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The best possible lower bound for the Perron root using traces

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Abstract

Let A be an $n \times n$ matrix with real eigenvalues. Wolkowicz and Styan presented bounds for the eigenvalues, using only n, $\operatorname{tr} A$, and $\operatorname{tr} A^2$. We show that their lower bound for the largest eigenvalue works also as a lower bound for the Perron root of A if A is nonnegative and its eigenvalues are not necessarily real. We also show that this bound is optimal under certain conditions. Finally, we solve completely the problem to find the optimal lower bound for the Perron root using only n, $\operatorname{tr} A$, and $\operatorname{tr} A^2$.

1. Introduction

Throughout this paper, we use the following notations:

$A = (a_{jk})$ is a real or complex $n \times n$ matrix, $n \geqslant 3$;
$\lambda_1 = \lambda_1(A), \dots, \lambda_n = \lambda_n(A)$ are the eigenvalues of A, ordered $\lambda_1 \geqslant \cdots \geqslant \lambda_n$ if they are real;
$A \geqslant 0$ means that A is real and nonnegative;
$r = r(A)$ is the Perron root of $A \geqslant 0$;
$a = \operatorname{tr} A$, $b = \operatorname{tr} A^2$.

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If a and b are real and $a^2 \leqslant nb$ (which happens, for example, if $\lambda_1, \ldots, \lambda_n$ are real or if $A \geqslant 0$), we denote

$$l = \frac{a}{n} + \sqrt{\frac{1}{n(n-1)}\left(b - \frac{a^2}{n}\right)}, \quad u = \frac{a}{n} + \sqrt{\frac{n-1}{n}\left(b - \frac{a^2}{n}\right)},$$

$$l' = \frac{a}{n} - \sqrt{\frac{n-1}{n}\left(b - \frac{a^2}{n}\right)}, \quad u' = \frac{a}{n} - \sqrt{\frac{1}{n(n-1)}\left(b - \frac{a^2}{n}\right)}.$$

We may use also the notation $l(A)$ etc.

Theorem 1 (Wolkowicz and Styan [10, Theorem 2.1]). *If $\lambda_1, \ldots, \lambda_n$ are real, then $l \leqslant \lambda_1 \leqslant u$ and $l' \leqslant \lambda_n \leqslant u'$. Equality holds on the left (right) of these inequalities if and only if the $n-1$ largest (smallest) eigenvalues are equal.*

Theorem 2 (The first part of [10, Theorem 2.3]). *If $\lambda_1, \ldots, \lambda_n$ are real, then, for $1 \leqslant k \leqslant n$,*

$$\lambda_1 + \cdots + \lambda_k \geqslant \begin{cases} kl & \text{if } k \leqslant \frac{1}{2}n, \\ u + (k-1)u' & \text{if } k \geqslant \frac{1}{2}n. \end{cases}$$

Equality holds if and only if

$$\begin{array}{ll} \lambda_1 = \cdots = \lambda_{n-1} & \text{for } k < \frac{1}{2}n, \\ \lambda_1 = \cdots = \lambda_{n-1} \text{ or } \lambda_2 = \cdots = \lambda_n & \text{for } k = \frac{1}{2}n, \\ \lambda_2 = \cdots = \lambda_n & \text{for } k > \frac{1}{2}n. \end{array}$$

For the origin of Theorem 1, see Jensen and Styan [4] and Jensen [3]. Theorem 2 (without matrix formulation) is due to Mallows and Richter [6, Corollary 6.1]. We omit the second part of [10, Theorem 2.3], since it follows directly from the first part.

Let a and b be arbitrary real numbers satisfying $a^2 \leqslant nb$. Then, for each inequality of Theorems 1 and 2, there exists a matrix A with $\operatorname{tr} A = a$, $\operatorname{tr} A^2 = b$, $\lambda_1, \ldots, \lambda_n$ real, such that equality holds. This follows from the equality conditions stated in these theorems. Therefore the eigenvalue bounds given by these inequalities are *optimal*. In other words, they are the best possible bounds, using only n, a, and b.

