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RESULTS ON BOUNDS OF THE SPECTRUM OF POSITIVE DEFINITE MATRICES BY PROJECTIONS

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ABSTRACT. In this paper, we develop further the theory of trace bounds and show that in some sense that the earlier bounds obtained by various authors on the spectrum of symmetric positive definite matrices are optimal. Our approach is by considering projection operators, from which several mathematical relationships may be derived. Also criteria for positive lower bounds are derived.

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1. INTRODUCTION

Eigenvalues and the extreme eigenvalues play an important role in many scientific applied fields [4]. The determination of the zeroes of the characteristic polynomial is a difficult and expensive task to perform, especially for large dimensions. In some cases, only knowledge of the extreme eigenvalues is necessary, for example the ratio of the largest to smallest eigenvalues for a symmetric positive definite matrix determines the conditioning of the associated linear system. Perhaps the most well known bound for the spectrum $\sigma(\mathbf{A})$ is the Gerschgorin bound, where the eigenvalues lie in the union of n disks in the complex plain, centred at the diagonal entries and having radii the sum of the absolute off diagonal entries. Zhan [12] bounded the spread $sp(\mathbf{A})$ of real symmetric interval matrices. Sun [10] bounded the minimal eigenvalue of positive definite matrices and improved the bounds of Dembo [3] and Ma and Zarowski [7]. Mirskey [8], Brauer and Mewbom [1] used traces to bound $sp(\mathbf{A})$. Wolcowicz and Styan [11] used a statistical approach to bound the extremal eigenvalues of complex matrices with real eigenvalues. Their approach naturally led to extensive use of trace bounds. Sharma et al.[9] extended and improved the work of Wolcowiz and Styan. Trace bounds are elegant as they are functions only of the diagonal entries of a matrix and its associated powers.

2. THEORY

Let $\boldsymbol{\lambda} = (\lambda_i) \in \mathbb{R}^n$ be the vector of eigenvalues of a symmetric positive definite matrix $\mathbf{A} \in \mathbb{R}^{n\times n}$ and $f : (0, \infty) \longrightarrow (0, \infty)$ be an increasing function. Order the eigenvalues such that

$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n.$$

Define $f(\boldsymbol{\lambda}) = [f(\lambda_1),\, f(\lambda_2),\, \cdots ,\, f(\lambda_n)]^t$.

Lemma 2.1.

$$\frac{trace\,(f(\mathbf{A}))^2}{n} \leq trace\,(f(\mathbf{A})^2)$$

We shall prove 2.1 in two different ways.

Proof 1.

$$\begin{aligned} trace\,(f(\mathbf{A}))^2 &= \left(\sum_{i=1}^{n} f(\lambda_i)\right)^2 \\ &= n^2\left(\frac{\sum_{i=1}^{n} f(\lambda_i)}{n}\right)^2 \\ &\leq \frac{n^2}{n}\sum_{i=1}^{n} f(\lambda_i)^2 \\ &= n\,trace\,(f(\mathbf{A})^2) \end{aligned}$$

Where we have Jensen's inequality [5] applied to the convex function $(\cdot)^2$. ∎

Proof 2. This is our innovative new proof. Consider

$$\mathbf{P} = \mathbf{I} - \frac{\mathbf{e}\mathbf{e}^{\mathbf{t}}}{n},$$

then $\mathbf{P}$ is an orthogonal symmetric projector on to the $n-1$ dimensional subspace range $R(\mathbf{P}) \subset \mathbb{R}^n$. Also an orthonormal basis for the nullspace $N(\mathbf{P})$ is $\left\{\frac{\mathbf{e}}{\sqrt{n}}\right\}$. Then

$$f(\boldsymbol{\lambda}) = \mathbf{P}f(\boldsymbol{\lambda}) + \left\langle f(\boldsymbol{\lambda}),\, \frac{\mathbf{e}}{\sqrt{n}} \right\rangle \frac{\mathbf{e}}{\sqrt{n}}$$

