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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What kind of functions have this property?
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Main reference:
A. Belton, D. Guillot, A. Khare, M. Putinar,  
*Matrix positivity preservers in fixed dimension. I*,  
Outline

1. Motivation

2. Functions preserving positivity
   - Schoenberg’s theorem
   - Horn’s necessary condition

3. Results in fixed dimension
   - Polynomials preserving positivity
   - Main characterization
   - Sketch of proof: Schur polynomials

4. Structured matrices
   - Hankel matrices
   - Real powers
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).
- Functions operating on Fourier transforms (see e.g. Helson, Kahane, Katznelson, and Rudin, Acta Math. 1959).
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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).
Covariance matrices

$$\Sigma = (\sigma_{j,k})_{j,k=1}^p.$$  
- Random vector: $ (X_1, \ldots, X_p) 
  \sigma_{j,k} = \text{Cov}(X_j, X_k) 
  = E((X_j - E(X_j))(X_k - E(X_k)))$$

- Estimation: $x_1, \ldots, x_n \in \mathbb{R}^p$.

- Sample covariance matrix
  $$S = \frac{1}{n-1} \sum_{j=1}^{n} (x_j - \bar{x})(x_j - \bar{x})^T, \quad \bar{x} = \frac{1}{n} \sum_{j=1}^{n} x_j.$$  

Pancaldi et al., 2010.


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- Modern approach via compressed sensing (Daubechies, Donoho, Tao, Candes).
- Uses convex optimization to obtain sparse estimates (of \(\Sigma\) or \(\Sigma^{-1}\)) – e.g. \(\ell_1\) 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

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\text{True } \Sigma = \begin{pmatrix}
1 & 0.2 & 0 \\
0.2 & 1 & 0.9 \\
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\end{pmatrix}
\quad \quad
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- Thresholding is equivalent to applying the function

\[
f_\epsilon(x) = x \cdot 1_{|x|>\epsilon}
\]
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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**Problem:** For what functions $f : \mathbb{R} \rightarrow \mathbb{R}$, does $f[-]$ preserve $\mathbb{P}_N$?
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Can we find any such functions?
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*Proof 1:* $A \circ B$ is a principal submatrix of $A \otimes B$. 
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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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As a consequence of the Schur product theorem:

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**Important observation:** The above functions preserve positivity on \( \mathbb{P}_N \) regardless of the dimension \( N \), i.e., on \( \cup_{N \geq 1} \mathbb{P}_N \).
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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 \( c_k \geq 0 \).
Preserving positivity in fixed dimension

- Schoenberg’s result characterizes functions preserving positivity entrywise on $\bigcup_{N \geq 1} \mathbb{P}_N$. 
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In applications: dimension of the problem is known. Unnecessarily restrictive to preserve positivity in all dimensions.
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- **Open** when $N \geq 3$. 
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  For fixed $N \geq 3$, necessary condition known due to Horn (who attributes it to Loewner):

Fix $I = (0, \rho)$ for $0 < \rho \leq \infty$, and $f : I \rightarrow \mathbb{R}$ and $N \geq 3$.

Suppose $f[A] \in \mathbb{P}_N$ for $A = a1_{N\times N} + uu^T \in \mathbb{P}_N(I)$ with $a \in I$. 


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

Implies Schoenberg’s theorem on $(0, \rho)$ via a result of Bernstein: 

**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 $D(b - a)$. 

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

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

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

Implies Schoenberg’s theorem on $(0, \rho)$ via a result of Bernstein:

**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 $D(a, b - a)$. 
Obtaining a nice characterization of functions preserving positivity on $\mathbb{P}_N$ for a fixed $N$ has remained open for 76 years.
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Observation: By Horn’s theorem, if

$$f(x) = c_0 + c_1 x + \cdots + c_{N-1} x^{N-1} + c_N x^N$$

preserves positivity on $\mathbb{P}_N((0, \rho))$, then $c_0, \ldots, c_{N-1} \geq 0$. 

