Outer Bounds for the Extremal Eigenvalues of Positive Definite Matrices

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Abstract—**In this paper, we show how the outer bounds of the extremal eigenvalues of real positive definite symmetric irreducible matrices may be improved by the simple application of optimizing the Gerschgorin bounds. The method is easy to apply and yields fairly accurate results with minimal effort.**

Index Terms—**positive definite matrix, eigenvalues, bounds.**

I. Introduction

THE role of the extremal eigenvalues of a matrix cannot be overemphasized. These values serve an important aspect in determining the conditioning of a linear algebraic system [1]. They are vital to the approximation of normal operators [2]. Their distribution on the complex plane determines the stability of the solution of a system of differential equations. As the solution of the characteristic equation of a matrix $\mathbf{A}$, is a difficult task for large dimensions, many methods have been proposed for approximating the extremal eigenvalues. Some crude bounds are obtained by an application of Gerschgorin's theorem [3], and the ovals of Cassini [4]. For positive definite symmetric matrices Dembo bounds [5] arise by examining the characteristic equation of $\mathbf{A}$ and rely on bounds of a principal submatrix. Ma and Zarowski [6] improved on Dembo's lower bound by ensuring that it was always positive. This idea was also used to further improve the lower bounds of the minimal eigenvalue [7] and to Toeplitz matrices by Melman [8] for both upper and lower bounds. Recently trace bounds [9], [10] have given reasonably good results. However the lower bound is not guaranteed to be positive as expected, for the class of positive definite real symmetric matrices. Also, an improvement using trace bounds [11] requires much more effort. The application of Rayleigh's theorem [3] provides good inner bounds. Recently, Huang et al. [12] bounded the minimum eigenvalue of the Hadamard product of an M matrix and its inverse. No single approach has proven dominant, so all are to be considered in the proper context to isolate the extremal eigenvalues.

II. Theory

Let $A \in \mathbb{R}^{n\times n}$ be a symmetric positive definite and irreducible matrix, and let $|\mathbf{A}| = |a_{ij}|$ denote the non-negative matrix derived from $\mathbf{A}$. Furthermore, let $\mathbf{D} = (\mathbf{a_{ii}})$ denote the diagonal part of $\mathbf{A}$ and note that $a_{ii} > 0$ follows from positive definiteness. Also, recall that the spectrum $\sigma(\mathbf{A}) > 0$ and $\mathbf{A}$ is diagonalizable with a real eigenbasis. Denote the distinct eigenvalues of $\mathbf{A}$ by $\lambda_i,\ i = 1, 2, \cdots, k$, where $k \le n$. Let m_i denote the algebraic multiplicity of λ_i, $\sum_{i=1}^{k} m_i = n$. Arrange the eigenvalues in descending order

$$\lambda_1 > \lambda_2 \ge \cdots \lambda_{k-1} > \lambda_k,$$

where we assume strict separation for the minimal and maximal eigenvalues. Since A is symmetric it is orthogonally diagonalizable and from the spectral theorem [3] we may write

$$\mathbf{I} = \sum_{i=1}^{k} \mathbf{G}_i$$
$$\mathbf{A} = \sum_{i=1}^{k} \lambda_i \mathbf{G}_i,$$

where $\mathbf{G}_i$ is the orthogonal projector onto the nullspace $N(\mathbf{A} - \lambda_i \mathbf{I})$. Consequently $\mathbf{G}_i\mathbf{G}_j = \delta_{ij}\mathbf{G}_i$ and

$$\mathbb{R}^n = \bigoplus_{i=1}^{k} N(\mathbf{A} - \lambda_\mathbf{i}\mathbf{I}).$$

Lemma 2.1 (Rayleigh): Let $\mathbf{x} \in \mathbb{R}^n$, where $\|\mathbf{x}\|_\mathbf{2} = \mathbf{1}$, then it follows that

$$\lambda_k \le R(\mathbf{x}) = \langle \mathbf{A}\mathbf{x}, \mathbf{x}\rangle \le \lambda_1. \tag{1}$$

