Fractional Hadamard Powers of Positive Definite Matrices

by

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1. Preamble.

Let $P(t) = (a_{ij}^t)$ be any $n \times n$ real symmetric matrix, where $a_{ij} \geq 0$ and $t \geq 1$. We consider the following conjecture.

Conjecture. If $P(1)$ is positive definite then $P(t)$ is also positive definite for all $t \geq 1$. (C)

This conjecture is relevant to the study of positive definite similarity matrices, such as correlation matrices, which arise in the analysis of psychological data. For such matrices, monotonic transformations of the coefficients are sought whose properties include the preservation of both the ordering of the coefficients and the positive definiteness of the matrices.

The conjecture (C) is always true when $n = 2$ or 3 and, in certain special cases, for all n. It is in general untrue when $n = 4$, and it is thus in general untrue when $n \geq 4$ since a real symmetric matrix is positive definite if and only if all of its principal minors are strictly positive.

Remark. Since $P(t) = (a_{ij}^t)$ is positive definite if and only if the real quadratic form $x^T P(t) x$ is positive definite, where $x = (x_i)$, the substitution $x_i = y_i/\sqrt{a_{ii}}$ shows that it will suffice to assume that $a_{ii} = 1$ for all i, and that $0 \leq a_{ij} < 1$ when $i \neq j$. (1.1)

2. Cases when the conjecture (C) is true.*

Let $P(t) = (a_{ij}^t)$ be any $n \times n$ real symmetric matrix which satisfies (1.1), let $t \geq 1$ and let $P(1)$ be positive definite. Then $P(t)$ is also positive definite in the following cases:

1. for all $t \geq 1$ when $n = 2$ and when $n = 3$;
2. for all n when t is any positive integer;
3. for all n provided that $t \geq T$, where the value of T depends upon the particular matrix;
4. for all $t \geq 1$ and for all n when $a_{ij} = \alpha_i \alpha_j$ and $\alpha_i > 0$, for $i \neq j$ and $i,j = 1,2,\ldots,n$;
5. for all t and any given n if and only if $P(t)$ is positive definite whenever $1 < t < 2$. (2.1)

Proofs. All of the proofs are elementary. In some of them use is made of the facts that a real symmetric matrix is positive definite if and only if all of its principal minors are strictly positive and that the Hadamard product of two positive definite matrices is also positive definite.

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* Some work in this section is due to AM Russell.

2. Conditions for the conjecture (C) to be false.

Let $n = 4$, let $P(1)$ be positive definite and satisfy (1.1), and let $t \geq 1$. Then, by (2.1), (C) will be untrue if and only if it is untrue for some t such that $1 < t < 2$. Now (C) is true for $n = 3$, so that all proper principal minors of $P(t)$ are strictly positive. Since $|P(1)| > 0$ and P is a continuous function of t, (C) will therefore be untrue if and only if there exists a smallest number t, t' say, such that

$$1 < t' < 2, \qquad |P(t')| = 0, \tag{3.1}$$

and

$$d|P(t)|/dt|_{t=t'} \leq 0. \tag{3.2}$$

We define t' by (3.1) and seek conditions for (3.2) to hold. Let $0 < a_{12}, a_{13}, a_{14}$ and put

$$\alpha_1 = a_{14}^{-2t'},\ \alpha_2 = a_{13}^{-2t'},\ \alpha_3 = a_{12}^{-2t'},\ \delta_1 = (a_{23}/a_{12}a_{13})^{t'},\ \delta_2 = (a_{24}/a_{12}a_{14})^{t'},\ \delta_3 = (a_{34}/a_{13}a_{14})^{t'}$$

and $s = t/t'$. Then $\alpha_i > 1$ and $\delta_i > 0$ for all i, $\delta_1 < \sqrt{(\alpha_2\alpha_3)}$, $\delta_2 < \sqrt{(\alpha_3\alpha_1)}$, $\delta_3 < \sqrt{(\alpha_1\alpha_2)}$ and $t = t'$ when $s = 1$. It is easy to show that $|P(t)| = |P(st')| = (1 - \alpha_1^{-s})(1 - \alpha_2^{-s})(1 - \alpha_3^{-s})\Delta(s)$, where

$$\Delta(s) = 1 - X_1^2(s) - X_2^2(s) - X_3^2(s) + 2X_1(s)X_2(s)X_3(s),$$

$X_1(s) = (\delta_1^s - 1)/\sqrt{[(\alpha_2^s - 1)(\alpha_3^s - 1)]}$, $X_2(s) = (\delta_2^s - 1)/\sqrt{[(\alpha_3^s - 1)(\alpha_1^s - 1)]}$ and

