

Moments in positivity:

metric geometry, covariance estimation, novel graph invariant

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(Partly based on joint works with Alexander Belton, Dominique Guillot,
Mihai Putinar, Bala Rajaratnam, and Terence Tao)

Working example

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

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Example: Consider the following 5×5 correlation matrices:

$$A = \begin{pmatrix} 1 & 0.6 & 0 & 0 & 0 \\ 0.6 & 1 & 0.5 & 0 & 0 \\ 0 & 0.5 & 1 & 0.4 & 0 \\ 0 & 0 & 0.4 & 1 & 0.3 \\ 0 & 0 & 0 & 0.3 & 1 \end{pmatrix}, \quad B = \begin{pmatrix} 1 & 0.6 & 0.5 & 0 & 0 \\ 0.6 & 1 & 0.6 & 0.5 & 0 \\ 0.5 & 0.6 & 1 & 0.6 & 0.5 \\ 0 & 0.5 & 0.6 & 1 & 0.6 \\ 0 & 0 & 0.5 & 0.6 & 1 \end{pmatrix}.$$

(Pattern of zeros according to graphs: tree, banded graph.)

Question: Raise each entry to the α th power for some $\alpha > 0$.
For which α are the resulting matrices positive?

Positivity and Analysis

Introduction

Positivity (and preserving it) studied in many settings in the literature.

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)
- Hilbert space kernels
- Positive definite functions on metric spaces, topological (semi)groups

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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 $N \geq 1$ 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 $f : I \rightarrow \mathbb{R}$, 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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- Anything else?

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Theorem (Schoenberg, *Duke Math. J.* 1942; Rudin, *Duke Math. J.* 1959)

Suppose $I = (-1, 1)$ and $f : I \rightarrow \mathbb{R}$. The following are equivalent:

- 1 $f[A] \in \mathbb{P}_N$ for all $A \in \mathbb{P}_N(I)$ 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 $c_k \geq 0$.

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Such functions f are said to be **absolutely monotonic** on $(0, 1)$.

Toeplitz and Hankel matrices

Motivations: Rudin was motivated by harmonic analysis and Fourier analysis on locally compact groups. On $G = S^1$, he studied preservers of *positive definite sequences* $(a_n)_{n \in \mathbb{Z}}$. This means the Toeplitz kernel $(a_{i-j})_{i,j \geq 0}$ is positive semidefinite.

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- Important parallel notion: **moment sequences**.

Given positive measures μ on $[-1, 1]$, with moment sequences

$$\mathbf{s}(\mu) := (s_k(\mu))_{k \geq 0}, \quad \text{where } s_k(\mu) := \int_{\mathbb{R}} x^k d\mu,$$

classify the moment-sequence transformers: $f(s_k(\mu)) = s_k(\sigma_\mu)$, $\forall k \geq 0$.

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- With Belton–Guillot–Putinar \rightsquigarrow a parallel result to Rudin:

Toeplitz and Hankel matrices (cont.)

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

Theorem (Rudin, *Duke Math. J.* 1959)

Given a function $f : I \rightarrow \mathbb{R}$, the following are equivalent:

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In other words, $f(x) = \sum_{k=0}^{\infty} c_k x^k$ on I with all $c_k \geq 0$.

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

Given a function $f : I \rightarrow \mathbb{R}$, the following are equivalent:

- 1 $f[-]$ preserves the set of **moment sequences** with entries in I .
- 2 $f[-]$ preserves positivity on **Hankel** matrices of all sizes and rank ≤ 3 .
- 3 f is analytic on I and has nonnegative Maclaurin coefficients.

Positive semidefinite kernels

- These two results greatly weaken the hypotheses of Schoenberg's theorem – only need to consider positive semidefinite matrices of rank ≤ 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 ≥ 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.

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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.)

Positivity and Metric geometry

Distance geometry

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- Now ubiquitous in science (mathematics, physics, economics, statistics, computer science. . .).

