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Improving Hadamard's Inequality*

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We study several bounds for the determinant of an $n \times n$ positive definite Hermitian matrix A. These bounds are the best possible given certain data about A. We find the best bounds in the cases that we are given: (i) the diagonal elements of A; (ii) the traces $\operatorname{tr} A$, $\operatorname{tr} A^2$ and n; and (iii) n, $\operatorname{tr} A$, $\operatorname{tr} A^2$ and the diagonal elements of A. In case (i) we get the well known Hadamard inequality. The other bounds are Hadamard type bounds. The bounds are found using optimization techniques.

1. INTRODUCTION

Given the $n \times n$ positive definite Hermitian matrix $A = (a_{ij})$, the Hadamard inequality yields the following upper bound for the deter-

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minant of A,

$$\det A \leqslant \prod_{i=1}^{n} a_{ii}. \tag{1.1}$$

For a general matrix A this implies

$$|\det A|^2 = (\det A^*A) \leqslant \prod_{i=1}^{n} \sum_{j=1}^{n} |a_{ij}|^2.$$

Equality is attained in (1.1) if and only if A is diagonal. Thus, increasing the off-diagonal terms of A (in modulus) decreases the determinant of A. We propose to use the sum of the squares of the modulii of the off diagonal terms to improve (1.1), as well as to find a lower bound for $\det A$.

The upper (lower) bounds for the determinant are based on finding upper (lower) bounds for the largest eigenvalue. In Section 2 we find a finite nested sequence of upper and lower bounds for the largest eigenvalues of an $n \times n$ Hermitian matrix A in terms of the traces $\operatorname{tr} A$, $\operatorname{tr} A^2$, n, and the diagonal elements, a_{ii}, of A. This improves the bound given in [7], which does not use the diagonal elements. The bound is obtained by applying the Karush–Kuhn–Tucker optimality conditions to an appropriate mathematical program, see [6]. The diagonal elements are introduced by using the majorization result of Horn [2]. The main result of this section is presented as Corollary 2.1. We also present a sequence of lower bounds for the smallest eigenvalue in Corollary 2.2.

In Section 3 we present the Hadamard type bounds for $\det A$. These are of the form

$$\alpha_l \prod_{i=1}^{n} a_{ii} \leqslant \det A \leqslant \prod_{i=1}^{n} a_{ii}\alpha_u,$$

for appropriate fractions α_l and α_u which depend on n, a_{ii}, $\operatorname{tr} A$ and $\operatorname{tr} A^2$. If $m = \operatorname{tr} A/n$ and $s^2 = \operatorname{tr} A^2/n - m^2$, then bounds of this type given in [1] state that

$$\left(m - s(n-1)^{1/2}\right)\left(m + s/(n-1)^{1/2}\right)^{n-1} \leqslant \det A$$
$$\leqslant \left(m + s(n-1)^{1/2}\right)\left(m - s/(n-1)^{1/2}\right)^{n-1}. \tag{1.2}$$

Various improvements of Hadamard's inequality (1.1) have appeared in the literature. A result of Schur (see e.g. [5, pg 224]) states that

$$0 \leqslant \prod a_{ii} - \det A \leqslant \frac{(\sum a_{ii})^{n-2}}{n-2} \frac{\operatorname{tr} A^2 - \sum a_{ii}^2}{2}.$$

Marcus [4] states that

$$\det A \leqslant \prod a_{ii} - \lambda_n^{n-1} \sum_{i \neq j} |a_{ij}|^2,$$

where λ_n is the smallest eigenvalue of A. In [3], Johnson discusses the problem of improving Hadamard's inequality by using more information about A other than just the diagonal.

2. AN UPPER BOUND FOR THE LARGEST EIGENVALUE

Let $A = (a_{ij})$ be an $n \times n$ nonzero Hermitian matrix (not necessarily positive definite) with eigenvalues $\lambda_1 \geqslant \cdots \geqslant \lambda_n$. Set

$$m = \operatorname{tr} A / n = \sum_{i=1}^{n} a_{ii} / n, \qquad s^2 = \operatorname{tr} A^2 / n - m^2. \tag{2.1}$$

In [7], it was shown that

$$\lambda_1 \leqslant m + s(n-1)^{1/2}, \tag{2.2}$$

with equality if and only if $\lambda_2 = \cdots = \lambda_n = m - s/(n-1)^{1/2}$. Thus, if we let

$$U(A) = \left\{ B = (b_{ij}) : B \text{ is Hermitian, } \operatorname{tr} B = \operatorname{tr} A, \text{ and } \operatorname{tr} B^2 = \operatorname{tr} A^2 \right\},$$

then (2.2) provides a *tight* upper bound for the largest eigenvalue $\lambda_1(B)$ for any $B \in U(A)$. The bound is independent of which $B \in U(A)$ is chosen. We now improve (2.2) (see Corollary 2.1) by considering the set

$$V(A) = U(A) \cap \{ B : b_{ii} = a_{ii}, i = 1, \ldots, n \},$$

and find the maximum of $\lambda_1(B)$ over all $B \in V(A)$. This leads to the following optimization problem:

$$\text{maximize} \left\{ \lambda_1(A) : \sum_{i,j} |a_{ij}|^2 \leqslant L, a_{11} = a_1 \geqslant \cdots \geqslant a_{nn} = a_n \right\}, \tag{P1}$$

