On the Extreme Eigenvalues of Certain Gram Matrices of Hermite Polynomials

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I. Hermite Polynomials

Motivation & Introduction

Monic Hermite polynomials (MHP)

$$
\begin{aligned}
h_0(x) &= 1, \\
h_1(x) &= x, \\
h_2(x) &= x^2 - 1, \\
h_3(x) &= x^3 - 3x, \\
h_4(x) &= x^4 - 6x^2 + 3, \\
h_5(x) &= x^5 - 10x^3 + 15x, \quad \dots
\end{aligned}
$$

given by recursive schemes

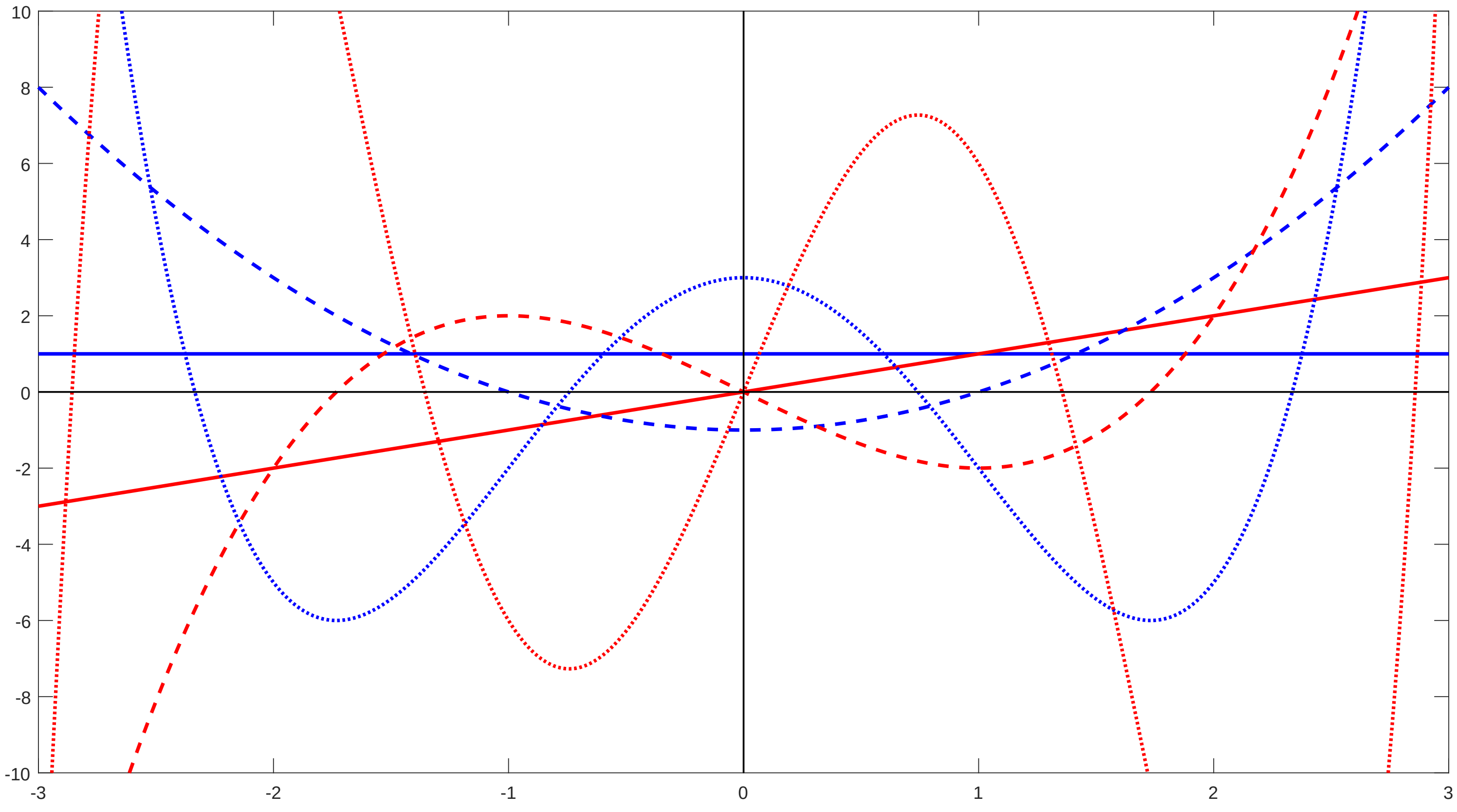
$$
\begin{aligned}
& h_0(x) = 1, \quad h_{m+1} = x h_m(x) - h'_m(x), \quad m = 0, 1, 2, \dots, \\
\text{or} \quad & h_0(x) = 1, \quad h_1(x) = x, \quad h_{m+1} = x h_m(x) - m h_{m-1}(x), \quad m = 1, 2, \dots,
\end{aligned}
$$

are orthogonal w.r.t. inner-product

$$
\langle f, g \rangle = \int_{\mathbb{R}} f(x) g(x) \varrho(x) \mathrm{d}x, \quad \varrho(x) = \mathrm{e}^{-\frac{x^2}{2}}. \qquad \|f\| = \sqrt{\langle f, f \rangle}.
$$

Sometimes $h_j(x)$ are called *probabilists'* HP's; the *physicists'* HP's use $\varrho(x) = \mathrm{e}^{-x^2}$.

The first six Hermite polynomials



Since

$$\langle h_m, h_m \rangle = \|h_m\|^2 = \sqrt{2\pi}\, m!\,, \qquad m = 0, 1, \dots,$$

then

$$p_m(x) = \frac{h_m(x)}{\|h_m(x)\|} = \frac{h_m(x)}{\sqrt[4]{2\pi}\,\sqrt{m!}}, \qquad \langle p_m, p_k \rangle = \delta_{m,k}, \qquad m, k = 0, 1, \dots,$$

are normalized Hermite polynomials (NHP).