Wolkowicz and Styan [10, Section 3] extended Theorems 1 and 2 and related results for the case when $\lambda_1, \ldots, \lambda_n$ are not necessarily real. We pursue this topic further by showing that if $A \geqslant 0$, then l is a lower bound for its Perron root r. We will also show that l is optimal under certain conditions (Theorem 8). Finally (Theorem 10), we will solve completely the problem to find the optimal lower bound for r, using only n, a, and b.

2. The lower bound l for r

If $\lambda_1, \ldots, \lambda_n$ are not necessarily real, we can modify Theorem 2 to hold for their real parts. In [10, Theorem 3.5], different bounds of the same kind are presented for normal matrices.

Theorem 3. *Order $\lambda_1, \ldots, \lambda_n$ so that $\operatorname{re}\lambda_1 \geqslant \cdots \geqslant \operatorname{re}\lambda_n$. Assume that $a = \operatorname{tr} A$ and $b = \operatorname{tr} A^2$ are real and that $a^2 \leqslant nb$. Then*

$$\operatorname{re}\lambda_1 + \cdots + \operatorname{re}\lambda_k \geqslant \begin{cases} kl & \text{if } k \leqslant \frac{1}{2}n, \\ u + (k-1)u' & \text{if } k \geqslant \frac{1}{2}n. \end{cases}$$

In particular,

$$\operatorname{re}\lambda_1 \geqslant l.$$

Equality holds if and only if $\lambda_1, \ldots, \lambda_n$ are real and satisfy the equality conditions of Theorem 2.

Proof. Since

$$a = \operatorname{tr} A = \operatorname{re}\operatorname{tr} A = \operatorname{re}\lambda_1 + \cdots + \operatorname{re}\lambda_n,$$
$$b = \operatorname{tr} A^2 = \operatorname{re}\operatorname{tr} A^2 = \operatorname{re}\lambda_1^2 + \cdots + \operatorname{re}\lambda_n^2 = \sum_{k=1}^{n} (\operatorname{re}\lambda_k)^2 - \sum_{k=1}^{n} (\operatorname{im}\lambda_k)^2,$$

we have

$$\operatorname{re}\lambda_1 + \cdots + \operatorname{re}\lambda_n = a, \quad (\operatorname{re}\lambda_1)^2 + \cdots + (\operatorname{re}\lambda_n)^2 = \beta \geqslant b.$$

Applying Theorem 2 to $B = \operatorname{diag}(\operatorname{re}\lambda_1, \ldots, \operatorname{re}\lambda_n)$ and noting that $l(B)$ is a strictly increasing function of β, the inequality follows. The equality conditions are obvious. □

Theorem 4. *The lower bounds for $\operatorname{re}\lambda_1 + \cdots + \operatorname{re}\lambda_k$ presented in Theorem 3 are optimal.*

Proof. If a and b are arbitrary real numbers satisfying $a^2 \leqslant nb$, there exists a matrix A with $\operatorname{tr} A = a$, $\operatorname{tr} A^2 = b$, such that equality holds in the relevant inequality of Theorem 3. This follows from the equality conditions stated in this theorem. □

Since the Perron root of a nonnegative matrix is greater than the real part of any other eigenvalue, Theorem 3 implies the following

Corollary 5. *If $A \geqslant 0$, then $r \geqslant l$.*

If $a^2 \geqslant nb$, then we have only the trivial result

$$\operatorname{re}\lambda_1 + \cdots + \operatorname{re}\lambda_k \geqslant \frac{k}{n}a.$$

