Mathematical
Inequalities
& Applications
Volume 1, Number 2 (1998), 153–169

ESTIMATING THE EXTREME SINGULAR VALUES OF MATRICES

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(*communicated by R. Horn*)

Abstract. Algorithms are derived to obtain upper and lower bounds for the largest and smallest singular values of a square complex matrix in terms of its eigenvalues and Frobenius norm. These bounds are best possible in the sense that they are attainable by some matrices with the prescribed eigenvalues and Frobenius norm. Numerical examples are given to compare them with those in the literature.

1. Introduction

Let $A \in M_n$, the algebra of $n \times n$ complex matrices. We shall always assume that $n \geqslant 2$ to avoid trivial considerations. Denote by $\lambda_i(A)$, $1 \leqslant i \leqslant n$, the eigenvalues of A arranged so that $|\lambda_1(A)| \geqslant \cdots \geqslant |\lambda_n(A)|$. The *singular values* of A, denoted by $s_1(A) \geqslant \cdots \geqslant s_n(A)$, are the nonnegative square roots of the eigenvalues of the positive semi-definite matrix A^*A. The singular values are very useful in the study of problems in different areas (see [HJ, Chapter 3], [S], and their references). Equip $\mathbb{C}^n$ with the standard norm $\|x\| = (x^*x)^{1/2}$. Then the *spectral norm* of A defined by

$$\|A\| = \max\{\|Ax\| : x \in \mathbb{C}^n,\ \|x\| = 1\}$$

is just $s_1(A)$. Moreover, if A is invertible then

$$\|A^{-1}\| = \max\{\|A^{-1}x\| : x \in \mathbb{C}^n,\ \|x\| = 1\}$$

is just $s_n(A)^{-1}$.

In the study of matrix theory, operator theory, and numerical analysis (see [G, Chapter 1], [HJ, Chapter 3], [Met], [MO, Chapters 9 & 10] and their references), one often needs to estimate $\|A\|$, $\|A^{-1}\|$, and other functions of singular values of A in terms of some partial information about A. Recall that the *Frobenius norm* of A is defined by $\|A\|_F = (\operatorname{tr} A^*A)^{1/2}$. The purpose of this paper is to study the following problem.

Problem: Obtain upper and lower bounds for the largest and smallest singular values of a complex square matrix based on its eigenvalues and Frobenius norm.

Mathematics subject classification (1991): 15A42.
Key words and phrases: Singular value, eigenvalue, Frobenius norm.
† Research supported by an NSF grant.

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Paper MIA-01-14

It turns out that one needs to focus only on the moduli of the eigenvalues and the Frobenius norm. Henceforth, let $\lambda = (\lambda_1, \dots, \lambda_n)^t \in \mathbb{C}^n$ be a given complex vector and let b be a given nonnegative real number such that

$$|\lambda_1| \geqslant \cdots \geqslant |\lambda_n| \quad \text{and} \quad b^2 \geqslant \sum_{j=1}^{n} |\lambda_j|^2.$$

Define

$$\mathscr{S}(\lambda, b) = \{A \in M_n : \lambda_j(A) = \lambda_j,\ j = 1, \dots, n,\ \|A\|_F = b\}.$$

Since

$$A = \begin{pmatrix} \lambda_1 & c \\ 0 & \lambda_n \end{pmatrix} \oplus \operatorname{diag}(\lambda_2, \dots, \lambda_{n-1}) \in \mathscr{S}(\lambda, b)$$

if $c = \{b^2 - \sum_{j=1}^{n} |\lambda_j|^2\}^{1/2}$, we see that $\mathscr{S}(\lambda, b)$ is nonempty. For notational convenience, define

$$a = |\lambda_1 \cdots \lambda_n|$$

and note that $a = |\det A|$ for any $A \in \mathscr{S}(\lambda, b)$.

We shall study the optimization problems:

$$\max s_1(X), \quad \min s_1(X), \quad \max s_n(X), \quad \min s_n(X)$$

over the compact set $\mathscr{S}(\lambda, b)$. Since the functions $s_1(X)$ and $s_n(X)$ are continuous, there are matrices in $\mathscr{S}(\lambda, b)$ that solve these optimization problems. We shall determine the entire vector of singular values of the optimal matrices.

To achieve our goal, we need a simple description of the singular values of a matrix in the set $\mathscr{S}(\lambda, b)$. Let $\mathbb{R}^n$ be the Euclidean space of $n \times 1$ or $1 \times n$ real vectors. Suppose $u = (u_1, \dots, u_n)$, $v = (v_1, \dots, v_n) \in \mathbb{R}^n$ have non-negative entries. We say that u is *log-majorized* by v, denoted by $u \prec_{\log} v$, if the product of the k largest entries of u is not larger than that of v for $k = 1, \dots, n-1$, and $\prod_{j=1}^{n} u_j = \prod_{j=1}^{n} v_j$. Note that if u and v have positive entries, an alternative definition for $u \prec_{\log} v$ is that the product of the k smallest entries of v is not smaller than that of v for $k = 1, \dots, n-1$, and $\prod_{j=1}^{n} u_j = \prod_{j=1}^{n} v_j$.

The following description of the singular values of a matrix in $\mathscr{S}(\lambda, b)$ is due to A. Horn ([HJ, 3.3.10] or [MO, 9.E.1]).

LEMMA 1.1. *There exists an $A \in \mathscr{S}(\lambda, b)$ with singular values $s_1 \geqslant \cdots \geqslant s_n \geqslant 0$ if and only if $b^2 = s_1^2 + \cdots + s_n^2$ and*

$$(|\lambda_1|, \dots, |\lambda_n|) \prec_{\log} (s_1, \dots, s_n).$$

The following result ([HJ, Corollary 3.3.10] or [MO, 3.D]) is also important in our discussion.

LEMMA 1.2. *Let* $u, v \in \mathbb{R}^n$ *have non-negative entries arranged in descending order and assume that* $u \prec_{\log} v$. *Then* $\|u\| \leqslant \|v\|$, *and equality holds if and only if* $u = v$.

In Sections 2 and 3, we shall determine bounds for the largest and smallest singular values of matrices in $\mathscr{S}(\lambda, b)$. Moreover, we give algorithms to determine the entire vector of singular values of all matrices that attain those bounds. In Section 4, we show that the algorithms can be used efficiently to compute the bounds, and we compare our results with estimates of other authors. Remarks and open problems are mentioned in Section 5.

2. Estimating the Largest Singular Value

We first consider an $\tilde{A} \in \mathscr{S}(\lambda, b)$ that satisfies $s_1(A) \leqslant s_1(\tilde{A})$ for all $A \in \mathscr{S}(\lambda, b)$. It is somewhat surprising that the vector $s(\tilde{A}) = (s_1(\tilde{A}), \ldots, s_n(\tilde{A}))$ of singular values of such a matrix is uniquely determined by λ and b.

THEOREM 2.1. *Let* $\tilde{A} \in \mathscr{S}(\lambda, b)$ *satisfy* $s_1(A) \leqslant s_1(\tilde{A})$ *for all* $A \in \mathscr{S}(\lambda, b)$. *Then* $s(\tilde{A})$ *can be determined by the following algorithm.*
Step 1. Let m *be the largest integer such that* $|\lambda_m| > 0$.
Step 2. If $m \geqslant 2$, *set* $k = m$ *and go to Step 3. Otherwise, set*

$$s(\tilde{A}) = (b, 0, \ldots, 0),$$

and stop.
Step 3. Construct

$$\Phi_k(x) = (k-1)x^2 + \left[\frac{|\lambda_1 \cdots \lambda_k|}{x^{k-1}}\right]^2 + \sum_{k<j\leqslant n} |\lambda_j|^2 - b^2, \quad x > 0.$$

Step 4. If $\Phi_k(|\lambda_k|) > 0$, *then set* $k = k-1$ *and go to Step 3. Otherwise, determine the smallest positive zero* $\tilde{r}$ *of* $\Phi_k(x)$, *set*

$$s(\tilde{A}) = \left(\frac{|\lambda_1 \cdots \lambda_k|}{\tilde{r}^{k-1}}, \underbrace{\tilde{r}, \ldots, \tilde{r}}_{k-1}, |\lambda_{k+1}|, \cdots, |\lambda_n|\right), \tag{1}$$

and stop.