$X_3(s) = (\delta_3^s - 1)/\sqrt{[(\alpha_1^s - 1)(\alpha_2^s - 1)]}$. Then $|X_i(s)| < 1$ for all i, and $|P(t')| = 0$ when $\Delta(1) = 0$ or

$$1 - X_1^2 - X_2^2 - X_3^2 + 2X_3X_2X_3 = 0,$$

where X_i denotes $X_i(1)$ for all i. Now $d|P|/dt|_{t=t'} = (t')^{-1} \prod_i (1 - \alpha_i^{-s}) d\Delta/ds|_{s=1}$, so that

$d|P|/dt|_{t=t'} \leq 0$ if and only if $d\Delta/ds|_{s=1} \leq 0$. If δ_1, δ_2 or $\delta_3 = 1$, it can easily be shown that (3.2) is not satisfied. Let $\delta_1, \delta_2, \delta_3 \neq 1$. Then it will follow that

$$d\Delta/ds|_{s=1} = x^*(X_1^2 - X_1X_2X_3) + y^*(X_2^2 - X_1X_2X_3) + z^*(X_3^2 - X_1X_2X_3).$$

4. Main Theorem.

Theorem Let $\phi(x) = [x\log x]/(x-1)$ for $x \neq 1$, let $\phi(1) = 1$, and let

$$x^* = (d/ds)[\log X_1^{-2}(s)]_{s=1} = \phi(\alpha_2) + \phi(\alpha_3) - 2\phi(\delta_1),$$

$$y^* = (d/ds)[\log X_2^{-2}(s)]_{s=1} = \phi(\alpha_3) + \phi(\alpha_1) - 2\phi(\delta_2),$$

and

$$z^* = (d/ds)[\log X_3^{-2}(s)]_{s=1} = \phi(\alpha_1) + \phi(\alpha_2) - 2\phi(\delta_3).$$

Then $x^*, y^*, z^* > 0$ and the conjecture (C) will be false for a continuum of values of a_{ij} if any one of the following inequalities is satisfied when $X_i^2 \approx 1$ for all i.

$$\sqrt{x^*} + \sqrt{y^*} < \sqrt{z^*}, \tag{4.1}$$

$$\sqrt{z^*} + \sqrt{x^*} < \sqrt{y^*}, \tag{4.2}$$

$$\sqrt{y^*} + \sqrt{z^*} < \sqrt{x^*}. \tag{4.3}$$

Proof. It suffices to suppose that $\delta_i \neq 1$ for all i and that

$$(\delta_1 - 1)(\delta_2 - 1) > 0 \quad \text{or} \quad (\alpha_3 - 1) \geq (1 - \delta_1)(\delta_2 - 1) > 0. \tag{4.4}$$

The other cases will follow by similar arguments. We first write $\Delta(s)$ as

$$\Delta(s) = X_1^2(s)\, X_2^2(s)\, [(A_1(s) - 1)(A_2(s) - 1) - (H(s) - 1)^2],$$

where $A_i(s) = X_i^{-2}(s)$ for all i, and $H(s) = X_3(s)/[X_1(s)X_2(s)]$. Since $|P(t')| = 0$, $\Delta(1) = 0$, and it follows that

$$H - 1 = \lambda(A_1 - 1)^{1/2}(A_2 - 1)^{1/2} = \lambda\rho(A_1 - 1) = \lambda\rho^{-1}(A_2 - 1),$$

where H denotes H(1), A_i denotes $A_i(1)$ for all i, $\lambda = \mathrm{sgn}\,(H - 1)$ and $\rho = [(A_2 - 1)/(A_1 - 1)]^{1/2}$, ($\rho \neq 1$ when $H > 1$). Then A_1 and A_2 can be expressed in terms of H and ρ. Now

$$dA_1(s)/ds = A_1(s)x^*, \quad dA_2(s)/ds = A_2(s)y^*, \text{ and } -2dH(s)/ds = H(s)(z^* - x^* - y^*),$$

so that

$$d\Delta(s)/ds|_{s=1} = X_1^2X_2^2(H - 1)L, \tag{4.5}$$

where

$$L = (z^* - x^* - y^*)H + \lambda(A_1\rho x^* + A_2\rho^{-1}y^*), \tag{4.6}$$

Now $L = L(x^*, y^*, z^*, \rho, A_1, A_2, H)$, and it can be shown that $L = L(\alpha_3, \delta_1, \delta_2, \rho, H)$, where the variables H, α_3, δ_1, and δ_2 satisfy the inequality $(\delta_1 - 1)(\delta_2 - 1)H + \alpha_3 > 1$.