In particular,

$$\operatorname{re}\lambda_1 \geqslant \frac{a}{n}.$$

Equality holds if and only if $\operatorname{re}\lambda_1 = \cdots = \operatorname{re}\lambda_n (= a/n)$. These lower bounds are clearly optimal if we know only n and a. The fact that $\operatorname{tr} A^2 = b$ does not now give further information, since if we know a, we can make b (with $a^2 \geqslant nb$) arbitrary. Simply take

$$\lambda_1 = \frac{a}{n} + x\mathrm{i}, \quad \lambda_2 = \cdots = \lambda_{n-1} = \frac{a}{n}, \quad \lambda_n = \frac{a}{n} - x\mathrm{i},$$

where

$$x = \sqrt{\frac{a^2 - nb}{2n}}.$$

An alternative proof of Corollary 5 is to define the *geometric symmetrization* of A as $G = (g_{jk})$ with $g_{jk} = \sqrt{a_{jk}a_{kj}}$. If A is irreducible, then by Schwenk [8, p. 261]

$$r(G) \leqslant r(A),$$

which holds also in the reducible case by a continuity argument. Since $\operatorname{tr} G = a$, $\operatorname{tr} G^2 = b$, we have $r(G) \geqslant l$ by Theorem 1, and so the corollary follows.

Another alternative proof is to apply to the spectral radius $\rho(A)$ an inequality of Horne [2, Theorem 1 (5)] reformulated as

$$\rho(A) \geqslant \max(|l|, |u'|),$$

and to note that, for $A \geqslant 0$, we have $r = \rho(A)$ (and $l = |l| \geqslant |u'|$).

Corollary 5 motivates us to ask whether $r \leqslant u$ holds. The answer is negative. In fact, we can say more.

Proposition 6. *If $A \geqslant 0$, there exists no upper bound for r, using only n, a, and b.*

Proof. Suppose that such an upper bound $f(n, a, b)$ exists. For $t \geqslant 0$, let

$$A_t = \begin{pmatrix} 0 & t & 0 \\ 0 & 0 & t \\ t & 0 & 0 \end{pmatrix}.$$

Then $r(A_t) = t$, $a = b = 0$, and so $t \leqslant f(3, 0, 0)$. This is a contradiction, since the left-hand side can be made arbitrarily large, while the right-hand side is a constant. □

3. Optimality of l ($A \geqslant 0$)

If $A \geqslant 0$, then $\sqrt{b/n}$ is a trivial lower bound for r. We compare l with it.

Lemma 7. *Let a and b be real numbers satisfying $a^2 \leqslant nb$. The following conditions are equivalent*:

(a) $l \geqslant \sqrt{\frac{b}{n}}$,

(b) $\frac{na^2}{(n-2)^2} \geqslant b$,

(c) $l \geqslant |l'|$,

(d) *There exists $A \geqslant 0$ with eigenvalues $l = l(A)$ of multiplicity $n-1$ and $l' = l'(A)$ of multiplicity one.*

Proof. To show (a) ⇔ (b) ⇔ (c) is elementary, but not quite easy. We omit it. We have (d) ⇒ (c) by the Perron–Frobenius theorem. If $l' \geqslant 0$, then (c) ⇒ (d) is trivial. If $l' < 0$, this implication follows by considering

$$A = lI_{n-2} \oplus \begin{pmatrix} l+l' & \sqrt{-ll'} \\ \sqrt{-ll'} & 0 \end{pmatrix}$$

where I_{n-2} denotes the identity matrix of order $n-2$. □

Now we can answer partially the question of optimality.

Theorem 8. *Let $A \geqslant 0$. Then l is optimal* (*i.e., the best possible lower bound for r, using only n, a, and b, and the information that $A \geqslant 0$*) *if and only if the equivalent conditions of Lemma 7 are satisfied.*

Proof. Let a and b be real numbers satisfying $a^2 \leqslant nb$. If (d) in Lemma 7 holds, then there exists $A \geqslant 0$ with $\operatorname{tr} A = a$, $\operatorname{tr} A^2 = b$, such that $l(A) = r(A)$, and therefore l is optimal. If (a) does not hold, then every $A \geqslant 0$ with $\operatorname{tr} A = a$, $\operatorname{tr} A^2 = b$ satisfies

$$l(A) < \sqrt{\frac{b}{n}} \leqslant r(A),$$

and therefore l is not optimal.