Note that HP's have symmetric distribution of roots:

$$0 = h_m(x) = p_m(x) \quad \Longleftrightarrow \quad p_m(-x) = h_m(-x) = 0.$$

Shifted inner-product

Let us consider

$$\langle f, g\rangle_\alpha = \int_{\mathbb{R}} f(x)g(x)\mathrm{e}^{-\frac{x^2}{2}+\alpha x}\mathrm{d}x, \qquad \alpha \in \mathbb{R}.$$

Since

$$-\frac{x^2}{2} + \alpha x = -\frac{x^2 - 2\alpha x + \alpha^2 - \alpha^2}{2} = -\frac{(x-\alpha)^2}{2} + \frac{\alpha^2}{2}$$

then

$$\begin{aligned}\langle f, g\rangle_\alpha &= \mathrm{e}^{\frac{\alpha^2}{2}} \int_{\mathbb{R}} f(x)g(x)\mathrm{e}^{-\frac{(x-\alpha)^2}{2}}\mathrm{d}x \\ &= \mathrm{e}^{\frac{\alpha^2}{2}} \int_{\mathbb{R}} f(x+\alpha)g(x+\alpha)\mathrm{e}^{-\frac{x^2}{2}}\mathrm{d}x = \mathrm{e}^{\frac{\alpha^2}{2}}\langle f(x+\alpha), g(x+\alpha)\rangle\end{aligned}$$

Trivially $\langle f, g\rangle_0 \equiv \langle f, g\rangle$.

Shifted inner-product of HP's $\equiv$ the standard inner-product of shifted HP's (up to the scaling factor).

Note that $\langle \cdot, \cdot\rangle$ and $\langle \cdot, \cdot\rangle_\alpha$ live on different spaces, but P's are subspaces of both;

let $\alpha > 0$, then try $f(x) = g(x) = \begin{cases} \mathrm{e}^{\frac{1}{2}(\frac{x^2}{2} - \alpha x)} & x \geq 0 \\ 0 & x < 0 \end{cases}$

Shifted Hermite polynomials

We are interested in spectral properties of Gram matrices of NHP's w.r.t. shifted inner-product.

Shifted MHP as linear combination of MHP's

$$
\begin{aligned}
h_0(x+\alpha) &= 1 &&= h_0(x),\\
h_1(x+\alpha) &= x+\alpha &&= h_1(x)+\alpha h_0(x),\\
h_2(x+\alpha) &= x^2+2\alpha x+\alpha^2-1 &&= h_1(x)+2\alpha h_1(x)+\alpha^2 h_0(x),\\
h_3(x+\alpha) &= x^3+3\alpha x^2+3\alpha^2 x+\alpha^3-3x-3\alpha &&= h_3(x)+3\alpha h_2(x)+3\alpha^2 h_1(x)+\alpha^3 h_0(x).
\end{aligned}
$$

There is a clear pattern

$$h_m(x+\alpha) = \sum_{\ell=0}^{m} \binom{m}{\ell} \alpha^{m-\ell} h_\ell(x).$$

Proof by induction employs recurrent formula $h_{s+1} = xh_s(x) - h'_s(x)$.

Shifted inner-product of HP's

Recalling $\|h_\ell(x)\| = \sqrt[4]{2\pi}\,\sqrt{\ell!}$, the shifted inner-products of MHP & NHP are

$$\begin{aligned}
\langle h_m, h_k\rangle_\alpha &= \mathrm{e}^{\frac{\alpha^2}{2}} \langle h_m(x+\alpha), h_k(x+\alpha)\rangle \\
&= \mathrm{e}^{\frac{\alpha^2}{2}} \left\langle \sum_{\ell=0}^{m} \binom{m}{\ell} \alpha^{m-\ell}\, h_\ell(x)\,,\, \sum_{\ell=0}^{k} \binom{k}{\ell} \alpha^{k-\ell}\, h_\ell(x) \right\rangle \\
&= \mathrm{e}^{\frac{\alpha^2}{2}} \sum_{\ell=0}^{\min(m,k)} \binom{m}{\ell}\binom{k}{\ell} \alpha^{m+k-2\ell}\, \|h_\ell(x)\|^2 \\
&= \mathrm{e}^{\frac{\alpha^2}{2}} \sum_{\ell=0}^{\min(m,k)} \binom{m}{\ell}\binom{k}{\ell} \alpha^{m+k-2\ell}\, \sqrt{2\pi}\,\ell!,
\end{aligned}$$

$$\langle p_m, p_k\rangle_\alpha = \frac{\langle h_m, h_k\rangle_\alpha}{\sqrt{2\pi}\,\sqrt{m!}\,\sqrt{k!}} = \frac{\mathrm{e}^{\frac{\alpha^2}{2}}}{\sqrt{m!}\,\sqrt{k!}} \sum_{\ell=0}^{\min(m,k)} \binom{m}{\ell}\binom{k}{\ell} \alpha^{m+k-2\ell}\, \ell!.$$

II. Gram Matrices

Gram matrix of NHP's. Basic properties

Let $A_\alpha \in \mathbb{R}^{(N+1)\times(N+1)}$,

$$(A_\alpha)_{m+1,k+1} = \langle p_m, p_k\rangle_\alpha = \frac{e^{\frac{\alpha^2}{2}}}{\sqrt{m!}\,\sqrt{k!}} \sum_{\ell=0}^{\min(m,k)} \binom{m}{\ell}\binom{k}{\ell}\,\alpha^{m+k-2\ell}\,\ell!, \qquad m,k = 0,1,\ldots,N.$$

