Moments in the history of positivity

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(Partly joint with Alexander Belton, Dominique Guillot, Mihai Putinar;
and partly with Terence Tao)

Entrywise functions preserving positivity

Definitions:

1. A real symmetric matrix $A_{n\times n}$ is *positive semidefinite* if its quadratic form is so: $x^T Ax \geq 0$ for all $x \in \mathbb{R}^n$. (Hence $\sigma(A) \subset [0,\infty)$.)
2. 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 $\mathbb{P}_n = \mathbb{P}_n(\mathbb{R})$.)

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3. A function $f : I \to \mathbb{R}$ acts *entrywise* on a matrix $A \in I^{n \times n}$ via: $f[A] := (f(a_{jk}))_{j,k=1}^n$.

Problem: For which functions $f : I \to \mathbb{R}$ is it true that

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- (Long history:) The Schur Product Theorem [Schur, *Crelle* 1911] says: If $A, B \in \mathbb{P}_n$, then so is $A \circ B := (a_{jk}b_{jk})$.
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- (Pólya–Szegö, 1925): Taking sums and limits, if $f(x) = \sum_{k=0}^\infty c_k x^k$ is convergent and $c_k \geq 0$, then $f[-]$ preserves positivity.

  Question: Anything else?

Schoenberg's theorem

Interestingly, the answer is **no**, for preserving positivity in *all* dimensions:

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* $n \geq 1$.
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* I, *with all* $c_k \geq 0$.

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- Schoenberg's result is the (harder) converse to that of his advisor: Schur.
- Vasudeva (*IJPAM* 1979) proved a variant, over $I = (0, \infty)$.
- *Upshot:* Preserving positivity in all dimensions is a rigid condition $\rightsquigarrow$ implies real analyticity, absolute monotonicity...

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- *Upshot:* Preserving positivity in all dimensions is a rigid condition $\rightsquigarrow$ implies real analyticity, absolute monotonicity. . .
- We show stronger versions of Vasudeva's and Schoenberg's theorems. (Outlined below.)

Schoenberg's motivations: metric geometry

Endomorphisms of matrix spaces with positivity constraints related to:

- matrix monotone functions (Loewner)
- preservers of matrix properties (rank, inertia, . . .)
- real-stable/hyperbolic polynomials (Borcea, Branden, Liggett, Marcus, Spielman, Srivastava. . .)
- positive definite functions (von Neumann, Bochner, Schoenberg . . .)

Definition

$f : [0, \infty) \to \mathbb{R}$ is *positive definite* on a metric space (X, d) if
$[f(d(x_j, x_k))]_{j,k=1}^n \in \mathbb{P}_n,$ for all $n \geq 1$ and all $x_1, \dots, x_n \in X$.

Distance geometry

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In the 1900s, the notion of a *metric space* emerged from the works of Fréchet and Hausdorff. . .

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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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- 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 $n, r \geq 1$, and a finite set $X = \{x_0, \dots, x_n\}$ together with a metric d on X. 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

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

is positive semidefinite of rank r.

Connects metric geometry and matrix positivity.

Schoenberg: from metric geometry to matrix positivity

Sketch of one implication: If (X, d) isometrically embeds into $(\mathbb{R}^r, \|\cdot\|)$, then

$$\begin{aligned}
& d(x_0, x_j)^2 + d(x_0, x_k)^2 - d(x_j, x_k)^2 \\
= \; & \|x_0 - x_j\|^2 + \|x_0 - x_k\|^2 - \|(x_0 - x_j) - (x_0 - x_k)\|^2 \\
= \; & 2\langle x_0 - x_j, x_0 - x_k\rangle.
\end{aligned}$$

But then the matrix A above, is the Gram matrix of a set of vectors in $\mathbb{R}^r$, hence is positive semidefinite, of rank $\leq r$.