is a decomposition of $f(\boldsymbol{\lambda})$ into it orthogonal components. Quite clearly

$$\|f(\boldsymbol{\lambda})\|^2 = \langle f(\boldsymbol{\lambda}),\, f(\boldsymbol{\lambda})\rangle \geq \left\langle f(\boldsymbol{\lambda}),\, \frac{\mathbf{e}}{\sqrt{n}} \right\rangle^2$$

by the Pythagorean theorem in an innerproduct space. This yields the desired result

$$trace\,(f(\mathbf{A})^2) \geq \frac{trace\,(f(\mathbf{A}))^2}{n}$$

∎

Theorem 2.2. *Let* $\mathbf{A}$ *be invertible so that* $\lambda_j \neq 0$ *and assume that* $f_j = f(\lambda_j) \neq 0$. *Also define* $h(f(\mathbf{A})) = trace\,(f(\mathbf{A}))^2 - (n-1)\,trace\,(f(\mathbf{A})^2)$ *and* $u_j = \frac{1}{f_j}$, *then the eigenvalues of* $f(\mathbf{A})$ *and* $f(\mathbf{A})^{-1}$ *satisfy the quadratic equations*

$$nf_j^2 - 2\,trace\,(f(\mathbf{A}))f_j + h(f(\mathbf{A})) \leq 0 \tag{2.1}$$

$$h(f(\mathbf{A}))u_j^2 - 2\,trace\,(f(\mathbf{A}))u_j + n \leq 0 \tag{2.2}$$

Proof. Let

$$\mathbf{P} = \mathbf{I} - \mathbf{e}_j\mathbf{e}_j^t - \frac{(\mathbf{e}-\mathbf{e}_j)(\mathbf{e}-\mathbf{e}_j)^t}{n-1}$$

Then $\mathbf{P}$ is a symmetric and orthogonal projector and it is easily verified that $R(\mathbf{P})$ has dimension $n-2$. Also a orthonormal basis for $N(\mathbf{P})$ is $\left\{\mathbf{e}_j,\, \frac{\mathbf{e}-\mathbf{e}_j}{\sqrt{n-1}}\right\}$. Write

$$f(\boldsymbol{\lambda}) = \mathbf{P}f(\boldsymbol{\lambda}) + \langle f(\boldsymbol{\lambda}),\, \mathbf{e}_j\rangle\mathbf{e}_j + \frac{\langle f(\boldsymbol{\lambda}),\, \mathbf{e}-\mathbf{e}_j\rangle}{\sqrt{n-1}}\frac{\mathbf{e}-\mathbf{e}_j}{\sqrt{n-1}}$$

Clearly

$$\langle f(\boldsymbol{\lambda}),\, f(\boldsymbol{\lambda})\rangle \geq f_j^2 + \frac{(\langle f(\boldsymbol{\lambda}),\, \mathbf{e}\rangle - f_j)^2}{n-1} \tag{2.3}$$

by the Pythagorean theorem. Thus

$$(n-1)\,trace\,(f(\mathbf{A})^2) \geq (n-1)f_j^2 + trace\,(f(\mathbf{A}))^2 - 2\,trace\,(f(\mathbf{A}))f_j + f_j^2$$

$$nf_j^2 - 2\,trace\,(f(\mathbf{A}))f_j + h(f(\mathbf{A})) \leq 0$$

Simply divide (2.1) by f_j^2 to get (2.2). ∎

Equation (2.2) has been derived by Huang and Xu [6] for the special case $f(x) = x$ and solved to give bounds for $\sigma(\mathbf{A}^{-1})$ and thus bounds for $\sigma(\mathbf{A})$.