Proof. We prove the right-hand side of (1) as the left-hand side is proved in a similar manner.

$$\begin{aligned}\langle \mathbf{A}\mathbf{x}, \mathbf{x}\rangle &= \sum_{i=1}^{k} \langle \lambda_i \mathbf{G_i}\mathbf{x}, \mathbf{x}\rangle \\ &\le \lambda_1 \left\langle \left(\sum_{i=1}^{k} \mathbf{G_i}\right)\mathbf{x}, \mathbf{x}\right\rangle \\ &= \lambda_1 \langle \mathbf{x}, \mathbf{x}\rangle \\ &= \lambda_1.\end{aligned}$$

Lemma 2.2: Let $\mathbf{x_p} \in N(\mathbf{A} - \lambda_p \mathbf{I})$ such that $\|\mathbf{x_p}\|_2 = 1$ and consider a perturbation of $\mathbf{x_p}$ given by

$$\mathbf{x_p}' = \frac{\mathbf{x_p} + \beta\mathbf{x}}{\sqrt{1+\beta^2}},$$

where $\|\mathbf{x}\|_2 = 1$, $\mathbf{x} \perp N(\mathbf{A} - \lambda_p \mathbf{I})$ and $\mathbf{x_p}'$ has been normalized to unity. Then

$$\lambda_p' - \lambda_p = \mathcal{O}(\beta^2)(\langle \mathbf{A}\mathbf{x}, \mathbf{x}\rangle - \lambda_p), \tag{2}$$

where $\lambda_p' = R(\mathbf{x_p}')$.

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Proof.

$$R(\mathbf{x_p}') = (1+\beta^2)^{-1}\langle \mathbf{A}(\mathbf{x}_p+\beta\mathbf{x}),\, \mathbf{x}_p+\beta\mathbf{x}\rangle$$
$$= (1+\beta^2)^{-1}(\langle \mathbf{A}\mathbf{x}_p,\, \mathbf{x}_p\rangle + 2\beta\langle \mathbf{A}\mathbf{x}_p,\, \mathbf{x}\rangle + \beta^2\langle \mathbf{A}\mathbf{x},\, \mathbf{x}\rangle)$$
$$= \frac{\lambda_p + \beta^2\langle \mathbf{A}\mathbf{x},\, \mathbf{x}\rangle}{(1+\beta^2)}.$$

Hence,

$$R(\mathbf{x_p}') - \lambda_p = \frac{\beta^2(\langle \mathbf{A}\mathbf{x},\, \mathbf{x}\rangle) - \lambda_p}{(1+\beta^2)}$$
$$= \mathcal{O}(\beta^2)(\langle \mathbf{A}\mathbf{x},\, \mathbf{x}\rangle) - \lambda_p).$$

Thus, an $\mathcal{O}(\beta)$ approximation to an eigenvector results in a "better" $\mathcal{O}(\beta^2)$ approximation to the corresponding eigenvalue. For $p = k$ in (2), we have an upper bound $\lambda'_k \geq \lambda_k$ and for $p = 1$ in (2), we have a lower bound $\lambda'_1 \leq \lambda_1$.

By Gerschgorin's theorem, the eigenvalues of $\mathbf{A}$ are all contained in the union of the n intervals given by

$$|\lambda - a_{ii}| \leq r_i = \sum_{\substack{p=1\\ p\neq i}}^{n} |a_{ip}|,$$

where $i = 1, 2, \cdots, n$. These radii are assembled in a vector $\mathbf{r}$ and are given by

$$\mathbf{r} = |\mathbf{A}|\mathbf{e} - \mathbf{D}\mathbf{e} = |\mathbf{A} - \mathbf{D}|\mathbf{e},$$

where $\mathbf{e} = \sum_{i=1}^{n} \mathbf{e_i} = [1,\, 1, \cdots, 1]^t$.
The left bound of the Gerschgorin intervals are given by

$$b_i = a_{ii} - r_i,$$

and can be written more compactly in a vector $\mathbf{b}$ as

$$\mathbf{b} = \mathbf{D}\mathbf{e} - \mathbf{r} = (2\mathbf{D} - |\mathbf{A}|)\mathbf{e}. \tag{3}$$

Note that if $b_i \leq 0$, for any i, then no information can be established regarding the lower bound for λ_k, which is already known to be positive.