To find the optimal bound in the case when l is not optimal, denote

$$N_k = n - 4k\frac{n-k-1}{n-1}, \quad 0 \leqslant k \leqslant \left\lfloor \frac{n-1}{2} \right\rfloor,$$

$$l_k = \frac{n-2k-1}{n-1}\frac{a}{N_k} + \sqrt{\frac{1}{N_k(n-1)}\left(b - \frac{a^2}{N_k}\right)},$$

$$K = \left\{ k \in \left\{0, \ldots, \left\lfloor \frac{n-1}{2} \right\rfloor \right\} \,\middle|\, \frac{na^2}{(n-2k)^2} \leqslant b \right\},$$

$$\kappa = \max K.$$

Note that $N_0 = n$, $l_0 = l$. Also note that $K \neq \emptyset$, since $0 \in K$. If $k \leqslant \kappa$, then l_k is real, since

$$N_k(n-1) = (-1-2k+n)^2 + n - 1 > 0$$

and

$$b - \frac{a^2}{N_k} \geqslant \frac{na^2}{(n-2k)^2} - \frac{a^2}{N_k} = a^2 \frac{4k^2}{(n-2k)^2} \frac{1}{N_k(n-1)} \geqslant 0. \qquad \square$$

Theorem 9. *Let $A \geqslant 0$. If*

$$\frac{na^2}{(n-2k)^2} \leqslant b; \quad i.e., \quad k \in K,$$

then $r \geqslant l_k$.

Theorem 10. *Let $A \geqslant 0$, $k \in K$. The following conditions are equivalent*:

(a) l_k *is optimal* (*i.e., the best possible lower bound for r, using only n, a, and b, and the information that $A \geqslant 0$*),
(b) $l_k = l_\kappa$,
(c) $l_k \geqslant \sqrt{\frac{b}{n}}$.

The proofs of Theorems 9 and 10 are quite long and technical. They are presented in Appendix A.

If $a = 0$, then $\kappa = \lfloor \frac{n-1}{2} \rfloor$, and we obtain

Corollary 11. *Let $A \geqslant 0$. If $a = 0$, then the optimal lower bound for r is*

$$\begin{cases} \sqrt{\frac{b}{n}} & \text{if } n \text{ is even,} \\ \sqrt{\frac{b}{n-1}} & \text{if } n \text{ is odd.} \end{cases}$$

Szulc [9, Theorem 1] presented the following lower bound for the Perron root:

$$r \geqslant \rho_S = \begin{cases} \rho_{S_1} & \text{if } n \text{ is even,} \\ \max\{\rho_{S_1}, \rho_{S_2}\} & \text{if } n \text{ is odd,} \end{cases}$$

where

$$\rho_{S_1} = \min_k a_{kk} + \sqrt{\frac{\operatorname{tr}(A - \min_k a_{kk} I)^2}{n}},$$

$$\rho_{S_2} = \min_k a_{kk} + \sqrt{\frac{2}{n-1} \sum_{1 \leqslant j < k \leqslant n} a_{jk} a_{kj}}.$$

If $a = 0$, then all diagonal elements of A are zero and $b = 0 + \operatorname{tr}(A - 0I)^2 = 2\sum_{1\leqslant j<k\leqslant n} a_{jk}a_{kj}$. It follows that in this case $\rho_S = l_\kappa$. Hence Corollary 11 shows that ρ_S is optimal when $a = 0$.

4. Examples

We compare our bounds with the following simple bounds:

$\rho_F = \max(\min_k r_k, \min_k c_k)$ (Frobenius, see e.g. [1, p. 492]),

$\rho_0 = \sqrt{\frac{b}{n}}$ (Lemma 7),

ρ_S (Szulc [9], see above),

$\rho_K = \frac{1}{n}\sum_j \sum_k g_{jk}$ (Kolotilina [5]).

Here $r_1, \ldots, r_n$ $(c_1, \ldots, c_n)$ are the row (column) sums and $G = (g_{jk})$ is the geometric symmetrization of A.