- A_α is symmetric positive definite.
- For $\begin{cases} \alpha > 0, & A_\alpha > 0, \\ \alpha = 0, & A_\alpha = I, \\ \alpha < 0, & A_\alpha \text{ has nonzero entries with chess-board structure of sign pattern, i.e.,} \end{cases}$

$$\begin{bmatrix} + & - & + & \cdots \\ - & + & - & \cdots \\ + & - & + & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}.$$

- Moreover $|A_\alpha| = |A_{-\alpha}|$.
- Consider a "sign" matrix $S = \mathrm{diag}(1,-1,1,\ldots)$, $S = S^T = S^{-1}$, then

$$A_\alpha = S A_{-\alpha} S, \quad \text{i.e.,} \quad \mathrm{sp}(A_\alpha) = \mathrm{sp}(A_{-\alpha}).$$

Modified Gram matrix

Note that each entry contains $e^{\frac{\alpha^2}{2}}$ factor.

Let $G_\alpha = e^{-\frac{\alpha^2}{2}} A_\alpha \in \mathbb{R}^{(N+1)\times(N+1)}$,

$$(G_\alpha)_{m+1,k+1} = \frac{1}{\sqrt{m!}\sqrt{k!}} \sum_{\ell=0}^{\min(m,k)} \binom{m}{\ell}\binom{k}{\ell} \alpha^{m+k-2\ell}\, \ell!, \quad m,k = 0,1,\ldots,N.$$

Observation: Denote $\chi_{N+1}(\lambda) = \det(\lambda I_{N+1} - G_\alpha)$, for $N = 0,1,2,3$ we have

$$\begin{aligned}
\chi_1(\lambda) &= \lambda - 1, \\
\chi_2(\lambda) &= \lambda^2 - (\alpha^2 + 2)\lambda + 1, \\
\chi_3(\lambda) &= \lambda^3 - (\tfrac{\alpha^4}{2} + 3\alpha^2 + 3)\lambda^2 + (\tfrac{\alpha^4}{2} + 3\alpha^2 + 3)\lambda - 1, \\
\chi_4(\lambda) &= \lambda^4 - (\tfrac{\alpha^6}{6} + 2\alpha^4 + 6\alpha^2 + 4)\lambda^3 + (\tfrac{\alpha^8}{12} + \tfrac{4\alpha^6}{3} + 7\alpha^4 + 12\alpha^2 + 6)\lambda^2 \\
&\qquad - (\tfrac{\alpha^6}{6} + 2\alpha^4 + 6\alpha^2 + 4)\lambda + 1.
\end{aligned}$$

The $\left\{ \begin{array}{l} \text{odd} \\ \text{even} \end{array} \right\}$ degree characteristic polynomial has $\left\{ \begin{array}{l} \text{anti-palindromic} \\ \text{palindromic} \end{array} \right\}$ coeff's.

Palindromic—anti-palindromic intermezzo

Polynomial of degree n

$$f(x) = \sum_{j=0}^{n} \varphi_j\, x^j \ \text{ is } \left\{ \begin{array}{ll} \text{palindromic (PP)} & \iff \quad \varphi_j = \varphi_{n-j} \\ \text{anti-palindromic (AP)} & \iff \quad \varphi_j = -\varphi_{n-j} \end{array} \right\} \ j = 0, 1, \ldots, n.$$

Since

$$\frac{1}{x^n}\, f(x) = \sum_{j=0}^{n} \frac{\varphi_j}{x^{n-j}} = \sum_{j=0}^{n} \frac{\pm\varphi_{n-j}}{x^{n-j}} = \pm\, f\left(\frac{1}{x}\right),$$

it has reciprocal roots, i.e.,

$$f(x) = 0 \quad \iff \quad f\left(\frac{1}{x}\right) = 0.$$

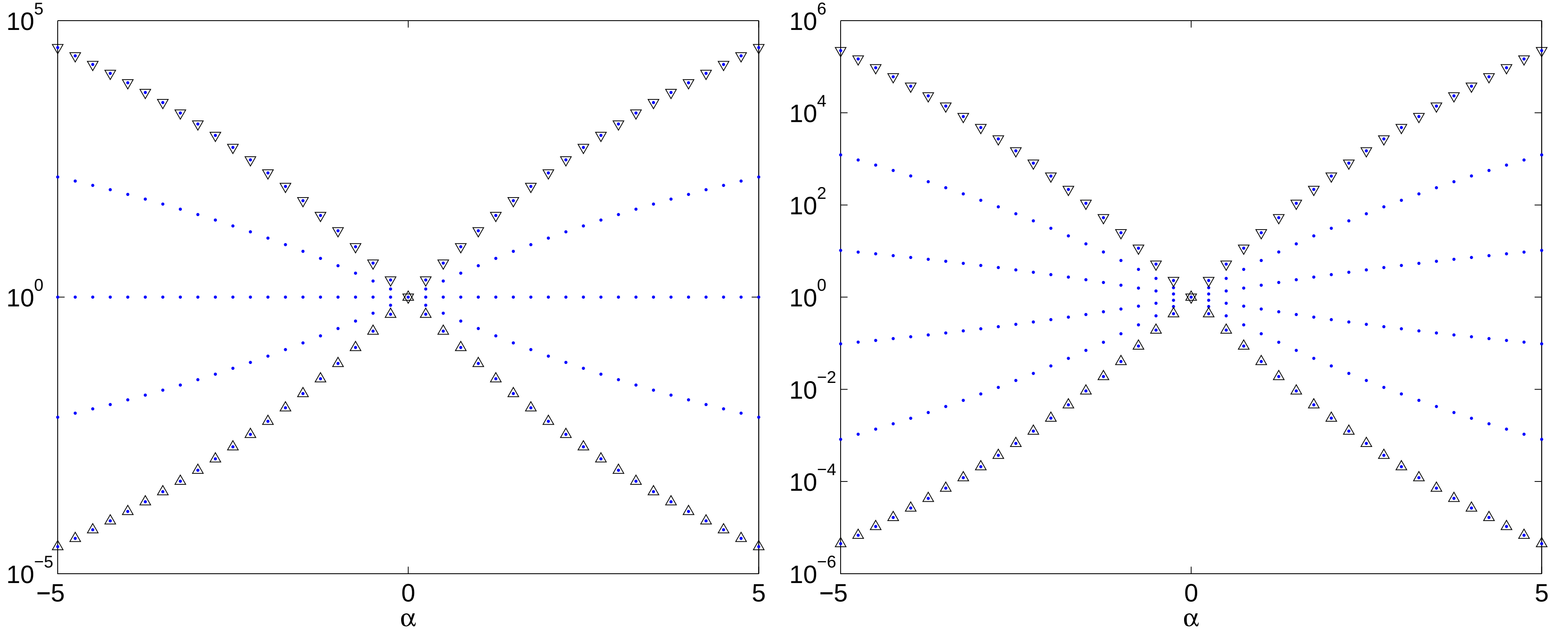
A lot of interesting properties, e.g.:

- AP has always root 1 (AP factor $(x-1)$),
- odd-degree PP has always root -1 (P factor $(x+1)$),
- PP-AP multiplication $\longrightarrow$

$\cdot$	PP	AP
PP	PP	AP
AP	AP	PP

Spectra of modified Gram matrices

Observation:



Decomposition of the modified Gram matrix

Recall the "sign" matrix

$$S = \mathrm{diag}(1, -1, 1, \ldots, (-1)^N) \in \mathbb{R}^{(N+1)\times(N+1)}, \qquad S = S^T = S^{-1}.$$

Consider an upper triangular matrix

$$U_\alpha = \begin{bmatrix} \binom{0}{0}\alpha^0 & \binom{1}{0}\alpha^1 & \binom{2}{0}\alpha^2 & \binom{3}{0}\alpha^3 & \cdots \\ 0 & \binom{1}{1}\alpha^0 & \binom{2}{1}\alpha^1 & \binom{3}{1}\alpha^2 & \cdots \\ 0 & 0 & \binom{2}{2}\alpha^0 & \binom{3}{2}\alpha^1 & \cdots \\ 0 & 0 & 0 & \binom{3}{3}\alpha^0 & \cdots \\ \vdots & \vdots & \vdots & \ddots & \ddots \end{bmatrix} = \begin{bmatrix} 1 & \alpha & \alpha^2 & \alpha^3 & \cdots \\ 0 & 1 & 2\alpha & 3\alpha^2 & \cdots \\ 0 & 0 & 1 & 3\alpha & \cdots \\ 0 & 0 & 0 & 1 & \cdots \\ \vdots & \vdots & \vdots & \ddots & \ddots \end{bmatrix} \in \mathbb{R}^{(N+1)\times(N+1)}.$$

Then

$$U_\alpha = SU_{-\alpha}S, \qquad U_\alpha U_{-\alpha} = I, \qquad \text{so} \qquad U_\alpha^{-1} = U_{-\alpha} = SU_\alpha S.$$

Finally consider also a "factorial" matrix

$$F = \mathrm{diag}(0!, 1!, 2!, \ldots, N!) \in \mathbb{R}^{(N+1)\times(N+1)}, \qquad F = F^T,$$

then ...

The modified Gram matrix $G_\alpha = \mathrm{e}^{-\frac{\alpha^2}{2}} A_\alpha \in \mathbb{R}^{(N+1)\times(N+1)}$ with entries

$$(G_\alpha)_{m+1,k+1} = \frac{1}{\sqrt{m!}\,\sqrt{k!}} \sum_{\ell=0}^{\min(m,k)} \binom{m}{\ell}\binom{k}{\ell} \alpha^{m+k-2\ell}\,\ell!, \qquad m,k = 0,1,\ldots,N,$$

can be then factorized as

$$G_\alpha = F^{-\frac{1}{2}} U_\alpha^T F U_\alpha F^{-\frac{1}{2}} = \underbrace{\left(F^{\frac{1}{2}} U_\alpha F^{-\frac{1}{2}}\right)^T \left(F^{\frac{1}{2}} U_\alpha F^{-\frac{1}{2}}\right)}_{\text{Cholesky factorization}}.$$

Its inverse can be factorized as

$$G_\alpha^{-1} = F^{\frac{1}{2}} U_\alpha^{-1} F^{-1} U_\alpha^{-T} F^{\frac{1}{2}}$$

$$= \left(F^{\frac{1}{2}} S\right) U_\alpha \left(S F^{-1} S\right) U_\alpha^T \left(S F^{\frac{1}{2}}\right) = S F^{\frac{1}{2}} U_\alpha F^{-1} U_\alpha^T F^{\frac{1}{2}} S = S \left(F^{\frac{1}{2}} U_\alpha F^{-\frac{1}{2}}\right) \left(F^{\frac{1}{2}} U_\alpha F^{-\frac{1}{2}}\right)^T S,$$

i.e.,

$$G_\alpha^{-1} \sim \left(F^{\frac{1}{2}} U_\alpha F^{-\frac{1}{2}}\right) \left(F^{\frac{1}{2}} U_\alpha F^{-\frac{1}{2}}\right)^T \sim \left(F^{\frac{1}{2}} U_\alpha F^{-\frac{1}{2}}\right)^T \left(F^{\frac{1}{2}} U_\alpha F^{-\frac{1}{2}}\right) = G_\alpha.$$