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- Also observe: the matrix $A := (d(x_0, x_j)^2 + d(x_0, x_k)^2 - d(x_j, x_k)^2)_{j,k=1}^n$ is positive semidefinite,
  if and only if the matrix $A'_{(n+1)\times(n+1)} := (-d(x_j, x_k)^2)_{j,k=0}^n$ is *conditionally positive semidefinite*: $u^T A' u \geq 0$ whenever $\sum_{j=0}^n u_j = 0$.
- This is how positive / conditionally positive matrices emerged from metric geometry.

Distance transforms: positive definite functions

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

What operations send distance matrices to positive semidefinite matrices?

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What operations send distance matrices to positive semidefinite matrices? These are the *positive definite functions*. **Example:** Gaussian kernel:

Theorem (Schoenberg, *Trans. AMS* 1938)

The function $f(x) = \exp(-x^2)$ *is positive definite on* $\mathbb{R}^r$, *for all* $r \geq 1$.

Schoenberg showed this using Bochner's theorem on $\mathbb{R}^r$, and the fact that the Gaussian function is its own Fourier transform (up to constants).

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Alternate proof (K.):
(1) An observation of Gantmakher and Krein: *Generalized Vandermonde matrices are totally positive*. In other words, if $0 < y_1 < \cdots < y_n$ and $x_1 < \cdots < x_n$ in $\mathbb{R}$, then $\det(y_j^{x_k})_{j,k=1}^n$ is positive.

(2) A result by Pólya: *The Gaussian kernel is positive definite on $\mathbb{R}^1$.* Indeed,

$$\left(\exp(-(x_j - x_k)^2)\right)_{j,k=1}^n = \operatorname{diag}(e^{-x_j^2}) \times \left(\exp(2x_j x_k)\right)_{j,k=1}^n \times \operatorname{diag}(e^{-x_k^2}).$$

(3) A result of Schur: *The Schur product theorem* implies the result for $\mathbb{R}^r$. $\square$

Spherical embeddings, via positive definite maps

In fact, Schoenberg [*Trans. Amer. Math. Soc.* 1938] showed: Euclidean spaces $\mathbb{R}^r$, or their direct limit $\mathbb{R}^\infty = \ell^2(\mathbb{N})$ (called *Hilbert space* by Schoenberg) are characterized by the property that the maps

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What about distinguished subsets of $\mathbb{R}^r$ or of $\mathbb{R}^\infty$? Can one find similar families of functions for them?

Schoenberg explored this question for **spheres**: $S^{r-1} \subset \mathbb{R}^r$ and $S^\infty \subset \mathbb{R}^\infty$. It turns out, the characterization now involves a *single* function!

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This is the cosine.

Spherical embeddings via cosines

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:

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

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

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

and this is a Gram matrix, so positive semidefinite.

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

A finite metric space (X,d) embeds isometrically into the Hilbert sphere S^∞ if and only if (a) $\cos(x)$ is positive definite on X, and (b) $\operatorname{diam} X \leq \pi$.

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- For more on the history/overview: survey article by Belton–Guillot–K.–Putinar, 2019.
- For full proofs of these and below results: lecture notes (K.), 2019.

Positive definite functions on spheres

These results characterize $\mathbb{R}^\infty$ and S^∞ in terms of positive definite functions.

At the same time (1930s), Bochner proved his famous theorem classifying all positive definite functions on Euclidean space [*Math. Ann.* 1933]. Simultaneously generalized in 1940 by Weil, Povzner, and Raikov to arbitrary locally compact abelian groups.

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After understanding that $\cos(\cdot)$ is positive definite on S^∞, Schoenberg was interested in classifying *positive definite functions on spheres*.
This is the main result – and the title! – of his 1942 paper:

Positive definite functions on spheres (cont.)

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

Suppose $f : [-1,1] \to \mathbb{R}$ *is continuous. Then* $f(\cos \cdot)$ *is positive definite on the Hilbert sphere* $S^\infty \subset \mathbb{R}^\infty = \ell^2(\mathbb{N})$ *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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Freeing this result from the sphere context, one obtains Schoenberg's theorem on entrywise positivity preservers: *If* f *is continuous, then*
$f[-] : \mathbb{P}_n \to \mathbb{P}_n$ *for all* $n \quad \iff \quad f$ *is a power series with all coefficients* ≥ 0.

