10-2016

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**Recommended Citation**  
Johnson, Ch. R.; Pena, J. M.; and Szulc, T., Optimal Gersgorin-Style Estimation Of The Largest Singular Value, Ii (2016).  
10.13001/1081-3810.3033
2016

Optimal Gersgorin-style estimation of the largest singular value. II

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Recommended Citation

Johnson, Charles R.; Pena, J. M.; and Szulc, Tomasz. (2016), "Optimal Gersgorin-style estimation of the largest singular value. II", *Electronic Journal of Linear Algebra*, Volume 31, pp. 679-685.  
DOI: [https://doi.org/10.13001/1081-3810.3033](https://doi.org/10.13001/1081-3810.3033)
OPTIMAL GERSGORIN-STYLE ESTIMATION OF THE LARGEST SINGULAR VALUE, II*

CH. R. JOHNSON†, J. M. PEÑA‡, AND T. SZULC§

Abstract. In estimating the largest singular value in the class of matrices equiradial with a given \( n \)-by-\( n \) complex matrix \( A \), it was proved that it is attained at one of \( n(n-1) \) sparse nonnegative matrices (see C.R. Johnson, J.M. Peña and T. Szulc, Optimal Gersgorin-style estimation of the largest singular value; *Electronic Journal of Linear Algebra Algebra Appl.*, 25:48–59, 2011). Next, some circumstances were identified under which the set of possible optimizers of the largest singular value can be further narrowed (see C.R. Johnson, T. Szulc and D. Wojtera-Tyrakowska, Optimal Gersgorin-style estimation of the largest singular value, *Electronic Journal of Linear Algebra Algebra Appl.*, 25:48–59, 2011). Here the cardinality of the mentioned set for \( n \)-by-\( n \) matrices is further reduced. It is shown that the largest singular value, in the class of matrices equiradial with a given \( n \)-by-\( n \) complex matrix, is attained at one of \( n(n-1)/2 \) sparse nonnegative matrices. Finally, an inequality between the spectral radius of a 3-by-3 nonnegative matrix \( X \) and the spectral radius of a modification of \( X \) is also proposed.

Key words. Equiradial class; Spectral norm; Singular values; Gersgorin set.

AMS subject classifications. 65F15, 15A18, 15A42, 15A48.

1. Introduction. Let \( M_n(\mathbb{C}) \) be the set of all \( n \)-by-\( n \) complex matrices. For a given matrix \( A = (a_{ij}) \in M_n(\mathbb{C}) \), we set \( P_k(A) = \sum_{j \neq k} |a_{kj}|, k = 1, \ldots, n \), and define the class \( \Lambda(A) \) of matrices equiradial with \( A \) by

\[
\Lambda(A) = \{ B = (b_{ij}) \in M_n(\mathbb{C}) : |D(B)| = |D(A)|, P_k(B) = P_k(A), k = 1, \ldots, n \},
\]

where, for an \( X = (x_{ij}) \in M_n(\mathbb{C}) \), \( D(X) = \text{diag}(x_{1,1}, \ldots, x_{n,n}) \). In particular, we will focus on the finite subset of \( \Lambda(A) \) that consists of \( n(n-1) \) nonnegative matrices

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*Received by the editors on April 11, 2013. Accepted for publication on June 7, 2015. Handling Editor: Bryan L. Shader.
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$A^{(s,k)} = (a_{i,j}^{(s,k)})$, in which $s, k \in \{1, \ldots, n\}$ and $s \neq k$, such that

$$a_{i,j}^{(s,k)} = \begin{cases} |a_{i,i}| & \text{for } i = j, \\ P_1(A) & \text{for } i \neq j \text{ and } j = s, \\ P_s(A) & \text{for } (i,j) = (s,k), \\ 0 & \text{otherwise.} \end{cases}$$