Example 1

$$A = \begin{pmatrix} 1 & 1 & 2 \\ 2 & 1 & x \\ 2 & 3 & 5 \end{pmatrix}, \quad x \geqslant 0.$$

If $x = 3$, then A is singular and therefore all its eigenvalues are real. Hence Wolkowicz and Styan [10, Example 2] could apply Theorem 1 in the case $x = 3$. We can study the general case.

If $x < 18$, then $\kappa = 0$ and the optimal lower bound for r using n, a, b is

$$l = \frac{7 + \sqrt{9x + 34}}{3}.$$

If $x \geqslant 18$, then $\kappa = 1$ and the optimal bound is

$$l_1 = \sqrt{3x - 5}.$$

The bounds listed above are

$$\rho_F = \begin{cases} x + 3 & \text{if } x < 1, \\ 4 & \text{if } x \geqslant 1, \end{cases}$$

$$\rho_0 = \sqrt{2x + 13},$$

$$\rho_{S_1} = 1 + \sqrt{\tfrac{6x+28}{3}},$$

$$\rho_{S_2} = 1 + \sqrt{3x + 6},$$

$$\rho_K = \tfrac{2\sqrt{3x}+2\sqrt{2}+11}{3}.$$

1. l and l_1 vs. ρ_{F}
   We have $l > \rho_{\mathrm{F}}$ for all x and $l_1 > l > \rho_{\mathrm{F}}$ for all $x > 18$. Giving $x \to \infty$, we see that l and l_1 can be made infinitely much better than ρ_{F}.
2. l and l_1 vs. ρ_0
   We note that $l \leqslant \rho_0 \Leftrightarrow x \geqslant 18 \Leftrightarrow l_1 \geqslant \rho_0$, confirming Theorem 10.
3. l and l_1 vs. ρ_{S}
   We have $l \geqslant \rho_{\mathrm{S}_1} \Leftrightarrow x \leqslant 3\frac{1}{3}$ and $l_1 \geqslant \rho_{\mathrm{S}_1} \Leftrightarrow x \geqslant \frac{2(29+6\sqrt{11})}{3} \approx 32.6$.
   Since ρ_{S_1} is obtained from ρ_0 by shifting, we include also the shifted bound $L_1 = t + l_1(A - tI)$, $t = \min_k a_{kk}$. Now $L_1 = \rho_{\mathrm{S}_2}$ (this is true whenever n is odd and at least $n-1$ diagonal elements of A are equal). We obtain
   $$\rho_{\mathrm{S}} = \begin{cases} \rho_{\mathrm{S}_1} & \text{if } x \leqslant 3\frac{1}{3}, \\ \rho_{\mathrm{S}_2} & \text{if } x \geqslant 3\frac{1}{3}, \end{cases}$$
   and
   $$\begin{cases} \rho_{\mathrm{S}} < l & \text{if } x < 3\frac{1}{3}, \\ \rho_{\mathrm{S}} = L_1 = l & \text{if } x = 3\frac{1}{3}, \\ \rho_{\mathrm{S}} = L_1 > \rho_{\mathrm{S}_1} > l & \text{if } x > 3\frac{1}{3}. \end{cases}$$
   Note that $l = t + l(A - tI)$ for all t.
4. l and l_1 vs. ρ_{K}
   We have $l < \rho_{\mathrm{K}}$ for all x and $l_1 > \rho_{\mathrm{K}} \Leftrightarrow x > \frac{2(951+286\sqrt{2}+6\sqrt{23{,}738+12{,}452\sqrt{2}})}{75} \approx 68.7$.

Example 2

$$A = \begin{pmatrix} 4 & 1 & 1 & 2 & 2 \\ 1 & 5 & 1 & 1 & 1 \\ 1 & 1 & 6 & 1 & 1 \\ 2 & 1 & 1 & 7 & 1 \\ 2 & 1 & 1 & 1 & 8 \end{pmatrix}.$$

The matrix A is symmetric and hence has real eigenvalues. Wolkowicz and Styan [10, Example 5] obtained the bound

$$l \approx 7.45 \leqslant r(A) \approx 11.17.$$

Now $\kappa = 0$ and hence l is the best possible lower bound using only $n = 5$, $\operatorname{tr} A = 30$, and $\operatorname{tr} A^2 = 222$. In particular, $\rho_0 \approx 6.66 < l$.

