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“Khare demonstrates an extensive knowledge of this material and has taken considerable responsibility in presenting a blend of classical and contemporary topics in an appealing style opening the text to a broad readership with an interest in matrix positivity and their associated preservers. I expect this reference will be indispensable for both new and active researchers in this subject area.”

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“The opening notes of this symphony of ideas were written by Schur in 1911. Schoenberg, Loewner, Rudin, Herz, Hiai, FitzGerald, Jain, Guillot, Rajaratnam, Belton, Putinar, and others composed new themes and variations. Now, Khare has orchestrated a masterwork that includes his own harmonies in an elegant synthesis. This is a work of impressive scholarship.”

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– Terence Tao, University of California, Los Angeles

Matrix Analysis and Entrywise Positivity Preservers

APOORVA KHARE
Indian Institute of Science



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To Amruta and Anandi

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Foreword

Matrix positivity in its broad sense was and remains a catalyst of algebraic statements with an analytic proof, and of analytic statements with an algebraic proof. Every working mathematician can provide relevant examples in both directions. One of the turning points in promoting matrix positivity as a substitute of analytic techniques is cast in the following quote from a letter of Hermite:

En poursuivant mes recherches sur le théorème de Mr. Sturm, j'ai réussi à traiter par les memes principes les équations à coefficients imaginaires; ce qui m'a conduit au théorème de Mr. Cauchy pour le cas du rectangle, du cercle, et d'une infinité d'autres courbes qui sont meme à branches infinies, comme l'hyperbole. La théorie des formes quadratiques vient ainsi donner pour ces théorèmes des demonstrations indépendantes de toute considération de continuité, comme celle que Vous avez déjà pu conclure Vous-meme de ce que j'ai dit au sujet du théorème de Mr. Sturm dans les Comptes rendus de l'Académie. (1853, 1er semestre p. 294). Extrait d'une lettre de Mr. Ch. Hermite de Paris Mr. Borchardt de Berlin, sur le nombre des racines d'une équation algébrique comprises entre les limites données, J. Reine Angew. Math. 52(1856), 39–51

The long-lasting impact of Sturm's sequence method and Hermite's quadratic forms on the development of mathematics is unquestionable. Think of Tarski's elimination of quantifiers principle for real closed fields, in itself the foundation stone of modern real algebraic geometry, respectively the role of Hermitian forms in spectral analysis or modern differential geometry. As a sign of vitality of these concepts, and their underlying matrix positivity characteristic, every new generation of scientists has unveiled fresh facets and striking applications. For instance, the data of a bounded analytic interpolation problem is encoded in the positivity of a Nevanlinna–Pick matrix, the power moments of a mass distribution on the line are characterized by the positivity of a Hankel matrix, the characteristic function of a probability distribution is

identified to a positive definite kernel, the stability of a dynamical system can be derived from a positive matrix certificate, and so on.

Coming closer to the topics in the present book, we single out two discoverers in the vast landscape of matrix positivity: Charles Loewner (1893–1968) and Isaac J. Schoenberg (1903–1990). To Loewner we owe the characterization of matrix monotone functions, that is, differentiable functions f which preserve via the natural functional calculus the monotonicity of self-adjoint matrices: if $A \leq B$, then $f(A) \leq f(B)$. Note that when allowing matrices A, B of arbitrary dimension, these matrix monotone functions are real analytic with an analytic continuation in the upper-half plane that contains a positive imaginary part. Matrix monotonicity continues to fascinate to the point that the recent Springer volume *Loewner's Theorem on Monotone Matrix Functions* by Barry Simon starts with the provocative sentence: “This book is a love poem to Loewner’s theorem.”

In a different vein, soon after defending his doctoral dissertation, Schoenberg started a lifelong exploration of total positivity and variation diminishing linear transformations. A motivation for his study was the classical Hermite–Poulain theorem which isolates linear difference operations preserving the class of polynomials with real roots. Schoenberg’s elaborate construct, masterfully combining matrix (total) positivity and the harmonic analysis of Laplace transforms, is unanimously accepted as the foundation of the theory of splines. A counterpart to Loewner’s theorem, this time for the entrywise functional calculus $f[A]$, is a byproduct of Schoenberg’s work: if $f[A] \geq 0$ for all matrices $A \geq 0$, then f is a real analytic function with nonnegative Taylor coefficients at zero.