Let $\mathbf{S^k}$ be a diagonal matrix with all the positive elements denoted by s^k_{ii}, and consider the similarity transformation $\mathbf{A}' = (\mathbf{S^k})^{-1}\mathbf{A}\mathbf{S^k}$, then clearly $\sigma(\mathbf{A})$ is preserved. The Gerschgorin left bounds are now given by the vector $\mathbf{b}'$,

$$\mathbf{b}' = (2\mathbf{D} - |(\mathbf{S^k})^{-1}\mathbf{A}\mathbf{S^k}|)\mathbf{e} = (2\mathbf{D} - (\mathbf{S^k})^{-1}|\mathbf{A}|\mathbf{S^k})\mathbf{e}.$$

Note that the diagonal elements of $\mathbf{A}'$ and $\mathbf{A}$ are identical, and the similarity transformation neither affects the signs of the elements of $\mathbf{A}$ nor makes any element zero.

Consider the matrix

$$\mathbf{C^k} = [2\mathbf{D} - \lambda'_k(1-\epsilon)\mathbf{I}]^{-1}|\mathbf{A}|, \tag{4}$$

where $0 \leq \epsilon < 1$, and λ'_k is a good upper bound approximation of λ_k. consequentially it follows from (1) that

$$\lambda_k \leq R(\mathbf{e_i}) = \langle \mathbf{A}\mathbf{e_i}, \mathbf{e_i}\rangle = a_{ii}.$$

Since $\mathbf{C^k}$ is non-negative and irreducible, it follows from the Perron Frobenius theorem for non-negative matrices [3] that $\mathbf{C^k}$ has a unique positive eigenvector $\mathbf{v^k}$ corresponding to the Perron root $\rho_k = \rho(\mathbf{C^k})$, which is the spectral radius of $\mathbf{C^k}$. Let $s^k_{ii} = v^k_i$ or equivalently write $\mathbf{v^k} = \mathbf{S^k}\mathbf{e}$ then,

$$[2\mathbf{D} - \lambda'_k(1-\epsilon)\mathbf{I}]^{-1}|\mathbf{A}|\mathbf{S^k}\mathbf{e} = \rho_k\mathbf{S^k}\mathbf{e}. \tag{5}$$

Rewrite (5) as

$$(\mathbf{S^k})^{-1}|\mathbf{A}|\mathbf{S^k}\mathbf{e} = \rho_k[2\mathbf{D} - \lambda'_k(1-\epsilon)I]\mathbf{e}$$
$$(2\mathbf{D} - (\mathbf{S^k})^{-1}|\mathbf{A}|\mathbf{S^k})\mathbf{e} = [2(1-\rho_k)\mathbf{D} + \rho_k\lambda'_k(1-\epsilon)I]\mathbf{e} = 2(1-\rho_k)\mathbf{D}\mathbf{e} + \rho_k\lambda'_k(1-\epsilon)\mathbf{e}.$$

Hence, it follows from (3) that

$$\mathbf{b}' = 2(1-\rho_k)\mathbf{D}\mathbf{e} + \rho_k\lambda'_k(1-\epsilon)\mathbf{e}. \tag{6}$$

Note that the elements of $\mathbf{b}'$, namely

$$b'_i = 2(1-\rho_k)a_{ii} + \rho_k\lambda'_k(1-\epsilon), \tag{7}$$

are not constant and vary with the value of a_{ii}, for fixed ϵ. An ideal requirement is that all components of $\mathbf{b}'$ be equal. If $b'_i = b'_j$, then

$$(1-\rho_k)(a_{ii} - a_{jj}) = 0. \tag{8}$$

Clearly $\rho_k = 1$, thus (6) simplifies to

$$\mathbf{b}' = \lambda'_k(1-\epsilon)\mathbf{e} > \mathbf{0},$$

which is a constant and represents a lower bound of λ_k, for suitable ϵ. However in practice it is not always possible to choose an ideal value for ϵ, hence for the value of ϵ such that ρ_k is close to unity, we choose the minimum component of $\mathbf{b}'$ as a lower bound of λ_k.