Using the information that $A \geqslant 0$ and $\min_k a_{kk} = 4$, we obtain a better lower bound $\rho_{\mathrm{S}} = \rho_{\mathrm{S}_1} \approx 7.52 \leqslant r(A)$ (note that $\rho_{\mathrm{S}_2} \approx 6.83 < l$) and, since $\kappa(A - 4I) = 1$, a still better lower bound

$$L_1 = l_1(A - 4I) + 4 \approx 7.72 \leqslant r(A).$$

However, $\rho_{\rm F} = 9$ and $\rho_{\rm K} = 10.8$ are much better lower bounds in this example. Since A is symmetric,

$$\rho_{\rm K} = \frac{1}{n}\sum_j\sum_k a_{jk}.$$

It is well-known [7] that this bound is often good.

Example 3. We compare $l = l_0$ with l_κ when $n = 4$. Since $r(cA) = cr(A)$ and $l_k(cA) = cl_k(A)$, we can assume without loss of generality that $\operatorname{tr} A = 1$ and $\operatorname{tr} A^2 = b \geqslant 1/4$. Then

$$\kappa = \begin{cases} 0 & \text{if } 1/4 \leqslant b < 1, \\ 1 & \text{if } 1 \leqslant b, \end{cases}$$

$$l = l(b) = \tfrac{1}{12}\left(3 + \sqrt{12b-3}\right) \quad \left(b \geqslant \tfrac{1}{4}\right),$$
$$l_1 = l_1(b) = \tfrac{1}{4}\left(1 + \sqrt{4b-3}\right) \quad (b \geqslant 1).$$

For all $b > 1$,

$$l(b) < l_1(b) < \sqrt{3}l(b),$$

$l_1(b)/l(b)$ increases, and $\lim_{b\to\infty} l_1(b)/l(b) = \sqrt{3}$:

b	$l(b)$	$l_1(b)$	$l_1(b)/l(b)$
1	0.50	0.50	1.00
10	1.15	1.77	1.54
100	3.13	5.23	1.67
1000	9.38	16.06	1.71
10,000	29.12	50.25	1.73

Note that for each $b \geqslant 1/4$ there exists such A that $\operatorname{tr} A = 1$, $\operatorname{tr} A^2 = b$, and $r(A) = l_\kappa$. For example, let $b = 10{,}000$. Then

$$A = \begin{pmatrix} 0 & x & 0 & 0 \\ x & 0 & 0 & 0 \\ 0 & 0 & x+y & \sqrt{-xy} \\ 0 & 0 & \sqrt{-xy} & 0 \end{pmatrix} \approx \begin{pmatrix} 0 & 50.25 & 0 & 0 \\ 50.25 & 0 & 0 & 0 \\ 0 & 0 & 1 & 49.75 \\ 0 & 0 & 49.75 & 0 \end{pmatrix},$$

where $x = (1 + \sqrt{39{,}997})/4$, $y = (3 - \sqrt{39{,}997})/4$, satisfies $\operatorname{tr} A = 1$, $\operatorname{tr} A^2 = 10{,}000$, and $r(A) = l_1 \approx 50.25$.

Example 4. We compare l_κ with ρ_0 when $n = 10$. Without loss of generality, we can assume that $\operatorname{tr} A^2 = 10$ and $\operatorname{tr} A = a$ $(0 \leqslant a \leqslant 10)$. Then $\rho_0 = 1$ and

	κ
$0 \leqslant a \leqslant 2$	4
$2 < a \leqslant 4$	3
$4 < a \leqslant 6$	2
$6 < a \leqslant 8$	1
$8 < a \leqslant 10$	0