Note in both examples above how purely algebraic and positivity statements imply the analyticity of the transformation. Apoorva Khare’s book resonates precisely with this string by adding pertinent advances to the theories of Loewner and Schoenberg. The main theme is the structure of “positivity preservers,” that is, entrywise transformations of positive matrices, them being of a prescribed finite size, infinite, structured, or even depending on a continuum of variables (better known as kernels). The source of this quest comes from the years the author spent among statisticians, and their pragmatic need of operating on large correlation matrices. Soon, however, the expertise of Professor Khare on group representation theory intervened, by considerably enlarging the scope and perspective of the inquiry.

The result is a highly original synthesis of a century of matrix positivity studies interlaced with very recent findings due to the author and his collaborators. The volume collects for the first time, in a surprisingly natural coordination, topics such as: distance geometry, moment problems, complete

monotonicity, total positivity, graphical models, network analysis, and Schur polynomials. Qualitative features of the determinant of a linear pencil of symmetric matrices form the gateway to an array of deep new results touching the representation theory of the symmetric group, but also very basic concepts of numerical matrix analysis. Two recurrent phenomena are worth mentioning: the striking rigidity of entrywise preservers of various positive cones of matrices or kernels and the existence of a critical exponent for fractional power transforms, that is, a boundary separating a discrete spectrum from a continuous one.

The text was forged during two rounds of semester-long courses delivered by the author. In this sense, the book is far from being a definitive monograph, rather marking the birth of a promising new interdisciplinary area of research. Most of the classical theorems are included with complete proofs. Informative historical notes and a careful selection of exercises, not excluding open questions, will delight and challenge the reader. The joy of fresh discovery permeates every page of the book.

Mihai Putinar
University of California at Santa Barbara
and University of Newcastle

Preface

This text arose out of the course notes for Math 341: Matrix Analysis and Positivity, a one-semester course on analysis and matrix positivity preservers – or, more broadly, composition operators preserving various kinds of positive kernels. The course was offered in Spring 2018 and Fall 2019 at the Indian Institute of Science (IISc). In the present text, we briefly describe some notions of positivity in matrix theory, followed by our main focus: a detailed study of the operations that preserve these notions (and, in the process, an understanding of some aspects of real functions). Several different notions of positivity in analysis, studied for classical and modern reasons, are touched upon in the text:

- Positive semidefinite and positive definite matrices.
- Entrywise positive matrices.
- A common strengthening of the first two notions, which involves totally positive (*TP*) and totally nonnegative (*TN*) matrices.
- Settings somewhat outside matrix theory. For instance, consider discrete data associated with positive measures on locally compact abelian groups G . E.g., for $G = \mathbb{R}$, one obtains moment-sequences, which are intimately related to positive semidefinite Hankel matrices. For $G = S^1$, the circle group, one obtains Fourier–Stieltjes sequences, which are connected to positive semidefinite Toeplitz matrices. (See works of Carathéodory, Hamburger, Hausdorff, Herglotz, and Stieltjes, among others.)
- More classically, functions and kernels with positivity structures have long been studied in analysis, including on locally compact groups and metric spaces (see Bochner, Schoenberg, von Neumann, Pólya, etc.). These include positive definite functions and Pólya frequency functions and sequences.

The text begins by discussing positive semidefinite and TN matrices and some of their basic properties, followed by some of the early results on preservers of positive semidefiniteness. The next two parts then study, in detail, classical and modern results on entrywise positivity preservers in fixed and all dimensions. Among other things, this journey involves going through many beautiful classical results by leading experts in analysis during the first half of the twentieth century.