Lemma 2.3. *The eigenvalues of* $f(\mathbf{A})$ *satisfy*

$$f_j \geq \frac{trace\,(f(\mathbf{A})) - \sqrt{trace\,(f(\mathbf{A}))^2 - nh(f(\mathbf{A}))}}{n} \tag{2.4}$$

$$f_j \leq \frac{trace\,(f(\mathbf{A})) + \sqrt{trace\,(f(\mathbf{A}))^2 - nh(f(\mathbf{A}))}}{n} \tag{2.5}$$

Proof. This is simply a case of solving the quadratic (2.1). However we check that the radical is positive.

$$trace\,(f(\mathbf{A}))^2 - nh(f(\mathbf{A})) = trace\,(f(\mathbf{A}))^2 - n\left[(trace\,(f(\mathbf{A}))^2 - (n-1)\,trace\,(f(\mathbf{A})^2)\right]$$

$$= (n-1)\left[n\,trace\,(f(\mathbf{A})^2) - trace\,(f(\mathbf{A}))^2\right] \tag{2.6}$$

$$\geq 0 \text{ by Lemma 2.1}$$

∎

We prefer writing (2.4) and (2.5) in the form

$$\left| f_j - \frac{trace\,(f(\mathbf{A}))}{n} \right| \leq \frac{\sqrt{(n-1)\left[n\,trace\,(f(\mathbf{A})^2) - trace\,(f(\mathbf{A}))^2\right]}}{n} \tag{2.7}$$

where we have used (2.6).

Lemma 2.4. *An upper bound for $f(\lambda_1)$ and a lower bound for $f(\lambda_n)$ are given by*

$$f_1 \leq m + S\sqrt{n-1} \tag{2.8}$$

$$f_n \geq m - S\sqrt{n-1} \tag{2.9}$$

where

$$m = \frac{\langle f(\boldsymbol{\lambda}),\, \mathbf{e}\rangle}{n} = \frac{trace\,(f(\mathbf{A}))}{n}$$

is the average and the variance S is given by

$$nS^2 = \langle f(\boldsymbol{\lambda}) - m\mathbf{e},\; f(\boldsymbol{\lambda}) - m\mathbf{e}\rangle$$

$$= \langle f(\boldsymbol{\lambda}),\; f(\boldsymbol{\lambda})\rangle - 2m\langle f(\boldsymbol{\lambda}),\, \mathbf{e}\rangle + m^2\langle \mathbf{e},\, \mathbf{e}\rangle$$

$$= trace\,(f(\mathbf{A})^2) - m^2 n$$

$$S^2 = \frac{trace\,(f(\mathbf{A})^2)}{n} - m^2$$

Proof. Simply set $j = 1$ and $j = n$ in (2.7) and note that

$$(n-1)\left[n\,trace\,(f(\mathbf{A})^2) - trace\,(f(\mathbf{A}))^2\right] = (n-1)\left[n^2(S^2 + m^2) - m^2 n^2\right] = (n-1)n^2 S^2$$

Thus (2.7) simplifies to

$$|f_j - m| \leq S\sqrt{n-1} \tag{2.10}$$

from which the result follows. ∎

Lemma 2.5. *A lower bound for $f(\lambda_1)$ and an upper bound for $f(\lambda_n)$ are given by*

$$f_1 \geq m + \frac{S}{\sqrt{n-1}} \tag{2.11}$$

$$f_n \leq m - \frac{S}{\sqrt{n-1}} \tag{2.12}$$

Proof. We use the fact that for real numbers f_i, $i = 1, 2, \cdots, n$ the variance S satisfies the inequality [2].

$$S^2 \leq (f_1 - m)(m - f_n). \tag{2.13}$$

Substitute (2.9) into (2.13) and solve for f_1, similarly substitute (2.8) into (2.13) and solve for f_n ∎

It is noted that (2.8),(2.9),(2.11) and (2.12) have been derived by Wolcowiz and Styan [11] for the special case $f(x) = x$, hence the result obtained later by Huang and Xu [6] is identical after rationalization of the latter's result.