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- Now ubiquitous in science (mathematics, physics, economics, statistics, computer science. . .).
- Fréchet [*Math. Ann.* 1910]. If (X, d) is a metric space with $|X| = n + 1$, then (X, d) isometrically embeds into $(\mathbb{R}^n, \ell_\infty)$.
- This avenue of work led to the exploration of metric space embeddings.
Natural question: *Which metric spaces isometrically embed into Euclidean space?*

Euclidean metric spaces and positive matrices

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Theorem (Schoenberg, *Ann. of Math.* 1935)

Fix a finite metric space (X, d) , where $X = \{x_0, \dots, x_n\}$. Then (X, d) isometrically embeds into some \mathbb{R}^m (with the Euclidean distance/norm) if and only if the $n \times n$ matrix

$$A := (d(x_0, x_i)^2 + d(x_0, x_j)^2 - d(x_i, x_j)^2)_{i,j=1}^n$$

is positive semidefinite.

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is positive semidefinite. Moreover, the smallest such m is the rank of A .

This is how Schoenberg connected metric geometry and matrix positivity.

Positive definite 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:

$$d(x, y) := \sphericalangle(x, y) = \arccos \langle x, y \rangle, \quad x, y \in S^\infty.$$

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- Applying $\cos[-]$ entrywise to any distance matrix on S^∞ yields:

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

and this is a Gram matrix, so $\cos(\cdot)$ is positive definite on S^∞ .

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

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

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 $\leq r$ correlation matrix $A = (a_{ij})_{i,j=1}^n$, i.e.,

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

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

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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 $f : [-1, 1] \rightarrow \mathbb{R}$ 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

$$f(\cos \theta) = \sum_{k \geq 0} c_k \cos^k \theta,$$

where $c_k \geq 0 \forall k$ are such that $\sum_k c_k < \infty$.

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Suppose $f : [-1, 1] \rightarrow \mathbb{R}$ 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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where $c_k \geq 0 \forall k$ are such that $\sum_k c_k < \infty$.

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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.)

Positivity and Statistics

Modern motivation: covariance estimation

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- **Important question:** Estimate Σ from data $x_1, \dots, x_n \in \mathbb{R}^p$.
- In modern-day settings (small samples, ultra-high dimension), covariance estimation can be very challenging.
- Classical estimators (e.g. sample covariance matrix (MLE)):

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

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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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- Not scalable to modern-day problems with 100,000+ variables (disease detection, climate sciences, finance...).

Thresholding and regularization

Thresholding covariance/correlation matrices

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

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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.

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

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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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Problems motivated by applications

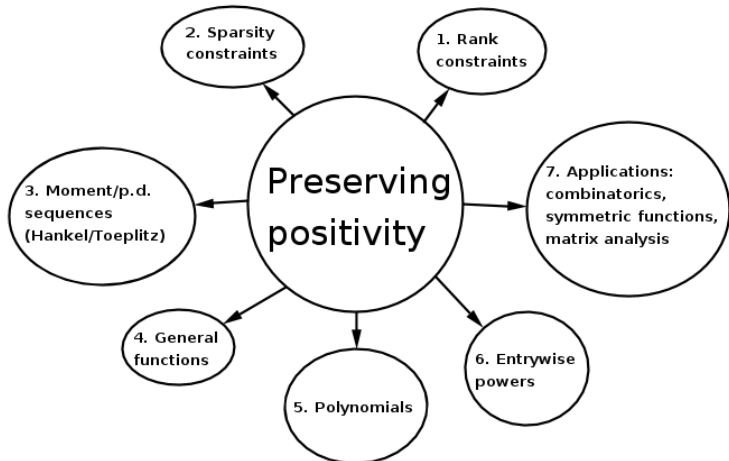
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Further connections: total positivity, symmetric functions

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- 1 *Total positivity*: Pólya frequency functions and sequences.

Rich history, from Laguerre and Fekete–Pólya, to Schoenberg, Gantmacher–Krein, Karlin. . .