REMARK 1. Note that Φ_k is a continuous function on $(0, \infty)$ satisfying $\Phi_k(x) \to \infty$ as $x \to 0$ from the right. If $\Phi_k(|\lambda_k|) \leqslant 0$, then Φ_k has at least one zero in $(0, |\lambda_k|]$. We shall show that the entries in the proposed $s(\tilde{A})$ in (1) are indeed in descending order and satisfy $(|\lambda_1|, \ldots, |\lambda_n|) \prec_{\log} s(\tilde{A})$ and $\|s(\tilde{A})\| = b$.

Also, observe that the algorithm must terminate in Step 2 if $\lambda_2 = 0$, or in Step 4 if $\lambda_2 \neq 0$, because

$$\Phi_2(|\lambda_2|) = \sum_{j=1}^{n} |\lambda_j|^2 - b^2 \leqslant 0.$$

Proof of Theorem 2.1. Let $\tilde{A} \in \mathscr{S}(\lambda, b)$ satisfy $s_1(A) \leqslant s_1(\tilde{A})$ for all $A \in \mathscr{S}(\lambda, b)$, and write $s(\tilde{A}) = (s_1, \ldots, s_n)$.

If $\lambda_2 = 0$, then

$$\hat{A} = \begin{bmatrix} \lambda_1 & \sqrt{b^2 - |\lambda_1|^2} \\ 0 & 0 \end{bmatrix} \oplus 0_{n-2} \in \mathscr{S}(\lambda, b)$$

has singular values $b, 0, \ldots, 0$. Since

$$b = s_1(\hat{A}) \leqslant s_1(\tilde{A}) = s_1 \leqslant \left\{ \sum_{j=1}^{n} s_j^2 \right\}^{1/2} = b,$$

it follows that $s(\tilde{A}) = (b, 0, \ldots, 0)$.

Now suppose $\lambda_m \neq 0 = \lambda_{m+1}$ for some positive integer m with $2 \leqslant m \leqslant n$. If $m < n$, we claim that $s_{m+1} = 0$. If not, then construct $(\hat{s}_1, \ldots, \hat{s}_n)$ as follows:

$$\hat{s}_j = \begin{cases} \{s_1^2 + \sum_{i>m} s_i^2\}^{1/2} & \text{if j} = 1, \\ s_j & \text{if j} = 2, \ldots, \text{m}, \\ 0 & \text{otherwise.} \end{cases}$$

Since $\tilde{A} \in \mathscr{S}(\lambda, b)$, its singular values satisfy the condition in Lemma 1.1. It follows that $(|\lambda_1|, \ldots, |\lambda_n|) \prec_{\log} (\hat{s}_1, \ldots, \hat{s}_n)$ and $\|(\hat{s}_1, \ldots, \hat{s}_n)\| = b$. By Lemma 1.1, there exists an $\hat{A} \in \mathscr{S}(\lambda, b)$ with $s(\hat{A}) = (\hat{s}_1, \ldots, \hat{s}_n)$. By construction, $s_1(\hat{A}) = \hat{s}_1 > s_1 = s_1(\tilde{A})$, which is a contradiction. Thus we have $s(\tilde{A}) = (s_1, \ldots, s_m, 0, \ldots, 0)$ with $s_m > 0$. Moreover, by Lemma 1.1, the conditions on $s_1, \ldots, s_m$, $\lambda_1, \ldots, \lambda_m$, and b ensure that there is a matrix $\tilde{B} \in M_m$ with these quantities as singular values, eigenvalues, and Frobenius norm, respectively. If $B \in M_m$ has the same eigenvalues and Frobenius norm as $\tilde{B}$, then $s_1(B) \leqslant s_1 = s_1(\tilde{B})$. Otherwise, $\hat{B} = B \oplus 0_{n-m} \in \mathscr{S}(\lambda, b)$ satisfies $s_1(\hat{B}) = s_1(B) > s_1 = s_1(\tilde{A})$, which is a contradiction. So, we can focus on studying $s(\tilde{B})$ with $\tilde{B} \in M_m$ so that $s_1(\tilde{B})$ is largest possible over all matrices in M_m with Frobenius norm b and eigenvalues $\lambda_1, \ldots, \lambda_m$.

For notational convenience, we assume that $m = n$, and $\tilde{B}$ is just $\tilde{A}$. Consider $\Phi_n(|\lambda_n|)$. We shall prove:

ASSERTION 1. *If $\Phi_n(|\lambda_n|) \leqslant 0$, then the smallest positive zero $\tilde{r}$ of $\Phi_n(x)$ lies in $(0, |\lambda_n|]$, and*

$$s(\tilde{A}) = (a/\tilde{r}^{n-1}, \tilde{r}, \ldots, \tilde{r}),$$

as suggested in Step 4 of the algorithm when $k = n$. If $\Phi_n(|\lambda_n|) > 0$, then there is no $A \in \mathscr{S}(\lambda, b)$ with

$$s(A) = (a/t^{n-1}, t, \ldots, t) \quad \textit{with } t \in (0, |\lambda_n|].$$

By Remark 1, we see that the smallest positive zero $\tilde{r}$ of $\Phi_n(x)$ lies in $(0, |\lambda_n|]$. Now consider

$$v(x) = (a/x^{n-1}, \underbrace{x, \ldots, x}_{n-1}), \qquad x \in (0, |\lambda_n|].$$

Then

$$(|\lambda_1|, \dots, |\lambda_n|) \prec_{\log} v(x) \quad \text{and} \quad \|v(x)\|^2 - b^2 = \Phi_n(x)$$

for all $x \in (0, |\lambda_n|]$. It follows that $(|\lambda_1|, \dots, |\lambda_n|) \prec_{\log} v(\tilde{r})$ and $\|v(\tilde{r})\| = b$. Moreover, since $\tilde{r} \leqslant |\lambda_n|$, we have $a = |\lambda_1 \cdots \lambda_n| \geqslant \tilde{r}^n$ and hence $1/\tilde{r}^{n-1} \geqslant \tilde{r}$. Thus the entries of $v(\tilde{r})$ are in descending order. By Lemma 1.1, there exists an $\hat{A} \in \mathscr{S}(\lambda, b)$ such that $s(\hat{A}) = v(\tilde{r}) = (a/\tilde{r}^{n-1}, \tilde{r}, \dots, \tilde{r})$.

Next, we show that $s(\tilde{A}) = s(\hat{A})$. Since

$$a/\tilde{r}^{n-1} = s_1(\hat{A}) \leqslant s_1(\tilde{A}) = s_1 = a/(s_2 \cdots s_n),$$

we have

$$r := (s_2 \cdots s_n)^{\frac{1}{n-1}} \leqslant \tilde{r}.$$

Hence

$$(a/\tilde{r}^{n-1}, \underbrace{\tilde{r}, \dots, \tilde{r}}_{n-1}) \prec_{\log} (a/r^{n-1}, \underbrace{r, \dots, r}_{n-1}). \tag{2}$$

Also, since $r^{n-1} = s_2 \cdots s_n$, we have

$$(\underbrace{r, \dots, r}_{n-1}) \prec_{\log} (s_2, \dots, s_n)$$

and hence

$$(s_1, \underbrace{r, \dots, r}_{n-1}) \prec_{\log} (s_1, \dots, s_n). \tag{3}$$

By (2), (3), and the fact that $a/r^{n-1} = s_1$, we have

$$s(\hat{A}) = (a/\tilde{r}^{n-1}, \underbrace{\tilde{r}, \dots, \tilde{r}}_{n-1}) \prec_{\log} (s_1, \dots, s_n) = s(\tilde{A}),$$

and thus $\|s(\hat{A})\| \leqslant \|s(\tilde{A})\|$ by Lemma 1.2. Since $b = \|\hat{A}\|_F = \|\tilde{A}\|_F$, we conclude that $s(\hat{A}) = s(\tilde{A})$ by Lemma 1.2.

