Pólya frequency sequences and functions

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Applied Matrix Positivity – II

1. Totally positive matrices and Pólya frequency sequences

Totally positive/nonnegative matrices

Definition. A rectangular matrix is *totally positive (TP)* if all minors are positive. (Similarly, totally nonnegative (TN).)

Thus all entries > 0, all 2×2 minors > 0, $\ldots$

These matrices occur widely in mathematics:

Totally positive matrices in mathematics

TP and TN matrices occur in

- analysis and differential equations (Aissen, Edrei, Schoenberg, Pólya, Loewner, Whitney)
- probability and statistics (Efron, Karlin, Pitman, Proschan, Rinott)
- interpolation theory and splines (Curry, Schoenberg)
- Gabor analysis (Gröchenig, Romero, Stöckler)
- interacting particle systems (Gantmacher, Krein)
- matrix theory (Ando, Cryer, Fallat, Garloff, Holtz, Johnson, Pinkus, Sokal)

- representation theory and the Grassmannian (Lusztig, Postnikov, Lam)
- cluster algebras (Berenstein, Fomin, Zelevinsky)
- integrable systems (Kodama, Williams)
- quadratic algebras (Borger, Davydov, Grinberg, Hô Hai)
- combinatorics (Branden, Brenti, Skandera, Sturmfels, Wagner, . . .)

$\vdots$

Examples of TP/TN matrices

1. Generalized Vandermonde matrices are TP: if $0 < x_1 < \cdots < x_n$ and $y_1 < y_2 < \cdots < y_n$ are real, then

$$\det(x_j^{y_k})_{j,k=1}^n > 0.$$

2. (Pólya:) The *Gaussian kernel* is TP: given $\sigma > 0$ and scalars

$$x_1 < x_2 < \cdots < x_n, \qquad y_1 < y_2 < \cdots < y_n,$$

the matrix $G[\mathbf{x};\mathbf{y}] := (e^{-\sigma(x_j - y_k)^2})_{j,k=1}^n$ is TP.

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3. The lower-triangular matrix $A = (\mathbf{1}_{j \geq k})_{j,k=1}^n$ is TN.
4. *Submatrices* and *Limits* of TN matrices are TN.
5. *Products* of TN/TP matrices are TN/TP, by the Cauchy–Binet formula.

Pólya frequency sequences

A real sequence $(a_n)_{n\in\mathbb{Z}}$ is a *Pólya frequency sequence* if for any integers

$$l_1 < l_2 < \cdots < l_n, \qquad m_1 < m_2 < \cdots < m_n,$$

the determinant $\det(a_{l_j - m_k})_{j,k=1}^n \geq 0$.

In other words, these are semi-infinite Toeplitz matrices

$$\begin{pmatrix} a_0 & a_{-1} & a_{-2} & a_{-3} & \cdots \\ a_1 & a_0 & a_{-1} & a_{-2} & \cdots \\ a_2 & a_1 & a_0 & a_{-1} & \cdots \\ a_3 & a_2 & a_1 & a_0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

which are totally nonnegative (TN).

Generating functions of Pólya frequency sequences

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Suppose $\mathbf{a} = (\dots, 0, 0, a_0, a_1, a_2, a_3, \dots)$ is one-sided. Its *generating function* is

$$\Psi_{\mathbf{a}}(s) := a_0 + a_1 s + a_2 s^2 + a_3 s^3 + \cdots, \qquad a_0 \neq 0.$$

Now if $\mathbf{a}, \mathbf{b}$ are one-sided PF sequences, then their Toeplitz "matrices" are TN:

$$T_{\mathbf{a}} := \begin{pmatrix} a_0 & 0 & 0 & \cdots \\ a_1 & a_0 & 0 & \cdots \\ a_2 & a_1 & a_0 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \qquad T_{\mathbf{b}} := \begin{pmatrix} b_0 & 0 & 0 & \cdots \\ b_1 & b_0 & 0 & \cdots \\ b_2 & b_1 & b_0 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

By the Cauchy–Binet formula, so also is $T_{\mathbf{a}} T_{\mathbf{b}} \rightsquigarrow$ **(Miracle 1?)** Toeplitz matrix.

