Entrywise positivity preservers:

covariance estimation, symmetric function identities, novel graph invariant

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Apoorva Khare

IISc and APRG (Bangalore, India)

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

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Question: Classify the positivity preservers in these settings.

Studied for the better part of a century.

Positivity and Analysis

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 $\mathbb{P}_N = \mathbb{P}_N(\mathbb{R})$.)

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

Suppose $I = (-1,1)$ and $f : I \to \mathbb{R}$. 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* $c_k \geqslant 0$.

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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 $(a_{i-j})_{i,j \geqslant 0}$ is positive semidefinite.

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- Important parallel notion: **moment sequences**.
  Given positive measures μ on $[-1,1]$, with moment sequences
  $$\mathbf{s}(\mu) := (s_k(\mu))_{k \geqslant 0}, \qquad \text{where } s_k(\mu) := \int_{\mathbb{R}} x^k \, d\mu,$$
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  classify the moment-sequence transformers: $f(s_k(\mu)) = s_k(\sigma_\mu), \ \forall k \geqslant 0.$
- With Belton–Guillot–Putinar $\rightsquigarrow$ a parallel result to Rudin:

Toeplitz and Hankel matrices (cont.)

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

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

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

1. $f[-]$ *preserves the set of positive definite sequences with entries in* I.
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Theorem (Belton–Guillot–K.–Putinar, 2016)

Given a function $f : I \to \mathbb{R}$, 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 $\leqslant 3$.*
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 $\leqslant 3$.
- 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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- 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 theorem in several variables

Let $I = (-\rho, \rho)$ for some $0 < \rho \leqslant \infty$ as above. Also fix $m \geqslant 1$.
Given matrices $A_1, \dots, A_m \in \mathbb{P}_N(I)$ and $f : I^m \to \mathbb{R}$, define

$$f[A_1, \dots, A_m]_{ij} := f(a_{ij}^{(1)}, \dots, a_{ij}^{(m)}), \qquad \forall i, j = 1, \dots, N.$$

Theorem (FitzGerald–Micchelli–Pinkus, *Linear Alg. Appl.* 1995)

Given $f : \mathbb{R}^m \to \mathbb{R}$, the following are equivalent:

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2. *The function f is real entire and absolutely monotonic: for all* $\mathbf{x} \in \mathbb{R}^m$,
$$f(\mathbf{x}) = \sum_{\alpha \in \mathbb{Z}_+^m} c_\alpha \mathbf{x}^\alpha, \qquad \text{where } c_\alpha \geqslant 0 \ \forall \alpha \in \mathbb{Z}_+^m.$$

($(2) \Rightarrow (1)$ by Schur Product Theorem.)

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($(2) \Rightarrow (1)$ by Schur Product Theorem.) The test set can again be reduced:

Theorem (Belton–Guillot–K.–Putinar, 2016)

The above two hypotheses are further equivalent to:

3. $f[-]$ *preserves positivity on m-tuples of Hankel matrices of rank* $\leqslant 3$.

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****?*

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- Menger [*Amer. J. Math.* 1931] and Fréchet [*Ann. of Math.* 1935] provided characterizations.
- Reformulated by Schoenberg, using... matrix positivity!

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

Fix integers $n, r \geqslant 1$, *and a finite metric space* (X, d), *where* $X = \{x_0, \dots, x_n\}$. *Then* (X, d) *isometrically embeds into* $\mathbb{R}^r$ *(with the Euclidean distance/norm) but not into* $\mathbb{R}^{r-1}$ *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 of rank r.

This is how Schoenberg connected metric geometry and matrix positivity.

Distance transforms: positive definite functions

- In the preceding result, the 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,

  if and only if the matrix $A'_{(n+1)\times(n+1)} := (-d(x_i, x_j)^2)_{i,j=0}^n$ is

  conditionally positive semidefinite: $u^T A' u \geqslant 0$ whenever $\sum_{j=0}^n u_j = 0$.

- Early instance of how (conditionally) positive matrices emerged from metric geometry.

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Now we move to *transforms* of positive matrices. Note that:

- Applying the function $-x^2$ *entrywise* sends any distance matrix from Euclidean space, to a conditionally positive semidefinite matrix A'.

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- Schoenberg was interested in embedding metric spaces into Euclidean spheres. This embeddability turns out to involve a *single* p.d. function! This is the cosine function.