Now, suppose $\Phi_n(|\lambda_n|) > 0$. If there exists an $A \in \mathscr{S}(\lambda, b)$ such that

$$s(A) = (a/t^{n-1}, t, \dots, t) \quad \text{with } t \in (0, |\lambda_n|],$$

then

$$(a/|\lambda_n|^{n-1}, |\lambda_n|, \dots, |\lambda_n|) \prec_{\log} (a/t^{n-1}, t, \dots, t).$$

By Lemma 1.2, we have

$$\|(a/|\lambda_n|^{n-1}, |\lambda_n|, \dots, |\lambda_n|)\| \leqslant \|(a/t^{n-1}, t, \dots, t)\| = b.$$

Thus

$$\Phi_n(|\lambda_n|) = \|(a/|\lambda_n|^{n-1}, |\lambda_n|, \dots, |\lambda_n|)\|^2 - b^2 \leqslant 0,$$

which is a contradiction. The proof of Assertion 1 is now complete.

By the second statement of Assertion 1, if $\Phi_n(|\lambda_n|) > 0$, then $s(\tilde{A})$ cannot be of the form

$$(a/t^{n-1}, t, \dots, t) \quad \text{with } t > 0,$$

and we can move on to consider other possibilities.

From now on assume that $\Phi_n(|\lambda_n|) > 0$. Consider $\Phi_{n-1}(|\lambda_{n-1}|)$. We shall prove:

ASSERTION 2. *If* $\Phi_{n-1}(|\lambda_{n-1}|) \leqslant 0$, *then the smallest positive zero* $\tilde{r}$ *of* $\Phi_{n-1}(x)$ *lies in* $(|\lambda_n|, |\lambda_{n-1}|]$, *and*

$$s(\tilde{A}) = (|\lambda_1 \cdots \lambda_{n-1}|/\tilde{r}^{n-2}, \tilde{r}, \ldots, \tilde{r}, |\lambda_n|) = (a/|\tilde{r}^{n-2}\lambda_n|, \tilde{r}, \ldots, \tilde{r}, |\lambda_n|),$$

as suggested in Step 4 of the algorithm when $k = n-1$. *If* $\Phi_{n-1}(|\lambda_{n-1}|) > 0$, *then there is no* $A \in \mathscr{S}(\lambda, b)$ *such that*

$$s(A) = (a/|t^{n-2}\lambda_n|, t, \ldots, t, |\lambda_n|) \quad \textit{with } t \in (|\lambda_n|, |\lambda_{n-1}|].$$

By Remark 1 again, we see that the smallest positive zero $\tilde{r}$ of $\Phi_{n-1}(x)$ lies in $(0, |\lambda_{n-1}|]$. Now consider

$$v(x) = (|\lambda_1 \cdots \lambda_{n-1}|/x^{n-2}, \underbrace{x, \ldots, x}_{n-2}, |\lambda_n|), \qquad x \in (0, |\lambda_{n-1}|].$$

Then

$$(|\lambda_1|, \ldots, |\lambda_n|) \prec_{\log} v(x) \quad \text{and} \quad \|v(x)\|^2 - b^2 = \Phi_{n-1}(x)$$

for all $x \in (0, |\lambda_{n-1}|]$. Thus $(|\lambda_1|, \ldots, |\lambda_n|) \prec_{\log} v(\tilde{r})$ and $\|v(\tilde{r})\| = b$.

If $\tilde{r} \leqslant |\lambda_n|$, then $v(|\lambda_n|) \prec_{\log} v(\tilde{r})$ and hence $\|v(|\lambda_n|)\| \leqslant \|v(\tilde{r})\| = b$. It follows that $\Phi_n(|\lambda_n|) = \|v(|\lambda_n|)\|^2 - b^2 \leqslant 0$, which is a contradiction. Thus $\tilde{r} \in (|\lambda_n|, |\lambda_{n-1}|]$. Moreover, we have $|\lambda_1 \cdots \lambda_{n-1}| \geqslant \tilde{r}^{n-1}$ and hence $|\lambda_1 \cdots \lambda_{n-1}|/\tilde{r}^{n-2} \geqslant \tilde{r}$. So, the entries of $v(\tilde{r})$ are in descending order. By Lemma 1.1, there exists an $\hat{A} \in \mathscr{S}(\lambda, b)$ such that

$$s(\hat{A}) = v(\tilde{r}) = (a/|\tilde{r}^{n-2}\lambda_n|, \underbrace{\tilde{r}, \ldots, \tilde{r}}_{n-2}, |\lambda_n|).$$

Next, we show that $s(\tilde{A}) = s(\hat{A})$. Since

$$a/|\tilde{r}^{n-2}\lambda_n| = s_1(\hat{A}) \leqslant s_1(\tilde{A}) = s_1,$$

we have

$$r := (a/|s_1\lambda_n|)^{\frac{1}{n-2}} \leqslant \tilde{r}.$$

Hence

$$(a/|\tilde{r}^{n-2}\lambda_n|, \underbrace{\tilde{r}, \ldots, \tilde{r}}_{n-2}, |\lambda_n|) \prec_{\log} (s_1, \underbrace{r, \ldots, r}_{n-2}, |\lambda_n|). \tag{4}$$

Also, since $r^{n-2} = a/|s_1\lambda_n| \leqslant a/(s_1 s_n) = s_2 \cdots s_{n-1}$, we have $r^l \leqslant s_2 \cdots s_{l+1}$ for $l = 1, \ldots, n-2$, and hence

$$(s_1, \underbrace{r, \ldots, r}_{n-2}, |\lambda_n|) \prec_{\log} (s_1, \ldots, s_n). \tag{5}$$

By (4) and (5), we have

$$s(\hat{A}) = (a/|\tilde{r}^{n-2}\lambda_n|, \tilde{r}, \ldots, \tilde{r}, |\lambda_n|) \prec_{\log} (s_1, \ldots, s_n) = s(\tilde{A}),$$

and thus $\|s(\hat{A})\| \leqslant \|s(\tilde{A})\|$ by Lemma 1.2. Since $b = \|\hat{A}\|_F = \|\tilde{A}\|_F$, we conclude that $s(\hat{A}) = s(\tilde{A})$ by Lemma 1.2.

Now suppose $\Phi_{n-1}(|\lambda_{n-1}|) > 0$. If there is an $A \in \mathscr{S}(\lambda, b)$ such that

$$s(A) = (a/|t^{n-2}\lambda_n|, t, \ldots, t, |\lambda_n|) \quad \text{with } t \in (|\lambda_n|, |\lambda_{n-1}|],$$

then

$$(|\lambda_1|, \ldots, |\lambda_n|) \prec_{\log} (a/|t^{n-2}\lambda_n|, t, \ldots, t, |\lambda_n|)$$

by Lemma 1.1. It follows that $t \leqslant |\lambda_{n-1}|$ and

$$(a/|\lambda_{n-1}^{n-2}\lambda_n|, |\lambda_{n-1}|, \ldots, |\lambda_{n-1}|, |\lambda_n|) \prec_{\log} (a/|t^{n-2}\lambda_n|, t, \ldots, t, |\lambda_n|).$$

By Lemma 1.2, we have

$$\|(a/|\lambda_{n-1}^{n-2}\lambda_n|, |\lambda_{n-1}|, \ldots, |\lambda_{n-1}|, |\lambda_n|)\| \leqslant \|(a/|t^{n-2}\lambda_n|, t, \ldots, t, |\lambda_n|)\| = b.$$

Thus

$$\Phi_{n-1}(|\lambda_{n-1}|) = \|(a/|\lambda_{n-1}^{n-2}\lambda_n|, |\lambda_{n-1}|, \ldots, |\lambda_{n-1}|, |\lambda_n|)\|^2 - b^2 \leqslant 0,$$

which is a contradiction. The proof of Assertion 2 is now complete.