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(Miracle 2?) This product matrix corresponds to the coefficients of the power series $\Psi_{\mathbf{a}}(s)\Psi_{\mathbf{b}}(s)$! I.e., $\mathcal{L} : T_{\mathbf{a}} \mapsto \Psi_{\mathbf{a}}(s)$ is an $\mathbb{R}$-*algebra* map.

Finite Pólya frequency sequences – and real-rootedness

"Atomic" **finite** PF sequences:

- The sequence $(\dots, 0, 0, a_0, 0, 0, \dots)$ and $(\dots, 0, 0, 1, \alpha, 0, 0, \dots)$ are PF sequences if $a_0, \alpha > 0$.
  Indeed, every "square submatrix" drawn from these sequences either has a zero row/column, or is triangular with positive diagonal entries.

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- The "atom" $(\dots, 0, 0, 1, \alpha, 0, 0, \dots)$ corresponds to $\Psi_{\mathbf{a}}(x) = 1 + \alpha x$.
- By previous slide, $a_0(1 + \alpha_1 x)(1 + \alpha_2 x) \cdots (1 + \alpha_m x)$ generates a PF sequence $\mathbf{a}_m$, when all $\alpha_j > 0$.

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- By previous slide, $a_0(1 + \alpha_1 x)(1 + \alpha_2 x) \cdots (1 + \alpha_m x)$ generates a PF sequence $\mathbf{a}_m$, when all $\alpha_j > 0$. In fact, these are *all finite PF sequences:*

Theorem (Aissen–Schoenberg–Whitney and Edrei, *J. d'Analyse Math.*, 1950s; and Schoenberg, *Ann. of Math.*, 1955)

Suppose $a_0, \dots, a_m > 0$. The following are equivalent.

1. $\mathbf{a} = (\dots, 0, 0, a_0, \dots, a_m, 0, 0, \dots)$ *is a PF sequence.*
2. *The generating function $\Psi_{\mathbf{a}}(x)$ has m negative real roots (i.e., the above form).*
3. *The generating function $\Psi_{\mathbf{a}}(x)$ has m real roots.*

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$$\Psi_{\mathbf{a}_1}(x) = 1 + x + x^2 + \cdots = \frac{1}{1-x}.$$

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Claim: The function $\mathbf{a}_\beta := (\dots, 0, 0, 1, \beta, \beta^2, \dots)$ is a PF sequence for $\beta > 0$.

Proof: Given increasing tuples of integers $(l_j), (m_k)$ for $1 \leq j, k \leq n$,

$$((\mathbf{a}_\beta)_{l_j - m_k}) = \mathrm{diag}(\beta^{l_j})_{j=1}^n \cdot (\mathbf{1}_{l_j \geq m_k})_{j,k=1}^n \cdot \mathrm{diag}(\beta^{-m_k})_{k=1}^n,$$

and this has a nonnegative determinant since $\mathbf{a}_1$ is PF. $\square$

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- Therefore $(1 - \beta x)^{-1}$ is a PF sequence for $\beta > 0$.

Limits: If $\mathbf{a}_m$ are PF sequences, converging "pointwise" to $\mathbf{a}$, then $\mathbf{a}$ is a PF sequence.

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- *Example:* Since $(1 + \delta x/m)^m$ generates a PF sequence for all $m \geq 1$, so does $e^{\delta x}$. (E.g. **Fekete:** $(\dots, 0, 0, 1, \frac{\delta}{1!}, \frac{\delta^2}{2!}, \dots)$ is a PF sequence.)

Infinite one-sided Pólya frequency sequences (cont.)

- More examples: if $\alpha_j, \beta_j \geq 0$ for all $j \geq 0$ are summable, then

$$\prod_{j=1}^{\infty} (1 + \alpha_j x), \qquad \prod_{j=1}^{\infty} (1 - \beta_j x)^{-1}$$

  both generate PF sequences.

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- Hence so does their product:

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Remarkably, these are *all* of the PF sequences!