We now consider the special case, when the diagonal elements of $\mathbf{A}$ are equal. Let $a_{ii} = a$ and note from (4), that

$$\rho_k = \frac{\rho(|\mathbf{A}|)}{2a - \lambda'_k(1-\varepsilon)}. \tag{9}$$

consequently, from (9), we obtain

$$\lambda'_k(1-\varepsilon) = \frac{2a\rho_k - \rho(|\mathbf{A}|)}{\rho_k}. \tag{10}$$

Substituting (10) into (6) we write

$$\mathbf{b}' = 2(1-\rho_k)a\mathbf{e} + \rho_k\lambda'_k(1-\epsilon)\mathbf{e} = (2a - 2a\rho_k)\mathbf{e} + (2a\rho_k - \rho(|\mathbf{A})|)\mathbf{e} = (2a - \rho(|\mathbf{A}))\mathbf{e}. \tag{11}$$

Thus, the lower bounds are independent of λ'_k, ε, and ρ_k.

Algorithm

(i) Use a few iterates of the inverse power method on $\mathbf{A}$ to generate an approximate eigenvector $\mathbf{x}'_k$, corresponding to λ_k, that is

$$\mathbf{A}\mathbf{z}_{i+1} = \mathbf{y}_i$$

$$\mathbf{y}_{i+1} = \frac{\mathbf{z}_{i+1}}{\|\mathbf{z}_{i+1}\|_2},$$

where $\mathbf{y}_0 = \dfrac{\mathbf{e}}{\sqrt{n}}$, $i = 0, 1, 2, \cdots, N_{\mathbf{A}} - 1$ and $\mathbf{x}'_k = \mathbf{y}_{N_{\mathbf{A}}-1}$.

(ii) Set $\lambda'_k = \langle \mathbf{A}\mathbf{x}'_k, \mathbf{x}'_k \rangle$ as an upper bound of λ_k.

(iii) Choose a suitable ϵ, where $0 < \epsilon < 1$, and use the power method on matrix $\mathbf{C}$ to get an approximation of ρ (close to 1) that corresponds to a positive eigenvector

$$\mathbf{z}_{i+1} = \mathbf{C}\mathbf{y}_i$$

$$\mathbf{y}_{i+1} = \frac{\mathbf{z}_{i+1}}{\|\mathbf{z}_{i+1}\|_2},$$

where $\mathbf{y}_0 = \dfrac{\mathbf{e}}{\sqrt{n}}$ and $i = 0, 1, 2, \cdots, N_{\mathbf{C}} - 1$.

(iv) Generate the lower bound vector $\mathbf{b}'$ from (6), then choose $\min_i b'_i$ as a lower bound of λ_k.

The right bound of the Gerschgorin intervals is given by

$$b_i = a_{ii} + r_i,$$

which can be written more compactly as a vector $\mathbf{b_1}$, given by

$$\begin{aligned} \mathbf{b_1} &= \mathbf{D}\mathbf{e} + \mathbf{r} \\ &= |\mathbf{A}|\mathbf{e}. \end{aligned} \tag{12}$$

Consider the matrix $\mathbf{C^1} = [\lambda'_1(1+\epsilon)]^{-1}|\mathbf{A}|$, where $0 \leq \epsilon < 1$, and λ'_1 is a good lower bound approximation of λ_1. Consequentially it follows from (1) that

$$\begin{aligned} \lambda_1 &\geq R(\mathbf{e_i}) \\ &= \langle \mathbf{A}\mathbf{e_i}, \mathbf{e_i} \rangle \\ &= a_{ii}. \end{aligned}$$