Positive definite functions on spheres

Notice that the Hilbert sphere S^∞ (hence every subspace such as S^{r-1}) has a rotation-invariant distance – *arc-length* along a great circle:

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

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

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

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

Positive definite functions on spheres

Notice that the Hilbert sphere S^∞ (hence every subspace such as S^{r-1}) has a rotation-invariant distance – *arc-length* along a great circle:

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

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

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

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

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Also follows from Bochner's work on compact homogeneous spaces [*Ann. of Math.* 1941] – but Schoenberg proved it directly with less 'heavy' machinery.

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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- 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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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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- 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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perform poorly, are singular/ill-conditioned, etc.
- 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 $p = 1,000,000$ and only, say, $\sim 1\%$ of the entries of the true Σ are nonzero.

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

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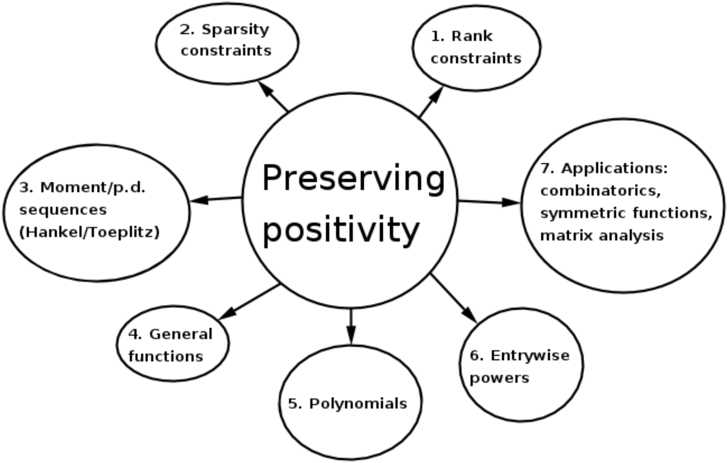

Positivity and Symmetric functions

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Can c_N be negative? Sharp bound? (Not known to date.)

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6. **Further applications:** Schubert cell-type stratifications, connections to Rayleigh quotients, thresholds for analytic functions and Laplace transforms, additional novel symmetric function identities, ...

Schur polynomials

Key ingredient in proof – representation theory / symmetric functions:

Given a decreasing N-tuple $n_{N-1} > n_{N-2} > \cdots > n_0 \geqslant 0$, the corresponding **Schur polynomial** over a field $\mathbb{F}$ is the unique polynomial extension to $\mathbb{F}^N$ of

$$s_{(n_{N-1},\dots,n_0)}(x_1,\dots,x_N) := \frac{\det(x_i^{n_{j-1}})}{\det(x_i^{j-1})}$$

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Example: If $N = 2$ and $\mathbf{n} = (m < n)$, then

$$s_{\mathbf{n}}(x_1,x_2) = \frac{x_1^n x_2^m - x_1^m x_2^n}{x_1 - x_2} = (x_1x_2)^m(x_1^{n-m-1}+x_1^{n-m-2}x_2+\cdots+x_2^{n-m-1}).$$

Basis of homogeneous symmetric polynomials in $x_1,\dots,x_N$.

By-product: novel symmetric function identity

- Well-known identity of Cauchy: if $f_0(t) = 1/(1-t) = \sum_{k \geqslant 0} t^k$, then

$$\det f_0[\mathbf{u}\mathbf{v}^T] = V(\mathbf{u})V(\mathbf{v}) \sum_{\mathbf{n}} s_{\mathbf{n}}(\mathbf{u}) s_{\mathbf{n}}(\mathbf{v}),$$

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- We show this for *every* power series
  $\rightsquigarrow$ obtained by generalizing a matrix positivity computation of Loewner:

Theorem (K., 2018)

Fix a commutative unital ring R and let t be an indeterminate. Let $f(t) := \sum_{M \geqslant 0} f_M t^M \in R[[t]]$ be an arbitrary formal power series. Given vectors $\mathbf{u}, \mathbf{v} \in R^N$ for some $N \geqslant 1$, we have:

$$\det f[t\mathbf{u}\mathbf{v}^T] = V(\mathbf{u})V(\mathbf{v}) \sum_{M \geqslant \binom{N}{2}} t^M \sum_{\mathbf{n}=(n_{N-1},\dots,n_0) \vdash M} s_{\mathbf{n}}(\mathbf{u}) s_{\mathbf{n}}(\mathbf{v}) \prod_{k=0}^{N-1} f_{n_k}.$$

Positivity and Combinatorics

Matrices with zeros according to graphs

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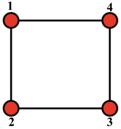

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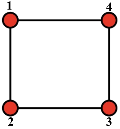

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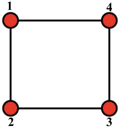

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Study matrices with zeros according to graphs:

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 $(i, j) \in E$.