Theorem (Aissen–Schoenberg–Whitney and Edrei, *J. d'Analyse Math.*, 1950s)

A one-sided sequence $\mathbf{a} = (\dots, 0, 0, a_0 = 1, a_1, \dots)$ *is a PF sequence, if and only if it is of the above form.*

(Uses Hadamard's thesis (1892) and Nevanlinna's refinement (1929) of Picard's theorem.)

From Pólya–Schur multipliers to Ramanujan graphs

What if $\Psi_{\mathbf{a}}(x)$ is an entire function? It must be $e^{\delta x} \prod_{j \geq 1}(1 + \alpha_j x)$.

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An entire function $\Psi(x) = \sum_{n \geq 0} a_n x^n$ with $\Psi(0) = 1$ generates a one-sided PF sequence,
if and only if $\Psi(x)$ is in the first Laguerre–Pólya class $\mathcal{LP}_1$,
if and only if the sequence $n! a_n$ is a multiplier sequence of the first kind.

In other words, if $\sum_{j \geq 0} c_j x^j$ is a real-rooted *polynomial*, so is $\sum_{j \geq 0} j! a_j c_j x^j$.

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- This circle of ideas – and classification of Pólya–Schur type multiplier sequences – has found far-reaching generalizations in work of Brändén with Borcea (late 2000s) and others.
- Taken forward by Marcus–Spielman–Srivastava (2010s):
    - Kadison–Singer conjecture.
    - Existence of bipartite Ramanujan (expander) graphs of every degree and every order.

2. Pólya frequency functions

Toeplitz TN kernels

Above: the Gaussian kernel $K_-(x,y) := \exp(-(x-y)^2)$ is TP.
More generally, a *totally nonnegative (TN) function* is $\Lambda : \mathbb{R} \to \mathbb{R}$ such that its Toeplitz kernel is TN:

$$T_\Lambda(x,y) := \Lambda(x-y), \qquad x,y \in \mathbb{R}.$$

"Representative" examples:

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4. $\Lambda(x) = \mathbf{1}_{x \geq 0}$. (Can be verified to be TN by explicit computation.)

Note: the last two examples are not integrable functions.

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Pólya Frequency Functions (PFFs) have a beautiful structure theory,[1] developed by Schoenberg and others. They connect to real function theory, PDEs, approximation theory (splines), Gabor analysis, ...

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Consequences of the definition: All Pólya frequency functions Λ are

- nonzero on a semi-axis, or nonzero on $\mathbb{R}$;
- continuous except at most at one point a (where $\Lambda(a^+), \Lambda(a^-)$ exist).
- All TN functions are an exponential $e^{ax+b} \times$ a Pólya frequency function.

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4. *Limits* of PF functions (if nonzero and integrable) are PF functions.

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- In the matrix/"discrete" case: given two matrices $A_{m\times n}$ and $B_{n\times p}$ which are both TN, *their product is also TN* – by Cauchy–Binet.

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- The Cauchy–Binet formula has a *continuous* version $\rightsquigarrow$ *Basic composition formula* (Pólya–Szegő). This implies:

Corollary: *If* $\Lambda_1, \Lambda_2 : \mathbb{R} \to [0,\infty)$ *are integrable Pólya frequency functions, then so is their convolution*

$$(\Lambda_1 * \Lambda_2)(x) := \int_{\mathbb{R}} \Lambda_1(t)\Lambda_2(x-t)\ dt, \qquad x \in \mathbb{R}.$$

This will help construct additional examples of Pólya frequency functions.

Pólya frequency functions and Laplace transforms

The bilateral Laplace transform of a PF function Λ is

$$\mathcal{L}(\Lambda)(s) := \int_{\mathbb{R}} e^{-sx} \Lambda(x) \, dx, \qquad s \in \mathbb{C}.$$

Fact: $\mathcal{L}$ is an algebra map: $\mathcal{L}(\Lambda_1 * \Lambda_2) = \mathcal{L}(\Lambda_1)\mathcal{L}(\Lambda_2)$!