Since $\mathbf{C^1}$ is non-negative and irreducible, it follows from the Perron Frobenius theorem for non-negative matrices [3] that $\mathbf{C^1}$ has a unique positive eigenvector $\mathbf{v^1}$, corresponding to the Perron root $\rho_1 = \rho\left(\mathbf{C^1}\right)$. Let $s^1_{ii} = v^1_i$ or equivalently write, $\mathbf{v^1} = \mathbf{S^1}\mathbf{e}$, then

$$\begin{aligned} \frac{|\mathbf{A}|}{\lambda'_1(1+\epsilon)}\mathbf{S^1}\mathbf{e} &= \rho_1\mathbf{S^1}\mathbf{e} \\ (\mathbf{S^1})^{-1}|\mathbf{A}|\mathbf{S^1}\mathbf{e} &= \rho_1\lambda'_1(1+\epsilon) \\ \left|(\mathbf{S^1})^{-1}\mathbf{A}\mathbf{S^1}\right|\mathbf{e} &= \rho_1\lambda'_1(1+\epsilon) \\ \mathbf{b_1}' &= \rho_1\lambda'_1(1+\epsilon). \end{aligned} \tag{13}$$

Hence, the upper bounds are all equal. In fact,

$$\begin{aligned} \rho_1 &= \rho(\mathbf{C^1}) \\ &= \frac{\rho(|\mathbf{A}|)}{\lambda'_1(1+\varepsilon)}, \end{aligned} \tag{14}$$

and consequently from (13),

$$\mathbf{b}'_1 = \rho(|\mathbf{A}|). \tag{15}$$

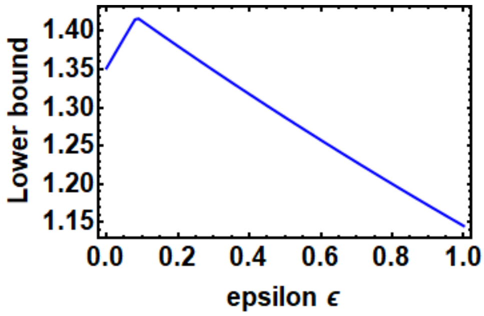

Fig. 1. Lower bound vs epsilon for example 3.1

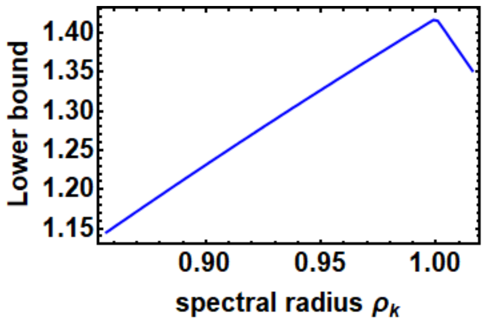

Fig. 2. Lower bound vs spectral radius for example 3.1

III. RESULTS

Example 3.1: Consider the test matrix [9], which is positive definite and irreducible,

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

with a minimum eigenvalue of $\mathbf{1.425687}$ and maximum eigenvalue of $\mathbf{9.375939}$, accurate to six decimal places. We use $N_{\mathbf{A}} = 3$ to determine $\mathbf{x}'_k$ and λ'_k from (ii). We use $N_{\mathbf{C}} = 10$ to determine ρ_k, for $\epsilon = 0.1$. The same parameters are used to determine the upper bound for λ_1. We obtain the following results

$$\begin{aligned} &\lambda'_k = 1.548137, \rho_k = 0.997039, \\ &\mathbf{b}' = [1.412885, 1.418807, 1.424728, 1.43065]^T, \\ &\lambda'_1 = 9.350228, \rho_1 = 0.91228, \end{aligned}$$

from which a lower bound of $\mathbf{1.412885}$ and an upper bound of $\mathbf{9.383023}$ is obtained.