By the last statement of Assertion 2, if $\Phi_{n-1}(|\lambda_{n-1}|) > 0$, then $s(\tilde{A})$ cannot be of the form

$$(a/|t^{n-2}\lambda_n|, t, \ldots, t, |\lambda_n|) \quad \text{with } t \in (|\lambda_n|, |\lambda_{n-1}|]$$

and we can move on to consider other possibilities.

From now on assume that $\Phi_{n-1}(|\lambda_{n-1}|) > 0$. One can use arguments similar to those in the previous cases to prove:

ASSERTION 3. *If* $\Phi_{n-2}(|\lambda_{n-2}|) \leqslant 0$, *then the smallest positive zero* $\tilde{r}$ *of* $\Phi_{n-2}(x)$ *lies in* $(|\lambda_{n-1}|, |\lambda_{n-2}|]$, *and*

$$\begin{aligned} s(\tilde{A}) &= (|\lambda_1 \cdots \lambda_{n-2}|/\tilde{r}^{n-3}, \underbrace{\tilde{r}, \ldots, \tilde{r}}_{n-3}, |\lambda_{n-1}|, |\lambda_n|) \\ &= (a/|\tilde{r}^{n-3}\lambda_{n-1}\lambda_n|, \underbrace{\tilde{r}, \ldots, \tilde{r}}_{n-3}, |\lambda_{n-1}|, |\lambda_n|), \end{aligned}$$

as suggested in Step 4 of the algorithm when $k = n-2$. *If* $\Phi_{n-2}(|\lambda_{n-2}|) > 0$, *then there is no* $A \in \mathscr{S}(\lambda, b)$ *such that*

$$s(A) = (|\lambda_1 \cdots \lambda_{n-2}|/t^{n-3}, \underbrace{t, \ldots, t}_{n-3}, |\lambda_{n-1}|, |\lambda_n|) \quad \textit{with } t \in (|\lambda_{n-1}|, |\lambda_{n-2}|].$$

Repeating these arguments, one gets the desired conclusion. □

Next, we turn to the lower bound for $s_1(A)$ with $A \in \mathscr{S}(\lambda, b)$.

THEOREM 2.2. *Define*

$$\Phi(x) = (n-1)x^2 + \left[\frac{a}{x^{n-1}}\right]^2 - b^2, \qquad x > 0.$$

Let $\tilde{A} \in \mathscr{S}(\lambda, b)$ satisfy $s_1(\tilde{A}) \leqslant s_1(A)$ for all $A \in \mathscr{S}(\lambda, b)$. Then exactly one of the following holds:

(a) *If $|\lambda_1| > 0$ and $\Phi(|\lambda_1|) \geqslant 0$, then $s_1(\tilde{A}) = |\lambda_1|$.*

(b) *If $\lambda_1 = 0$, or if $\lambda_1 \neq 0$ and $\Phi(|\lambda_1|) < 0$, then $s(\tilde{A}) = (\tilde{r}, \ldots, \tilde{r}, a/\tilde{r}^{n-1})$, where $\tilde{r}$ is the largest positive zero of $\Phi(x)$.*

Note that Φ is a continuous function on $(0, \infty)$ satisfying $\Phi(x) \to \infty$ if $x \to \infty$. If $\lambda_1 \neq 0$ and $\Phi(|\lambda_1|) < 0$, then Φ has a zero in $(|\lambda_1|, \infty)$. If $\lambda_1 = 0$, then $a = 0$ and $\Phi(x)$ has a positive zero, namely, $\sqrt{b^2/(n-1)}$.

Proof of Theorem 2.2. Let $\tilde{A} \in \mathscr{S}(\lambda, b)$ satisfy $s_1(\tilde{A}) \leqslant s_1(A)$ for all $A \in \mathscr{S}(\lambda, b)$, and write $s(\tilde{A}) = (s_1, \ldots, s_n)$.

Suppose $|\lambda_1| > 0$, and $\Phi(|\lambda_1|) = (n-1)|\lambda_1|^2 + \left[\frac{a}{|\lambda_1^{n-1}|}\right]^2 - b^2 \geqslant 0$. We construct $\hat{A} \in \mathscr{S}(\lambda, b)$ with $s_1(\hat{A}) = |\lambda_1|$ as follows:

Let A_1 have singular values $|\lambda_1|, \ldots, |\lambda_n|$. If $|\lambda_1|^2 + \cdots + |\lambda_n|^2 = b^2$, then let $\hat{A} = A_1$. If $|\lambda_1|^2 + \cdots + |\lambda_n|^2 < b^2$, then consider $A_2(t) \in M_n$ with singular values

$$|\lambda_1|, t, |\lambda_3|, \ldots, |\lambda_{n-1}|, |\lambda_2\lambda_n|/t$$

with $|\lambda_2| < t \leqslant |\lambda_1|$. If $A_2(t)$ has Frobenius norm b for some t, then let $\hat{A} = A_2(t)$. Otherwise, we have $|\lambda_1|^2 + |\lambda_1|^2 + |\lambda_3|^2 + \cdots + |\lambda_{n-1}|^2 + \left|\frac{\lambda_2\lambda_n}{t}\right|^2 < b^2$. Consider $A_3(t) \in M_n$ with singular values

$$|\lambda_1|, |\lambda_1|, t, |\lambda_4|, \ldots, |\lambda_{n-1}|, |(\lambda_2\lambda_3\lambda_n)/(t\lambda_1)|$$

with $|\lambda_3| < t \leqslant |\lambda_1|$. If $A_3(t)$ has Frobenius norm b for some t, then let $\hat{A} = A_3(t)$.

Since $(n-1)|\lambda_1|^2 + \left[\frac{a}{|\lambda_1^{n-1}|}\right]^2 \geqslant b^2$, we can continue this process until we get $\hat{A} = A_k(t)$ for some integer k between 1 and n such that $A_k(t)$ has Frobenius norm b and singular values

$$\underbrace{|\lambda_1|, \ldots, |\lambda_1|}_{k-1}, t, |\lambda_{k+1}|, \ldots, |\lambda_{n-1}|, |\lambda_2 \cdots \lambda_k\lambda_n/(t\lambda_1^{k-2})|,$$

with $|\lambda_{k+1}| < t \leqslant |\lambda_1|$. Thus, $\hat{A} \in M_n$ satisfies $s_1(\hat{A}) = |\lambda_1|$. Since $|\lambda_1| \leqslant s_1(A)$ for all $A \in \mathscr{S}(\lambda, b)$, we have $|\lambda_1| \leqslant s_1(\tilde{A}) \leqslant s_1(\hat{A}) = |\lambda_1|$.

Suppose $\lambda_1 = 0$. Then every $A \in \mathscr{S}(\lambda, b)$ is singular, i.e., $s_n(A) = 0$, and we have

$$s_1(A)^2 + \cdots + s_{n-1}(A)^2 = b^2.$$

It follows that $s_1(A)^2 \geqslant b^2/(n-1)$, and equality holds if and only if $s_1(A) = s_{n-1}(A)$. By Lemma 1.1, there indeed exists an $\hat{A} \in \mathscr{S}(\lambda, b)$ with singular values $r, \ldots, r, 0$ with $r = b/\sqrt{n-1}$. Hence $\tilde{A}$ must satisfy $s(\tilde{A}) = (r, \ldots, r, 0)$.