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Now consider *one-sided* PF functions: $\varphi_a(x) := \frac{1}{a} e^{-x/a} \mathbf{1}_{x \geq 0} \rightsquigarrow$ Laplace transform $\mathcal{L}(\varphi_a)(s) = 1/(1+as)$.

- Let $a_j \geq 0$ with $\sum_{j=1}^\infty a_j < \infty$. Then for each n, the convolution $\varphi_{a_1} * \cdots * \varphi_{a_n}$ is a one-sided PF function (Hirschman–Widder density), with Laplace transform

$$\mathcal{L}(\varphi_{a_1} * \cdots * \varphi_{a_n})(s) = \frac{1}{\prod_{j=1}^n (1 + a_j s)}.$$

Laguerre–Pólya class and Schoenberg's results: I. One-sided

- Shifting the origin of $\varphi_{a_1} * \cdots * \varphi_{a_n}$ to $\delta \geq 0$ yields a one-sided PF function with Laplace transform $e^{-\delta s} / \prod_{j=1}^{n} (1 + a_j s)$.

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- Taking limits of PF functions gives a PF function $\rightsquigarrow$ a PF function with Laplace transform $e^{-\delta s} / \prod_{j=1}^{\infty}(1 + a_j s)$.
- Its reciprocal is the analytic (entire) function $e^{\delta s} \prod_{j=1}^{\infty}(1 + a_j s)$.

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Remarkably, *every* one-sided PF function shares this property:

Theorem (Schoenberg, *J. d'Analyse Math.*, 1951)

A function $\Lambda : \mathbb{R} \to \mathbb{R}$, continuous on $(0, \infty)$ and with $\int_{\mathbb{R}} \Lambda(x)\ dx = 1$, is a one-sided PF function vanishing on $(-\infty, 0)$, if and only if

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This is the limit of the polynomials $(1 + \dfrac{\delta s}{n})^n \displaystyle\prod_{j=1}^{n} (1 + a_j s)$, with negative roots.

Laguerre–Pólya class and Schoenberg's results: II. Two-sided

Similarly, using the Gaussian kernel and "oppositely directed" variants of $e^{-x}\mathbf{1}_{x\geq 0}$, Schoenberg proved:

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where $\gamma \geq 0$ and $\delta, a_j \in \mathbb{R}$ are such that $0 < \gamma + \sum_j a_j^2 < \infty$.

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These two classes of entire functions were very well-studied by Laguerre, Pólya, and Schur in the early 20th century:

1. The first class of entire functions are limits – uniform on compact sets – of real polynomials with real non-positive roots. ("One-sided")

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2. The second class $\rightsquigarrow$ limits of real polynomials with real roots.

$\rightsquigarrow$ *Laguerre–Pólya functions* (allowing for a factor of cs^m, $c \geq 0, m \in \mathbb{Z}^{\geq 0}$).

From the Laguerre–Pólya class to the Riemann Hypothesis

Pólya initiated the study of functions $\Lambda(t)$ such that $\mathcal{L}(\Lambda)(s)$ has only pure imaginary zeros. His work alludes to the following result:

Theorem (Pólya, *J. reine angew. Math.*, 1927)

The following statements are equivalent:

1. *The Riemann Xi-function* $\Xi(s) = \xi(1/2 + iz)$ *is in the Laguerre–Pólya class, where* $\xi(s) := \binom{s}{2}\pi^{-s/2}\Gamma(s/2)\zeta(s)$.
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Combined with Schoenberg's result above, this yields:

Theorem (Gröchenig, *Appl. Numer. Harm. Anal.*, 2020)

Let $\xi(s) = \binom{s}{2}\pi^{-s/2}\Gamma(s/2)\zeta(s)$ *be the Riemann xi-function. If*

$$\Lambda(x) := \int_{\mathbb{R}} \xi(u + 1/2)^{-1} e^{-ixu} \, du$$

is a Pólya frequency function, then the Riemann Hypothesis is true.

The Laguerre–Pólya class is thus a distinguished one in several areas.