So, in particular, for a given 3-by-3 complex matrix $A = (a_{ij})$, the mentioned subset consists of the following 6 matrices:

$$A^{(1,2)} = \begin{pmatrix} |a_{1,1}| & P_1(A) & 0 \\ P_2(A) & |a_{2,2}| & 0 \\ P_3(A) & 0 & |a_{3,3}| \end{pmatrix}, \quad A^{(2,1)} = \begin{pmatrix} |a_{1,1}| & P_1(A) & 0 \\ P_2(A) & |a_{2,2}| & 0 \\ 0 & P_3(A) & |a_{3,3}| \end{pmatrix},$$

$$A^{(1,3)} = \begin{pmatrix} |a_{1,1}| & 0 & P_1(A) \\ P_2(A) & |a_{2,2}| & 0 \\ P_3(A) & 0 & |a_{3,3}| \end{pmatrix}, \quad A^{(3,1)} = \begin{pmatrix} |a_{1,1}| & 0 & P_1(A) \\ 0 & |a_{2,2}| & P_2(A) \\ P_3(A) & 0 & |a_{3,3}| \end{pmatrix},$$

$$A^{(2,3)} = \begin{pmatrix} |a_{1,1}| & P_1(A) & 0 \\ 0 & |a_{2,2}| & P_2(A) \\ 0 & P_3(A) & |a_{3,3}| \end{pmatrix}, \quad A^{(3,2)} = \begin{pmatrix} |a_{1,1}| & 0 & P_1(A) \\ 0 & |a_{2,2}| & P_2(A) \\ 0 & P_3(A) & |a_{3,3}| \end{pmatrix}.$$

**Remark 1.** For our purposes, throughout this paper, it will be assumed that $A$ has at least one nonzero off-diagonal entry in each row and that all its diagonal entries are nonzero. Then, it is easy to observe that any matrix $A^{(s,k)} (s, k \in \{1, \ldots, n\}$ and $s \neq k$) has exactly $2n$ nonzero entries, i.e. all diagonal entries, all off-diagonal entries of the $s$th column and the $(k, s)$th entry.

We now describe how the matrices $A^{(s,k)}$ play an important role in estimation of the largest singular value among matrices equiradial with $A$ (see [3]). Upper bounds for the largest singular value $\sigma_1(A)$ of a square matrix $A$ in terms of possible simple functions of the entries of a matrix have many potential theoretical and practical applications. By simple functions we mean those which use “Gersgorin-type” data related to a matrix, i.e., diagonal entries and sums of the moduli of off-diagonal entries. Observe that for a given $A \in M_n(\mathbb{C})$ all matrices from $\Lambda(A)$ share this type of information and therefore, from this point of view, they can be equal. So, the above comment motivates us to state the following question, which was studied in [3] and we refer to as the “motivating question”: Given a matrix $A$, what is the maximum singular value among the matrices that are equivalent with $A$? I.e.,

“what is $\max_{X \in \Lambda(A)} \{\sigma_1(X)\}$,”

where $\sigma_1(X)$ is the largest singular value of an $n$-by-$n$ complex matrix $X$ (equiradial with $A$). It was proved in [3] (Theorem 3) that one of the $n(n - 1)$ matrices $A^{(s,k)}$ attains this maximum.
Here, we show that the number \( n(n - 1) \) of candidates for a maximum can be reduced to \( n(n - 1)/2 \).

2. Results. We start with the main result of the paper.

**Theorem 2.** Consider \( n \times n \) matrices \( A^{(k,l)} \) and \( A^{(l,k)} \) and suppose that

\[
|a_{k,k}|^2 + P_1^2(A) > |a_{i,l}|^2 + P_k^2(A).
\]

Then

\[
\sigma_1(A^{(k,l)}) > \sigma_1(A^{(l,k)}).
\]

**Proof.** Without loss of generality, we set \( (k, l) = (1, 2) \). Applying the Perron-Frobenius theorem to the nonnegative matrix \( (A^{(2,1)})^T A^{(2,1)} \), we can deduce that there exists a nonnegative unit vector \( x = (x_1, \ldots, x_n)^T \) such that \( \|A^{(2,1)}x\|_2 = \|A^{(2,1)}\|_2 \).