The purpose of this text is to study the post-composition transforms that preserve positivity on various classes of kernels. When the kernel has finite domain – i.e., is a matrix, as is the case in most of this book – then this amounts to studying *entrywise* preservers of various notions of positivity. The question of why this entrywise calculus was studied – as compared to the usual holomorphic functional calculus – has a rich and classical history in the analysis literature, beginning with the work of Schoenberg, Rudin, Loewner, and Horn (these results are proved in Part II of the text), but also drawing upon earlier works of Menger, Schur, Bochner, and others. (In fact, the entrywise calculus was introduced, and the first such result proved, by Schur in 1911.) Interestingly, this entrywise calculus also arises in modern-day applications from high-dimensional covariance estimation; we elaborate on this in Section 7.1, and briefly also in Chapter 8. Furthermore, this evergreen area of mathematics continues to be studied in the literature, drawing techniques from – and also contributing to – symmetric function theory, statistics and graphical models, combinatorics, and linear algebra (in addition to analysis).

As a historical curiosity, the course and this text arose in a sense out of research carried out in significant measure by mathematicians at Stanford University (including their students) over the years. This includes Loewner, Karlin, and their students FitzGerald, Horn, Micchelli, and Pinkus. Less directly, there was also Katznelson, who had previously worked with Helson, Kahane, and Rudin, leading to Rudin’s strengthening of Schoenberg’s theorem. (Coincidentally, Pólya and Szegő, who made the original observation on entrywise preservers of positivity using the Schur product theorem, were again colleagues at Stanford.) On a personal note, the author’s contributions to this area also have their origins in his time spent at Stanford University, collaborating with Alexander Belton, Dominique Guillot, Mihai Putinar, Bala Rajaratnam, and Terence Tao (though the collaboration with the last-named colleague was carried out almost entirely at IISc).

We now discuss the course, the notes that led to this text, and their mathematical contents. The notes were scribed by the students taking the

course in Spring 2018 at IISc, followed by extensive “homogenization” by the author – and, in several chapters, addition of material. Each chapter was originally intended to cover the notes of roughly one 90-minute lecture, or occasionally two; that said, some material has subsequently been moved around for logical, mathematical, and expositional reasons. The notes, and the course itself, require an understanding of basic linear algebra and analysis, with a bit of measure theory as well. Beyond these basic topics, we have tried to keep these notes as self-contained as possible, with full proofs. To that end, we have included proofs of “preliminary” results, including:

- (i) results of Schoenberg, Menger, von Neumann, Fréchet, and others connecting metric geometry and positive definite functions to matrix positivity;
- (ii) results in Euclidean geometry (including on triangulation), Heron’s formula for triangles, and linking Cayley–Menger matrices to simplicial volumes;
- (iii) results of Boas–Widder and Bernstein on functions with positive differences;
- (iv) Sierpiński’s result: midconvexity and measurability imply continuity;
- (v) an extension to normed linear spaces, of (a special case of) a classical result of Ostrowski on midconvexity and local boundedness implying continuity;
- (vi) Descartes’ rule of signs;
- (vii) Fekete’s result on TP matrices via positive contiguous minors;
- (viii) Sylvester’s criterion and the Schur product theorem for positive definite and semidefinite matrices (also, the Jacobi formula);
- (ix) the Rayleigh–Ritz theorem;
- (x) a special case of Weyl’s inequality on eigenvalues;
- (xi) the Cauchy–Binet formula and a continuous generalization;
- (xii) the discreteness of zeros of real analytic functions (and a sketch of the continuity of roots of complex polynomials); and
- (xiii) the equivalence of Cauchy’s and Littlewood’s definitions of Schur polynomials (and of the Jacobi–Trudi and von Nägelsbach–Kostka identities) via Lindström–Gessel–Viennot bijections.

As the reader will notice, the exposition herein has left out some proofs. These include proofs of theorems by Hamburger/Hausdorff/Stieltjes, Fubini, Tonelli, Cauchy, Montel, and Morera; a Schur positivity phenomenon for ratios of Schur polynomials; Lebesgue’s dominated convergence theorem; as well as the closure of real analytic functions under composition. Most of these can be

found in standard textbooks in mathematics. Nevertheless, as the previous and current paragraphs indicate, these notes cover many classical results by past experts and acquaint the reader with a variety of tools in analysis (especially the study of real functions) and in matrix theory – many of these tools are not found in more “traditional” courses on these subjects.