Now suppose $|\lambda_1| > 0$ and $\Phi(|\lambda_1|) = (n-1)|\lambda_1|^2 + \left[\frac{a}{|\lambda_1^{n-1}|}\right]^2 - b^2 < 0$. By Lemma 1.1, we have $\|(s_1, \ldots, s_n)\| = b$ and

$$(|\lambda_1|, \ldots, |\lambda_n|) \prec_{\log} (s_1, \ldots, s_n) \prec_{\log} (s_1, \ldots, s_1, a/s_1^{n-1}).$$

Since $(s_1, \ldots, s_n) \prec_{\log} (s_1, \ldots, s_1, a/s_1^{n-1})$, $b = \|(s_1, \ldots, s_n)\| \leqslant \|(s_1, \ldots, s_1, a/s_1^{n-1})\|$ by Lemma 1.2. If strict inequality holds, there exists a $t > 1$ such that

$$\|(s_1/t, \ldots, s_1/t, a/(s_1/t)^{n-1})\| = b.$$

Since $(n-1)|\lambda_1|^2 + (a/|\lambda_1^{n-1}|)^2 < b^2$, we see that $s_1/t > |\lambda_1|$, and hence

$$(|\lambda_1|, \ldots, |\lambda_n|) \prec_{\log} (s_1/t, \ldots, s_1/t, t^{n-1}a/s_1^{n-1}).$$

By Lemma 1.1, there exists an $A \in \mathscr{S}(\lambda, b)$ with singular values $s_1/t, \ldots, s_1/t, t^{n-1}a/s_1^{n-1}$. It follows that $s_1(A) = s_1/t < s_1 = s_1(\tilde{A})$, which is a contradiction. Thus, we have $\|(s_1, \ldots, s_n)\| = \|(s_1, \ldots, s_1, a/s_1^{n-1})\|$, and $(s_1, \ldots, s_n) = (s_1, \ldots, s_1, a/s_1^{n-1})$ by Lemma 1.2. $\square$

3. Estimating the Smallest Singular Value

If $\lambda_n = 0$, then $s_n(A) = 0$ for all $A \in \mathscr{S}(\lambda, b)$. Thus we assume $|\lambda_n| > 0$, or equivalently, $a > 0$, when we study upper and lower bounds for $s_n(A)$ with $A \in \mathscr{S}(\lambda, b)$.

THEOREM 3.1. *Suppose $a > 0$. Define*

$$\Psi(x) = (n-1)x^2 + \left[\frac{a}{x^{n-1}}\right]^2 - b^2, \qquad x > 0.$$

Let $\tilde{A} \in \mathscr{S}(\lambda, b)$ satisfy $s_n(A) \leqslant s_n(\tilde{A})$ for all $A \in \mathscr{S}(\lambda, b)$. Then exactly one of the following holds:

(a) $\Psi(|\lambda_n|) \geqslant 0$ *and* $s_n(\tilde{A}) = |\lambda_n|$.

(b) $\Psi(|\lambda_n|) < 0$ *and* $s(A) = (a/\tilde{r}^{n-1}, \tilde{r}, \ldots, \tilde{r})$, *where $\tilde{r}$ is the smallest positive zero of* $\Psi(x)$.

Note that Ψ is a continuous function on $(0, \infty)$ satisfying $\Psi(x) \to \infty$ if $x \to 0$ from the right. If $\lambda_n \neq 0$ satisfies $\Phi(|\lambda_n|) < 0$, then Ψ has a zero in $(0, |\lambda_n|]$.

Proof of Theorem 3.1. Let $\tilde{A} \in \mathscr{S}(\lambda, b)$ satisfy $s_n(A) \leqslant s_n(\tilde{A})$ for all $A \in \mathscr{S}(\lambda, b)$, and write $s(\tilde{A}) = (s_1, \ldots, s_n)$.

If $\Psi(|\lambda_n|) = (n-1)|\lambda_n|^2 + \left[\frac{a}{|\lambda_n^{n-1}|}\right]^2 - b^2 \leqslant 0$, construct $\hat{A}$ with $s_n(\hat{A}) = |\lambda_n|$ as follows:

Let A_1 have singular values $|\lambda_1|, \dots, |\lambda_n|$. If $|\lambda_1|^2 + \cdots + |\lambda_n|^2 = b^2$, then set $\hat{A} = A_1$. Otherwise, we have $|\lambda_1|^2 + \cdots + |\lambda_n|^2 < b^2$. Consider $A_2(t) \in M_n$ with singular values

$$\left|\frac{\lambda_1\lambda_{n-1}}{t}\right|, |\lambda_2|, \dots, |\lambda_{n-2}|, t, |\lambda_n|$$

where $|\lambda_{n-1}| \geqslant t \geqslant |\lambda_n|$. If $A_2(t)$ has Frobenius norm b for some $t \in [|\lambda_n|, |\lambda_{n-1}|]$, then set $\hat{A} = A_2(t)$. Otherwise, we have $\left|\frac{\lambda_1\lambda_{n-1}}{\lambda_n}\right|^2 + |\lambda_2|^2 + \cdots + |\lambda_{n-2}|^2 + 2|\lambda_n|^2 < b^2$. Consider $A_3(t) \in M_n$ with singular values

$$\left|\frac{\lambda_1\lambda_{n-2}\lambda_{n-1}}{t\lambda_n}\right|, |\lambda_2|, \dots, |\lambda_{n-3}|, t, |\lambda_n|, |\lambda_n|$$

where $|\lambda_{n-2}| \geqslant t \geqslant |\lambda_n|$. If $A_3(t)$ has Frobenius norm b for some $t \in [|\lambda_{n-1}|, |\lambda_{n-2}|]$, then set $\hat{A} = A_3(t)$.

Since

$$\left[\frac{a}{|\lambda_n^{n-1}|}\right]^2 + (n-1)|\lambda_n|^2 \geqslant b^2,$$

we can continue this process until we get $A_k(t)$, $1 \leqslant k < n$, with singular values

$$\left|\frac{\lambda_1\lambda_{n-k+1}\cdots\lambda_{n-1}}{t|\lambda_n|^{k-1}}\right|, |\lambda_2|, \dots, |\lambda_{n-k}|, t, \underbrace{|\lambda_n|, \dots, |\lambda_n|}_{k-1}$$

with $|\lambda_{n-k+1}| \geqslant t \geqslant |\lambda_n|$ so that $\hat{A} = A_k(t)$ has Frobenius norm b. Thus, we have $s_n(\hat{A}) = |\lambda_n|$. Since $s_n(A) \leqslant |\lambda_n|$ for all $A \in \mathscr{S}(\lambda, b)$, we have $|\lambda_n| = s_n(\hat{A}) \leqslant s_n(\tilde{A}) \leqslant |\lambda_n|$.

Next, assume that $\Psi(|\lambda_n|) = (n-1)|\lambda_n|^2 + \left[\frac{a}{|\lambda_n^{n-1}|}\right]^2 - b^2 < 0$. By Lemma 1.1, the singular values of $\tilde{A}$ satisfy $\sum_{j=1}^n s_j^2 = b^2$ and $(|\lambda_1|, \dots, |\lambda_n|) \prec_{\log} (s_1, \dots, s_n)$. Thus, we have

$$(|\lambda_1|, \dots, |\lambda_n|) \prec_{\log} (s_1, \dots, s_n) \prec_{\log} \left(a/s_n^{n-1}, s_n, \dots, s_n\right),$$

and hence $b = \|(s_1, \dots, s_n)\| \leqslant \| \left(a/s_n^{n-1}, s_n, \dots, s_n\right) \|$. If strict inequality holds, there exists a $t \in (0,1)$ such that $\| \left(t^{n-1}a/s_n^{n-1}, s_n/t, \dots, s_n/t\right) \| = b$. Since $\left[a/|\lambda_n^{n-1}|\right]^2 + (n-1)|\lambda_n|^2 > b^2$, we see that $s_n/t < |\lambda_n|$, and hence

$$(|\lambda_1|, \dots, |\lambda_n|) \prec_{\log} (s_1, \dots, s_n) \prec_{\log} \left(t^{n-1}a/s_n^{n-1}, s_n/t, \dots, s_n/t\right).$$

By Lemma 1.1, there exists an $A \in \mathscr{S}(\lambda, b)$ with singular values $t^{n-1}a/s_n^{n-1}, s_n/t, \dots, s_n/t$. It follows that $s_n(A) = s_n/t > s_n = s_n(\tilde{A})$, which is a contradiction. Thus, we have $\|(s_1, \dots, s_n)\| = \| \left(a/s_n^{n-1}, s_n, \dots, s_n\right) \|$, and hence $(s_1, \dots, s_n) = \left(a/s_n^{n-1}, s_n, \dots, s_n\right)$ by Lemma 1.2. $\square$

Next, we turn to those $\tilde{A} \in \mathscr{S}(\lambda, b)$ that satisfy $s_n(\tilde{A}) \leqslant s_n(A)$ for all $A \in \mathscr{S}(\lambda, b)$. It is again interesting to note that the vector of singular values of $\tilde{A}$ is uniquely determined by λ and b.