Example 3.2: Consider the test matrix below, which is positive definite and irreducible,

$$\mathbf{A} = \begin{bmatrix} 10 & 3 & 2 & -0.5 \\ 3 & 4 & 3.5 & 5 \\ 2 & 3.5 & 10 & 1.5 \\ -0.5 & 5 & 1.5 & 12 \end{bmatrix}$$

with a minimum eigenvalue of $\mathbf{6.323996}$ and a maximum eigenvalue of $\mathbf{20.250466}$, accurate to six decimal places. We use $N_{\mathbf{A}} = 3$ to determine $\mathbf{x}'_k$ and λ'_k is determined from step from (ii) in the algorithm. We use $N_{\mathbf{C}} = 10$ to determine ρ_k, for $\epsilon = 0.5$. The same parameters are used to determine

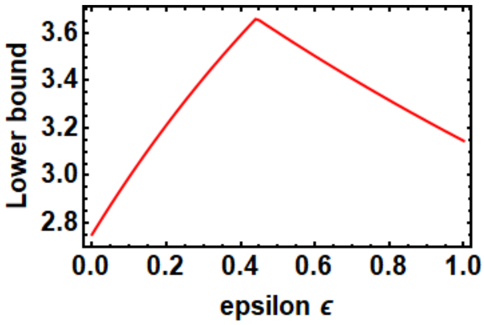

Fig. 3. Lower bound vs epsilon for example 3.2

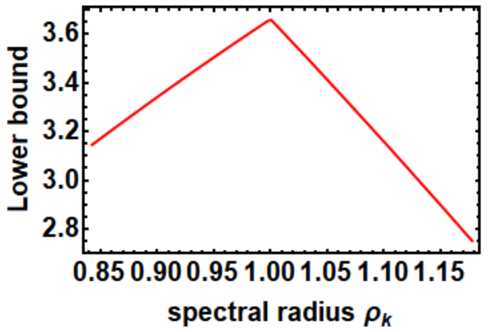

Fig. 4. Lower bound vs spectral radius for example 3.2

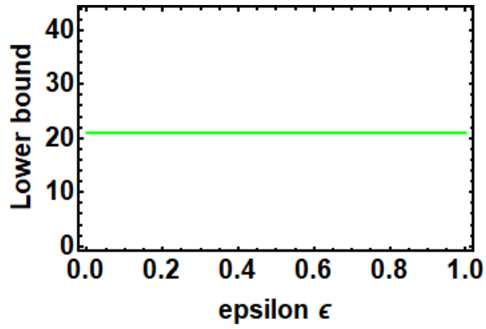

Fig. 5. Lower bound vs epsilon for example 3.3

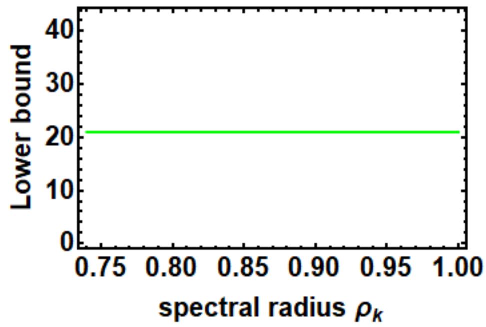

Fig. 6. Lower bound vs spectral radius for example 3.3

the upper bound of λ_1. We obtain the following results:

$$\lambda_k' = 6.562099, \rho_k = 0.980824,$$
$$\mathbf{b}' = [3.60166, 3.755072, 3.60166, 3.678366]^T,$$
$$\lambda_1' = 20.236249, \rho_1 = 0.676565,$$

from which a lower bound $\mathbf{3.60166}$ and an upper bound $\mathbf{20.536707}$ is obtained.

From figures 1 and 3, we can determine the optimal value of ε for which the lower bound is maximum. Examining figures 2 and 4, we note that the lower bound is maximized when ρ_k is close to unity, as discussed in equation 8. Although we have shown in equation (15) that it is theoretically and practically possible to have the upper bound components equal, the same statement is only true for the lower bounds, if a suitable value for ε is known in advance, where $\rho_k = 1$. However in practice the lower bound components differ slightly from each other, even if ε is not optimal.

