Entrywise positivity preservers

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Joint work with Alexander Belton (Lancaster), Apoorva Khare (Indian Institute of Sciences, Bangalore), and Mihai Putinar (UCSB and Newcastle)

- **The psd cone:** Let

$$\mathbb{P}_N := \{A \in \mathbb{M}_N(\mathbb{R}) \text{ symmetric} : x^T A x \geq 0 \ \forall x \in \mathbb{R}^N\}$$

- More generally, given $S \subset \mathbb{C}$, we let

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Main reference:
A. Belton, D. Guillot, A. Khare, M. Putinar,
Matrix positivity preservers in fixed dimension. I,
Adv. Math., 298, 2016, Pages 325–368.

Outline

Motivation for entrywise calculus

Classical motivation:

- Schoenberg's original motivation: invariant distances on homogeneous spaces which are isometrically equivalent to a Hilbert-space (see e.g. Bochner, Ann. Math. 1941).
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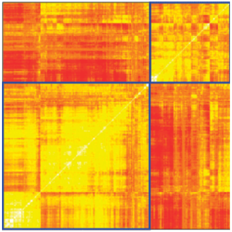
Recent interest:

- Applications to data science (e.g. covariance estimation).
- Interpolation problems involving positive definite kernels (climate science, machine learning; see e.g. Gneiting, 2013).
- Semidefinite programming.
- Construction of sparse probability models (see e.g. Bai and Zhang, SIAM J. Matrix Anal. 2007).



Pancaldi et al., 2010.

Covariance matrices

$\Sigma = (\sigma_{j,k})_{j,k=1}^{p}$.

- Random vector: $(X_1, \ldots, X_p)$

$$\begin{aligned}\sigma_{j,k} &= \mathrm{Cov}(X_j, X_k) \\ &= E((X_j - E(X_j))(X_k - E(X_k)))\end{aligned}$$

- Estimation: $x_1, \ldots, x_n \in \mathbb{R}^p$.
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$$S = \frac{1}{n-1}\sum_{j=1}^{n}(x_j - \overline{x})(x_j - \overline{x})^T, \quad \overline{x} = \frac{1}{n}\sum_{j=1}^{n} x_j.$$

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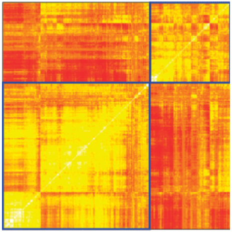

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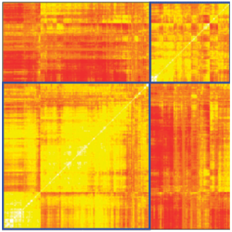

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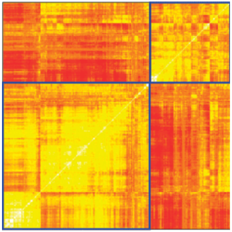
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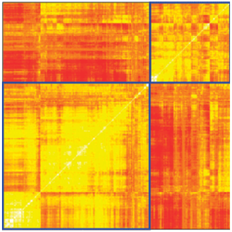

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- Modern approach via compressed sensing (Daubechies, Donoho, Tao, Candes).
- Uses convex optimization to obtain sparse estimates (of Σ or Σ^{-1}) – e.g. ℓ_1 penalized estimation.
- Works very well, but usually too computationally intensive in modern applications with 100,000+ variables (genomics, climate science, finance, etc.).

Thresholding and regularization

Thresholding covariance/correlation matrices

$$\text{True } \Sigma = \begin{pmatrix} 1 & 0.2 & 0 \\ 0.2 & 1 & 0.9 \\ 0 & 0.9 & 1 \end{pmatrix} \quad S = \begin{pmatrix} 0.95 & 0.18 & 0.02 \\ 0.18 & 0.96 & 0.87 \\ 0.02 & 0.87 & 0.98 \end{pmatrix}$$

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- Resulting matrix typically have much better properties (e.g. non-singular).
- Thresholding is equivalent to applying the function $f_\epsilon(x) = x \cdot \mathbf{1}_{|x|>\epsilon}$ to the entries of the matrix, for some $\epsilon > 0$

More generally, can apply a function $f : \mathbb{R} \to \mathbb{R}$ to the elements of S

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References:

1. Guillot, Khare, and Rajaratnam, *Preserving positivity for rank-constrained matrices*, Trans. Amer. Math. Soc, 2017.
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From Schur to Schoenberg