Toeplitz and Hankel matrices

- Rudin (1959) strengthened Schoenberg's theorem to *all functions*.

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
  $$\mathbf{s}(\mu) := (s_k(\mu))_{k \geqslant 0}, \qquad \text{where } s_k(\mu) := \int_{\mathbb{R}} x^k \, d\mu,$$
  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 $I = (-\rho, \rho)$.

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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:

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- Natural refinement of original problem of Schoenberg.
- Known for $n = 2$ (Vasudeva [*Indian J. Pure Appl. Math.* 1979]). **Open** when $n \geq 3$.

To date, there is essentially *only one result* for fixed $n \geq 3$, due to Charles Loewner. It appeared in the [*Trans. Amer. Math. Soc.* 1969] paper of his student, Roger A. Horn:

Theorem (Loewner/Horn, 1969)

Suppose $I = (0, \infty)$*, and a continuous function* $f : I \to \mathbb{R}$ *entrywise preserves positivity on* $\mathbb{P}_n(I)$ *for fixed* $n \geq 3$*. Then* $f \in C^{n-3}(I)$*, and*

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

If $n \geq 1$ *and* $f \in C^{n-1}(I)$ *then this holds for all* $0 \leq k \leq n-1$.

Horn's 1969 paper

We observe that if the quadratic form $\langle x, Ax\rangle$ assumes only real values for $x \in \boldsymbol{C}^n$, then A is necessarily Hermitian ($A = A^*$). In particular, if $A \succeq 0$, then A must be Hermitian. All functions and products of matrices will be taken in the pointwise sense, i.e., $f(A) \equiv (f(a_{ij}))_{i,j=1}^n$ and $A \circ B \equiv (a_{ij}b_{ij})_{i,j=1}^n$, and we recall the *Schur product theorem* (vid. [14, p. 14], or [1, p. 94]):

THEOREM 1.1. *If $A \succeq 0$ and $B \succeq 0$, then $A \circ B \succeq 0$. Furthermore, if $A \gg 0$ and $B \gg 0$, then $A \circ B \gg 0$.*

This theorem shows that if $f(t) \equiv t^n$, $n = 1, 2, \ldots$, then $f(A) \succeq 0$ whenever $A \succeq 0$, so it is not unnatural to ask what other functions share this property of leaving invariant the convex cone of nonnegative quadratic forms. C. Loewner has found (oral communication) certain necessary conditions, and we have the

THEOREM 1.2. *Let $f \in C(\boldsymbol{R}^+)$, let $n \geqq 1$ be an integer, and suppose that $f(A) \succeq 0$ for every $n \times n$ matrix A such that $A > 0$ and $A \succeq 0$. Then $f \in C^{n-3}(\boldsymbol{R}^+)$, $f^{(k)}(x) \geqq 0$ for all $x \in \boldsymbol{R}^+$ and all $k = 0, 1, 2, \ldots, n-3$, and $f^{(n-3)}$ is a convex and monotone nondecreasing function on $\boldsymbol{R}^+$. In particular, if $f \in C^{n-1}(\boldsymbol{R}^+)$, then $f^{(k)}(x) \geqq 0$ for all $x \in \boldsymbol{R}^+$ and all $k = 0, 1, 2, \ldots, n-1$.*

Stronger form of the Loewner/Horn result

- Define a *special Hankel matrix* to be $((a + tx^{j+k}))_{j,k=0}^{n-1}$, where $a, t, x \geq 0$ and $n \geq 1$. (This is a rank ≤ 2 Hankel psd matrix.)