Lemma 2.6. *A condition for the lower bound on f_n to be positive is that $h(f(\mathbf{A})) > 0$.*

Proof. It follows from (2.9) that

$$m^2 > S^2(n-1)$$

$$m^2 - \left[\frac{trace\,(f(\mathbf{A})^2)}{n} - m^2\right](n-1) > 0$$

$$m^2 n - (n-1)\,\frac{trace\,(f(\mathbf{A})^2)}{n} > 0$$

$$m^2 n^2 - (n-1)\,trace\,(f(\mathbf{A})^2) > 0$$

$$trace\,(f(\mathbf{A}))^2 - (n-1)\,trace\,(f(\mathbf{A})^2) > 0$$

which completes the proof. ∎

Lemma 2.7. *If $f(x)$ is replaced by $\alpha f(x) + \beta$, where $\alpha,\ \beta > 0$ are constants then the bounds are unchanged.*

Proof. The bounds result from (2.1). Let $T_1 = trace\,(f(\mathbf{A}))$ and $T_2 = trace\,(f(\mathbf{A})^2)$ then

$$n(\alpha f_j + \beta)^2 - 2\,trace\,(\alpha f(\mathbf{A}) + \beta I)(\alpha f_j + \beta) + trace\,(\alpha f(\mathbf{A}) + \beta I)^2$$
$$- (n-1)\,trace((\alpha f(\mathbf{A}) + \beta I)^2) \leq 0$$

$$n(\alpha f_j + \beta)^2 - 2(\alpha T_1 + \beta n)(\alpha f_j + \beta) + (\alpha T_1 + \beta n)^2$$
$$- (n-1)(\alpha^2 T_2 + 2\alpha\beta T_1 + \beta^2 n) \leq 0$$

$$\alpha^2[n f_j^2 - 2T_1 f_j + T_1^2 - (n-1)T_2] \leq 0$$

$$n f_j^2 - 2T_1 f_j + T_1^2 - (n-1)T_2 \leq 0$$

which is identical to (2.1). ∎

Comment 1. *Thus translating $f(\boldsymbol{\lambda})$ will not change the magnitude of the projections onto $N(\mathbf{P})$ and $R(\mathbf{P})$. Also amplifying $f(\boldsymbol{\lambda})$ will result in a similar amplification on the projected components onto $N(\mathbf{P})$ and $R(\mathbf{P})$.*

Theorem 2.8. *Replacing the j_{th} component of $f(\boldsymbol{\lambda})$ by $g(\lambda_j)$ will not change the bounds.*

Proof. Let

$$\widetilde{g}(\boldsymbol{\lambda}) = [f(\lambda_1),\, f(\lambda_2),\, \cdots,\, f(\lambda_{j-1}),\, g(\lambda_j),\, f(\lambda_{j+1}),\, \cdots,\, f(\lambda_j)]^t$$

or equivalently

$$\widetilde{g}(\boldsymbol{\lambda}) = f(\boldsymbol{\lambda}) - f(\lambda_j)\mathbf{e}_j + g(\lambda_j)\mathbf{e}_j$$

$$m_g = \frac{trace\,(\widetilde{g}(\mathbf{A}))}{n} \tag{2.14}$$

$$= \frac{trace\,(f(\mathbf{A})) - f_j + g_j}{n} \tag{2.15}$$

$$= m - \frac{f_j}{n} + \frac{g_j}{n} \tag{2.16}$$

$$nm_g = mn - f_j + g_j \tag{2.17}$$

$$n^2 m_g = mn^2 - nf_j + ng_j \tag{2.18}$$

$$n^2 m_g^2 = m^2 n^2 - 2mnf_j + 2mng_j - 2f_j g_j + f_j^2 + g_j^2 \tag{2.19}$$

$$S_g^2 = \frac{trace\,(\widetilde{g}(\mathbf{A}))^2}{n} - m_g^2 \tag{2.20}$$

$$= \frac{trace\,(f(\mathbf{A}))^2 - f_j^2 + g_j^2}{n} - m_g^2 \tag{2.21}$$

$$= (S^2 + m^2) - \frac{f_j^2}{n} + \frac{g_j^2}{n} - m_g^2 \tag{2.22}$$

From (2.10) it follows that

$$|g_j - m_g| \le \sqrt{n-1}S_g$$

$$g_j^2 - 2g_j m_g + m^2 g \le (n-1)S_g^2$$

$$= (n-1)\left(S^2 + m^2 - \frac{f_j^2}{n} + \frac{g_j^2}{n} - m_g^2\right) \tag{2.23}$$