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Proof 2: If $A = \sum_{j=1}^n \lambda_j v_j v_j^T$ and $B = \sum_{k=1}^n \mu_k w_k w_k^T$, then

$$A \circ B = \sum_{j,k=1}^n \lambda_j \mu_k (v_j v_j^T) \circ (w_k w_k)^T = \sum_{j,k=1}^n \lambda_j \mu_k (v_j \circ w_k)(v_j \circ w_k)^T.$$

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Theorem (Schoenberg, Duke 1942; Rudin, Duke 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 Taylor 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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For fixed $N \geq 3$, necessary condition known due to Horn (who attributes it to Loewner):

Horn's thesis

Theorem (Horn, Trans. Amer. Math. Soc. 1969; Guillot-Khare-Rajaratnam, Trans. Amer. Math. Soc., 2015)

Fix $I = (0, \rho)$ *for* $0 < \rho \leq \infty$, *and* $f : I \to \mathbb{R}$ *and* $N \geq 3$.
Suppose $f[A] \in \mathbb{P}_N$ *for* $A = a\mathbf{1}_{N\times N} + uu^T \in \mathbb{P}_N(I)$ *with* $a \in I$.

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Then $f \in C^{N-3}(I)$, *and*

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

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Theorem (Bernstein). Suppose $-\infty < a < b \leq \infty$. If $f : [a, b) \to \mathbb{R}$ is continuous at a and absolutely monotonic on (a, b), then f can be extended analytically to the complex disc $D(a, b-a)$.

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7. The allowed signs in the coefficients of polynomials preserving positivity on $\mathbb{P}_N$ were characterized by A. Khare and T. Tao.
Theorem.(A. Khare, T. Tao, 2017)
Let $N > 0$ and $0 \leq n_0 < n_1 < \cdots < n_{N-1}$ be natural numbers, and for each $M > n_{N-1}$, let $\epsilon_M \in \{-1, 0, 1\}$ be a sign. Let $0 < \rho < \infty$, and let $c_{n_0}, \ldots, c_{n_{N-1}}$ be positive reals. Then there exists a convergent power series

$$f(x) = c_{n_0} x^{n_0} + c_{n_1} x^{n_1} + \cdots + c_{n_{N-1}} x^{n_{N-1}} + \sum_{M > n_{N-1}} c_M x^M$$

on $(0, \rho)$ that is an entrywise positivity preserver on $\mathbb{P}_N((0, \rho))$, such that for each $M > n_{N-1}$, c_M has the sign ϵ_M.

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Problem: Find smallest t such that $p(t) \geq 0$ for all $A = \mathbf{u}\mathbf{u}^T$.

Schur polynomials

Given an integer partition (i.e., a non-increasing N-tuple of non-negative integers, $n_N \geq \cdots \geq n_1$), the corresponding **Schur polynomial** over a field $\mathbb{F}$ is the unique polynomial extension to $\mathbb{F}^N$ of

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Let $M \geq N \geq 1$ 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

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$$\det p_t[\mathbf{u}\mathbf{v}^T] =$$

$$t^{N-1}\Delta_N(\mathbf{u})\Delta_N(\mathbf{v}) \prod_{j=0}^{N-1} c_j \times \Big(t - \sum_{j=0}^{N-1} \frac{s_{\mu(M,N,j)}(\mathbf{u}) s_{\mu(M,N,j)}(\mathbf{v})}{c_j}\Big).$$

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For more details: Belton, Guillot, Khare, Putinar, *Matrix positivity preservers in fixed dimension. I*, Advances in Mathematics, 2016.

Reformulation: Linear matrix inequalities (LMI)

- For $A \in \mathbb{P}_N$ and f as in the Theorem, note:

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For $A \in \mathbb{P}_N(\overline{D}(0,1))$, this holds with

$$c = \sum_{j=0}^{N-1} \binom{M}{j}^2 \binom{M-j-1}{N-j-1}^2 \qquad \text{(sharp bound)}.$$

Reformulation: Linear matrix inequalities (LMI)

- For $A \in \mathbb{P}_N$ and f as in the Theorem, note:

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

- $f[A]$ is positive semidefinite $\Leftrightarrow$ linear matrix inequality

$$c_M A^{\circ M} \leq c_0 \mathbf{1}_{N\times N} + c_1 A + \cdots + c_{N-1} A^{\circ(N-1)},$$

- Bound higher powers using lower ones. E.g.