Consequently

$$\mathrm{sp}(G_\alpha) = \mathrm{sp}(G_\alpha^{-1}).$$

Perron–Frobenius theory

Entries of G_α are positive and increasing for $\alpha \in (0, \infty)$, i.e.,

$$\forall \epsilon > 0, \quad G_{\alpha+\epsilon} > G_\alpha > 0.$$

Perron–Frobenius theory then gives

$$\lambda_{\text{max}}(G_{\alpha+\epsilon}) > \lambda_{\text{max}}(G_\alpha).$$

Since $\text{sp}(G_\alpha) = \text{sp}(G_\alpha^{-1})$, then

$$\lambda_{\text{min}}(G_\alpha) = (\lambda_{\text{max}}(G_\alpha))^{-1} \quad \text{and} \quad \kappa(G_\alpha) = \frac{\lambda_{\text{max}}(G_\alpha)}{\lambda_{\text{min}}(G_\alpha)} = \lambda_{\text{max}}(G_\alpha)^2,$$

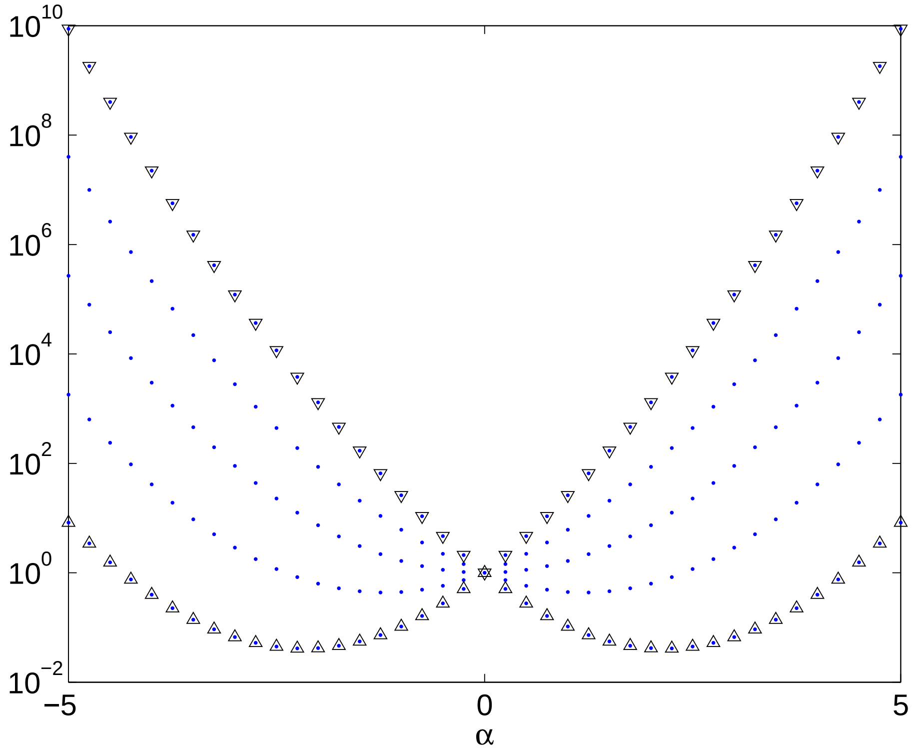
and thus

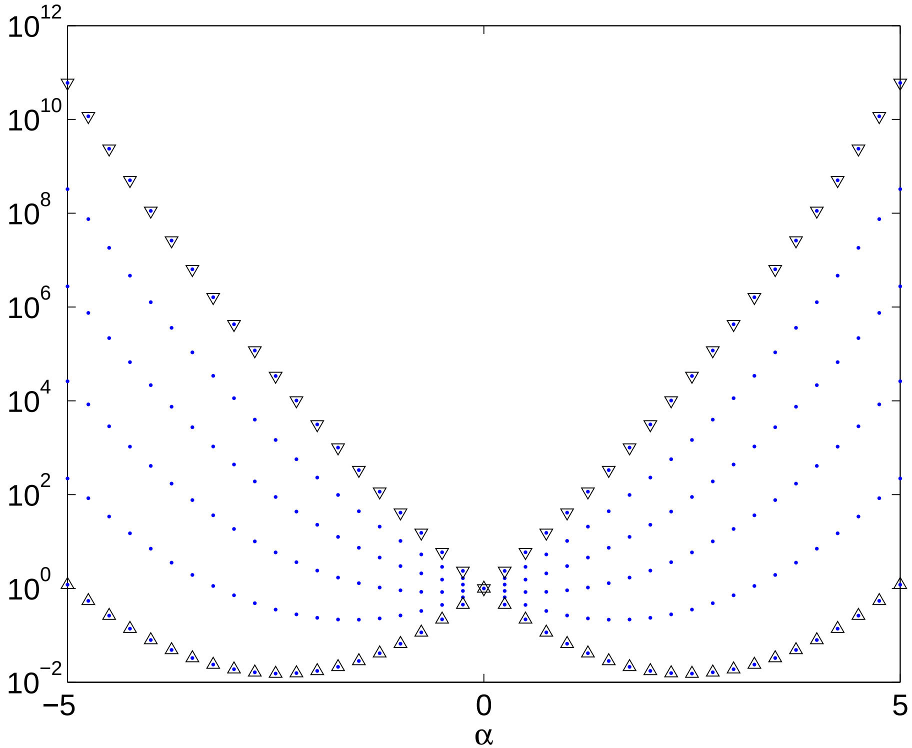
$$\lambda_{\text{min}}(G_{\alpha+\epsilon}) < \lambda_{\text{min}}(G_\alpha) \quad \text{and} \quad \kappa(G_{\alpha+\epsilon}) > \kappa(G_\alpha).$$

Since $\text{sp}(G_\alpha) = \text{sp}(G_{-\alpha})$, then analogous results can be obtained for $\alpha \in (-\infty, 0)$.

