Entrywise positivity preservers in fixed dimension: I

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(Joint with Alexander Belton, Dominique Guillot, and Mihai Putinar;
and with Terence Tao)

Introduction

Definition. A real symmetric matrix $A_{N \times N}$ is *positive semidefinite* if all eigenvalues of A are $\geqslant 0$. (Equivalently, $u^T A u \geqslant 0$ for all $u \in \mathbb{R}^N$.)

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Different flavors of positivity:

- Positive semidefinite matrices (correlation and covariance matrices)
- Positive definite sequences/Toeplitz matrices (measures on S^1)
- Moment sequences/Hankel matrices (measures on $\mathbb{R}$)
- Totally positive matrices and kernels (Pólya frequency functions/sequences)
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Question: Classify the positivity preservers in these settings.

Studied for the better part of a century.

Entrywise functions preserving positivity

Given $N \geqslant 1$ and $I \subset \mathbb{R}$, let $\mathbb{P}_N(I)$ denote the $N \times N$ positive semidefinite matrices, with entries in I. (Say $\mathbb{P}_N = \mathbb{P}_N(\mathbb{R})$.)

Problem: Given a function $f : I \to \mathbb{R}$, when is it true that

$$f[A] := (f(a_{ij})) \in \mathbb{P}_N \text{ for all } A \in \mathbb{P}_N(I)?$$

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(Long history!) The *Hadamard product* (or Schur, or entrywise product) of two matrices is given by: $A \circ B = (a_{ij} b_{ij})$.

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Theorem (Schoenberg, *Duke Math. J.* 1942)

If $f : [-1,1] \to \mathbb{R}$ is continuous, the following are equivalent:

1. $f[A] \in \mathbb{P}_N$ *for all* $A \in \mathbb{P}_N([-1,1])$ *and all* N.
2. f *is analytic on* I *and has nonnegative Maclaurin coefficients. In other words,* $f(x) = \sum_{k=0}^{\infty} c_k x^k$ *on* $[-1,1]$ *with all* $c_k \geqslant 0$.

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Schoenberg's theorem is the far harder converse to the result of his advisor (Schur).

Rudin (a) removed the continuity hypothesis, and (b) greatly reduced the test set:

Toeplitz and Hankel matrices (cont.)

Let $0 < \rho \leqslant \infty$ be a scalar, and set $I = (-\rho, \rho)$.

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Theorem (Belton–Guillot–K.–Putinar, *J. Eur. Math. Soc.*, accepted)

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Positive semidefinite kernels

- These two results greatly weaken the hypotheses of Schoenberg's theorem – only need to consider positive semidefinite matrices of rank $\leqslant 3$.
- Note, such matrices are precisely the Gram matrices of vectors in a 3-dimensional Hilbert space. Hence Rudin (essentially) showed:

  Let $\mathcal{H}$ be a real Hilbert space of dimension $\geqslant 3$. If $f[-]$ preserves positivity on all Gram matrices in $\mathcal{H}$, then f is a power series on $\mathbb{R}$ with non-negative Maclaurin coefficients.

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- But such functions are precisely the *positive semidefinite kernels on* $\mathcal{H}$! (Results of Pinkus et al.) Such kernels are important in modern day machine learning, via RKHS.
- Thus, Rudin (1959) classified positive semidefinite kernels on $\mathbb{R}^3$, which is relevant in machine learning. (Now also via our parallel 'Hankel' result.)

Schoenberg's motivations: pos. def. functions on spheres

Schoenberg was interested in embedding metric spaces into Euclidean spheres.

- Notice that every sphere S^{r-1} – whence the Hilbert sphere S^∞ – has a rotation-invariant distance. Namely, the *arc-length* along a great circle:

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$$\cos[(d(x_i, x_j))_{i,j\geqslant 0}] = (\langle x_i, x_j\rangle)_{i,j\geqslant 0},$$

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Schoenberg then classified *all* continuous f such that $f\circ\cos(\cdot)$ is p.d.:

Theorem (Schoenberg, *Duke Math. J.* 1942)

Suppose $f:[-1,1]\to\mathbb{R}$ is continuous, and $r\geqslant 2$. Then $f(\cos\cdot)$ is positive definite on the unit sphere $S^{r-1}\subset\mathbb{R}^r$ if and only if

$$f(\cdot) = \sum_{k\geqslant 0} a_k C_k^{(\frac{r-2}{2})}(\cdot) \qquad \text{for some } a_k\geqslant 0,$$

where $C_k^{(\lambda)}(\cdot)$ are the ultraspherical / Gegenbauer / Chebyshev polynomials.