Can $c_N$ be negative? If so, how large can $c_N$ be? Sharp bound?
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Fix $\rho > 0$ and integers $M \geq N \geq 1$, and let

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Polynomials preserving positivity in fixed dimension

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Then the following are equivalent.

1. $f[-]$ preserves positivity on $\mathbb{P}_N(\overline{D}(0, \rho))$.
2. The coefficients $c_j$ satisfy either $c_0, \ldots, c_{N-1}, c' \geq 0$, 

\[
C(c; z^M; N, \rho) := N - 1 \sum_{j=0}^{N-1} (M - j - 1)^2 (N - j - 1) \rho^{M - j - 1} c_j.
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\]

3. \( f[\cdot] \) preserves positivity on rank-one matrices in \( \overline{P}_N((0, \rho)) \).
Consequences

1. Quantitative version of Schoenberg’s theorem in fixed dimension for polynomials.
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Can use the theorem to obtain bounds on the coefficients of analytic functions preserving positivity.
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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 $\epsilon_M$. 
Let $c_0, \ldots, c_{N-1}, c' \in \mathbb{R}$ and $M \geq N \geq 1$. If $f(z) = \sum_j c_j z^j + c' z^M$, TFAE:

1. $f[-]$ preserves positivity on $\mathbb{P}_N(D(0, \rho))$.
2. Either $c_j, c' \geq 0$ or $c_0, \ldots, c_{N-1} > 0 > c' \geq -\mathcal{C}(c; z^M; N, \rho)^{-1}$.
3. $f[-]$ preserves positivity on $\mathbb{P}_{1_N}^1((0, \rho))$.

Sketch of the Proof of (3) $\implies$ (2):
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Sketch of the proof of the main result

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Study the determinants of linear pencils

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p(t) = p_t[A] := \det \left( t(c_0 \mathbf{1}_{N \times N} + c_1 A + \cdots + c_{N-1} A^{\circ(N-1)}) - A^{\circ M} \right)
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for rank-one matrices \( A = uv^T \), with \( t = |c'|^{-1} \).
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Problem: Find smallest $t$ such that $p(t) \geq 0$ for all $A = uu^T$. 
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

$$S(n_N, \ldots, n_1)(x_1, \ldots, x_N) := \frac{\det(x_i^{n_j+j-1})}{\det(x_i^{j-1})}$$

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- **Weyl Character Formula in Type A:**
  $$s(n_N, \ldots, n_1)(1, \ldots, 1) = \prod_{1 \leq i < j \leq N} \frac{n_j - n_i + j - i}{j - i}.$$
Sketch of the proof of the main result (cont.)

Technical heart of the proof: Jacobi-Trudi type identity for $p_t$. 
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**Theorem (Belton, Guillot, Khare, Putinar, 2016)**

Let $M \geq N \geq 1$ be integers, and $c_0, \ldots, c_{N-1} \in \mathbb{F}^\times$ be non-zero scalars in any field $\mathbb{F}$. Define the polynomial

$$p_t(x) := t(c_0 + \cdots + c_{N-1}x^{N-1}) - x^M,$$

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$$\mu(M, N, j) := (M - N + 1, 1, \ldots, 1, 0, \ldots, 0).$$

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$(N - j - 1$ ones, $j$ zeros). The following identity holds for all $u, v \in \mathbb{F}^N$:

$$\det p_t[uv^T] =$$

$$t^{N-1} \Delta_N(u) \Delta_N(v) \prod_{j=0}^{N-1} c_j \times \left( t - \sum_{j=0}^{N-1} \frac{s_{\mu(M,N,j)}(u)s_{\mu(M,N,j)}(v)}{c_j} \right).$$
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Reformulation: Linear matrix inequalities (LMI)

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

$$f[A] = c_0 1_{N \times N} + \cdots + c_{N-1} A^{o(N-1)} - c_M A^{oM}, \quad A^o := (a^o_{ij}).$$
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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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Consider the Hankel matrix associated to $\mu$:

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Preserving positivity on Hankel matrices (of all dimensions).
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**Interesting consequence:** $f$ preserve positivity (entrywise) on Hankel matrices iff it maps moment sequences to themselves:

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

for some positive Borel measure $s_\mu$. 
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Can prove several variants for measures with other supports.