Multiply (2.23) by n and simplify using (2.17)-(2.19) to get

$$\begin{aligned} &ng_j^2 - 2g_j(mn - f_j + g_j) + m^2n^2 - 2mnf_j + 2mng_j^2 \\ &- 2f_jg_j + f_j^2 + g_j^2 \\ &\leq n(n-1)S^2 + n(n-1)m^2 - (n-1)f_j^2 + (n-1)g_j \end{aligned}$$

$$nf_j^2 - 2mnf_j + nm^2 \leq n(n-1)S^2$$

$$(f_j - m)^2 \leq (n-1)S^2$$

$$|f_j - m| \leq S\sqrt{n-1}$$

∎

Theorem 2.9. *Replacing the i_{th} component of $f(\boldsymbol{\lambda})$ by $g(\lambda_i)$, optimal outer bounds given by*

$$f_n \geq \frac{mn - f_1}{n-1} - \sqrt{(n-1)S^2 - (m - f_1)^2} \tag{2.24}$$

$$f_1 \leq \frac{mn - f_n}{n-1} + \sqrt{(n-1)S^2 - (m - f_n)^2} \tag{2.25}$$

are satisfied.

Proof. If the i_{th} component of $f(\boldsymbol{\lambda})$ is replaced by $g(\lambda_i)$ then this is equivalent to a new function $r(\boldsymbol{\lambda})$ given by

$$r(\boldsymbol{\lambda}) = f(\boldsymbol{\lambda}) - f(\lambda_i)\mathbf{e_i} + g(\lambda_i)\mathbf{e_i} \tag{2.26}$$

$$= f(\boldsymbol{\lambda}) + (g_i - f_i)\mathbf{e_i} \tag{2.27}$$

As

$$\langle r(\boldsymbol{\lambda}), r(\boldsymbol{\lambda})\rangle = T_2 + 2f_i(g_i - f_i) + (g_i - f_i)^2 \tag{2.28}$$

$$\langle r(\boldsymbol{\lambda}), \mathbf{e}\rangle = T_2 + g_i - f_i \tag{2.29}$$

and $r(\boldsymbol{\lambda})$ satisfies (2.3), it follows that

$$(n-1)[T_2 + 2f_i(g_i - f_i) + (g_i - f_i)^2] \geq (n-1)f_j^2 + (T_1 - f_j + g_i - f_i)^2 \tag{2.30}$$

Equation (2.30) may be written as a quadratic in f_j of the form

$$\begin{aligned} &nf_j^2 - 2(T_1 + g_i - f_i)f_j + T_1^2 - (n-1)T_2 \\ &+ 2(g_i - f_i)[T_1 - (n-1)f_i] - (n-2)(g_i - f_i)^2 \leq 0 \end{aligned} \tag{2.31}$$

Let $\beta = g_i - f_i$ and simplify (2.31) to

$$nf_j^2 - 2(nm + \beta)f_j + nm^2 - n(n-1)S^2 + 2\beta[nm - (n-1)f_i] - (n-2)\beta^2 \leq 0 \tag{2.32}$$

The zeroes of (2.32) are given by

$$f_j^{\pm} = m + \alpha \pm \sqrt{n-1}\sqrt{(n-1)\alpha^2 - 2\alpha(m - f_i) + S^2} \tag{2.33}$$

where $\alpha = \frac{\beta}{n}$. Hence

$$|f_j - m - \alpha| \leq (n-1)\sqrt{q(\alpha)} \tag{2.34}$$

where

$$q(\alpha) = \alpha^2 - 2\alpha\frac{m-f_i}{n-1} + \frac{S^2}{n-1} \tag{2.35}$$

$$= \left(\alpha - \frac{m-f_i}{n-1}\right)^2 + \frac{(n-1)S^2-(m-f_i)^2}{(n-1)^2} \tag{2.36}$$

$$\geq \frac{(n-1)S^2-(m-f_i)^2}{(n-1)^2} \tag{2.37}$$

$$\geq 0 \tag{2.38}$$

Substituting $\alpha = \frac{m-f_i}{n-1}$ and (2.37) into (2.34), $q(\alpha)$ is minimized to give

$$\left|f_j - \frac{mn-f_i}{n-1}\right| \leq \sqrt{(n-1)S^2-(m-f_i)^2} \tag{2.39}$$