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- 2 Connections of positivity preservers, as well as of total positivity, to \longleftrightarrow algebraic combinatorics, Schur polynomials. (K.–Tao)

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

Fix $I = (0, \infty)$ and $f : I \rightarrow \mathbb{R}$ of class C^{N-1} . Suppose $f[A] \in \mathbb{P}_N$ for all $A \in \mathbb{P}_N(I)$ **Hankel of rank ≤ 2 , with N fixed.**

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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. ~~$f(t) \geq 0, f'(t) \geq 0$~~ that if f is $(n-1)$ times differentiable the following conditions are necessary

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

The functions t^p ($p \geq 1$) do not satisfy these conditions for all p if $n \geq 3$.

The proof is obtained by considering matrices of the

form $a_{ij} = \alpha \frac{1}{|x_i - x_j|}$ with $\alpha \in (a, b)$ ≥ 0 and the x_i arbitrary. Then $(f(a_{ij})) > 0$ and hence the determinant $\Delta(\omega)$ is > 0 . The first term in the Taylor expansion of $\Delta(\omega)$ at $\omega = 0$ is $f(\alpha) f'(\alpha) \dots f^{(n-1)}(\alpha) \cdot (\prod (x_i - x_j))^2$ and hence $f(\alpha) f'(\alpha) \dots f^{(n-1)}(\alpha) \geq 0$, from which one easily deduces that (C) must hold.

Entrywise polynomial preservers in fixed dimension

Consequence: Let $N \in \mathbb{N}$ and $c_0, \dots, c_{2N} \neq 0$. Suppose

$$f(x) = \sum_{j=0}^{N-1} c_j x^j + c_N x^N + \sum_{j=N+1}^{2N} c_j x^j$$

preserves positivity on \mathbb{P}_N . Then:

- By considering $f(x)$, we obtain $c_0, \dots, c_{N-1} > 0$.
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Theorem (K.–Tao, *Amer. J. Math.*, accepted)

There exists a polynomial preserver of positivity on \mathbb{P}_N , with a (sufficiently small) negative coefficient, if and only if there are N positive coefficients occurring 'before' it, and N positive coefficients occurring 'after' it.

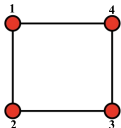
Positivity and Combinatorics

Matrices with zeros according to graphs

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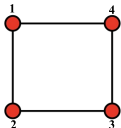
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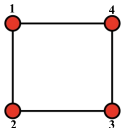


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Study matrices with zeros according to graphs:

Given a graph $G = (V, E)$ on N vertices, and $I \subset \mathbb{R}$, define

$$\mathbb{P}_G(I) := \{A = (a_{ij}) \in \mathbb{P}_N(I) : a_{ij} = 0 \text{ if } i \neq j, (i, j) \notin E\}.$$

Note: a_{ij} can be zero if $(i, j) \in E$.

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Raise each entry to the α th power for some $\alpha > 0$.
When is the resulting matrix positive semidefinite?

Intriguing “phase transition” discovered by two students of Loewner:

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Raise each entry to the α th power for some $\alpha > 0$.
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Intriguing “phase transition” discovered by two students of Loewner:

Theorem (FitzGerald–Horn, *J. Math. Anal. Appl.* 1977)

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Distinguished family of functions: the power maps x^α , $\alpha \in \mathbb{R}$, $x \geq 0$.
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Can we do better?

Digression: the Pólya frequency function of Karlin

In fact when FitzGerald–Horn were students (at Stanford), in the next building S. Karlin had discovered this same ‘Wallach set’ of powers, via total positivity!

- Karlin studied powers of the Pólya frequency function $\Omega(x) := xe^{-x}\mathbf{1}_{x \geq 0}$, and showed that if $n \geq 0$ is an integer, $\Omega(x)^n$ has the following property:

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For all $N \geq 1$, the function $\Omega(x)^n$ is totally non-negative of order N .

That is, for all scalars $x_1 < \dots < x_N$, $y_1 < \dots < y_N$, the matrix

$$\begin{pmatrix} \Omega(x_1 - y_1)^n & \Omega(x_1 - y_2)^n & \cdots & \Omega(x_1 - y_N)^n \\ \Omega(x_2 - y_1)^n & \Omega(x_2 - y_2)^n & \cdots & \Omega(x_2 - y_N)^n \\ \vdots & \vdots & \ddots & \vdots \\ \Omega(x_N - y_1)^n & \Omega(x_N - y_2)^n & \cdots & \Omega(x_N - y_N)^n \end{pmatrix}$$

has all $1 \times 1, \dots, N \times N$ minors non-negative.