i.e. we want to find the largest eigenvalue among all Hermitian matrices A satisfying $\operatorname{tr} A^2 \leqslant L$ and given the nonincreasing diagonal a_{ii}, $i = 1, \ldots, n$. Let $\lambda_1 \geqslant \lambda_n$ be the eigenvalues of A. Using the majorization of the diagonal by the eigenvalues, see [2], (P1) becomes equivalent to

$$\begin{aligned} \text{maximize}\quad & \lambda_1 \\ \text{s.t.}\quad & a_1 \leqslant \lambda_1, \\ & a_1 + a_2 \leqslant \lambda_1 + \lambda_2, \\ & \cdots\cdots\cdots\cdots \\ & a_1 + \ldots + a_{n-1} \leqslant \lambda_1 + \ldots + \lambda_{n-1}, \\ & a_1 + \ldots + a_n = \lambda_1 + \ldots + \lambda_n, \quad \text{and} \\ & \sum_{i=1}^{n} \lambda_i^2 \leqslant L, \lambda_1 \geqslant \lambda_2 \geqslant \ldots \geqslant \lambda_n . \end{aligned} \tag{P2}$$

By using the inequality constraint $\sum \lambda_i^2 \leqslant \mathrm{L}$, rather than the equality constraint $\sum \lambda_i^2 = \mathrm{L}$, we maintain the convexity of the problem (P2).

We now state the solution of (P2). Let

$$A_k := \sum_{i=1}^{k} a_i ; \qquad \Lambda_k := \sum_{i=1}^{k} \lambda_i ; \qquad L_k := L - \sum_{i=k+1}^{n} a_i^2 ;$$
$$m_k := A_k / k ; \qquad s_k^2 := L_k / k - m_k^2 .$$

THEOREM 2.1 *Suppose that the constants* L, $a_1 \geqslant \cdots \geqslant a_n > a_{n+1} = -\infty$ *are given such that*

$$\sum_{i=1}^{n} a_i^2 \leqslant L. \tag{2.4}$$

Let

$$\mu_k := m_k - s_k/(k-1)^{1/2}, \qquad k \geqslant 2.$$

Then there exists an integer t such that

$$2 \leqslant t \leqslant n; \qquad a_t \geqslant \mu_t \geqslant a_{t+1} \tag{2.5}$$

and the solution of $(P2)$ *is*

$$\lambda_1 = m_t + s_t(t-1)^{1/2} \tag{2.6}$$

$$\lambda_2 = \cdots = \lambda_t = m_t - s_t/(t-1)^{1/2} \tag{2.7}$$

$$\lambda_i = a_i , \qquad i = t+1, \ldots, n. \tag{2.8}$$

Proof The Karush–Kuhn–Tucker optimality conditions, e.g. [6], for (P2) are

$$\begin{bmatrix} -1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} + \alpha \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix} + \beta \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \vdots \\ \lambda_n \end{bmatrix} - \alpha_1 \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} - \dots - \alpha_{n-1} \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \\ 0 \end{bmatrix} = 0, \quad (2.9)$$

$$\beta \geqslant 0, \quad \beta\left(\sum_{i=1}^{n} \lambda_i^2 - L\right) = 0,$$

$$\alpha_j \geqslant 0, \quad \alpha_j(\Lambda_j - A_j) = 0, \quad j = 1, \dots, n-1, \quad (2.10)$$

$$\Lambda_n = A_n, \quad (2.11)$$

where the solution vector (λ_i) must satisfy the majorization constraint as well as

$$\lambda_1 \geqslant \cdots \geqslant \lambda_n \quad \text{and} \quad \sum_{i=1}^{n} \lambda_i^2 \leqslant L. \quad (2.12)$$

First, suppose $\beta = 0$. Then, from the last equation in (2.9), we have $\alpha = 0$. Similarly $\alpha_{n-1} = \alpha_{n-2} = \cdots = \alpha_2 = 0$. The first equation is now $-1 - \alpha_1 = 0$, which is impossible since $\alpha_1 \geqslant 0$. Therefore

$$\beta > 0 \quad \text{and} \quad \sum_{i=1}^{n} \lambda_i^2 = L. \quad (2.13)$$

We can now solve for the λ_i to get

$$\begin{aligned} \lambda_1 &= \frac{1}{\beta} - \frac{\alpha}{\beta} + \sum_{i=1}^{n-1} \frac{\alpha_i}{\beta} \\ \lambda_2 &= \frac{-\alpha}{\beta} + \sum_{i=2}^{n-1} \frac{\alpha_i}{\beta} \\ &\dots \quad \dots \quad \dots \\ \lambda_{n-1} &= \frac{-\alpha}{\beta} + \frac{\alpha_{n-1}}{\beta} \\ \lambda_n &= \frac{-\alpha}{\beta}. \end{aligned} \quad (2.14)$$

We also have

$$\alpha_j(\Lambda_j - A_j) = 0, \qquad j = 1, \dots, n-1,$$

so that

$$\alpha_j > 0 \quad \text{implies} \quad \Lambda_j = A_j, \quad j = 1, \ldots, n-1. \tag{2.15}$$

But by (2.14)

$$\alpha_j = 0 \quad \text{implies} \quad \lambda_j = \lambda_{j+1}, \quad j = 2, \ldots, n-1. \tag{2.16}$$

