathbf{u}\mathbf{u}^T] = t^{N-1} \Delta_N(\mathbf{u})^2 c_0 \cdots c_{N-1} \left( t - \sum_{j=0}^{N-1} \frac{s_{\lambda(M,N,j)}(\mathbf{u})^2}{c_j} \right). \quad (5)$$

Letting  $u_k \rightarrow \sqrt{\rho}$  for all  $k$  with  $u_l \neq u_m$  for  $l \neq m$ , we conclude that

$$t = |c_M|^{-1} \geq \sum_{j=0}^{N-1} \frac{s_{\lambda(M,N,j)}(\sqrt{\rho}, \dots, \sqrt{\rho})^2}{c_j} = \sum_{j=0}^{N-1} s_{\lambda(M,N,j)}(1, \dots, 1)^2 \frac{\rho^{M-j}}{c_j} = \mathfrak{C}(\mathbf{c}; z^M; N, \rho). \quad (6)$$

### 3. Consequences and extensions of the main result

In this section, we set out three remarkable corollaries of Theorem 2.1.

#### 3.1. Linear matrix inequalities

For  $A \in \mathcal{P}_N(K)$  and  $f$  as in the statement of Theorem 2.1, note that

$$f[A] = c_0 \mathbf{1}_{N \times N} + \cdots + c_{N-1} A^{\circ(N-1)} + c_M A^{\circ M},$$

where  $A^{\circ k} := (a_{ij}^k)$  denotes the  $k$ th Hadamard power of  $A$ . Understanding when  $f[A]$  is positive semidefinite is thus equivalent to obtaining linear inequalities for Hadamard powers. As an immediate consequence of our main result, we provide a sharp bound for controlling the Hadamard powers of positive semidefinite matrices using lower order powers.

**Corollary 3.1** *Fix  $\rho > 0$ , integers  $M \geq N \geq 1$ , and scalars  $c_0, \dots, c_{N-1} > 0$ . Then*

$$A^{\circ M} \leq \mathfrak{C}(\mathbf{c}; z^M; N, \rho) \cdot (c_0 \mathbf{1}_{N \times N} + c_1 A + \cdots + c_{N-1} A^{\circ(N-1)}) \quad (7)$$

for all  $A \in \mathcal{P}_N(\overline{D}(0, \rho))$ . Moreover, the constant  $\mathfrak{C}(\mathbf{c}; z^M; N, \rho)$  is sharp.

We note that Corollary 3.1 is also sharp in the sense that the right-hand side of (7) cannot be replaced by a linear combination of fewer than  $N$  Hadamard powers of  $A$ . This can be shown using matrices of the form  $A = \mathbf{u}\mathbf{u}^T$  for a vector  $\mathbf{u}$  with distinct real entries.

#### 3.2. Spectrahedra and matrix cubes

Our main result is also connected to the study of spectrahedra [4] and the matrix cube problem [20]. Recall that given real symmetric  $N \times N$  matrices  $A_0, \dots, A_{M+1}$ , the corresponding matrix cubes are

$$\mathcal{U}[\eta] := \left\{ A_0 + \sum_{m=1}^{M+1} u_m A_m : u_m \in [-\eta, \eta] \right\} \quad (\eta > 0). \quad (8)$$

The matrix cube problem consists of determining whether  $\mathcal{U}[\eta] \subset \mathcal{P}_N$ , and finding the largest  $\eta$  for which this is the case. As another consequence of our main result, we obtain an asymptotically sharp bound for the matrix cube problem when the matrices  $A_j$  are Hadamard powers.

**Corollary 3.2** *Fix  $\rho > 0$ , integers  $M \geq 0, N \geq 1$ , and  $c_0, \dots, c_{N-1} > 0$ . Given a matrix  $A \in \mathcal{P}_N(\overline{D}(0, \rho))$ , let*

$$A_0 := c_0 \mathbf{1}_{N \times N} + c_1 A + \cdots + c_{N-1} A^{\circ(N-1)}, \quad A_m := A^{\circ(N-1+m)} \quad (1 \leq m \leq M+1).$$

Then

$$\eta \leq \left( \sum_{m=0}^M \mathfrak{C}(\mathbf{c}; z^{N+m}; N, \rho) \right)^{-1} \Rightarrow \mathcal{U}[\eta] \subset \mathcal{P}_N(\mathbb{C}) \Rightarrow \eta \leq \mathfrak{C}(\mathbf{c}; z^{N+M}; N, \rho)^{-1}. \quad (9)$$

The upper and lower bounds for  $\eta$  are asymptotically equal as  $N \rightarrow \infty$ , i.e.,

$$\lim_{N \rightarrow \infty} \mathfrak{C}(\mathbf{c}; z^{N+M}; N, \rho)^{-1} \sum_{m=0}^M \mathfrak{C}(\mathbf{c}; z^{N+m}; N, \rho) = 1. \quad (10)$$

### 3.3. Extension to other classes of functions

Theorem 2.1 naturally extends to general polynomials.