Set $j = n$ and $i = 1$ to obtain the lower bound (2.24) and $j = 1$ and $i = n$ to obtain the upper bound (2.25). ∎

One may also obtain the inner bounds

$$f_n \leq \frac{mn-f_1}{n-1} + \sqrt{(n-1)S^2-(m-f_1)^2} \tag{2.40}$$

$$f_1 \geq \frac{mn-f_n}{n-1} - \sqrt{(n-1)S^2-(m-f_n)^2} \tag{2.41}$$

from (2.39). It is easily shown that these bounds (2.40) and (2.41) are slightly worse than the bounds from (2.11) and (2.12), whilst the outer bounds (2.24) and (2.25) are comparable to those in (2.8) and (2.9). Outer bounds can then be obtained from (2.13) of the form

$$f_n \leq m - \frac{S^2}{f_1-m} \tag{2.42}$$

$$f_1 \geq m + \frac{S^2}{m-f_n} \tag{2.43}$$

These bounds are only useful if either f_n or f_1 are known. We have shown in some sense that the bounds derived by Wolkowicz and Styan for $f(x) = x$ are in some sense optimal, however for different choices of $f(x)$, the bounds may be improved as we shall illustrate with an example.

3. RESULTS

Consider the test matrix [11]

$$\mathbf{A} = \begin{bmatrix} 4 & 0 & 2 & 3 \\ 0 & 5 & 0 & 1 \\ 2 & 0 & 6 & 0 \\ 3 & 1 & 0 & 7 \end{bmatrix}$$

with spectrum $\sigma(\mathbf{A}) = \{1.425687, 4.775356, 6.423019, 9.375939\}$ accurate to six decimal places. We choose $f(x) = x^k,\ k \in \mathbb{N}$ as polynomial functions of $\mathbf{A}$ are easy to evaluate. We then take the k_{th} root to recover the bounds. If the lower bound is negative we bound below by zero.

k	**L**-(2.9)	**L**-(2.24)	**U**-(2.12)	**U**- (2.42)
1	0.525063	1.089191	3.841688	3.371483
2	0	0	4.492841	4.258399
3	0	0	4.897759	4.776953
4	0	0	5.155153	5.087181

*Table 3.1: Lower (**L**) and upper (**U**) bounds for* λ_n

k	**L**-(2.11)	**L**-(2.43)	**U**-(2.8)	**U**- (2.25)
1	7.158312	7.524881	10.474937	9.712920
2	7.537532	8.129768	9.6666	9.578714
3	7.846080	8.605355	9.467244	9.509757
4	8.083989	8.917644	9.408333	9.472481

*Table 3.2: Lower (**L**) and upper (**U**) bounds for* λ_1

As observed from columns three and five of table 3.1 slightly superior results are obtained for the lower and upper bounds of λ_n when λ_1 is known. Similarly from columns three and five of table 3.2 when λ_n is known, better bounds are attained for λ_1 for $k = 1, 2$. Also the bounds from columns two and four are fairly accurate. However one would not use large k as this will necessitate evaluation of larger powers of $\mathbf{A}$.

4. CONCLUSION

We have shown that slightly superior bounds are obtained for small k when either of the extremal eigenvalues are known. It is noted that if $f : (-\infty, \infty) \longrightarrow (-\infty, \infty)$ is an increasing function, then the bounds may be applied to real symmetric matrices, without regards for positive definiteness, for example $f(x) = x^{2k-1}, k \in \mathbb{N}$.

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