Similar to Rudin's strengthening of Schoenberg's theorem, we now weaken the hypotheses of Loewner's theorem:

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

Let $0 < \rho \leq \infty$ and set $I = (0, \rho)$. Given any function $f : I \to \mathbb{R}$, suppose $f[-]$ preserves positivity on $\mathbb{P}_2(I)$ and the special Hankel matrices in $\mathbb{P}_n(I)$ for fixed $n \geq 3$. Then the same conclusions as above hold: $f \in C^{n-3}(I)$, and

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

If $n \geq 1$ and $f \in C^{n-1}(I)$ then this holds for all $0 \leq k \leq n-1$.

The proof for smooth functions: Loewner's calculation

Suppose f **smooth**, entrywise preserves positivity on $\mathbb{P}_n((0,\rho))$. Why are $f, f', \dots, f^{(n-1)}$ non-negative on $(0,\rho)$?

- Proceed by induction on n; for $n = 1$ there is nothing to prove.

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- Now define $f_\epsilon(x) := f(x) + \epsilon x^{n-1}$ for $\epsilon > 0$. Then f_ϵ satisfies the hypotheses, and $f_\epsilon, f'_\epsilon, \dots, f_\epsilon^{(n-2)} > 0$ on I.

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$$\Delta(t) := \det f_\epsilon[A(a,x,t)] \geq 0, \quad \text{so } \frac{\Delta(t)}{t^N} \geq 0, \quad \text{where } N = \binom{n}{2}.$$

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- Now Loewner computed:

$$0 = \Delta(0) = \Delta'(0) = \cdots = \Delta^{(N-1)}(0),$$

whence by L'Hopital's Rule,

$$0 \leq \lim_{t \to 0^+} \frac{\Delta(t)}{t^N} = \lim_{t \to 0^+} \frac{\Delta'(t)}{N t^{N-1}} = \cdots = \lim_{t \to 0^+} \frac{\Delta^{(N)}(t)}{N!} = \frac{\Delta^{(N)}(0)}{N!}.$$

Smooth functions: Loewner's calculation (cont.)

But now Loewner also computed:

$$\Delta^{(N)}(0) = \binom{N}{0, 1, \ldots, n-1} \prod_{0 \leq j < k \leq n-1} (x^j - x^k)^2 \cdot f_\epsilon(a) f'_\epsilon(a) \cdots f_\epsilon^{(n-1)}(a).$$

Hence $f_\epsilon^{(n-1)}(a) \geq 0$ for all $\epsilon > 0$, so $f^{(n-1)}(a) \geq 0$. $\square$

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- Loewner's computation can be made completely algebraic, using the derivation ∂_t over any unital commutative ring. (K., 2018 preprint.) This leads to novel symmetric function identities *arising out of analysis*.
- This line of attack is useful in classifying the entrywise polynomials preserving positivity. (Belton–Guillot–K.–Putinar, [*Adv. in Math.* 2016], K.–Tao, 2017 preprint).

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- 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 $(a_{ij}) \geq 0$* of order n with elements $a_{ij} \in (a,b)$. What properties must f have in order that the matrices $(f(a_{ij})) \geq 0$.

I found ~~as necessary conditions: $f(t) \geq 0$, $f'(t)$~~ that if f 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 $\alpha \in (a,b)$, $\omega \geq 0$ and the α_i arbitrary.
Then $(f(a_{ij})) \geq 0$ for sufficiently small ω and hence the determinant $\Delta(\omega) = \det(f(a_{ij})) \geq 0$.
The first term in the Taylor expansion of $\Delta(\omega)$ at $\omega = 0$ is $f(\alpha) f'(\alpha) \cdots f^{(n-1)}(\alpha) \cdot \left(\prod (\alpha_i - \alpha_\beta)\right)^2$ and hence
$f(\alpha) f'(\alpha) \cdots f^{(n-1)}(\alpha) \geq 0$, from which one easily derives that (C) must hold.