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**Proposition** Suppose $f(s_k(\mu)) = s_k(\sigma \mu)$ for all $k \geq 0$ and all $\mu$ with $\text{supp} \mu \subseteq [-1, 1]$. Then $f$ is continuous.
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Proof of the Proposition

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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 $\mu$ and $p$. 

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- 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

$$a := \beta + bv_0, \quad \mu := a\delta_{-1} + b\delta_{v_0}.$$
Key identity: $0 \leq \sum_{k=0}^{d} a_k f(s_k(\mu))$. 
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We compute the first moments of $\mu$:

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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.
References:


Work partially supported by the Simons foundation, a University of Delaware Research Foundation grant, and a University of Delaware Research Foundation strategic initiative grant.

Happy Birthday Tom!!!
Recall that $f(x) = x^k$ preserves positivity on $\bigcup_{N \geq 1} \mathbb{P}_N$ 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 $\alpha$th power for some $\alpha > 0$.

When is the resulting matrix positive semidefinite?

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Can we do better?
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Proof:

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Use Induction. $n = 2$ is easy.

Now,

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

Note that

$$A/a_{nn} = B - \zeta \zeta^T \in \mathbb{P}_{n-1}.$$
FitzGerald and Horn’s result (Sketch of proof)

**Theorem:** (FitzGerald and Horn, 1977) Let $n \geq 2$. Then:
1. $f(x) = x^\alpha$ preserves positivity on $\mathbb{P}_n((0, \infty))$ if $\alpha \geq n - 2$.
2. If $\alpha < n - 2$ is not an integer, there is a matrix $A \in \mathbb{P}_n$ such that $A^{\circ \alpha} \not\in \mathbb{P}_n$.

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**Goal:** Show that

$$A^{\circ \alpha}/a_{nn}^{\alpha} = B^{\circ \alpha} - \zeta^{\circ \alpha} \zeta^{\circ \alpha T}$$

$$= B^{\circ \alpha} - (\zeta \zeta^T)^{\circ \alpha} \in \mathbb{P}_{n-1}.$$
**Theorem:** (FitzGerald and Horn, 1977) Let \( n \geq 2 \). Then:

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Proof of (1). By elementary calculus, for any \( x, y \in \mathbb{R} \),

\[
f(x) - f(y) = \int_0^1 (x - y)f'(\lambda x + (1 - \lambda)y) \, d\lambda.
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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 $V = \{1, \ldots, N\}$, define a subset of $\mathbb{P}_N$ by

$$\mathbb{P}_G := \{ A \in \mathbb{P}_N : a_{jk} = 0 \text{ if } (j, k) \not\in E \text{ and } j \neq k \}. $$
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Example:

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* & * & 0 & *\\
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Define the set of powers preserving positivity for $G$:

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

$$CE(G) := \text{smallest } \alpha_0 \text{ s.t. } x^\alpha \text{ preserves positivity on } \mathbb{P}_G, \forall \alpha \geq \alpha_0.$$
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**Problem 1:** Compute $\mathcal{H}_G$ and $CE(G)$.

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**Problem 1:** Compute $\mathcal{H}_G$ and $CE(G)$.
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**Problem 2:** How does the structure of $G$ relate to the set of powers preserving positivity?
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Clearly, the maximal clique is \( K_3 \). However, we can show that \( \mathcal{H}_{K_4^{(1)}} = \{1\} \cup [2, \infty) \).
Theorem. (Guillot, Khare, Rajaratnam, 2016) $CE(T) = 1$ for any tree $T$. 
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![Chordal vs Not Chordal](chordal_not_chordal.png)
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![Chordal vs. Not Chordal](image)

- 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

$$\mathcal{H}_G = \mathbb{N} \cup [r - 2, \infty).$$

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