We conclude that

$$\Lambda_j = A_j \quad \text{or} \quad \lambda_j = \lambda_{j+1}, \qquad j = 2, \ldots, n-1. \tag{2.17}$$

Now suppose that

$$\Lambda_j = A_j, \qquad j = n, n-1, \ldots, n-k, \tag{2.18}$$

and

$$\Lambda_j > A_j, \qquad j = n-k-1, \ldots, n-k-l. \tag{2.19}$$

Let us show that either $\Lambda_j > A_j$, for $j = n-k-l-1$, or that $n - k - l = 1$. Suppose not, i.e. suppose

$$\Lambda_j = A_j, \qquad j = n-k-l-1. \tag{2.20}$$

From (2.18), we have

$$\lambda_j = \Lambda_j - \Lambda_{j-1} = A_j - A_{j-1} = a_j, \qquad j = n, \ldots, n-k+1, \tag{2.21}$$

while (2.19) implies that $\alpha_j = 0$ so that (2.16) yields

$$\lambda_j = \lambda_{j+1}, \qquad j = n-k-1, \ldots, n-k-l. \tag{2.22}$$

Now (2.20) and (2.19) imply

$$\lambda_j = \Lambda_j - \Lambda_{j-1} > A_j - A_{j-1} = a_j, \qquad j = n-k-l,$$

i.e., by (2.22),

$$\lambda_{n-k-1} = \cdots = \lambda_{n-k-l} > a_{n-k-l} \geqq \cdots \geqslant a_{n-k-1}. \tag{2.23}$$

Therefore

$$\begin{aligned} \Lambda_{n-k} &= \Lambda_{n-k-l-1} + \lambda_{n-k-l} + \ldots + \lambda_{n-k-1} + \lambda_{n-k} \\ &= A_{n-k-l-1} + \lambda_{n-k-l} + \ldots + \lambda_{n-k}, && \text{by (2.20)}, \\ &= A_{n-k-l-1} + (l+1)\lambda_{n-k-l}, && \text{by (2.22)}, \\ &> A_{n-k-l-1} + (l+1)a_{n-k-l} \geqslant A_{n-k}, && \text{by (2.23)}, \end{aligned}$$

which contradicts (2.18). Therefore, we conclude that strict inequality holds in (2.20). Continuing, we get

$$\Lambda_j > A_j, \qquad m = n-k-1, \ldots, 2, 1. \tag{2.24}$$

By (2.16) we now have

$$\lambda_2 = \lambda_3 = \cdots = \lambda_{n-k} := \lambda, \tag{2.25}$$

and

$$\lambda_j = a_j, \qquad j = n-k+1, \ldots, n. \tag{2.26}$$

This, together with (2.13) and $\Lambda_n = A_n$, yields an explicit solution for the λ_i, i.e. we solve

$$\begin{aligned} \lambda_1 + (n-k-1)\lambda &= \Lambda_{n-k} = A_{n-k} \\ \lambda_1^2 + (n-k-1)\lambda^2 &= \sum_{i=1}^{n-k} \lambda_i^2 = L - \sum_{i=n-k+1}^{n} a_i^2 = L_{n-k}. \end{aligned} \tag{2.27}$$

The solution is

$$\lambda_1 = \frac{A_{n-k}}{n-k} + (n-k-1)^{1/2}\left\{ \frac{L_{n-k}}{n-k} - \left(\frac{A_{n-k}}{n-k}\right)^2 \right\}^{1/2}, \tag{2.28}$$

$$\lambda = \frac{A_{n-k}}{n-k} - \frac{1}{(n-k-1)^{1/2}}\left\{ \frac{L_{n-k}}{n-k} - \left(\frac{A_{n-k}}{n-k}\right)^2 \right\}^{1/2}. \tag{2.29}$$

This is the given solution with $n - k = t$.

Now, except for the trivial case when $L = na_n^2$, the Slater constraint qualification, see e.g. [6], is satisfied for the convex (bounded) program (P2). Therefore, the Karush–Kuhn–Tucker conditions are necessary and sufficient for optimality. This implies that a feasible solution satisfying (2.28) and (2.29) *must* exist. Moreover, this solution must satisfy (2.5) by the above arguments.

The Karush–Kuhn–Tucker conditions are used above not only to prove the result but also to generate it (see [6]). Once the structure of the solution is found a simpler proof can be constructed. The structure of the solution

$$\lambda_2 = \ldots = \lambda_t, \qquad \lambda_i = a_i, \qquad i = t+1, \ldots, n$$

uniquely determines the solution (2.6)–(2.8), using $\sum_{i=1}^n \lambda_i = A_n$ and $\sum_{i=1}^n \lambda_i^2 = L$. Now, suppose that the optimal solution does not have this structure, i.e. suppose that for some $t > 2$, we have

$$\lambda_{t-1} > \lambda_t \neq a_t, \qquad \lambda_i = a_i, \qquad i = t+1, \ldots, n. \tag{2.30}$$

Then necessarily,

$$\lambda_t < a_t, \quad A_t = \Lambda_t \quad \text{and} \quad A_{t-1} < \Lambda_{t-1}.$$