Let us consider two cases. First, we assume that \( x_2 > x_1 \). Then

\[
\sigma_1^2(A^{(2,1)}) = \|A^{(2,1)}x\|_2^2 = \langle |a_{11}|^2 + P_2^2(A)\rangle x_1^2 + \left( |a_{22}|^2 + P_1^2(A) + \sum_{i=3}^n P_i^2(A) \right) x_2^2 + \sum_{i=3}^n |a_{ii}|^2 x_i^2 \]

\[

+ 2(|a_{11}P_1(A) + |a_{22}P_2(A)|)x_1x_2 + 2\sum_{i=3}^n |a_{ii}|P_i(x_2x_i).
\]

From (1) we have

\[
|a_{11}|^2 + P_2^2(A) = \alpha + |a_{22}|^2 + P_1^2(A),
\]

where \( \alpha \) is a positive number. So, by (3), (2) becomes

\[
\sigma_1^2(A^{(2,1)}) = \langle |a_{22}|^2 + P_1^2(A) + \alpha \rangle x_1^2 + \left( |a_{11}|^2 + P_2^2(A) - \alpha + \sum_{i=3}^n P_i^2(A) \right) x_2^2 + \sum_{i=3}^n |a_{ii}|^2 x_i^2 \]

\[

+ 2(|a_{11}P_1(A) + |a_{22}P_2(A)|)x_1x_2 + 2\sum_{i=3}^n |a_{ii}|P_i(x_2x_i),
\]

which can be written as

\[
(|a_{22}|^2 + P_1^2(A))x_1^2 + \alpha(x_1^2 - x_2^2) + \left( |a_{11}|^2 + P_2^2(A) + \sum_{i=3}^n P_i^2(A) \right) x_2^2 + \sum_{i=3}^n |a_{ii}|^2 x_i^2 +
\]

\[

2(|a_{11}P_1(A) + |a_{22}P_2(A)|)x_1x_2 + 2\sum_{i=3}^n |a_{ii}|P_i(A)x_2x_i.
\]
from which, keeping in mind that $x_2 > x_1$, we obtain

\begin{equation}
\sigma_1^2(A^{(2,1)}) < \left( |a_{11}|^2 + P_2^n(A) + \sum_{i=3}^n P_i^n(A) \right) x_2^2 + (|a_{22}|^2 + P_1^n(A)) x_1^2 + \sum_{i=3}^n |a_{ii}|^2 x_i^2 + 2(|a_{11} P_1(A) + |a_{22}| P_2(A)) x_1 x_2 + 2 \sum_{i=3}^n |a_{ii}| P_i(A) x_2 x_i = \|A^{(1,2)} P x\|_2^2,
\end{equation}

where $P$ is the permutation matrix $P = (e_2, e_1, e_3, \ldots, e_n)^T$ with $e_i$ the $i$-th row of the identity $n \times n$ matrix. So, from (4), we obtain

\begin{equation}
\sigma_1^2(A^{(2,1)}) < \|A^{(1,2)} P x\|_2^2 \leq \max_{\|x\|_2 = 1} \|A^{(1,2)} P x\|_2^2 = \sigma_1^2(A^{(1,2)} P)
\end{equation}

and, as $P$ is a unitary matrix, we finally get

\begin{equation}
\sigma_1^2(A^{(2,1)}) < \sigma_1^2(A^{(1,2)}).
\end{equation}

To prove the remaining case, assume that $x_1 \geq x_2$. Then we have

\begin{equation}
\|A^{(1,2)} x\|_2^2 = \left( |a_{11}|^2 + \sum_{i=2}^n P_i^n(A) \right) x_1^2 + (|a_{22}|^2 + P_1^n(A)) x_2^2 + \sum_{i=3}^n |a_{ii}|^2 x_i^2 + 2(|a_{11} P_1(A) + |a_{22}| P_2(A)) x_1 x_2 + 2 \sum_{i=3}^n |a_{ii}| P_i(A) x_2 x_i,
\end{equation}

which, as $x_1 \geq x_2$, becomes

\begin{equation}
\|A^{(1,2)} x\|_2^2 \geq (|a_{11}|^2 + P_2^n(A)) x_1^2 + \left( |a_{22}|^2 + P_1^n(A) + \sum_{i=3}^n P_i^n(A) \right) x_2^2 + \sum_{i=3}^n |a_{ii}|^2 x_i^2 + 2(|a_{11} P_1(A) + |a_{22}| P_2(A)) x_1 x_2 + 2 \sum_{i=3}^n |a_{ii}| P_i(A) x_2 x_i = \|A^{(2,1)} x\|_2^2 = \|A^{(2,1)}\|_2^2 = \sigma_1^2(A^{(2,1)}).
\end{equation}