$$\begin{aligned} & A^{\circ M} \leq c(\mathbf{1}_{N\times N} + A + \cdots + A^{\circ(N-1)}) \\ \iff & c\mathbf{1}_{N\times N} + cA + \cdots + cA^{\circ(N-1)} - A^{\circ M} \geq 0 \\ \iff & \mathbf{1}_{N\times N} + A + \cdots + A^{\circ(N-1)} - \frac{1}{c} A^{\circ M} \geq 0 \end{aligned}$$

For $A \in \mathbb{P}_N(\overline{D}(0,1))$, this holds with

$$c = \sum_{j=0}^{N-1} \binom{M}{j}^2 \binom{M-j-1}{N-j-1}^2 \qquad \text{(sharp bound)}.$$

Special Case $M = N$: $c = \sum_{j=0}^{N-1} \binom{N}{j}^2 = \binom{2N}{N} - 1 \sim \frac{4^N}{\sqrt{\pi N}}$.

Preserving positivity on Hankel matrices (of all dimensions).

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Let μ a non-negative measure on $\mathbb{R}$, with moments of all orders

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

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- Consider the Hankel matrix associated to μ:

$$H_\mu := \begin{pmatrix} s_0 & s_1 & s_2 & \cdots \\ s_1 & s_2 & s_3 & \cdots \\ s_2 & s_3 & s_4 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

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Theorem (Hamburger). A sequence $(s_k)_{k \geq 0}$ is the moment sequence of a positive Borel measure on $\mathbb{R}$ if and only if its associated Hankel matrices are positive semidefinite.

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Interesting consequence: f preserve positivity (entrywise) on Hankel matrices iff it maps moment sequences to themselves:

$$f(s_k(\mu)) = s_k(\sigma_\mu) \qquad (k \geq 0)$$

for some positive Borel measure s_μ.

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Proposition Suppose $f(s_k(\mu)) = s_k(\sigma_\mu)$ for all $k \geq 0$ and all μ with $\operatorname{supp} \mu \subseteq [-1, 1]$. Then f is continuous.

Proof of the Proposition

Step 1. f is continuous on $(0,\infty)$. Let $0 < x \leq y$.

$$\begin{pmatrix} y & x \\ x & y \end{pmatrix} \in \mathbb{P}_2 \implies \begin{pmatrix} f(y) & f(x) \\ f(x) & f(y) \end{pmatrix} \in \mathbb{P}_2 \implies f(x) \leq f(y).$$

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Next, for $a, b \in (0, \infty)$,

$$\begin{pmatrix} a & \sqrt{ab} \\ \sqrt{ab} & b \end{pmatrix} \in \mathbb{P}_2 \Rightarrow \begin{pmatrix} f(a) & f(\sqrt{ab}) \\ f(\sqrt{ab}) & f(b) \end{pmatrix} \in \mathbb{P}_2 \Rightarrow f(\sqrt{ab})^2 \leq f(a)f(b),$$

i.e., f is multiplicatively mid-convex.

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This implies $\log f(e^x)$ is convex and so f is continuous on $(0,\infty)$.

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Key Idea: If $p(t) = a_0 + a_1 t + \cdots + a_d t^d \geq 0$ on $[-1, 1]$. Then

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- We discover properties of f by applying the above identity for carefully chosen μ and p.
- Let $p_\pm(t) = (1 \pm t)(1 - t^2)$. Then $p_\pm \geq 0$ on $[-1, 1]$.
- Fix $v_0 \in (0, 1)$, let $b, \beta \geq 0$ and define

$$a := \beta + b v_0, \qquad \mu := a\delta_{-1} + b\delta_{v_0}.$$

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Letting $b \to 0^+$ we obtain that f is left-continuous at $-\beta$.
Can use a similar argument to obtain right-continuity. □

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Happy Birthday Tom!!!

Critical exponents

- Recall that $f(x) = x^k$ preserves positivity on $\cup_{N \geq 1} \mathbb{P}_N$ when $k \in \mathbb{N}$.
- What about other powers $f(x) = x^\alpha$ for $\alpha \in \mathbb{R}$?

Example. Suppose

$$A = \begin{pmatrix} 1 & 0.6 & 0.5 & 0 & 0 \\ 0.6 & 1 & 0.6 & 0.5 & 0 \\ 0.5 & 0.6 & 1 & 0.6 & 0.5 \\ 0 & 0.5 & 0.6 & 1 & 0.6 \\ 0 & 0 & 0.5 & 0.6 & 1 \end{pmatrix}.$$

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Raise each entry to the αth power for some $\alpha > 0$.

When is the resulting matrix positive semidefinite?