We now fix $\bar{\lambda}_i = \lambda_i$, for all $i \neq 1, t-1, t$ and set, for $\epsilon, \delta > 0$,

$$\bar{\lambda}_1 = \lambda_1 + \epsilon, \qquad \bar{\lambda}_t = \lambda_t + \delta, \qquad \bar{\lambda}_{t-1} = \lambda_{t-1} - \epsilon - \delta.$$

For sufficiently small ϵ, δ, all the majorization constraints are satisfied by $(\bar{\lambda}_i)$. Moreover, by solving $\bar{\lambda}_1^{2} + \bar{\lambda}_{t-1}^{2} + \bar{\lambda}_t^{2} = \lambda_1^2 + \lambda_{t-1}^2 + \lambda_t^2$, with $\epsilon, \delta \geqslant 0$, the constraint $\sum_{i=1}^{n} \bar{\lambda}_i^{2} = L$ is also satisfied. Note that we get

$$\epsilon = \frac{-(\lambda_1 \lambda_{t-1})}{2} + \frac{\sqrt{(\lambda_1 - \lambda_{t-1})^2 + 4\delta(\lambda_{t-1} - \lambda_t) - 4\delta^2}}{2}$$

$$> 0, \qquad \text{for small} \quad \delta > 0, \quad \text{since} \quad \lambda_{t-1} > \lambda_t . \tag{2.31}$$

■

The above theorem yields a nested sequence of upper bounds for the largest eigenvalue of a Hermitian matrix A.

COROLLARY 2.1 *Given A Hermitian with $L = tr A^2$ and t defined in (2.5), let*

$$u_k := m_k + (k-1)^{1/2} s_k .$$

Then

$$\lambda_1 \leqslant u_t \leqslant u_{t+1} \leqslant \cdots \leqslant u_n . \tag{2.32}$$

Proof After applying the unitary similarity $P^t A P$, where P is a permutation matrix, we can assume that $a_{11} \geqslant \ldots \geqslant a_{nn}$. We now set $L = \operatorname{tr} A^2$ and apply the theorem. Adding one constraint $\sum_{i=1}^{k} a_{ii} \leqslant \sum_{i=1}^{k} \lambda_i$, at a time, for $k = n-1, n-2, \ldots, t$, provides the nested bounds. ■

Note that when $t = n$ is chosen by (2.5), the bound reduces to the one in [7]. Thus choosing $t = n$ always provides an upper bound for λ_1. Similarly, choosing t to be any integer ($\leqslant n$) larger than the t satisfying (2.5) provides an upper bound for λ_1. The best of these, of course, is the t satisfying (2.5). A procedure for calculating these bounds efficiently is given in Section 3.

We can also obtain a lower bound for the smallest eigenvalue λ_n by looking at the largest eigenvalue of $-A$. for this, let

$$A_{-k} := \sum_{i=n-k+1}^{n} a_i, \qquad L_{-k} := L - \sum_{i=1}^{n-k} a_i^2;$$

$$m_{-k} := A_{-k}/k; \qquad s_{-k}^2 := L_{-k}/k - m_{-k}^2.$$

COROLLARY 2.2 *Given A Hermitian with $L = tr A^2$, and $\infty = a_0 > a_1 \geqslant \cdots \geqslant a_n$ representing the* ordered *diagonal elements of A, let*

$$v_{-k} := m_{-k} + s_{-k}/(k-1)^{1/2}$$

$$b_{-k} := m_{-k} - s_{-k}(k-1)^{1/2}.$$

Then there exists an integer r such that

$$2 \leqslant r \leqslant n; \qquad a_{n-r+1} \leqslant v_{-r} \leqslant a_{n-r} \tag{2.33}$$

and

$$\lambda_n \geqslant b_{-r} \geqslant b_{-(r+1)} \geqslant \cdots \geqslant b_{-n}.$$

3. HADAMARD TYPE BOUNDS

Given the $n \times n$ positive definite Hermitian matrix $A = (a_{ij})$, then Hadamard's inequality states that the determinant

$$\det A \leqslant \prod_{i=1}^{n} a_{ii}. \tag{1.1}$$

Upper and lower bounds for the determinant given in [1] state that

$$\left(m - s(n-1)^{1/2}\right)\left(m + s/(n-1)^{1/2}\right)^{n-1} \leqslant \det A$$

$$\leqslant \left(m + s(n-1)^{1/2}\right)\left(m - s/(n-1)^{1/2}\right)^{n-1}. \tag{1.2}$$

Equality holds on the right iff $\lambda_2 = \cdots = \lambda_n$, in which case

$$\lambda_n = m - s/(n-1)^{1/2}; \qquad \lambda_1 = m + s(n-1)^{1/2}.$$

In the case that $m - s(n-1)^{1/2} \geqslant 0$, equality holds on the left iff $\lambda_1 = \cdots = \lambda_{n-1}$, in which case

$$\lambda_n = m - s(n-1)^{1/2}; \qquad \lambda_1 = m + s/(n-1)^{1/2}.$$

These latter bounds are the best possible bounds one can obtain given only the three facts n, $\operatorname{tr} A$ and $\operatorname{tr} A^2$. We now improve these bounds by using the ordered diagonal elements of A, i.e. we find the best upper and lower bounds for $\det A$ given only $n, \operatorname{tr} A, \operatorname{tr} A^2$ and the ordered diagonal elements $a_1 \geqslant \cdots \geqslant a_n$, see Theorem 3.1. We also consider the bound obtained by applying (1.2) to the matrix $B = DAD$, where D is the diagonal matrix with diagonal entries $d_i = 1/\sqrt{a_i}$.