From spheres to correlation matrices

- Any Gram matrix of vectors $x_j \in S^{r-1}$ is the same as a rank $\leqslant r$ correlation matrix $A = (a_{ij})_{i,j=1}^n$, i.e.,

$$A = \begin{pmatrix} 1 & & * & \\ & 1 & & \\ & * & 1 & \\ & & & 1 \end{pmatrix} = \begin{pmatrix} — & x_1^T & — \\ — & x_2^T & — \\ & \vdots & \\ — & x_n^T & — \end{pmatrix} \begin{pmatrix} | & | & & | \\ x_1 & x_2 & \dots & x_n \\ | & | & & | \end{pmatrix} = (\langle x_i, x_j \rangle)_{i,j=1}^n.$$

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- So,

$$\begin{aligned} f(\cos\cdot) \text{ positive definite on } S^{r-1} \quad &\iff \quad (f(\cos d(x_i, x_j)))_{i,j=1}^n \in \mathbb{P}_n \\ &\iff \quad (f(\langle x_i, x_j \rangle))_{i,j=1}^n \in \mathbb{P}_n \\ &\iff \quad (f(a_{ij}))_{i,j=1}^n \in \mathbb{P}_n \ \forall n \geqslant 1, \end{aligned}$$

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- If instead $r = \infty$, such a result would classify the entrywise positivity preservers on all correlation matrices. Interestingly, 70 years later the subject has acquired renewed interest because of its immediate impact in high-dimensional covariance estimation, in several applied fields.

Schoenberg's theorem on positivity preservers

And indeed, Schoenberg did make the leap from S^{r-1} to S^∞:

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Suppose $f : [-1,1] \to \mathbb{R}$ *is continuous. Then* $f(\cos \cdot)$ *is positive definite on the Hilbert sphere* $S^\infty \subset \mathbb{R}^\infty = \ell^2$ *if and only if*

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For more information: *A panorama of positivity* – arXiv, Dec. 2018.
(Survey, 80+ pp., by A. Belton, D. Guillot, A.K., and M. Putinar.)

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- Covariance/correlation is a fundamental measure of dependence between random variables:

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- In modern-day settings (small samples, ultra-high dimension), covariance estimation can be very challenging.
- Classical estimators (e.g. sample covariance matrix (MLE)):

$$S = \frac{1}{n} \sum_{j=1}^{n} (x_j - \overline{x})(x_j - \overline{x})^T$$

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- Require some form of *regularization* – and resulting matrix has to be positive semidefinite (in the parameter space) for applications.

Motivation from high-dimensional statistics

Graphical models: Connections between statistics and combinatorics.

Let $X_1, \dots, X_p$ be a collection of random variables.

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  Works well for dimensions of a few thousands.
- Not scalable to modern-day problems with $100,000+$ variables (disease detection, climate sciences, finance...).

Thresholding and regularization

Thresholding covariance/correlation matrices

$$\text{True } \Sigma = \begin{pmatrix} 1 & 0.2 & 0 \\ 0.2 & 1 & 0.5 \\ 0 & 0.5 & 1 \end{pmatrix}, \qquad S = \begin{pmatrix} 0.95 & 0.18 & 0.02 \\ 0.18 & 0.96 & 0.47 \\ 0.02 & 0.47 & 0.98 \end{pmatrix}$$

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Can be significant if $p = 100,000$ and only, say, $\sim 1\%$ of the entries of the true Σ are nonzero.

Entrywise functions – regularization

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Problem: For what functions $f : \mathbb{R} \to \mathbb{R}$, does $f[-]$ preserve $\mathbb{P}_N$?

Preserving positivity in fixed dimension

Schoenberg's result characterizes functions preserving positivity for matrices of *all* dimensions: $f[A] \in \mathbb{P}_N$ for all $A \in \mathbb{P}_N$ and **all** N.

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Fixed $N \geqslant 3$ and general $f \rightsquigarrow$ only known necessary condition, by Loewner:

Theorem (Horn–Loewner, Guillot–K.–Rajaratnam, *Trans. AMS* 1969, 2017)

*Fix $I = (0, \infty)$ and $f : I \to \mathbb{R}$. Suppose $f[A] \in \mathbb{P}_N$ for all $A \in \mathbb{P}_N(I)$ Hankel of rank $\leqslant 2$, with N **fixed**.*

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If $f \in C^{N-1}(I)$ then $f^{(N-2)}, f^{(N-1)} \geqslant 0$ on I.

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- Implies Schoenberg–Rudin result for matrices with positive entries.
- Loewner had initially summarized these computations in a letter to Josephine Mitchell (Penn. State University) on October 24, 1967:

Loewner's computations

when I got interested in the following question: Let $f(t)$ be a function defined in some interval (a,b), $a \geq 0$ and consider all real symmetric matrices $(a_{ij}) > 0^{*}$ of order n with elements $a_{ij} \in (a,b)$. What properties must ~~f~~ have in order that the matrices $(f(a_{ij})) > 0$.
I found ~~as necessary conditions: $f(t) \geq 0$,~~ $f'(t)$ that if is $(n-1)$ times differentiable the following conditions are necessary

(C) $f(t) \geq 0,\ f'(t) \geq 0,\ \ldots\ f^{(n-1)}(t) \geq 0$

The functions t^{ρ} $(\rho > 1)$ do not satisfy these conditions for all $\rho > 1$ if $n > 3$.
The proof is obtained by considering matrices of the

form $a_{ij} = \alpha + \omega \alpha_i \alpha_j$ with $\alpha \in (a,b)$, $\omega > 0$ and the α_i arbitrary
Then $(f(a_{ij})) > 0$ for sufficiently small ω and hence the determinant $\Delta(\omega)$ $(f(a_{ij})) \geq 0$
The first ~~term~~ term in the Taylor expansion of $\Delta(\omega)$ at $\omega = 0$ is $f(\alpha) f'(\alpha) \ldots f^{(n-1)}(\alpha) \cdot \left(\prod (\alpha_i - \alpha_\beta)\right)^2$ and hence $f(\alpha) f'(\alpha) \ldots f^{(n-1)}(\alpha) \geq 0$, from which one easily derives that (C) must hold.