THEOREM 3.2. *Suppose* $a > 0$. *Let* $\tilde{A} \in \mathscr{S}(\lambda, b)$ *satisfy* $s_n(\tilde{A}) \leqslant s_n(A)$ *for all* $A \in \mathscr{S}(\lambda, b)$. *Then* $s(\tilde{A})$ *can be determined by the following algorithm.*
Step 1. Set $k = 1$.
Step 2. Construct

$$\Psi_k(x) = (n-k)x^2 + \left[\frac{|\lambda_k \cdots \lambda_n|}{x^{n-k}}\right]^2 + \sum_{1 \leqslant j < k} |\lambda_j|^2 - b^2, \quad x > 0.$$

Step 3. If $\Psi_k(|\lambda_k|) > 0$, *then set* $k = k+1$ *and go to Step 2. Otherwise, determine the largest positive zero* $\tilde{r}$ *of* $\Psi_k(x)$, *set*

$$s(\tilde{A}) = \left(|\lambda_1|, \ldots, |\lambda_{k-1}|, \underbrace{\tilde{r}, \ldots, \tilde{r}}_{n-k}, \frac{|\lambda_k \cdots \lambda_n|}{\tilde{r}^{n-k}}\right), \tag{6}$$

and stop.

REMARK 2. Note that Ψ_k is a continuous function on $(0, \infty)$ satisfying $\Psi_k(x) \to \infty$ as $x \to \infty$. If $\Psi_k(|\lambda_k|) \leqslant 0$, then Ψ_k has at least one zero in $[|\lambda_k|, \infty)$. We shall show that the entries in the proposed $s(\tilde{A})$ in (6) are indeed in descending order order satisfying $(|\lambda_1|, \ldots, |\lambda_n|) \prec_{\log} s(\tilde{A})$ and $\|s(\tilde{A})\| = b$.

Also, observe that the algorithm must terminate in finitely many iterations because

$$\Psi_{n-1}(|\lambda_{n-1}|) = \sum_{j=1}^{n} |\lambda_j|^2 - b^2 \leqslant 0.$$

Proof of Theorem 3.2. Let $\tilde{A} \in \mathscr{S}(\lambda, b)$ satisfy $s_n(\tilde{A}) \leqslant s_n(A)$ for all $A \in \mathscr{S}(\lambda, b)$, and write $s(\tilde{A}) = (s_1, \ldots, s_n)$. Consider, $\Psi_1(|\lambda_1|)$. We shall prove:

ASSERTION 1. *If* $\Psi_1(|\lambda_1|) > 0$, *then the largest positive zero* $\tilde{r}$ *of* $\Psi_1(x)$ *lies in* $[|\lambda_1|, \infty)$, *and*

$$s(\tilde{A}) = (\tilde{r}, \ldots, \tilde{r}, a/\tilde{r}^{n-1}),$$

as suggested in Step 3 of the algorithm when $k = 1$. *If* $\Psi_1(|\lambda_1|) > 0$, *then there is no* $A \in \mathscr{S}(\lambda, b)$ *such that*

$$s(A) = (t, \ldots, t, a/t^{n-1}) \quad \textit{with } t \in [|\lambda_1|, \infty).$$

By Remark 2, we see that the largest positive zero $\tilde{r}$ of $\Psi_1(x)$ lies in $[|\lambda_1|, \infty)$. Now consider

$$v(x) = (\underbrace{x, \ldots, x}_{n-1}, a/x^{n-1}), \qquad x \geqslant |\lambda_1|.$$

Then

$$(|\lambda_1|, \ldots, |\lambda_n|) \prec_{\log} v(x) \quad \text{and} \quad \|v(x)\|^2 - b^2 = \Psi_1(x)$$

for all $x \geqslant |\lambda_1|$. Thus $(|\lambda_1|, \ldots, |\lambda_n|) \prec_{\log} v(\tilde{r})$ and $\|v(\tilde{r})\| = b$. Since $\tilde{r} \geqslant |\lambda_1|$, we have $\tilde{r}^n \geqslant |\lambda_1 \cdots \lambda_n| = a$ and hence $\tilde{r} \geqslant a/\tilde{r}^{n-1}$. Thus the entries of $v(\tilde{r})$

are in descending order. By Lemma 1.1, there exists an $\hat{A} \in \mathscr{S}(\lambda, b)$ such that $s(\hat{A}) = v(\tilde{r}) = (\tilde{r}, \dots, \tilde{r}, a/\tilde{r}^{n-1})$.

Next, we show that $s(\tilde{A}) = s(\hat{A})$. Since

$$a/\tilde{r}^{n-1} = s_n(\hat{A}) \geqslant s_n(\tilde{A}) = s_n = a/(s_1 \cdots s_{n-1}),$$

we have

$$r := (s_1 \cdots s_{n-1})^{\frac{1}{n-1}} \geqslant \tilde{r}.$$

Hence

$$(\underbrace{\tilde{r}, \dots, \tilde{r}}_{n-1}, a/\tilde{r}^{n-1}) \prec_{\log} (\underbrace{r \dots, r}_{n-1}, s_n). \tag{7}$$

Also, since $r^{n-1} = s_1 \cdots s_{n-1}$, we have

$$(\underbrace{r, \dots, r}_{n-1}) \prec_{\log} (s_1, \dots, s_{n-1})$$

and hence

$$(\underbrace{r, \dots, r}_{n-1}, s_n) \prec_{\log} (s_1, \dots, s_n). \tag{8}$$

By (7) and (8), we have

$$s(\hat{A}) = (\underbrace{\tilde{r}, \dots, \tilde{r}}_{n-1}, a/\tilde{r}^{n-1}) \prec_{\log} (s_1, \dots, s_n) = s(\tilde{A}),$$

and thus $\|s(\hat{A})\| \leqslant \|s(\tilde{A})\|$ by Lemma 1.2. Since $b = \|\hat{A}\|_F = \|\tilde{A}\|_F$, we conclude that $s(\hat{A}) = s(\tilde{A})$ by Lemma 1.2.

Suppose $\Psi_1(|\lambda_1|) > 0$. If there is an $A \in \mathscr{S}(\lambda, b)$ such that

$$s(A) = (t, \dots, t, a/t^{n-1}) \quad \text{with } t \geqslant |\lambda_1|,$$

then

$$(|\lambda_1|, \dots, |\lambda_1|, a/|\lambda_1|^{n-1}) \prec_{\log} (t, \dots, t, a/t^{n-1}).$$

By Lemma 1.2, we have

$$\|(|\lambda_1|, \dots, |\lambda_1|, a/|\lambda_1|^{n-1})\| \leqslant \|(t, \dots, t, a/t^{n-1})\| = b.$$

Thus

$$\Psi_1(|\lambda_1|) = \|(|\lambda_1|, \dots, |\lambda_1|, a/|\lambda_1|^{n-1})\|^2 - b^2 \leqslant 0,$$

which is a contradiction. The proof of Assertion 1 is now complete.

By the last statement of Assertion 1, if $\Psi_1(|\lambda_1|) > 0$, then $s(\tilde{A})$ cannot be of the form

$$(t, \dots, t, a/t^{n-1}) \quad \text{with } t > |\lambda_1|,$$

and we can move on to consider other possibilities.