Back to the original Gram matrix

Recall that $A_\alpha = e^{\frac{\alpha^2}{2}} G_\alpha$ is a scalar mutliple of G_α, i.e., $\mathrm{sp}(A_\alpha) = e^{\frac{\alpha^2}{2}} \mathrm{sp}(G_\alpha)$. Thus $\lambda_{\max}(A_\alpha)$ and $\kappa(A_\alpha)$ are still increasing for $\alpha \in (0, \infty)$.





III. Optimal Diagonal Scaling

Optimal diagonal scaling

Let $B = (b_{i,j}) \in \mathbb{R}^{n \times n}$ be symmetric positive definite, and

$$D_* \equiv \text{diag}\left(\frac{1}{\sqrt{b_{1,1}}}, \ldots, \frac{1}{\sqrt{b_{n,n}}}\right).$$

Then

$$\kappa(D_* B D_*) \leq n \min_{D \text{ diagonal}} \kappa(DBD).$$

See [A van der Sluis, 1969] or [N Higham, 2002].

Note that

$$(D_* B D_*)_{i,j} = \frac{b_{i,j}}{\sqrt{b_{i,i}}\sqrt{b_{j,j}}}, \quad (D_* B D_*)_{i,i} = 1.$$

Recall that

$$(A_\alpha)_{m+1,k+1} = \langle p_m, p_k \rangle_\alpha = \frac{e^{\frac{\alpha^2}{2}}}{\sqrt{m!}\,\sqrt{k!}} \sum_{\ell=0}^{\min(m,k)} \binom{m}{\ell}\binom{k}{\ell} \alpha^{m+k-2\ell}\, \ell!,$$

$$(A_\alpha)_{m+1,m+1} = \frac{e^{\frac{\alpha^2}{2}}}{m!} \sum_{i=0}^{m} \binom{m}{i}^2 \alpha^{2(m-i)}\, i!, \qquad (A_\alpha)_{k+1,k+1} = \frac{e^{\frac{\alpha^2}{2}}}{k!} \sum_{j=0}^{k} \binom{k}{j}^2 \alpha^{2(k-j)}\, j!,$$

Denote the $\overline{A_\alpha}$ the optimally diagonally scaled A_α (and also G_α),

$$(\overline{A_\alpha})_{m+1,k+1} = \frac{\langle p_m, p_k \rangle_\alpha}{\sqrt{\langle p_m, p_m \rangle_\alpha}\,\sqrt{\langle p_k, p_k \rangle_\alpha}} = \frac{\displaystyle\sum_{\ell=0}^{\min(m,k)} \binom{m}{\ell}\binom{k}{\ell} \alpha^{m+k-2\ell}\, \ell!}{\sqrt{\displaystyle\sum_{i=0}^{m} \binom{m}{i}^2 \alpha^{2(m-i)}\, i!}\,\sqrt{\displaystyle\sum_{j=0}^{k} \binom{k}{j}^2 \alpha^{2(k-j)}\, j!}}.$$

Properties of scaled Gram matrix

The optimally diagonally scaled matrix $\overline{A_\alpha} \in \mathbb{R}^{(N+1)\times(N+1)}$ is symmetric positive definite, positive $\overline{A_\alpha} > 0$ for $\alpha > 0$ (and $\overline{A_{-\alpha}} = S\overline{A_\alpha}S$),

$$1 \geq |(\overline{A_\alpha})_{m+1,k+1}| \geq 0 \qquad \text{(Cauchy–Schwarz ineq.)}$$

and

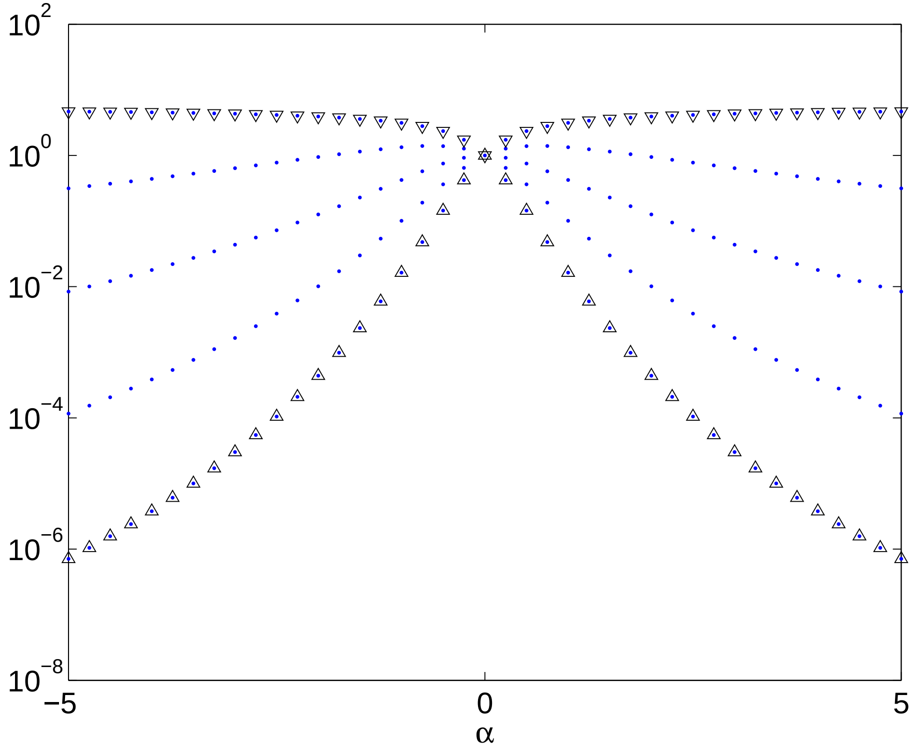
$$N+1 \geq \|\overline{A_\alpha}\|_1 \geq \lambda_{\max}(\overline{A_\alpha}) > 0 \qquad \text{(Perron–Frobenius theory).}$$