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

Let $N \geq 2$. *Then:*

1. $f(x) = x^\alpha$ *preserves positivity on* $\mathbb{P}_N((0,\infty))$ *if* $\alpha \geq N-2$.

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In other words, $f(x) = x^\alpha$ *preserves positivity on* $\mathbb{P}_N((0,\infty))$ *if and only if* $\alpha \in \mathbb{N} \cup [N-2,\infty)$.

Critical exponent: $N-2 =$ smallest α_0 such that $\alpha \geq \alpha_0$ preserves positivity on $\mathbb{P}_N$.

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So for $A = \begin{pmatrix} 1 & 0.6 & 0.5 & 0 & 0 \\ 0.6 & 1 & 0.6 & 0.5 & 0 \\ 0.5 & 0.6 & 1 & 0.6 & 0.5 \\ 0 & 0.5 & 0.6 & 1 & 0.6 \\ 0 & 0 & 0.5 & 0.6 & 1 \end{pmatrix}$, all powers $\alpha \in \mathbb{N} \cup [3, \infty)$ work.

Can we do better?

FitzGerald and Horn's result (Sketch of proof)

The proof of FitzGerald and Horn's result is easy, but very ingenious.

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Proof:

$$M = \begin{pmatrix} I_m & BD^{-1} \\ 0 & I_n \end{pmatrix} \begin{pmatrix} A - BD^{-1}C & 0 \\ 0 & D \end{pmatrix} \begin{pmatrix} I_m & 0 \\ D^{-1}C & I_n \end{pmatrix}$$

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Use Induction. $n = 2$ is easy.

Now,

$$A = \begin{pmatrix} B & \xi \\ \xi^T & a_{nn} \end{pmatrix} \qquad \zeta := \frac{1}{\sqrt{a_{nn}}}\xi.$$

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Goal: Show that

$$\begin{aligned} A^{\circ\alpha}/a_{nn}^\alpha &= B^{\circ\alpha} - \zeta^{\circ\alpha}\zeta^{\circ\alpha T} \\ &= B^{\circ\alpha} - (\zeta\zeta^T)^{\circ\alpha} \in \mathbb{P}_{n-1}. \end{aligned}$$

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1. $f(x) = x^\alpha$ preserves positivity on $\mathbb{P}_n((0,\infty))$ if $\alpha \geq n-2$.
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Proof of (1). By elementary calculus, for any $x, y \in \mathbb{R}$,

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Apply the identity entrywise:

$$B^{\circ\alpha} - (\zeta\zeta^T)^{\circ\alpha} = \int_0^1 (B - \zeta\zeta^T) \circ (\lambda B + (1-\lambda)\zeta\zeta^T)^{\circ(\alpha-1)}\, d\lambda.$$

Done by induction.

Critical exponent of graphs

Given $G = (V, E)$ with $V = \{1, \dots, N\}$, define a subset of $\mathbb{P}_N$ by

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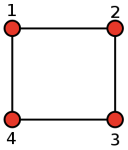

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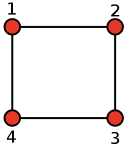

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Define the set of powers preserving positivity for G:

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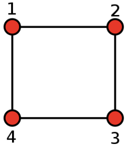

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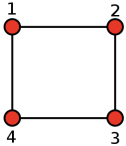

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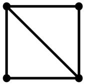

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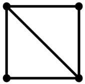

$K_4^{(1)}$

Clearly, the maximal clique is K_3. However, we can show that $\mathcal{H}_{K_4^{(1)}} = \{1\} \cup [2,\infty)$.

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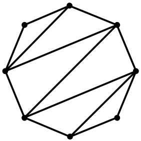

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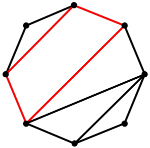

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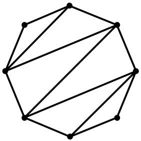

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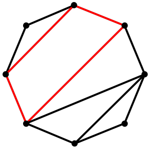

Not Chordal

- Occur in many *applications*: positive definite completion problems, maximum likelihood estimation in graphical models, Gaussian elimination, etc.

Theorem. (Guillot, Khare, Rajaratnam, J. Combin. Theory Ser. A, 2016)
Let G be any chordal graph with at least 2 vertices and let r be the largest integer such that either K_r or $K_r^{(1)}$ is an induced subgraph of G. Then

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Note: 1 is the largest integer such that K_r or $K_r^{(1)}$ is contained in C_n or in a bipartite!

Reference: Guillot, Khare, Rajaratnam, *Critical Exponents of Graphs*, J. Combin. Theory Ser. A, 2016.