**Corollary 3.3** Fix a bounded  $K \subset \mathbb{C}$  and integers  $M \geq N \geq 1$ . There exists a universal constant  $\mathfrak{h}_{N,M}(K) > 0$ , with the following property: if the polynomial  $f(z) = \sum_{k=0}^M c_k z^k$  has real coefficients with (i)  $c_0, \dots, c_{N-1} > 0$ , and (ii)  $\min\{c_k : 0 \leq k \leq N-1\} \geq \mathfrak{h}_{N,M}(K) \cdot \max\{|c_l| : c_l < 0, N \leq l \leq M\}$ , then  $f[-] : \mathcal{P}_N(K) \rightarrow \mathcal{P}_N(\mathbb{C})$ .

Our main result also extends to analytic functions.

**Theorem 3.4** Fix  $\rho > 0$  and an integer  $N \geq 1$ . Let  $\mathbf{c} := (c_0, \dots, c_{N-1}) \in (0, \infty)^N$ , and suppose  $g(z) := \sum_{M=N}^{\infty} c_M z^M$  is analytic on  $D(0, \rho + \epsilon)$  for some  $\epsilon > 0$ , with real coefficients. Then

$$t(c_0 \mathbf{1}_{N \times N} + c_1 A + \dots + c_{N-1} A^{\circ(N-1)}) - g[A] \in \mathcal{P}_N(\mathbb{C}) \quad (11)$$

for all  $A \in \mathcal{P}_N(\overline{D}(0, \rho))$  and all  $t \geq \mathfrak{C}(\mathbf{c}; g(z); N, \rho) := \sum_{M \geq N: c_M > 0} c_M \mathfrak{C}(\mathbf{c}; z^M; N, \rho)$ . Moreover,

$$\mathfrak{C}(\mathbf{c}; g(z); N, \rho) \leq \frac{g_2^{(2N-2)}(\sqrt{\rho})}{2^{N-1}(N-1)!^2} \sum_{j=0}^{N-1} \binom{N-1}{j}^2 \frac{\rho^{N-j-1}}{c_j} < \infty, \quad (12)$$

where  $g_2(z) := g_+(z^2)$  and  $g_+(z) := \sum_{M \geq N: c_M > 0} c_M z^M$ .

## 4. Extremal problems and generalized Rayleigh quotients

Understanding which polynomials preserve positivity can naturally be reformulated as an extremal problem involving Rayleigh quotients. The following result is therefore equivalent to Theorem 2.1.

**Theorem 4.1** Fix  $\rho > 0$ , integers  $M \geq N \geq 1$ , and positive scalars  $c_0, \dots, c_{N-1} > 0$ . Then

$$\inf_{u \in \mathcal{K}(A)^\perp} \frac{u^* \left( \sum_{j=0}^{N-1} c_j A^{\circ j} \right) u}{u^* A^{\circ M} u} \geq \mathfrak{C}(\mathbf{c}; z^M; N, \rho)^{-1},$$

for all  $A \in \mathcal{P}_N(\overline{D}(0, \rho))$ , where  $\mathcal{K}(A) := \ker(c_0 \mathbf{1}_{N \times N} + c_1 A + \dots + c_{N-1} A^{\circ(N-1)})$ . Moreover, the bound  $\mathfrak{C}(\mathbf{c}; z^M; N, \rho)$  is sharp, and may be obtained by considering only the set of rank-one matrices  $\mathcal{P}_N^1(\overline{D}(0, \rho))$ .

When considering the analogue of Theorem 4.1 for a single matrix, one can first show that  $\mathcal{K}(A) \subset \ker A^{\circ M}$  and immediately conclude that there exists a constant  $\mathfrak{C}(\mathbf{c}; z^M; A)$  such that

$$u^* \left( \sum_{j=0}^{N-1} c_j A^{\circ j} \right) u \geq \mathfrak{C}(\mathbf{c}; z^M; A)^{-1} \cdot u^* A^{\circ M} u \quad (\forall u \in \mathbb{C}^N).$$

The subtlety in attempting to prove Theorems 2.1 and 4.1 via this approach lies in the fact that the map  $A \mapsto \mathfrak{C}(\mathbf{c}; z^M; A)$  is not continuous. In fact, it is not continuous at the matrix  $A = \rho \mathbf{1}_{N \times N} \in \mathcal{P}_N^1(\overline{D}(0, \rho))$ .

Complete proofs and more ramifications of these results will appear in [1].

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