If $(\delta_1 - 1)(\delta_2 - 1) > 0$, then $\quad -(\alpha_3 - 1)/[(\delta_1 - 1)(\delta_2 - 1)] < H < \infty$,

and, if $(\delta_1 - 1)(\delta_2 - 1) < 0$, then $\quad -\infty < H < (\alpha_3 - 1)/[(1 - \delta_1)(\delta_2 - 1)]$. (4.7)

We fix the variables α_3, δ_1, δ_2 and ρ. Then it can be shown from (4.6) that $dL/dH = \log(\alpha_1\alpha_2/\delta_3^2)$ and thus that L increases monotonically with H, since $\alpha_1\alpha_2 > \delta_3^2$.

Now $d|P(t)|/dt|_{t=t'}$ has the same sign as $d\Delta(s)/ds|_{s=1}$ and, by (4.5), it has the same sign as λL. Let $H > 1$. Then $\lambda > 0$, $d(\lambda L)/dH > 0$ and

$$\inf\{\lambda L): H > 1\} = \lim_{H \to 1+} \lambda L(\alpha_3, \delta_1, \delta_2, \rho, H) = \lambda L(\alpha_3, \delta_1, \delta_2, \rho, 1+).$$

Thus $d|P|/dt|_{t=t'} < 0$ in some interval $1 < H < H^*$ if and only if

$$L(\alpha_3, \delta_1, \delta_2, \rho, 1+) < 0.$$

That H can attain the value 1+ follows from (4.4) and (4.7).

Next, let $H < 1$. Then $\lambda < 0$, $d(\lambda L)/dH < 0$ and

$$\inf\{\lambda L): H < 1\} = \lim_{H \to 1-} \lambda L(\alpha_3, \delta_1, \delta_2, \rho, H) = \lambda L(\alpha_3, \delta_1, \delta_2, \rho, 1-).$$

Therefore $d|P|/dt|_{t=t'} < 0$ in some interval $H_* < H < 1$ if and only if

$$L(\alpha_3, \delta_1, \delta_2, \rho, 1\text{-}) > 0.$$

That H can attain the value 1- follows again from (4.4) and (4.7). Since α_3, δ_1, δ_2 and ρ (> 0) are fixed and $H = 1\pm$ if and only if $A_1 = A_2 = 1+$, it can be shown from (4.6) that

$$\begin{aligned} \lim_{H\to 1\pm} \lambda L(\alpha_3, \delta_1, \delta_2, \rho, H) & \\ &= (z^* - x^* - y^*)\lambda + \rho x^* + \rho^{-1} y^* \\ &= [\sqrt{(\rho x^*)} - \sqrt{(y^*/\rho)}]^2 + L_0(\alpha_3, \delta_1, \delta_2, \lambda), \qquad (4.8) \end{aligned}$$

where $\quad L_0 = L_0(\alpha_3, \delta_1, \delta_2, \lambda) = (\sqrt{y^*} + \lambda\sqrt{z^*} - \lambda\sqrt{x^*})(\sqrt{x^*} + \sqrt{z^*} - \lambda\sqrt{y^*})$.

Now $H = 1\pm$ if and only if $X_1{}^2 = X_2{}^2 = X_3{}^2 = 1\text{-}$, so that $X_i{}^2 = 1$ for all i, as required. Also, if ρ is now allowed to vary, (4.8) shows that, when $H = 1\pm$, the infimum of λL is given by $L_0(\alpha_3, \delta_1, \delta_2, \pm 1)$, and it will be negative if and only at least one of $L_0(\alpha_3, \delta_1, \delta_2, \pm 1)$ is negative. Now

$$\begin{aligned} L_0(\alpha_3, \delta_1, \delta_2, -1) < 0 & \\ &\Leftrightarrow (\sqrt{y^*} - \sqrt{z^*} + \sqrt{x^*})(\sqrt{x^*} + \sqrt{z^*} + \sqrt{y^*}) < 0 \\ &\Leftrightarrow \sqrt{y^*} + \sqrt{x^*} - \sqrt{z^*} < 0. \qquad (4.9) \end{aligned}$$

Also

$$\begin{aligned} L_0(\alpha_3, \delta_1, \delta_2, 1) < 0 & \\ &\Leftrightarrow (\sqrt{y^*} + \sqrt{z^*} - \sqrt{x^*})(\sqrt{x^*} + \sqrt{z^*} - \sqrt{y^*}) < 0, \end{aligned}$$

which cannot be satisfied when $x^* = y^*$. If, then, $x^* < y^*$,

$$L_0(\alpha_3, \delta_1, \delta_2, 1) < 0 \Leftrightarrow \sqrt{x^*} + \sqrt{z^*} < \sqrt{y^*}, \qquad (4.10)$$

while, if $x^* > y^*$, then

$$L_0(\alpha_3, \delta_1, \delta_2, 1) < 0 \Leftrightarrow \sqrt{y^*} + \sqrt{z^*} < \sqrt{x^*}. \qquad (4.11)$$

The inequalities (4.9), (4.10) and (4.11) are (4.1), (4.2) and (4.3), respectively. If none of them are satisfied, then $d|P|/dt|_{t=t'} > 0$ for all values of H.