So, from (6), we get

\begin{equation}
\sigma_1^2(A^{(1,2)}) \geq \|A^{(1,2)} x\|_2^2 \geq \sigma_1^2(A^{(2,1)}),
\end{equation}

which, together with (5), completes the proof.
Estimation of extremal singular values

Clearly, in the case that

\[ |a_{il}|^2 + P_l(A)^2 \neq |a_{kk}|^2 + P_k(A)^2 \quad (l, k \in \{1, 2, \ldots, n\}, l \neq k), \]

then the number \(n(n-1)\) of possible optimizers for the largest singular value, obtained in [3], can be reduced to the number \(n(n-1)/2\). The reduction of the number of possible optimisers for the largest singular value to \(n(n-1)/2\) is also valid in the case when \(|a_{il}|^2 + P_l(A)^2 = |a_{kk}|^2 + P_k(A)^2\) for some \(l\) and \(k\) because in this case the singular values of \(A^{(k,l)}\) and \(A^{(l,k)}\) are equal. To see it assume, without loss of generality, that \(|a_{11}|^2 + P_1(A)^2 = |a_{22}|^2 + P_1(A)^2\) and let \(P = [e_2, e_1, e_3, \ldots, e_n]\) be a permutation \(n\)-by-\(n\) matrix, where \(e_i\) is the \(i\)th unit vector in \(\mathbb{R}^n\). Observing that matrices \(A^{(1,2)}\) and \(A^{(2,1)}P\) differ only in the upper left 2-by-2 block, and by a direct calculation and our assumption, we get

\[ (A^{(1,2)})^T A^{(1,2)} = P^T (A^{(2,1)})^T A^{(2,1)} P, \]

which implies the equality of singular values of \(A^{(1,2)}\) and \(A^{(2,1)}\).

**Example 3.** [3]. Let

\[ A = \begin{pmatrix} 3 & 1 & 1 \\ 4 & 7 & 1 \\ 2 & 1 & 4 \end{pmatrix}. \]

Then (see Theorem 3 in [3]) the candidates for a solution of the “Motivating question” of the Introduction are the matrices

\[ A^{(1,2)} = \begin{pmatrix} 3 & 2 & 0 \\ 5 & 7 & 0 \\ 3 & 0 & 4 \end{pmatrix}, \quad A^{(2,1)} = \begin{pmatrix} 3 & 2 & 0 \\ 5 & 7 & 0 \\ 0 & 3 & 4 \end{pmatrix}, \]

\[ A^{(1,3)} = \begin{pmatrix} 3 & 0 & 2 \\ 5 & 7 & 0 \\ 3 & 0 & 4 \end{pmatrix}, \quad A^{(3,1)} = \begin{pmatrix} 3 & 0 & 2 \\ 0 & 7 & 5 \\ 3 & 0 & 4 \end{pmatrix}, \]

\[ A^{(2,3)} = \begin{pmatrix} 3 & 2 & 0 \\ 0 & 7 & 5 \\ 0 & 3 & 4 \end{pmatrix}, \quad A^{(3,2)} = \begin{pmatrix} 3 & 0 & 2 \\ 0 & 7 & 5 \\ 0 & 3 & 4 \end{pmatrix}. \]