Preserving positivity with sparsity constraints

Given a subset $I \subset \mathbb{R}$ and a graph $G = (V, E)$, define for $A \in \mathbb{P}_G(I)$:

$$(f_G[A])_{ij} := \begin{cases} f(a_{ij}) & \text{if } i = j \text{ or } (i,j) \in E, \\ 0 & \text{otherwise.} \end{cases}$$

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We now explain how *powers* preserving positivity $\rightsquigarrow$ a novel graph invariant.

Powers preserving positivity: Working example

Distinguished family of functions: the power maps $x^\alpha, \alpha \in \mathbb{R},\ x \geqslant 0$.
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So for T_5 as above, all powers $\alpha \in \mathbb{N} \cup [3, \infty)$ work.

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Distinguished family of functions: the power maps $x^\alpha, \alpha \in \mathbb{R},\ x \geqslant 0$.
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Example: Suppose $T_5 = \begin{pmatrix} 1 & 0.6 & 0.5 & 0 & 0 \\ 0.6 & 1 & 0.6 & 0.5 & 0 \\ 0.5 & 0.6 & 1 & 0.6 & 0.5 \\ 0 & 0.5 & 0.6 & 1 & 0.6 \\ 0 & 0 & 0.5 & 0.6 & 1 \end{pmatrix}$.

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

Intriguing "phase transition" discovered by FitzGerald and Horn:

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

*Let $N \geqslant 2$. Then $f(x) = x^\alpha$ preserves positivity on $\mathbb{P}_N([0,\infty))$ if and only if $\alpha \in \mathbb{N} \cup [N-2, \infty)$. The threshold $N-2$ is called the **critical exponent**.*

So for T_5 as above, all powers $\alpha \in \mathbb{N} \cup [3, \infty)$ work. Can we do better?

Critical exponent of a graph

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

Problem: Compute the set of powers preserving positivity on $\mathbb{P}_G$:

$$\mathcal{H}_G := \{\alpha \geqslant 0 : A^{\circ\alpha} \in \mathbb{P}_G \text{ for all } A \in \mathbb{P}_G([0,\infty))\}$$

$$CE(G) := \text{ smallest } \alpha_0 \text{ s.t. } x^\alpha \text{ preserves positivity on } \mathbb{P}_G, \forall \alpha \geqslant \alpha_0.$$

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- How do $CE(G)$ and $\mathcal{H}_G$ depend on the geometry of G? Compute $CE(G)$ for a family containing complete graphs and trees?

Chordal graphs – powers preserving positivity

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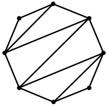
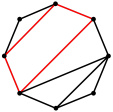
Definition: G is *chordal* if it does not contain induced cycles of length $n \geqslant 4$.



Chordal



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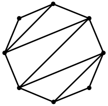

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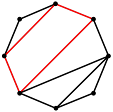

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Theorem (Guillot–K.–Rajaratnam, *J. Combin. Theory Ser. A* 2016)

Let $K_r^{(1)}$ be the 'almost complete' graph on r nodes – missing one edge. Let $r = r(G)$ be the largest integer such that either K_r or $K_r^{(1)}$ is an induced subgraph of G.

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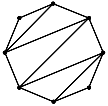

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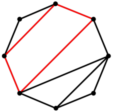

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Let $K_r^{(1)}$ be the 'almost complete' graph on r nodes – missing one edge. Let $r = r(G)$ be the largest integer such that either K_r or $K_r^{(1)}$ is an induced subgraph of G.

If G is chordal with $|V| \geqslant 2$, then $\mathcal{H}_G = \mathbb{N} \cup [r-2, \infty)$.

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

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

Non-chordal graphs

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

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Other graphs? (Talk by *Dominique Guillot* in MS18-iii.)

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Other graphs? (Talk by *Dominique Guillot* in MS18-iii.)
$CE(G)$ **in terms of other graph invariants?** Not clear.

American Institute of Mathematics
NSF
SERB INDIA
Taylor & Francis
DARPA
ICMS International Centre for Mathematical Sciences
Infosys Foundation
Indian Institute of Science भारतीय विज्ञान संस्थान
ILAS International Linear Algebra Society

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.

[4] *Complete characterization of Hadamard powers preserving Loewner positivity, monotonicity, and convexity*, J. Math. Anal. Appl., 2015.

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

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

[6] *Moment-sequence transforms*, Preprint, 2016.

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

---

[8] *On the sign patterns of entrywise positivity preservers in fixed dimension*, (With T. Tao) Preprint, 2017.

[9] *Smooth entrywise positivity preservers, a Horn–Loewner master theorem, and Schur polynomials*, Preprint, 2018.