Digression: the Pólya frequency function of Karlin (cont.)

Karlin asked: What if we consider non-integer powers $\alpha > 0$? These are never TN , but are TN_N for various N :

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Let $2 \leq N \in \mathbb{Z}$, and $\alpha \in \mathbb{N} \cup [N - 2, \infty)$.

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Theorem (K., 2020)

Let $\alpha \in (0, N - 2) \setminus \mathbb{Z}$. Then $x^\alpha e^{-\alpha x} \mathbf{1}_{x \geq 0}$ is not TN_N .

(Key ingredient in proof: 2020 results of Tanvi Jain.)

Critical exponent of a graph

Back to entrywise powers preserving *positivity*. E.g., can we improve on the set

of powers $\mathbb{N} \cup [3, \infty)$ for $T_5 = \begin{pmatrix} 1 & 0.6 & 0.5 & 0 & 0 \\ 0.6 & 1 & 0.6 & 0.5 & 0 \\ 0.5 & 0.6 & 1 & 0.6 & 0.5 \\ 0 & 0.5 & 0.6 & 1 & 0.6 \\ 0 & 0 & 0.5 & 0.6 & 1 \end{pmatrix}$?

Exploit the sparsity structure of \mathbb{P}_G .

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- Guillot–K.–Rajaratnam [*Trans. AMS* 2016] studied trees: $CE(T) = 1$.
- Compute $CE(G)$ for a family containing complete graphs and trees?

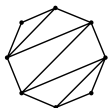
Chordal graphs – powers preserving positivity

Trees have no cycles of length $n \geq 3$.

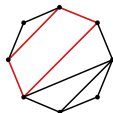
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Chordal



Not Chordal

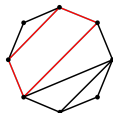
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Let $K_r^{(1)}$ be the ‘almost complete’ graph on r nodes – missing one edge.
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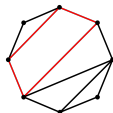
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If G is chordal with $|V| \geq 2$, then $\mathcal{H}_G = \mathbb{N} \cup [r - 2, \infty)$.

In particular, $CE(G) = r - 2$.

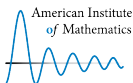
Unites complete graphs, trees, band graphs, split graphs. . .

Open to date: non-chordal graphs

Example: Band graphs with bandwidth d : $CE(G) = \min(d, n - 2)$.

So for $T_5 = \begin{pmatrix} 1 & 0.6 & 0.5 & 0 & 0 \\ 0.6 & 1 & 0.6 & 0.5 & 0 \\ 0.5 & 0.6 & 1 & 0.6 & 0.5 \\ 0 & 0.5 & 0.6 & 1 & 0.6 \\ 0 & 0 & 0.5 & 0.6 & 1 \end{pmatrix}$ as above, all powers $\geq 2 = d$ work.

Non-chordal graphs? $CE(G)$ in terms of 'known' graph invariants?
Not known to date.



Selected publications

D. Guillot, A. Khare, and B. Rajaratnam:

- [1] *Preserving positivity for rank-constrained matrices*, Trans. AMS, 2017.
 - [2] *Preserving positivity for matrices with sparsity constraints*, Tr. AMS, 2016.
 - [3] *Critical exponents of graphs*, J. Combin. Theory Ser. A, 2016.
-

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

- [4] *Matrix positivity preservers in fixed dimension. I*, Advances in Math., 2016.
 - [5] *Moment-sequence transforms*, J. Eur. Math. Soc., accepted.
 - [6] *A panorama of positivity (survey)*, Shimorin volume + Ransford-60 proc.
-

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

[8] *Matrix analysis and entrywise positivity preservers*,
Lecture notes (website); forthcoming book – Cambridge Univ. Press, 2021.