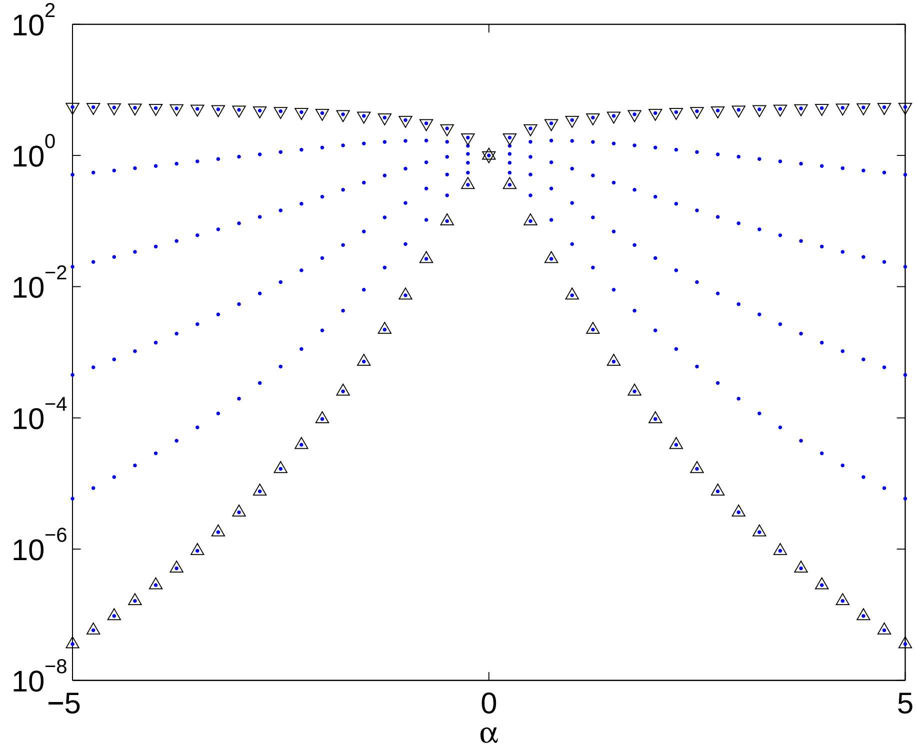
Moreover $\overline{A_0} = A_0 = I_{N+1}$ and

$$\lim_{\alpha\longrightarrow\infty} (\overline{A_\alpha})_{m+1,k+1} = \lim_{\alpha\longrightarrow\infty} \frac{\displaystyle\sum_{\ell=0}^{\min(m,k)} \binom{m}{\ell}\binom{k}{\ell} \alpha^{m+k-2\ell}\,\ell!}{\sqrt{\displaystyle\sum_{i=0}^{m} \binom{m}{i}^2 \alpha^{2(m-i)}\,i!}\sqrt{\displaystyle\sum_{j=0}^{k} \binom{k}{j}^2 \alpha^{2(k-j)}\,j!}} = 1,$$

$$\overline{A_\infty} = \begin{bmatrix} 1 & 1 & 1 & \cdots \\ 1 & 1 & 1 & \cdots \\ 1 & 1 & 1 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$ with simple $\lambda_{\max}(\overline{A_\infty}) = N+1$ and N-tuple $\lambda_{\min}(\overline{A_\infty}) = 0$.

Spectra of scaled Gram matrices





Monotonicity of λ_{min}, λ_{max}, κ?

Clearly

$$\lambda_{\text{min}}(\overline{A_\alpha}) = \frac{1}{\lambda_{\text{max}}\left((\overline{A_\alpha})^{-1}\right)}, \quad \text{moreover} \quad \overline{A_\alpha} = D_*^A\, A_\alpha\, D_*^A = D_*^G\, G_\alpha\, D_*^G.$$