The bound (1.1) is extremely easy to calculate. It requires exactly $n-1$ multiplications. The other bounds require knowing $\operatorname{tr} A^2 = \sum_{i,j} |a_{ij}|^2$ and so require of the order of n^2 multiplications.

To improve (1.2), we again solve an optimization problem:

$$\text{maximize}\{\det A : A \text{ is } n \times n \text{ Hermitian positive definite, } \operatorname{tr} A^2 = L,$$
$$\text{and } a_{11} = a_1 \geqslant \ldots \geqslant a_{nn} = a_n > 0\}, \qquad \text{(P3)}$$

where the a_i and L are given positive numbers satisfying

$$\sum_{i=1}^{n} a_i^2 \leqslant L \leqslant \left(\sum_{i=1}^{n} a_i \right)^2. \qquad (3.1)$$

We also solve (P3) with maximize replaced by minimize. First, let us note that:

PROPOSITION 3.1 *An $n \times n$ Hermitian positive semi-definite matrix A exists with diagonal $a_{ii} = a_i > 0$ and $\operatorname{tr} A^2 = L$ if and only if* (3.1) *holds.*

Proof Since $\sum_{i=1}^{n} \lambda_i = \operatorname{tr} A$ and $\sum_{i=1}^{n} \lambda_i^2 = \operatorname{tr} A^2$, necessity of (3.1) follows from

$$\sum_{i=1}^{n} a_{ii}^2 \leqslant \sum_{i,j} |a_{ij}|^2 = L = \sum_{i=1}^{n} \lambda_i^2$$
$$\leqslant \left(\sum_{i=1}^{n} \lambda_i \right)^2 \leqslant n \left(\sum_{i=1}^{n} \lambda_i^2 \right) = nL.$$

The last inequality follows from applying the Cauchy–Schwarz inequality to the vector (λ_i). To prove sufficiency, we use the majorization result of Horn [2]. Thus we need only find an ordered vector (λ_i) which majorizes (a_i). The solution is given by the solution of (P2) in Theorem 2.1. Note that $\lambda_t \geqslant a_{t+1} > 0$ if $t < n$ and $\mu_t = m_t - s_t/(n-1)^{1/2} > 0$, by (3.1), if $t = n$. Note that the extremal case is given by the matrix $a_{ij} = \sqrt{a_i a_j}$. This matrix has $\operatorname{tr} A^2 = (\sum_{i=1}^{n} a_i)^2$ and rank $= 1$. ■

The determinantal bounds are obtained using Theorem 2.1 and the somewhat isotonic property of $\det A$ and $\lambda_1(A)$. More precisely, we show that if $B \in V(A)$ does not solve (P2), then there exists $C \in V(A)$ such that $\det C > \det B$. The following lemma shows the isotonic character of $\det A$ and $\lambda_1(A)$.

LEMMA 3.1 *Suppose that $K, L > 0$ are given and consider the set*

$$\left\{(\lambda_1, \lambda_2, \lambda_3) : \lambda_1 \geqslant \lambda_2 \geqslant \lambda_3 \geqslant 0,\ \sum \lambda_i = K,\ \sum \lambda_i^2 = L.\right\}.$$

Then, on this set, the product $\lambda_1\lambda_{/2}\lambda_3$ is isotonic in each of λ_1 and λ_3 and is reverse isotonic in λ_2.

Proof Applying implicit differentiation on $\sum\lambda_i = K$ and $\sum\lambda_i^2 = L$ and solving, yields

$$\frac{\partial\lambda_i}{\partial\lambda_j} = \frac{\lambda_j - \lambda_k}{\lambda_k - \lambda_i}, \qquad i, j, k \text{ distinct.} \tag{3.2}$$

Differentiating the product, yields

$$\frac{\partial\lambda_1\lambda_2\lambda_3}{\partial\lambda_k} = (\lambda_k - \lambda_j)(\lambda_k - \lambda_i), \qquad i, j, k \text{ distinct.} \tag{3.3}$$

Since the derivatives exist, except possibly at the points where $\lambda_i = \lambda_k$, we get the isotonic properties from their signs.

Alternatively, $\lambda_1, \lambda_2, \lambda_3$ are the roots of

$$p(\lambda) = \lambda^3 - K\lambda^2 + P\lambda - c = 0$$

where $P = \frac{1}{2}(K^2 - L)$ and $c = \lambda_1\lambda_2\lambda_3$. Differentiating with respect to λ yields

$$3\lambda^2 - 2K\lambda = P = \frac{dc}{d\lambda}.$$

The discriminant $4K^2 - 12P = 2(3L - K^2) \geqslant 0$, by the Cauchy–Schwarz inequality. Thus $dc/d\lambda$ has exactly two sign changes and must be positive for large λ. This implies

$$\frac{dc}{d\lambda_i} = \begin{cases} \geqslant 0 & i = 1 \\ \leqslant 0 & i = 2 \\ \geqslant 0 & i = 3. \end{cases} \qquad \blacksquare$$