Denote here $l_k = l_k(a)$. Now $l_\kappa(a) = 1 = \rho_0$ for $a = 0, 2, \dots, 10$. By calculating $\max_{a\in[0,2]} l_4(a)$, $\max_{a\in]2,4]} l_3(a)$, etc., we find that

$$\rho_0 = 1 \leqslant l_\kappa(a) \leqslant \sqrt{10}/3 \approx 1.054\rho_0 \quad \text{for all } a \in [0, 10].$$

To see that $l_\kappa(a) = \sqrt{10}/3$ is attained, let $A = (a_{jk})$, where $a_{jk} = \sqrt{10}/3$ for

$$(j, k) \in \{(1, 1), (3, 4), (4, 3), (5, 6), (6, 5), (7, 8), (8, 7), (9, 10), (10, 9)\}$$

and $a_{jk} = 0$ otherwise. Then

$$\rho_0 = 1 < 1.054 \approx l_4(A) = r(A) = \sqrt{10}/3.$$

Discussion. Our bounds are in some cases better than other well-known simple bounds, see Examples 1 and 2. The bound l_1 may clearly improve l, see Example 3. If n is not very small, then l_κ improves ρ_0 only marginally, see Example 4, but we still found interesting to settle the question of optimality.

Appendix A. The proofs of Theorems 9 and 10

We recall the notations

$$K(b) = K = \left\{k \in \left\{0, \dots, \left\lfloor \frac{n-1}{2} \right\rfloor\right\} \,\middle|\, \frac{na^2}{(n-2k)^2} \leqslant b\right\},$$
$$\kappa(b) = \kappa = \max K(b),$$
$$N_k = n - 4k\frac{n-k-1}{n-1}, \quad 0 \leqslant k \leqslant \left\lfloor \frac{n-1}{2} \right\rfloor,$$
$$l_k(b) = l_k = \frac{n-2k-1}{n-1}\frac{a}{N_k} + \sqrt{\frac{1}{N_k(n-1)}\left(b - \frac{a^2}{N_k}\right)}.$$

We omit the proofs of the following three simple lemmas.

Lemma 12. *Let $k \leqslant \kappa$. For $k < \lfloor \frac{n-1}{2} \rfloor$,*

$$l_k(b) = \sqrt{\frac{b}{n}}$$

if and only if

$$b = \frac{na^2}{(n-2k)^2} \quad \text{or} \quad b = \frac{na^2}{(n-2k-2)^2}.$$

For $k = \lfloor \frac{n-1}{2} \rfloor$, exclude the last equality.

Lemma 13. *Let $k \leqslant \lfloor \frac{n-1}{2} \rfloor$. If*

$$b = \frac{na^2}{(n-2k-2)^2},$$

then $\kappa = k + 1$ *and*

$$l_k(b) = \sqrt{\frac{b}{n}} = l_{k+1}(b).$$

Lemma 14. *Let* $k \leqslant \kappa$. *If* $\kappa < \left\lfloor \frac{n-1}{2} \right\rfloor$, *then the following conditions are equivalent*:

(a) $|a - (n - 2k - 1)l_k| \leqslant l_k$,

(b) $\frac{a}{n-2k} \leqslant l_k \leqslant \frac{a}{n-2k-2}$,

(c) $\frac{na^2}{(n-2k)^2} \leqslant b \leqslant \frac{na^2}{(n-2k-2)^2}$,

(d) $\kappa = k$ *or* $\left(\kappa = k + 1 \text{ and } b = \frac{na^2}{(n-2k-2)^2}\right)$.

If $\kappa = \left\lfloor \frac{n-1}{2} \right\rfloor$, *exclude the latter inequality in* (b) *and* (c), *and the bracketed sentence in* (d).

A simple calculation shows that $(n - 1)l_k^2 + (a - (n - 2k - 1)l_k)^2 = b$ for $0 \leqslant k \leqslant \kappa$. Lemma 14 implies that if $k < \kappa$, then $|a - (n - 2k - 1)l_k| \geqslant l_k$, and so

$$b = (n - 1)l_k^2 + (a - (n - 2k - 1)l_k)^2 \geqslant nl_k^2.$$

If $k = \kappa$, we have $|a - (n - 2k - 1)l_k| \leqslant l_k$, and, similarly, $b \leqslant nl_k^2$.