5. Examples.

Let $\alpha_i{}^* = \log(\alpha_i - 1)$ and $\delta_i{}^* = \log(\delta_i - 1)$ for all i. Then examples can be found in the following cases when $\alpha_3 = \delta_1 = \delta_2$.

Case 1. Let $\alpha_3{}^* = \delta_1{}^* = \delta_2{}^*$, let $(1 <)\ \alpha_3 < \delta_1 < \delta_2$ and $\alpha_3 < \alpha_2 < \alpha_1$. Then $\alpha_3{}^* < \delta_1{}^* < \delta_2{}^*$.

Since we require that $X_1{}^2 = X_2{}^2 = X_3{}^2 = 1$, $(\delta_1 - 1)^2 = (\alpha_2 - 1)(\alpha_3 - 1)$ and

$(\delta_2 - 1)^2 \approx (\alpha_1 - 1)(\alpha_3 - 1)$, and it follows that $\alpha_1 \approx \alpha_2 \approx \alpha_3 \approx \delta_1 \approx \delta_2 \approx \delta_3$.

Similar examples arise when $\alpha_3^* \approx \delta_1^* \approx \delta_2^*$ and α_3, δ_1 and δ_2 are ordered differently.

Case 2. Let $\delta_1, \delta_2, \delta_3 > 1$, let $\alpha_3^*, \delta_1^*, \delta_2^* << -1$, and let $H \approx 1$ Then $\alpha_3 \approx \delta_1 \approx \delta_2 \approx 1$ and $X_1 \approx X_2 \approx X_3 \approx 1$. In particular, let $\alpha_3^*, \delta_1^*, \delta_2^* \to -\infty$ in such a way that, in the limit, $X_1 = X_2 = X_3 = 1-$ and the corresponding limiting values of α_1^* and α_2^* both exist and are finite. Then the limiting values of α_1 and α_2 will also be finite. For example, if α_3, δ_1 and δ_2 are chosen suitably close to 1 and are such that

$$(\alpha_3 - 1)/(\delta_1 - 1)^2 \quad [\approx 1/(\alpha_2 - 1)] \text{ and } (\alpha_3 - 1)/(\delta_2 - 1)^2 \quad [\approx 1/(\alpha_1 - 1)]$$

are small, then α_1 and α_2 are large and the inequality $\alpha_1^* \alpha_2^* < \delta_3^{*2}$ holds approximately. This can be attained for large α_1 and α_2 whose closeness is restricted by $\delta_3 - 1 = \sqrt{[(\alpha_1 - 1)(\alpha_2 - 1)]}$ when $X_i^2 \approx 1$ for all i .

6. Numerical examples.

Let P(t) be a real symmetric matrix with not more than three distinct off-diagonal elements, and let $a_{12} = a_{23} = a_{34} = p$, $a_{13} = a_{24} = q$ and $a_{14} = r$. Then the conjecture (C) will be false for some $t \in (1, 2)$ if $p = 0.875$, $q = 0.54$ and $r = 0.09$.

If T(p,q,r) is considered as a point in $\mathbf{R}^3$, then a continuity argument shows that T will lie in some region S in $\mathbf{R}^3$ such that the conjecture is false at all points of S. The boundary of S is not known, but T certainly lies inside the parallelpiped (within S) whose vertices are the points

$$(0.875 \pm 0.001, 0.5392 \pm 0.0001, 0.087 \pm 0.004).$$

It can be shown that P(t) satisfies the criterion $\sqrt{z^*} + \sqrt{x^*} < \sqrt{y^*}$.

If Q(t) is obtained from P(t) by simultaneous interchanging rows and columns, then Q(t) can take twelve distinct forms (including P(t)) and for all of these the corresponding real quadratic form is the same. Hence each of the forms of Q(t) demonstrates that the conjecture (C) will be false for some $t \in (1, 2)$ when p,q and r take the same values as above. Each of the criteria (4.1), (4.2) and (4.3) is satisfied by exactly four of these twelve forms.

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