THEOREM 3.1 *Let $A = (a_{ij})$ be an $n \times n$ positive definite Hermitian matrix with eigenvalues $\lambda_1 \geqslant \cdots \geqslant \lambda_n > 0$; let $\infty = a_0 \geqslant a_1 \geqslant \cdots$*

$\geqslant a_n \geqslant a_{n+1} = -\infty$ *contain the ordered diagonal elements of A; let*

$$\begin{aligned} \mu_k &:= m_k - s_k/(k-1)^{1/2}, \\ u_k &:= m_k + s_k(k-1)^{1/2}, \\ v_j &:= m_{-j} + s_{-j}/(j-1)^{1/2}, \\ b_j &:= m_{-j} - s_{-j}(j-1)^{1/2}. \end{aligned} \tag{3.4}$$

Then there exists integers t and r such that

$$\mu_k > a_k, \qquad k = n, n-1, \ldots, t+1; \qquad a_{t+1} \leqslant \mu_t \leqslant a_t; \tag{3.5}$$

$$v_{-j} < a_{n-j+1}, \qquad j = n, n-1, \ldots, r+1; \qquad a_{n-r} \geqslant v_{-r} \geqslant a_{n-r+1}$$

and we get

$$\begin{aligned} \det A &\leqslant u_t(\mu_t)^{t-1} a_{t+1} \ldots a_n \\ &\leqslant u_{t+1}(\mu_{t+1})^t a_{t+2} \ldots a_n \\ &\ldots \ldots \ldots \\ &\leqslant u_n(\mu_n)^{n-1}. \end{aligned} \tag{3.6}$$

Equality holds throughout the first j inequalities if $\lambda_2 = \cdots = \lambda_t = \cdots = \lambda_{t+j-1}$ and $\lambda_{t+j+i} = a_{t+j+i}$, $i = 0, 1, \ldots, n-t-j$; in this case $\lambda_2 = \mu_{t+j-1}$ and $\lambda_1 = u_{t+j-1}$;

$$\begin{aligned} \det A &\geqslant b_{-r}(v_{-r})^{r-1} a_1 \ldots a_{n-r} \\ &\geqslant b_{-(r+1)}(v_{-(r+1)})^r a_1 \ldots a_{n-r-1} \\ &\ldots \ldots \ldots \\ &\geqslant b_{-n}(v_{-n})^{n-1}. \end{aligned} \tag{3.7}$$

Equality holds throughout the last j inequalities iff $\lambda_{n-1} = \cdots = \lambda_{n-r} = \cdots = \lambda_{n-r-j+1}$ and $\lambda_i = a_i$, $i = 1, \ldots, n-r-j$; in this case $\lambda_{n-1} = v_{-(r+j)}$ and $\lambda_n = b_{-(r+j)}$.

Proof To prove the inequalities, we need only show that the determinant is a maximum (minimum) in (P3) only if λ_1 (resp. λ_n) is a maximum (resp. minimum). Suppose not, i.e. suppose that A solves (P3) but the eigenvalues (λ_i) of A do not have the structure of the solution of (P2). Then, as in the second proof of Theorem 2.1, we keep all the λ_i's fixed except for λ_i, $i = 1, t-1$, and t. Then the result follows from Lemma 3.1. ∎

Let us review the procedure for calculating upper (and then lower) bounds for $\det A$, from Theorem 3.1. We use pseudo-programming language. We include the subscripts for A_k, L_k etc. . . . , for clarity only.

Comment Calculate upper bounds for $\det A$ from (3.6). The diagonal elements of A are assumed ordered.

INITIALIZATION

$$A_n = \sum_{i=1}^{n} a_{ii}, \qquad L_n = \sum_{i=1}^{n} a_{ii}^2 + 2\sum_{i<j} |a_{ij}|^2;$$

$$m_n = A_n/n; \qquad s_n^2 = L_n/n - m_n^2;$$

$$\mu_n = m_n - s_n/(n-1)^{1/2}; \qquad u_n = m_n + s_n(n-1)^{1/2};$$

Set $k = n$

Write The first (upper) estimates for $\lambda_1, \lambda_2, \lambda_n$ and $\det A$ are:

$$\lambda_1 \leqslant u_k; \qquad \lambda_2 \geqq \mu_k \geqslant \lambda_k;$$

$$\det A \leqslant u_k(\mu_k)^{(k-1)}.$$

LOOP *While* $\mu_k > a_k$ and $k \geqslant 3$ do:

set $k = k - 1$

$$A_k = A_{k+1} - a_{k+1}; \qquad L_k = L_{k+1} - a_{k+1}^2;$$

$$m_k = A_k/k; \qquad s_k^2 = L_k/k - m_k^2;$$

$$\mu_k = m_k - s_k/(k-1)^{1/2}; \qquad u_k = m_k + s_k(k-1)^{1/2};$$

Write Improved (upper) estimates for $\lambda_1, \lambda_2, \lambda_3$ and $\det A$ are:

$$\lambda_1 \leqslant u_k; \qquad \lambda_2 \geqslant \mu_k \geqslant \lambda_k$$

$$\det A \leqslant u_k(\mu_k)^{k-1} a_{k+1} \ldots a_n$$

End while

Set $t = k$.