The Riemann Hypothesis

For the same reason, Pólya frequency sequences connect to number theory:

Theorem (Katkova, *Comput. Meth. Funct. Th.*, 2007)

Let $\xi(s) = \binom{s}{2}\pi^{-s/2}\Gamma(s/2)\zeta(s)$ *be the Riemann xi-function. If*

$$\xi_1(s) := \xi(1/2 + \sqrt{s})$$

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Katkova proved that ξ_1 is PF of order at least 43, and is "asymptotically PF" of all orders.

Pólya frequency functions are probability densities

Reformulation via probability:

- Traditionally: "frequency functions" $\longleftrightarrow$ *densities* of (continuous) random variables.
- Convolutions of these $\longleftrightarrow$ adding the (independent) random variables.

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(1) One-sided variant:
Pólya frequency functions vanishing on $(-\infty, 0)$ and positive on $(0, \infty)$ are precisely the densities of $\sum_{j \geq 1} \alpha_j X_j$,
where $\alpha_j \geq 0$ are summable and X_j are i.i.d. $\exp(1)$ variables (these are TN).

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For Pólya frequency functions not vanishing on a semi-axis, one simply needs to
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(3) "General" PF functions: are the above, up to shift of origin and scale.

3. Total positivity preservers: Joint with Belton, Guillot, Putinar

1. Preservers of 2×2 TN matrices

Question (Deift, 2017): Which transforms preserve total positivity?

Setting 1: *Preservers of* 2×2 *TN matrices*

Fix $x, y \geq 0$, and let $A = \begin{pmatrix} x & xy \\ 1 & y \end{pmatrix}, \quad B = \begin{pmatrix} xy & x \\ y & 1 \end{pmatrix}$. These are TN.

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Applying $0 \leq \det F[-]$, we get:

$$F(x)F(y) \geq F(xy)F(1), \qquad F(xy)F(1) \geq F(x)F(y),$$

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$$G(xy) = G(x)G(y).$$

This gives that $G(x)$ is either a power function x^α $(\alpha \geq 0)$ or the Heaviside function $\mathbf{1}_{x>0}$. (Conversely, these are preservers.) $\square$

2. Preservers of TN kernels of order 2

Setting 2: *Preservers of TN kernels of order 2*

- Can define TN of "finite order":

  Let X, Y be nonempty totally ordered sets. A kernel $K : X \times Y \to \mathbb{R}$ is totally nonnegative of order k, denoted TN$^{(k)}_{X \times Y}$, if all minors of $K(\cdot, \cdot)$ of size $\leq k$ are nonnegative.

- What are the preservers of such kernels? I.e., if K is TN$^{(2)}_{X \times Y}$, so is $F \circ K$.

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Theorem (Belton–Guillot–K.–Putinar, *J. d'Analyse Math.*, 2023)

For all X, Y of size ≥ 2, the transform $F \circ -$ preserves the class of TN$^{(2)}_{X \times Y}$ kernels if and only if $F(x) = cx^{\alpha}$ for some $c, \alpha \geq 0$, or $F(x) = c\mathbf{1}_{x>0}$ for some $c > 0$.

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Proof: These functions are all preservers. Conversely, act by any preserver on every 2×2 TN matrix *padded on $X \times Y$ by zeros.* $\square$

3. Preservers of 2×2 TP matrices

Setting 3: *Preservers of 2×2 TP matrices*

Here we use *Whitney's density theorem*: $\mathrm{TP}_{m \times n}$ matrices are dense in $\mathrm{TN}_{m \times n}$ matrices. Thus,

1. First prove F is increasing, by applying $F[-]$ to $\begin{pmatrix} x & y \\ y & x \end{pmatrix}$ for $x > y > 0$.

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3. Hence by Whitney density, now $F[-]$ preserves 2×2 TN matrices.

Thus, F is as above; and cannot be constant on an interval. So $F(x) = x^\alpha$ for some $\alpha > 0$. (Conversely, all such powers are preservers.) $\square$

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Setting 4: *Preservers of TP kernels of order 2*

- Can define TP of "finite order" similar to the TN version.
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For all X, Y of size ≥ 2, the transform $F \circ -$ preserves the class of $\mathrm{TP}^{(2)}_{X \times Y}$ kernels, if and only if $F(x) = cx^\alpha$ for some $c, \alpha > 0$.