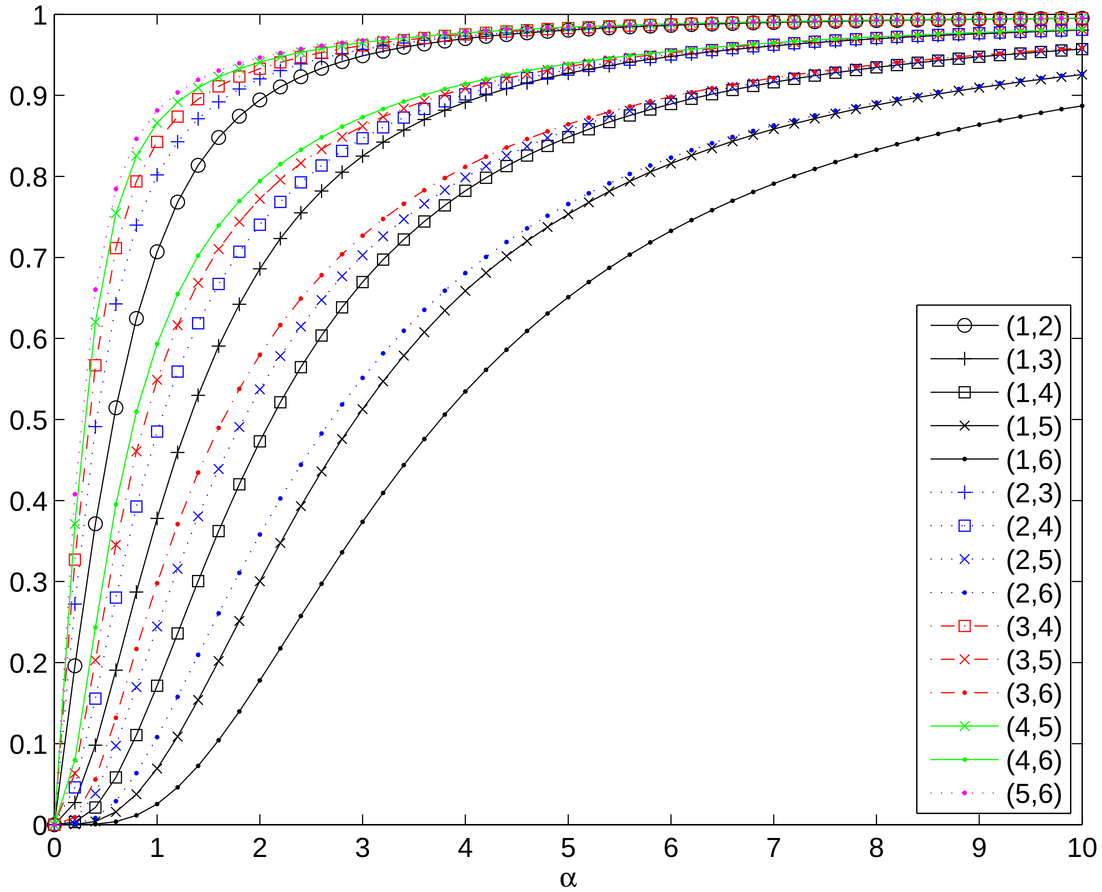
Thus

$$\begin{aligned}(\overline{A_\alpha})^{-1} &= (D_*^G)^{-1}\, \overbrace{F^{\frac{1}{2}} U_\alpha^{-1} F^{-1} U_\alpha^{-T} F^{\frac{1}{2}}}^{G_\alpha^{-1}}\, (D_*^G)^{-1} \\ &= \left((D_*^G)^{-1}\, F^{\frac{1}{2}} S\right) U_\alpha \left(S F^{-1} S\right) U_\alpha^T \left(S F^{\frac{1}{2}}\, (D_*^G)^{-1}\right) \\ &\sim\ (D_*^G)^{-1}\, F^{\frac{1}{2}} U_\alpha F^{-1} U_\alpha^T F^{\frac{1}{2}}\, (D_*^G)^{-1}\end{aligned}$$

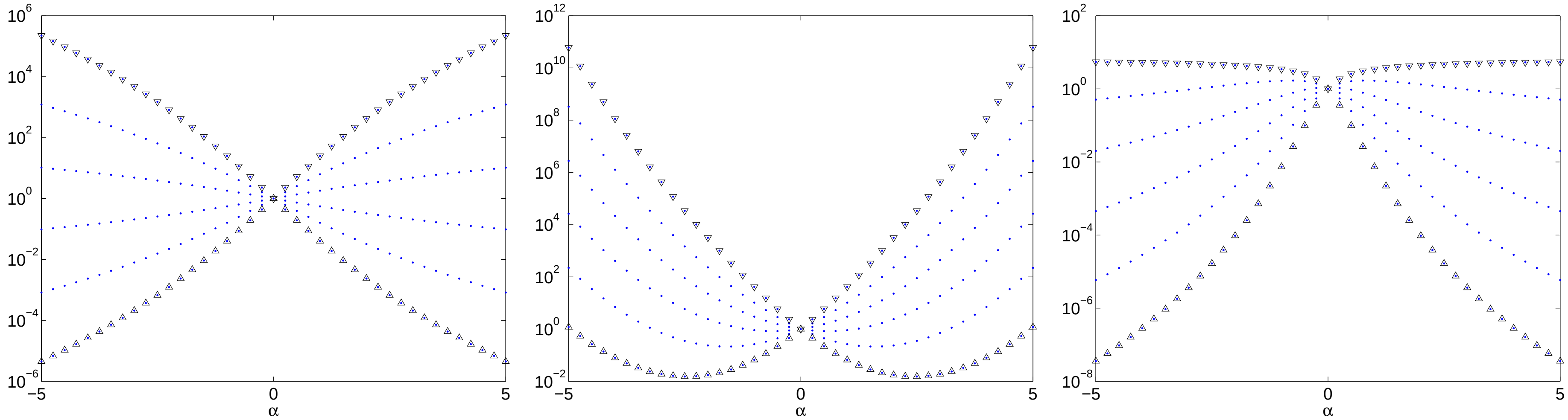
which is a positive matrix with increasing entries for $\alpha > 0$ (recall $D_*^B = \text{diag}(b_{i,i}^{-1/2})$).
From Perron–Frobenius theory: $\lambda_{\text{max}}((\overline{A_\alpha})^{-1})$ is increasing and

$$\kappa(\overline{A_\alpha}) = \frac{\lambda_{\text{max}}(\overline{A_\alpha})}{\lambda_{\text{min}}(\overline{A_\alpha})} \leq \frac{N+1}{\lambda_{\text{min}}(\overline{A_\alpha})}, \qquad \text{where} \qquad \lambda_{\text{min}}(\overline{A_\alpha}) \text{ is decreasing.}$$

Enries of scaled Gram matrices



That's all Folks!



MP, I Pultarová, LAA 546 (2018), pp. 50–66