We see that it takes $(n^2 + n)/2 + 8$ multiplications and $(n^2 + n)/2 + 3$ additions for the first estimates. Each improvement takes 8 multiplications and 5 additions. There are at most $n - 2$ improvements.

Comment Calculate lower bounds for $\det A$ from (3.7). The diagonal elements of A are assumed ordered.

Initialization

$$A_{-n} = A_n; \qquad L_{-n} = L_n; \qquad m_{-n} = m_n; \qquad s^2_{-n} = s^2_n;$$

$$v_{-n} = m_{-n} + s_{-n}/(n-1)^{1/2}; \qquad b_{-n} = m_{-n} - s_{-n}(n-1)^{1/2}$$

Set $k = n$

Write The first (lower) estimates for $\lambda_n; \lambda_{n-1}, \lambda_1$ and $\det A$ are:

$$\lambda_n \geqslant b_{-n}; \qquad \lambda_{k-1} \leqslant v_{-k} \leqslant \lambda_1;$$

$$\det A \geqslant \max\{0, b_{-k}(v_{-k})^{k-1}\}$$

LOOP *While* $v_k < a_{n-k+1}$ and $k \geqslant 3$ do:

Set $k = k - 1$

$$A_{-k} = A_{-(k+1)} - a_{n-k}; \qquad L_{-k} = L_{-(k+1)} - a^2_{n-k};$$

$$m_{-k} = A_{-k}/k; \qquad s^2_{-k} = L_{-k}/k - m^2_{-k};$$

$$v_{-k} = m_{-k} + s_{-k}/(k-1)^{1/2}; \qquad b_{-k} = m_{-k} - s_{-k}(k-1)^{1/2};$$

Write Improved (lower) estimates for $\lambda_n, \lambda_{n-1}, \lambda_{n-k+1}$ and $\det A$ are:

$$\lambda_n \geqslant b_{-k}; \qquad \lambda_{n-1} \leqslant v_{-k} \leqslant \lambda_{n-k+1}$$

$$\det A \geqslant \max\{0, b_{-k}(v_{-k})^{k-1}\} a_1 \ldots a_k$$

End while

Set $r = k$.

We have taken the lower estimates as a maximum with 0, since the lower estimates for λ_n, denoted b_{-k}, can be negative. The complexity of calculating these bounds compares with the upper bounds. Of course, we do not have to redo the bulk of the work, which is to calculate $L_{-n} = L_n$.

In the above theorem, we see that we can obtain improved estimates as long as $\mu_k > a_k$. Moreover, the last estimate satisfies $a_{t+1} \leqslant \mu_t a_t$. Thus, we cannot obtain any improvements if the diagonal elements of A are all equal, i.e. $a_1 = \cdots = a_n$. We now scale A to obtain equal diagonal elements and apply (2.1). This yields very good estimates for $\det A$.

THEOREM 3.2 *Let $A = (a_{ij})$ be an $n \times n$ Hermitian positive definite* *matrix; let*

$$\bar{L} = \sum_{i,j} |a_{ij}|^2/(a_{ii}a_{jj}); \qquad \bar{s}^2 = \bar{L}/n - 1;$$

$$u = 1 + \bar{s}(n-1)^{1/2}; \qquad \mu = 1 - \bar{s}/(n-1)^{1/2};$$

$$b = 1 - \bar{s}(n-1)^{1/2}; \qquad v = 1 + \bar{s}/(n-1)^{1/2}.$$

Then

$$bv^{n-1}\prod_{i=1}^{n} a_{ii} \leqslant \det A \leqslant u\mu^{n-1}\prod_{i=1}^{n} a_{ii} \tag{3.8}$$

Proof Let $B = DAD$, where D is the diagonal matrix with elements $1/\sqrt{a_{ii}}$. Then the diagonal elements of B are all equal to 1 and $\operatorname{tr} B^2 = \bar{L}$. Moreover $\det A = \det B \prod_{i=1}^{n} a_{ii}$. Applying (1.2) to B, yields the result. ■

The bounds in (3.8) require $(3n^2 - n)/2 + 8$ multiplications and so are still of the order of n^2 multiplications.

4. EXAMPLES

We now present several examples illustrating our bounds. Let us number the bounds as follows:

1. the bound from Hadamard's inequality (1.1);
2. the bounds from (1.2);
3. the bounds from (3.6) and (3.7) in Theorem 3.1;
4. the bounds from (3.8) in Theorem 3.2.

Bound 1 is the best possible bound given the diagonal elements of A. Equality is attained if and only if A is diagonal. Bounds 2 are the best possible bounds given n, $\operatorname{tr} A$ and $\operatorname{tr} A^2$. Conditions for equality depend on the eigenvalues of A (see Theorem 3.1). The upper bound from bound 2 can be better than bound 1 and vice-versa.

Example 4.1 If A is diagonal, then bound 1 is exact. This is not true for bound 2. Let $A = \operatorname{diag}(1, 2, 3)$. Then

$$\det A = 6 = \text{bound } 1 < \text{bound } 2 = 6.385$$

Conversely, bound 2 might be better than bound 1. Let

$$A = \begin{bmatrix} 5 & 1 & 1 \\ 1 & 4 & 1 \\ 1 & 1 & 3 \end{bmatrix}.$$

Then the upper bounds are

$$\det A = 50 < \text{bound } 2 = 51.065 < \text{bound } 1 = 60.$$

Bounds 3 improve on bound 1 and also improve on bounds 2 by using the diagonal elements of A. Bounds 3 give the best possible bounds given n, $\operatorname{tr} A$, $\operatorname{tr} A^2$ and the ordered diagonal elements of A. Conditions for equality again depend on the eigenvalues (see Theorem 3.1).