Example 3.3: Consider the Stieltjes matrix [13], which is irreducible, given by

$$\mathbf{A} = \begin{bmatrix} 2n & -1 & -1 & -1 & \cdots & -1 \\ -1 & 2n & -1 & -1 & \cdots & -1 \\ -1 & -1 & 2n & -1 & \cdots & -1 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ -1 & -1 & -1 & -1 & 2n & -1 \\ -1 & -1 & -1 & -1 & -1 & 2n \end{bmatrix},$$

where n is the dimension of $\mathbf{A}$. The matrix $\mathbf{A}$ can be written in the form $\mathbf{A} = (2n+1)\mathbf{I} - \mathbf{ee^t}$. The matrix $\mathbf{ee^t}$ has a rank of unity which implies that $\sigma(\mathbf{ee^t}) = \{0, n\}$, with zero having a multiplicity of $n-1$. Note that the eigenvalue n corresponds to the eigenvector $\mathbf{e}$. Hence, $\sigma(\mathbf{A}) = \{n+1, 2n+1\}$, where the eigenvalue $2n+1$ has a multiplicity o $n-1$. We illustrate the validity of (11), in figures 5 and 6, for $n = 20$, that is the independence of the lower bound on ϵ and ρ_k. We obtain exactly $\mathbf{21}$ and $\mathbf{59}$, for the lower and upper bound, respectively, which is in agreement with (15).

Example 3.4: When the Poisson partial differential equation is discretized by a five-point finite different scheme, it results in a $n \times n$ Stieltjes tridiagonal matrix $\mathbf{A}$, that has the form

$$\mathbf{A} = \begin{bmatrix} 4 & -1 & 0 & 0 & \cdots & 0 \\ -1 & 4 & -1 & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \ddots & 0 & \\ \vdots & \vdots & \ddots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & -1 & 4 & -1 \\ 0 & 0 & 0 & 0 & -1 & 4 \end{bmatrix}.$$

Clearly $\mathbf{A}$ is irreducible and the eigenvalues are explicitly given by [14]

$$\lambda_k = 4 - 2\cos\left(\frac{k\pi}{n+1}\right), \quad k = 1, 2, \cdots, n.$$

Thus, $\sigma(\mathbf{A}) \in [\lambda_1, \lambda_n] \approx [2.152241, 5.847759]$, for $n = 7$.

Once again, we observe from figure 7 and figure 8 that since the diagonal elements are equal, the lower bound is independent of ε and ρ_k. This further validates (11). We obtain $\mathbf{2.109941}$ for the lower bound and $\mathbf{5.890058}$ for the upper bound.

IV. Conclusion

We have presented a simple and relatively cost-effective method of improving the outer bounds of real symmetric positive definite matrices, which are irreducible. Some important matrices from engineering, as well as special cases have been considered. We have also shown that our method does indeed yield the outer bounds.

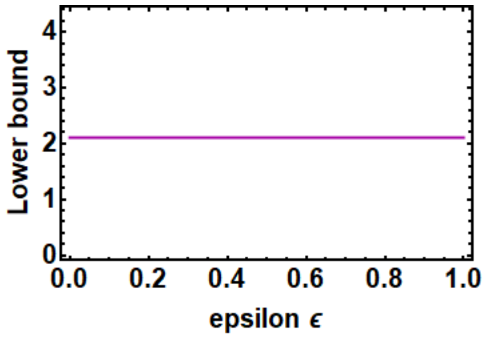

Fig. 7. Lower bound vs epsilon for example 3.4

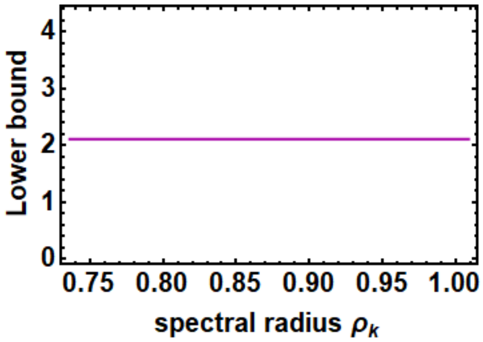

Fig. 8. Lower bound vs spectral radius for example 3.4

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