From now on assume that $\Psi_1(|\lambda_1|) > 0$. Consider $\Psi_2(|\lambda_2|)$. We shall prove:

ASSERTION 2. *If* $\Psi_2(|\lambda_2|) \leqslant 0$, *then the largest positive zero* $\tilde{r}$ *of* $\Psi_2(x)$ *lies in* $[|\lambda_2|, |\lambda_1|)$, *and*

$$s(\tilde{A}) = (|\lambda_1|, \tilde{r}, \dots, \tilde{r}, |\lambda_2 \cdots \lambda_n|/\tilde{r}^{n-2}),$$

as suggested in Step 3 of the algorithm when $k = 2$. *If* $\Psi_2(|\lambda_2|) > 0$, *then there is no* $A \in \mathscr{S}(\lambda, b)$ *such that*

$$s(A) = (|\lambda_1|, t, \dots, t, a/|t^{n-2}\lambda_1|) \quad \textit{with } t \in [|\lambda_2|, |\lambda_1|).$$

By Remark 2 again, we see that the largest positive zero $\tilde{r}$ of $\Psi_2(x)$ lies in $[|\lambda_2|, \infty)$. Now consider

$$v(x) = (|\lambda_1|, \underbrace{x, \dots, x}_{n-2}, |\lambda_2 \cdots \lambda_n|/x^{n-2}), \qquad x \geqslant |\lambda_2|.$$

Then

$$(|\lambda_1|, \dots, |\lambda_n|) \prec_{\log} v(x) \quad \text{and} \quad \|v(x)\|^2 - b^2 = \Psi_2(x)$$

for all $x \geqslant |\lambda_2|$. Thus $(|\lambda_1|, \dots, |\lambda_n|) \prec_{\log} v(\tilde{r})$ and $\|v(\tilde{r})\| = b$.

If $\tilde{r} \geqslant |\lambda_1|$, then $v(|\lambda_1|) \prec_{\log} v(\tilde{r})$, and hence $\|v(|\lambda_1|)\| \leqslant \|v(\tilde{r})\| = b$. It follows that $\Psi(|\lambda_1|) = \|v(|\lambda_1|)\|^2 - b^2 \leqslant 0$, which is a contradiction. Thus $\tilde{r} \in [|\lambda_2|, |\lambda_1|)$. Moreover, we have $\tilde{r}^{n-1} \geqslant |\lambda_2 \cdots \lambda_n|$ and hence $\tilde{r} \geqslant |\lambda_2 \cdots \lambda_n|/\tilde{r}^{n-2}$. So, the entries in $v(\tilde{r})$ are in descending order. By Lemma 1.1, there exists an $\hat{A} \in \mathscr{S}(\lambda, b)$ such that

$$s(\hat{A}) = v(\tilde{r}) = (|\lambda_1|, \underbrace{\tilde{r}, \dots, \tilde{r}}_{n-2}, a/|\tilde{r}^{n-2}\lambda_1|).$$

Next, we show that $s(\tilde{A}) = s(\hat{A})$. Since

$$a/|\tilde{r}^{n-2}\lambda_1| = s_n(\hat{A}) \geqslant s_n(\tilde{A}) = s_n,$$

we have

$$r := (a/|s_n\lambda_1|)^{\frac{1}{n-2}} \geqslant \tilde{r}.$$

Hence

$$(|\lambda_1|, \underbrace{\tilde{r}, \dots, \tilde{r}}_{n-2}, a/|\tilde{r}^{n-2}\lambda_1|) \prec_{\log} (|\lambda_1|, \underbrace{r, \dots, r}_{n-2}, a/|r^{n-2}\lambda_1|). \tag{9}$$

Also, since $r^{n-2} = a/|s_n\lambda_1| \geqslant a/(s_1 s_n) = s_2 \cdots s_{n-1}$, we have $r^l \geqslant s_l \cdots s_{n-1}$ for $l = 2, \dots, n-1$, and hence

$$(|\lambda_1|, \underbrace{r, \dots, r}_{n-2}, s_n) \prec_{\log} (s_1, \dots, s_n). \tag{10}$$

By (9), (10), and the fact that $a/|r^{n-2}\lambda_1| = s_n$, we have

$$s(\hat{A}) = (|\lambda_1|, \underbrace{\tilde{r}, \dots, \tilde{r}}_{n-2}, a/|\tilde{r}^{n-2}\lambda_1|) \prec_{\log} (s_1, \dots, s_n) = s(\tilde{A}),$$

and thus $\|s(\hat{A})\| \leqslant \|s(\tilde{A})\|$ by Lemma 1.2. Since $b = \|\hat{A}\|_F = \|\tilde{A}\|_F$, we conclude that $s(\hat{A}) = s(\tilde{A})$ by Lemma 1.2.

Now, suppose $\Psi_2(|\lambda_2|) > 0$. If there is an $A \in \mathscr{S}(\lambda, b)$ such that

$$s(A) = (|\lambda_1|, t, \ldots, t, a/|t^{n-2}\lambda_1|) \quad \text{with } t \geqslant |\lambda_2|,$$

then

$$(|\lambda_1|, |\lambda_2|, \ldots, |\lambda_2|, a/|\lambda_2^{n-2}\lambda_1|) \prec_{\log} (|\lambda_1|, t, \ldots, t, a/|t^{n-2}\lambda_1|).$$

By Lemma 1.2, we have

$$\|(|\lambda_1|, |\lambda_2|, \ldots, |\lambda_2|, a/|\lambda_2^{n-2}\lambda_1|)\| \leqslant \|(|\lambda_1|, t, \ldots, t, a/|t^{n-2}\lambda_1|)\| = b.$$

Thus

$$\Psi_2(|\lambda_2|) = \|(|\lambda_1|, |\lambda_2|, \ldots, |\lambda_2|, a/|\lambda_2^{n-2}\lambda_1|)\|^2 - b^2 \leqslant 0,$$

which is a contradiction. The proof of Assertion 2 is now complete.

By the last statement of Assertion 2, if $\Psi_2(|\lambda_2|) > 0$, $s(\tilde{A})$ cannot be of the form

$$(|\lambda_1|, t, \ldots, t, a/|t^{n-2}\lambda_1|) \quad \text{with } t \geqslant |\lambda_2|,$$

and we can move on to consider other possibilities.

From now on assume that $\Psi_2(|\lambda_2|) > 0$. One can use arguments similar to those in the previous cases to prove:

ASSERTION 3. *If* $\Psi_3(|\lambda_3|) \leqslant 0$, *then the largest positive zero* $\tilde{r}$ *of* $\Psi_3(x)$ *lies in* $[|\lambda_3|, |\lambda_2|)$, *and*

$$s(\tilde{A}) = (|\lambda_1|, |\lambda_2|, \underbrace{\tilde{r}, \ldots, \tilde{r}}_{n-3}, |\lambda_3 \cdots \lambda_n|/\tilde{r}^{n-3}),$$

as suggested in Step 3 of the algorithm when $k = 3$. *If* $\Psi_3(|\lambda_3|) > 0$, *then there is no* $A \in \mathscr{S}(\lambda, b)$ *such that*

$$s(A) = (|\lambda_1|, |\lambda_2|, \underbrace{t, \ldots, t}_{n-3}, |\lambda_3 \cdots \lambda_n|/t^{n-3}) \text{ with } t \in [|\lambda_3|, |\lambda_2|).$$

Repeating these arguments, one gets the desired conclusion. □

4. Numerical Examples

To use the theorems in the previous sections, we often have to find the positive zeros of a function of the form

$$f(x) = mx^2 + \left[\frac{c_1}{x^m}\right]^2 - c_2$$

for a positive integer m and positive constants c_1 and c_2. Note that r is a positive zero of $f(x)$ if and only if $r > 0$ and r^2 is a zero of the polynomial

$$p(y) = my^{m+1} - c_2 y^m + c_1^2.$$

Since $p(y)$ has only one positive turning point, at $y_0 = c_2/(m+1)$, we see that $p(y)$ has at most two positive zeros, and so does $f(x)$.