Bounds 4 are obtained by applying bounds 2 to the matrix $B = DAD$, obtained by scaling A. Here $D^{-1} = \operatorname{diag}(\sqrt{a_{11}}, \ldots, \sqrt{a_{nn}})$. Equality is attained if and only if equality is attained when applying bounds 2 to B. Thus, equality depends on the eigenvalues of B. Since the diagonal elements of B are all 1, bounds 2 and bounds 3 are equal when applied to B. Moreover, bound 1 is exactly 1, so the upper bound 2, for B, must be $\leqslant 1$. Thus the upper bound 4 is always an improvement on bound 1. However, this is not the case for bounds 2 (and so not for bounds 3).

Example 4.2 Let

$$A = \begin{bmatrix} 11/6 & 1/3 & 1/6 \\ 1/3 & 4/3 & -1/3 \\ 1/6 & -1/3 & 11/6 \end{bmatrix}$$

Then, the lower bounds are

$$\det A = 4 = \text{bound } 2 = \text{bound } 3 = 4 > \text{bound } 4 = 3.983$$

Thus bound 2 is better than bound 4. However the reverse is true for the upper bound in this example, i.e.

$$\det A = 4 < \text{bound } 4 = 4.091 < \text{bound } 2 = \text{bound } 3 = 4.148$$

The eigenvalues of A are $1, 2, 2$. Thus equality holds for the lower bound 2. If we choose A with eigenvalues $1, 1, 2$, then we would get equality for the upper bound 2 which would now be better than the upper bound 4.

However, it appears that the bounds 4 usually yield the best estimates. We see this in the following examples.

Example 4.3 Let

$$A = \begin{bmatrix} 5 & -2 & 3 \\ -2 & 2 & -3 \\ 3 & -3 & 10 \end{bmatrix}$$

Then the eigenvalues are 3.682, 12.607, .711; and $\det A = 33$.

bound 1: $\det A \leqslant 100$
bound 2: $\det A \leqslant 56.092$
bound 3: $\det A \leqslant 56. \leqslant 56.092$
bound 4: $\det A \leqslant 37.235$

The lower bounds 2, 3, 4 are all negative. The eigenvalues of $B = DAD$ are 2.158, .577, .265. The upper bound 3 was improved once.

Example 4.4 Let

$$A = \begin{bmatrix} 15 & 3 & 1 & 1 \\ 3 & 10 & 2 & 1 \\ 1 & 2 & 5 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix}$$

Then the eigenvalues are 16.813, 9.081, .705, 4.401; and $\det A = 474$.

bound 1: $\det A \leqslant 750$
bound 2: $\det A \leqslant 1421.42$
bound 3: $\det \mathrm{A} \leqslant 655. \leqslant 684.766 \leqslant 1421.42$
bound 4: $190.019 \leqslant \det A \leqslant 496.184$

The lower bounds 2, 3 are negative. The eigenvalues of $B = DAD$ are 1.852, .908, .527, .714. The upper bound 3 was improved twice.

Example 4.5 Let

$$A = \begin{bmatrix} 15 & 3 & 1 \\ 3 & 10 & 2 \\ 1 & 2 & 5 \end{bmatrix}$$

Then the eigenvalues are 16.674, 9.028, 4.299; and $\det A = 647$.

bound 1: $\det A \leqslant 750$
bound 2: $516.256 \leqslant \det \mathrm{A} \leqslant 703.743$
bound 3: $516.256 \leqslant 540. \leqslant \det A \leqslant 680. \leqslant 703.743$
bound 4: $617.667 \leqslant \det A \leqslant 652.333$

The eigenvalues of $B = DAD$ are 1.436, .886, .678. The bounds 3 were improved once.

In the last three examples, the bounds 4 were distinctly better than the other bounds. The scaling $B = DAD$ appears to 'average' the eigenvalues; i.e. the variance of the eigenvalues of B is smaller than that of A. Thus, we are closer to the conditions for equality when the bounds 2 are applied to B. This raises the question of which is the best scaling and suggests that if we are interested in a good upper bound, then we should scale to get closer to the condition $\lambda_2 = \cdots = \lambda_n$; while if we are interested in a good lower bound then we should scale to get closer to the condition $\lambda_1 = \cdots = \lambda_{n-1}$. Intuitively, we could let $D_1^{-1} = \operatorname{diag}(1\sqrt{a_{22}}, \ldots, \sqrt{a_{nn}})$ or $D_2^{-1} = \operatorname{diag}(\sqrt{a_{11}}, \ldots, \sqrt{a_{n-1}}, 1)$. (Where we have assumed that the a_{ii} are ordered.) For example, if we apply the second scaling $D^{-1} = \operatorname{diag}(\sqrt{5}, 1, \sqrt{10})$ to A in Example 4.3, we get that $\det A \leqslant 34.333$ which improves our previous bounds. The eigenvalues of B in this case are 3.047, .578, .265; so that we see we have come closer to the condition $\lambda_2 = \lambda_3$.

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