Note: now we cannot use "padding by zeros" (since the kernels are TP).

4. Preservers of TP kernels of order 2 (cont.)

Thus we make two observations [B–G–K.–P, 2023] :

1. If there exist $\mathrm{TP}^{(2)}$ (or TP) kernels on $X \times Y$, then how big can such totally ordered sets X, Y be?

   Answer: *They must embed into* $(0, \infty)$*!*

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2. Can we "embed" every 2×2 TP matrix into a TP$^{(2)}$ kernel on $X \times Y$? Or more ambitiously, into a TP kernel on arbitrary X, Y?
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   - Unlike the TN-case, we cannot pad by zeros.
   - Nevertheless, the answer is: *Yes!* Because. . .

4. Preservers of TP kernels of order 2 (cont.)

. . . we come back full circle – to our very first example of TP matrices:

Lemma (Belton–Guillot–K.–Putinar, *J. d'Analyse Math.*, 2023)

Every 2×2 TP matrix is – up to rescaling by some $c > 0$ – a generalized Vandermonde matrix.

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Therefore, any preserver in $\mathrm{TP}^{(2)}_{X \times Y}$ must preserve 2×2 TP matrices. By above, it is a power function. (Conversely, all powers are $\mathrm{TP}^{(2)}$ preservers.) $\square$

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In fact, in our paper we *classified the preservers in $TP^{(k)}_{X \times Y}$, for all integers $1 \leq k \leq \infty$, and all nonempty partially ordered sets X, Y.*

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Question: If $\Lambda(x)$ is a PF function, for which $F : [0, \infty) \to [0, \infty)$ is $F \circ \Lambda$ also one?

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- Choose $\Lambda_1(x) =$ exponential density $=$ PF function. First show $F \circ \Lambda_1$ is also discontinuous, so by Schoenberg's classification again an exp-density:

$$F \circ \mathbf{1}_{x \geq 0} e^{-x} = \mathbf{1}_{x \geq 0} c e^{-b_0 x}, \qquad c, b_0 > 0 \quad \text{(except at 0)}.$$

- So $F(t) = ct^{b_0}$ for $0 < t < t_0$. Now show that $F(t) = ct^{b_0}$ for all $t > 0$.

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- Apply $F \circ -$ to the PF function $\Lambda_2(x) := x \cdot \mathbf{1}_{x \geq 0} e^{-x} = (\Lambda_1 * \Lambda_1)(x)$ = density of sum of two i.i.d. exp-variables $\rightsquigarrow$
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- Applying F to $\Lambda_0(x) = 2e^{-|x|} - e^{-2|x|}$, conclude: $b_0 = 1$. In summary:

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$$F \circ \mathbf{1}_{x \geq 0} e^{-x} = \mathbf{1}_{x \geq 0} c e^{-b_0 x}, \qquad c, b_0 > 0 \quad \text{(except at 0)}.$$

- So $F(t) = ct^{b_0}$ for $0 < t < t_0$. Now show that $F(t) = ct^{b_0}$ for all $t > 0$.
- Apply $F \circ -$ to the PF function $\Lambda_2(x) := x \cdot \mathbf{1}_{x \geq 0} e^{-x} = (\Lambda_1 * \Lambda_1)(x)$ $=$ density of sum of two i.i.d. exp-variables $\rightsquigarrow$
  Also a PF function, so $G(s) := 1/\mathcal{L}(F \circ \Lambda_2)(s)$ is in the Laguerre–Pólya class. But $G(s) = (s + b_0)^{1+b_0}/\Gamma(b_0 + 1)$, so $b_0 > 0$ must be an integer.
- Applying F to $\Lambda_0(x) = 2e^{-|x|} - e^{-2|x|}$, conclude: $b_0 = 1$. In summary:

Theorem (Belton–Guillot–K.–Putinar, *J. d'Analyse Math.*, 2023)

The transform $F \circ -$ preserves the class of (one-sided) Pólya frequency functions, if and only if $F(x) = cx$ for some $c > 0$.

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