Clearly, $f(x)$ is continuous on $(0,\infty)$, $\lim_{x\to 0^+} f(x) = \infty$, and $\lim_{x\to\infty} f(x) = \infty$. If there exists an $x_0 > 0$ such that $f(x_0) \leqslant 0$, then $f(x)$ has at least one zero in $(0, x_0]$ and one zero in $[x_0, \infty)$. If $f(\sqrt{y}_0) \leqslant 0$, where $y_0 = c_2/(m+1)$ is the positive turning point of $p(y)$ defined in the preceding paragraph, then each of the intervals $(0, \sqrt{y}_0]$ and $[\sqrt{y}_0, \infty)$ contains exactly one zero of $f(x)$. With this background in mind, one easily derives iterative methods, or one can use standard software such as Maple or Matlab, to solve for the desired zero of $f(x)$ in the specific interval when our theorems are used.

In the following, we consider several numerical examples and compare our results with some estimates of other authors.

EXAMPLE 4.1. Take $|\lambda_1| = |\lambda_2| = |\lambda_3| = 1$ and $b = \sqrt{7}$.

Theorems 2.1, 2.2, 2.3, and 2.4 all require studying the zeros of

$$f(x) = 2x^2 + \left(\frac{1}{x^2}\right)^2 - 7.$$

Let r_1 and r_2 be the smallest and largest positive zeros of $f(x)$, respectively.

To determine the optimal upper bound for $s_1(A)$ with $A \in \mathscr{S}(\lambda, b)$, we use Theorem 2.1 and find the smaller positive zero of $\Phi_3(x) = f(x)$. We conclude that an optimal matrix A_1 has $s_2(A_1) = s_3(A_1) = r_1 \approx 0.6338$ and $s_1(A_1) = 1/r_1^2 \approx 2.489$.

A known upper bound [G, Example 1.2.5] for $s_1(A)$ with $A \in \mathscr{S}(\lambda, b)$ is given by

$$s_1(A) \leqslant |\lambda_1| + g(A),$$

where $g(A) = \left(b^2 - \sum_{i=1}^{3} |\lambda_i(A)|^2\right)^{1/2}$. For this example, $|\lambda_1| + g(A) = 1 + (7 - 3)^{1/2} = 3$, and our estimate gives an improvement of $\frac{3-2.489}{3} \approx 17\%$.

To determine the optimal lower bound for $s_1(A)$ with $A \in \mathscr{S}(\lambda, b)$, we use Theorem 2.2 and find the largest positive zero of the function $\Phi(x) = f(x)$. We conclude that an optimal matrix A_2 has $s_1(A_2) = s_2(A_2) = r_2 \approx 1.8595$, and $s_3(A_2) = 1/r_2^2 \approx 0.2892$.

Next, we determine the optimal upper bound for $s_3(A)$ with $A \in \mathscr{S}(\lambda, b)$. Using Theorem 3.1, we compute the smallest positive zero of the function $\Psi(x) = f(x)$. We conclude that an optimal matrix A_3 has $s_3(A_3) = s_2(A_3) = r_1 \approx 0.6338$ and $s_1 = 1/r_1^2 \approx 2.4893$.

Finally, we determine the optimal upper bound for $s_3(A)$ with $A \in \mathscr{S}(\lambda, b)$. Using Theorem 3.2, we compute the largest positive zero of $\Psi_1(x) = f(x)$. We conclude that an optimal matrix A_4 has $s_1(A_4) = s_2(A_4) = r_2 \approx 1.8595$, and $s_3(A_4) = 1/r_2^2 \approx 0.2892$.

Using the formula in [G, Example 1.2.7], we get the lower bound 0.2000 for $s_n(A)$. Thus, we get an improvement of $\frac{0.2892-0.2000}{0.2892} \approx 30\%$.

We give two more examples showing that $|\lambda_1|$ and $|\lambda_n|$ can be used as the bounds for some $\mathscr{S}(\lambda, b)$.

EXAMPLE 4.2. Suppose $|\lambda_1| = 2, |\lambda_2| = |\lambda_3| = 1,$ and $b = \sqrt{7}$.

To get the optimal lower bound for $s_1(A)$ with $A \in \mathscr{S}(\lambda, b)\}$, we apply Theorem 2.2. Suppose $\tilde{A}$ is an optimal matrix such that $s(\tilde{A}) = (s_1, s_2, s_3)$. Since

$$(n-1)|\lambda_1|^2 + \left[\frac{a}{|\lambda_1^{n-1}|}\right]^2 = (2)(2)^2 + (2/2^2)^2 = 8.25 > 7 = b^2,$$

we have $s_1 = |\lambda_1| = 2$. To find s_2 and s_3, we solve the equations

$$s_1^2 + s_2^2 + s_3^2 = 7 = b^2 \quad \text{and} \quad s_1 s_2 s_3 = 2$$

to get $s_2 \approx 1.618$ and $s_3 \approx 0.618$.

EXAMPLE 4.3. Suppose $|\lambda_1| = |\lambda_2| = 4, |\lambda_3| = 2,$ and $b = \sqrt{50}$.

To get the optimal upper bound for $s_n(A)$ with $A \in \mathscr{S}(\lambda, b)$, we apply Theorem 3.1. Suppose $\tilde{A}$ is an optimal matrix such that $s(\tilde{A}) = (s_1, s_2, s_3)$. Since

$$\left[\frac{a}{|\lambda_n^{n-1}|}\right]^2 + (n-1)|\lambda_n|^2 = \left(32/2^2\right)^2 + (2)(2^2) = 72 > 50 = b^2,$$

we have $s_3 = |\lambda_3| = 2$. To find s_1 and s_2, we solve the equations

$$s_1^2 + s_2^2 + s_3^2 = s_1^2 + s_2^2 + |\lambda_3|^2 = 50 \quad \text{and} \quad s_1 s_2 s_3 = s_1 s_2 |\lambda_3| = 32$$

to get $s_1 \approx 6.2867$ and $s_2 \approx 2.455$.

5. Remarks and Open Problems

In the previous sections, we have obtained upper and lower bounds for the extreme singular values of a square matrix in terms of its Frobenius norm and eigenvalues (actually, only the absolute values of the eigenvalues). In addition to these results, the important contribution of this paper is the idea of reducing problems of finding bounds on functions of singular values of matrices to certain optimization problems on $\mathbb{R}^n$ by means of Lemma 1.1. In fact, our technique can be used to study other functions of singular values of matrices with prescribed eigenvalues and Frobenius norm. For example, one may consider

(a) the function $g(s_1(A), \ldots, s_n(A)) = s_1(A) + \cdots + s_k(A)$ corresponding to the *Ky Fan k-norm* of A where $1 \leqslant k \leqslant n$,

(b) the function $g(s_1(A), \ldots, s_n(A)) = 1/s_n(A) + \cdots + 1/s_{n-k+1}(A)$ corresponding to the Ky Fan k-norm of A^{-1},

(c) the function $g(s_1(A), \ldots, s_n(A)) = \{s_1(A)^p + \cdots + s_n(A)^p\}^{1/p}$ corresponding to the *Schatten p-norm* of A where $p \geqslant 1$,

(d) the function $g(s_1(A), \ldots, s_n(A)) = \{1/s_n(A)^p + \cdots + 1/s_n(A)^p\}^{1/p}$ corresponding to the Schatten p-norm of A^{-1}.

One may see, for example, [HJ, Chapter 3] for general background of these functions. Another interesting function would be

(e) the *condition number* of A with respect to a given unitarily invariant norm $|||\cdot|||$, say, the Ky Fan k-norm or the Schatten p-norm, defined by $k(|||\cdot|||, A) = |||A||| \cdot |||A^{-1}|||$.

An upper bound for the condition number of a square matrix with respect to the spectral norm based on its determinant and Frobenius norm was obtained in [Me].

Of course, the analysis for these functions will be much more involved. However, in applications, one may use some software packages to solve the optimization problems numerically instead of obtaining the theoretical results.

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(Received August 20, 1997)

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