Corollary: Schoenberg–Rudin theorem on $(0, \infty)$

- Using mollifiers, pass from smooth functions to all continuous functions.
- By a result of Ostrowski (1925), every preserver must be continuous. $\square$

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

Suppose $0 < \rho \leq \infty$ *and* $I = (0, \rho)$*. The following are equivalent for any function* $f : I \to \mathbb{R}$*:*

1. $f[A] \in \mathbb{P}_n$ *for all* $A \in \mathbb{P}_n(I)$ *and all* n*.*
2. $f[-]$ *preserves positivity on special Hankel matrices in* $\mathbb{P}_n(I)$, $\forall n \geq 1$*.*
3. f *is analytic on* I *and has nonnegative Maclaurin coefficients. 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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Sketch: By the stronger Loewner theorem, f is smooth and all derivatives are ≥ 0 on I. Extend f continuously to 0^+, then apply Bernstein's theorem: such an f can be extended analytically to the complex disc $D(0, \rho)$. □

Stronger Schoenberg theorem: outline of proof

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Step 3: Use three Ms (Mollifiers, Montel, Morera) to pass from smooth functions to continuous functions. $\square$

Preservers in fixed dimensions: polynomials

- Recall: classifying the entrywise preservers of $\mathbb{P}_N$ for fixed $N \geq 3$ is open to date. For $\bigcup_N \mathbb{P}_N$ it was $\sum_{k \geq 0} c_k x^k$ with $c_k \geq 0$.
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  (a) we found the first such examples,
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- The proofs use representation-theoretic tools: Schur polynomials, Harish-Chandra–Itzykson–Zuber integrals, Gelfand–Tsetlin patterns, and Schur positivity.
- It is the **mixing of positivity and representation theory / algebra** that led us to the first examples and characterization results.

Schur polynomials

Key ingredient in computations – representation theory / symmetric functions:

(Cauchy's definition:) Given a non-increasing n-tuple $m_{n-1} \geq m_{n-2} \geq \cdots \geq m_0 \geq 0$, the corresponding **Schur polynomial** equals the integer-coefficient polynomial

$$s_{(m_{n-1},\dots,m_0)}(u_1,\dots,u_n) := \frac{\det(u_j^{m_{k-1}})}{\det(u_j^{k-1})}.$$

Note that the denominator is precisely the Vandermonde determinant $V(\mathbf{u})$.

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Example: If $n = 2$ and $\mathbf{m} = (k > l)$, then

$$s_{\mathbf{m}}(u_1,u_2) = \frac{u_1^k u_2^l - u_1^l u_2^k}{u_1 - u_2} = (u_1 u_2)^l (u_1^{k-l-1} + u_1^{k-l-2} u_2 + \cdots + u_2^{k-l-1}).$$

Basis of homogeneous symmetric polynomials in $u_1,\dots,u_n$.

From positivity and algebra, to inequalities

Treat Schur polynomials as **functions** on the positive orthant:

Let $s_{\mathbf{m}}(\mathbf{u}) := \det(u_i^{m_j}) / \det(u_i^{j-1})$ be the Schur polynomial corresponding to $\mathbf{m}$ (abusing notation). Using deep results in representation theory, (K.–Tao:)

$$\frac{s_{\mathbf{m}}(\mathbf{u})}{s_{\mathbf{n}}(\mathbf{u})}$$

is coordinatewise nondecreasing for $\mathbf{u}$ in the positive orthant $(0, \infty)^N$, whenever $\mathbf{m} \geq \mathbf{n}$ coordinatewise.

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Using this (with the H-C–I–Z integral) yields a **novel characterization of weak majorization** for real tuples:

Theorem (K.–Tao, 2017)

Suppose $\mathbf{m}, \mathbf{n}$ *are* N*-tuples of pairwise distinct non-negative real powers. Then*

$$\frac{|\det(\mathbf{u}^{\circ m_0} | \cdots | \mathbf{u}^{\circ m_{N-1}})|}{|V(\mathbf{m})|} \geq \frac{|\det(\mathbf{u}^{\circ n_0} | \cdots | \mathbf{u}^{\circ n_{N-1}})|}{|V(\mathbf{n})|}, \qquad \forall \mathbf{u} \in [1, \infty)^N,$$

if and only if $\mathbf{m}$ *weakly majorizes* $\mathbf{n}$.

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