For matrices \(A^{(1,2)}\) and \(A^{(2,1)}\), \(A^{(1,3)}\) and \(A^{(3,1)}\), and \(A^{(2,3)}\) and \(A^{(3,2)}\), by Theorem 2 we get \(3^2+5^2 < 7^2+2^2, 3^2+3^2 < 2^2+4^2\) and \(7^2+3^2 > 5^2+4^2\), respectively, and therefore \(\sigma_1(A^{(1,2)}) < \sigma_1(A^{(2,1)}), \quad \sigma_1(A^{(1,3)}) < \sigma_1(A^{(3,1)})\) and \(\sigma_1(A^{(2,3)}) > \sigma_1(A^{(3,2)})\). So, we may reduce the number of candidates for a solution of the “Motivating question” to the three matrices \(A^{(2,1)}, A^{(3,1)}, A^{(2,3)}\) (in fact we have: \(\sigma_1(A^{(1,2)}) = 9.4957, \quad \sigma_1(A^{(2,1)}) = 9.6217, \quad \sigma_1(A^{(1,3)}) = 9.1407, \quad \sigma_1(A^{(3,1)}) = 9.1892, \quad \sigma_1(A^{(2,3)}) = 9.995, \quad \sigma_1(A^{(3,2)}) = 9.9559\).
We also give a result on the spectral radius of a 3-by-3 nonnegative matrix that is similar in character to the 3-by-3 case of Theorem 2 (note that for the case \( n = 3 \) the assertion of Theorem 2 can be delivered by considering a relation between the largest roots of characteristic polynomials of \( A^{(k,l)} \) and \( A^{(l,k)} \)).

**Lemma 4.** Let \( f_1(x) = x^3 - a_1x^2 + a_2x - a_3 \) and \( f_2(x) = x^3 - a_1x^2 + a_2x - b_3 \) be real polynomials such that their maximum modulus roots \( \tilde{x}_1 \) and \( \hat{x}_1 \), respectively, are real and positive and let

\[
\begin{align*}
    a_3 &> b_3.
\end{align*}
\]

Then we have \( \tilde{x}_1 > \hat{x}_1 \).

**Proof.** It is easy to see that both \( f_1 \) and \( f_2 \) are increasing functions either for any \( x \) if \( a_1^2 - 3a_2 < 0 \) or for \( x \geq \frac{a_1 + \sqrt{a_1^2 - 3a_2}}{3} \), otherwise. Then, by (7) and the forms of \( f_1 \) and \( f_2 \), we get \( f_2(\tilde{x}_1) = a_3 - b_3 > 0 \) which, by the monotonicity of \( f_2 \), completes the proof.

**Theorem 5.** Let \( A = (a_{i,j}) \) be a 3-by-3 nonnegative matrix and let \( \tilde{A} = (\tilde{a}_{i,j}) \) be obtained from \( A \) by replacing an off-diagonal entry \( a_{i,j} \) by \( a_{j,i} \) and vice versa. If \( \det A > \det \tilde{A} \) then

\[
\rho(A) > \rho(\tilde{A}),
\]

where \( \rho(X) \) denotes the spectral radius of a square matrix \( X \).

**Proof.** We first observe that characteristic polynomials of \( A \) and \( \tilde{A} \) differ at most in the constant term. So, using the Perron-Frobenius theory [1], the assertion follows by applying Lemma 4.

**Example 6.** Let

\[
    A = \begin{pmatrix} 2 & 1 & 5 \\ 2 & 2 & 4 \\ 3 & 5 & 0 \end{pmatrix}.
\]

Then, since \( A \) is nonnegative with row sums 8, \( \rho(A) = 8 \) (see also [4]). In this case we have

\[
    \tilde{A}_1 = \begin{pmatrix} 2 & 2 & 5 \\ 1 & 2 & 4 \\ 3 & 5 & 0 \end{pmatrix}, \quad \tilde{A}_2 = \begin{pmatrix} 2 & 1 & 3 \\ 2 & 2 & 4 \\ 5 & 5 & 0 \end{pmatrix}, \quad \tilde{A}_3 = \begin{pmatrix} 2 & 1 & 5 \\ 2 & 2 & 5 \\ 3 & 4 & 0 \end{pmatrix}.
\]

A direct calculation yields: \( \det A = -8 \), \( \det \tilde{A}_1 = -21 \), \( \det \tilde{A}_2 = -20 \), and \( \det \tilde{A}_3 = -15 \). So, following Theorem 5, we have the following inequalities:

\[
    \rho(A) > \rho(\tilde{A}_3) > \rho(\tilde{A}_2) > \rho(\tilde{A}_1).
\]

In fact we have: \( \rho(\tilde{A}_3) = 7.92514 \), \( \rho(\tilde{A}_2) = 7.870156 \), \( \rho(\tilde{A}_1) = 7.859002 \).
Acknowledgments. The authors thank the anonymous referee whose suggestions have helped to improve this work.

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