This text is broadly divided into three parts, each with detailed bibliographic notes (these are given at the end of the text). In Part I, the key objects of interest – positive semidefinite and Hankel TN matrices – are introduced via basic results and important classes of examples. We then begin the study of functions acting entrywise on such matrices and preserving the relevant notion of positivity. Here, we will mostly restrict ourselves to studying power functions that act on various sets of matrices of a *fixed* size. This is a long-studied question, including by Bhatia, Elsner, Fallat, FitzGerald, Hiai, Horn, Jain, Johnson, Sokal, and the author together with Guillot and Rajaratnam. An interesting highlight is a construction by Jain of individual (pairs of) matrices, which encode the entire set of entrywise powers preserving Loewner positivity, monotonicity, and convexity. We also obtain certain necessary conditions on general entrywise functions that preserve positivity, including multiplicative midconvexity and continuity. We explain some of the modern motivations to study entrywise preservers, and we end with some unsolved problems.

Part II deals with the foundational results on matrix positivity preservers. We begin with the early history – including related work by Menger, Fréchet, Bochner, and Schoenberg. We then classify the entrywise functions that preserve positive semidefiniteness (= positivity) in all dimensions, or total nonnegativity on Hankel matrices of *all* sizes. This is a celebrated result of Schoenberg – later strengthened by Rudin – which is a converse to the Schur product theorem, and we prove a stronger version by using a rank-constrained test set. The proof here is different from previous approaches of Schoenberg and Rudin, is essentially self-contained, and uses relatively less sophisticated machinery compared to the works of Schoenberg and Rudin. Moreover, it also proves a variant by Vasudeva for matrices with only positive entries, and it lends itself to a multivariate generalization (which will not be covered here). The starting point of these proofs is a necessary condition for entrywise preservers in a fixed dimension, proved by Loewner (and Horn) in the late 1960s. To this day, this result remains essentially the only known condition in a fixed dimension $n \geq 3$, and a proof of a (rank-constrained, as above) stronger version is also provided in these notes. In addition to techniques and ingredients introduced by the above authors, the text also borrows from the author’s joint work with Belton, Guillot, and Putinar.

Following this development, this part of the text ends with several related results and follow-ups:

- (i) Chapters 18 and 19 classify “dimension-free” preservers of Loewner positivity, monotonicity, and convexity (on kernels over infinite domains).
- (ii) We next cover – in Chapter 20 – recent work by Vishwakarma on an “off-diagonal” variant of the positivity preserver problem.
- (iii) Chapter 21 covers a result by Boas and Widder, which shows a converse “mean value theorem” for divided differences.
- (iv) Finally, Chapter 22 explores the theme of Euclidean distance geometry, with a focus on some classical results by Menger.

The final Part III can be read directly following Chapter 5 and the statements of Theorems 11.2 and 12.1. Part III deals with entrywise functions preserving positivity in a fixed dimension. This is a challenging problem – it is still open in general, even for 3×3 matrices – and we restrict the discussion here to studying polynomial preservers. According to the Schur product theorem (1911), if the polynomial has all nonnegative coefficients, then it is at once a preserver; but, interestingly, until 2016 not a single other example was known in any fixed dimension $n \geq 3$. Very recently, this question has been answered to some degree of satisfaction by the author, in collaboration first with Belton, Guillot, and Putinar, and subsequently with Tao. The text ends by covering some of this recent progress, and it comes back full circle to Schur through symmetric function theory.

Also in this text, historical notes and further questions serve to acquaint the reader with past work(er)s, related areas, and possible avenues for future work – and can be accessed from the Index. See also the Exercises after each part of the text, and the Bibliographic Notes and References at the end of the text. The former include additional results not covered in the course or this text.

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