Entrywise polynomial preservers in fixed dimension

Consequence: Suppose $c_0, c_1, c_2 \neq 0$ are real, $M \geqslant 3$, and

$$c_0 + c_1 x + c_2 x^2 + c_M x^M$$

entrywise preserves positivity on 3×3 correlation matrices.
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General case:

Let $M \geqslant N \in \mathbb{N}$ and $c_0, \dots, c_{N-1} \neq 0$. Suppose $f(x) = \sum_{j=0}^{N-1} c_j x^j + c_M x^M$ preserves positivity on $\mathbb{P}_N((0, \rho))$. Then $c_0, \dots, c_{N-1} > 0$. **Can $c_M < 0$?**

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Reformulation: Multiplying by $t = |c_M|^{-1}$, does

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Main result

Theorem (Belton, Guillot, K., Putinar, *Adv. Math.* 2016)

Fix integers $M \geqslant N \geqslant 1$, *and real scalars* $\rho > 0$ *and* $c_0, \dots, c_{N-1}$.
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Then the following are equivalent.

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Consequences

1. Quantitative version of Schoenberg's theorem in fixed dimension: first examples of polynomials that work for $\mathbb{P}_N$ but not for $\mathbb{P}_{N+1}$. ("The Loewner–Horn theorem is sharp.")

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5. **Corollary:** By the Schur product theorem, functions of the form $t(c_2 x^2 + c_3 x^3 + c_4 x^4) - x^M$ can be preservers on $\mathbb{P}_3((0, \rho))$ for $c_j > 0$, $M > 4$, and large $t \gg 0$.

Sketch of the proof

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Study the determinants of linear pencils

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

for rank-one matrices $A = \mathbf{u}\mathbf{v}^T$.

Schur polynomials

Given an increasing N-tuple of integers $0 \leqslant n_0 < \cdots < n_{N-1}$, the corresponding **Schur polynomial** over a field $\mathbb{F}$ is the unique polynomial extension to $\mathbb{F}^N$ of

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- Weyl Character (Dimension) Formula in Type A:

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Theorem (Belton, Guillot, K., Putinar, *Adv. Math.* 2016)

Let $M \geqslant N \geqslant 1$ be integers, and $c_0, \dots, c_{N-1} \in \mathbb{F}^\times$ be non-zero scalars in any field $\mathbb{F}$. Define the polynomial

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

and the hook partition

$$\mu(M, N, j) := (0, 1, \dots, j-1; \quad j+1, \dots, N-1; \quad M).$$

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The following identity holds for all $\mathbf{u}, \mathbf{v} \in \mathbb{F}^N$:

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

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Proof of **(3)** $\implies$ **(2).**

- If $p_t[\mathbf{u}\mathbf{u}^T] \in \mathbb{P}_N$ for all $\mathbf{u} \in (0, \sqrt{\rho})^N$, and $t, c_0, \dots, c_{N-1} > 0$, then

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$$t \geqslant \sum_{j=0}^{N-1} \frac{s_{\mu(M,N,j)}(\sqrt{\rho}, \dots, \sqrt{\rho})^2}{c_j} = \sum_{j=0}^{N-1} \binom{M}{j}^2 \binom{M-j-1}{N-j-1}^2 \frac{\rho^{M-j}}{c_j},$$

and this is precisely $\mathcal{K}_{\rho,M}$ by the Weyl Dimension Formula. □

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Analogue of Loewner's necessary condition implies:

Suppose $c_0, c_2, c_3 \neq 0$ are real, $M \geqslant 4$, and

$$c_0 + c_2 x^2 + c_3 x^3 + c_M x^M$$

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- The same question, for sums of real powers.

Selected publications

A. Belton, D. Guillot, A. Khare, and M. Putinar:

[1] *Matrix positivity preservers in fixed dimension. I,* Advances in Math., 2016.

[2] *Moment-sequence transforms,* J. Eur. Math. Soc., accepted.

[3] *A panorama of positivity* (survey), Shimorin volume + Ransford-60 proc.

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[4] *On the sign patterns of entrywise positivity preservers in fixed dimension,* (With T. Tao) Amer. J. Math., in press.

[5] *Matrix analysis and preservers of (total) positivity,* 2020+, Lecture notes (website); forthcoming book – Cambridge Press + TRIM.