Hence we have

Lemma 15. *If* $k < \kappa$, *then*

$$r \geqslant \sqrt{\frac{b}{n}} \geqslant l_k,$$

and if $k = \kappa$, *then*

$$\sqrt{\frac{b}{n}} \leqslant l_k.$$

Next we prove that $l_\kappa \leqslant r$. We begin with the following lemma.

Lemma 16. *If* $\lambda_1, \ldots, \lambda_n$ *are real*, *then* $r \geqslant l_\kappa$.

Proof. Assume, on the contrary, that $\lambda_1 < l_\kappa$. Then $\lambda_n > -l_\kappa$. By Lemma 14, $l_\kappa \geqslant a - (n - 2\kappa - 1)l_\kappa \geqslant -l_\kappa$. Hence the vector $(\lambda_1, \ldots, \lambda_n)$ is strictly majorized by the vector $(l_\kappa^{(n-\kappa-1)}, a - (n - 2\kappa - 1)l_\kappa, -l_\kappa^{(\kappa)})$ where $x^{(p)}$ denotes $x, \ldots, x$ (p times). Since the function $(x_1, x_2, \ldots, x_n) \mapsto \sum x_i^2$ is strictly Schur-convex, then

$$b = \sum_j \lambda_j^2 < (n - 1)l_\kappa^2 + (a - (n - 2\kappa - 1)l_\kappa)^2 = b,$$

a contradiction. □

Using Lemma 13, it is easy to see that the function $g(y) = l_{\kappa(y)}(y)$ is continuous when $y \geqslant a^2/n$. Since $l_k(y)$ is increasing for a fixed $k \leqslant \kappa(y)$, it follows that g increases on the interval $\left[\frac{a^2}{n}, \infty\right[$.

Let

$$\beta = (\mathrm{re}\,\lambda_1)^2 + \cdots + (\mathrm{re}\,\lambda_n)^2.$$

Since $\mathrm{re}\,\lambda_1 + \cdots + \mathrm{re}\,\lambda_n = a$, then $r = \max_j \, \mathrm{re}\,\lambda_j \geqslant g(\beta)$ by Lemma 16. Further, since $\beta \geqslant b$, we have $g(\beta) \geqslant g(b) = l_\kappa$. We can now state Lemma 16 without assuming the reality of the eigenvalues.

Lemma 17. *Let* $A \geqslant 0$. *Then* $r \geqslant l_\kappa$.

Theorem 9 follows from Lemmas 15 and 17. Lemmas 12 and 15 imply that if $l_k(b) \neq l_\kappa(b)$, then $l_k(b) < \sqrt{b/n}$. To complete the proof of Theorem 10, we need the following lemma.

Lemma 18. *Let a and b be real numbers satisfying* $a^2 \leqslant nb$. *Then there exists* $A \geqslant 0$ *with* $\mathrm{tr}\, A = a$, $\mathrm{tr}\, A^2 = b$, *such that* $r(A) = l_\kappa$.

Proof. Let $x = l_\kappa$, $y = a - (n - 2\kappa - 1)x$, and

$$B = \begin{pmatrix} 0 & x \\ x & 0 \end{pmatrix} \oplus \cdots \oplus \begin{pmatrix} 0 & x \\ x & 0 \end{pmatrix} \quad (\kappa \text{ times}).$$

If $y \geqslant 0$, define

$$A = \mathrm{diag}\left(x^{(n-2\kappa-1)}, y\right) \oplus B,$$

and if $y < 0$,

$$A = \mathrm{diag}\left(x^{(n-2\kappa-2)}\right) \oplus \begin{pmatrix} x + y & \sqrt{-xy} \\ \sqrt{-xy} & 0 \end{pmatrix} \oplus B.$$

Now $\mathrm{tr}\, A = a$ and $\mathrm{tr}\, A^2 = b$. Further, by Lemma 14, $x \geqslant |y|$, and hence $A \geqslant 0$ and $r(A) = x = l_\kappa$. $\square$

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