The Relation between Two Types of Error Bounds for Computed Matrix Eigenvalues*

Shinya Miyajima

Faculty of Engineering, Gifu University, 1-1 Yanagido, Gifushi, Gifu 501-1193, Japan

miyajima@gifu-u.ac.jp

Abstract

Two types of error bounds are considered for numerically enclosing all eigenvalues of a matrix. A theorem is presented for clarifying the relation between these two error bounds under an assumption. We discuss the validity of this assumption, and report some numerical results illustrating the presented theorem and showing that this assumption is satisfied in many cases.

Keywords: matrix eigenvalue, numerical enclosure, verified error bound **AMS subject classifications:** 65F15, 65G20, 65G50

1 Introduction

In this paper, we are concerned with accuracy of computed eigenvalues for

$$Ax = \lambda x, \qquad A \in \mathbb{C}^{n \times n}, \quad \lambda \in \mathbb{C}, \quad x \in \mathbb{C}^n, \tag{1}$$

where λ is an eigenvalue and $x \neq 0$ is an eigenvector corresponding to λ .

There are several methods for enclosing eigenvalues and eigenvectors, e.g., [4, 5, 7, 9, 12, 13, 14]. For enclosing eigenvectors, see [9]. For enclosing eigenvalues in the case when *A* is Hermitian, see [4, 10, 12] and [5, Algorithm 3]. *A few specified* eigenvalues and eigenvectors can be enclosed by applying the methods in [7, 13, 14], even when *A* is *not* Hermitian.

In this paper, we consider a method for enclosing *all* eigenvalues which is applicable even when *A* is *not* Hermitian. Such a method, proposed in [5, Algorithm 2], is based on the following theorem:

Theorem 1 (Oishi [5]) Let λ be an eigenvalue of A. Assume, as a result of numerical computation, we have an $n \times n$ complex diagonal matrix \tilde{D} and an $n \times n$ complex matrix \tilde{X} such that $A\tilde{X} \approx \tilde{X}\tilde{D}$. Let $\tilde{\lambda}_i$, i = 1, ..., n be the (i, i) element of \tilde{D} and $\|\cdot\| := \|\cdot\|_p$, $1 \le p \le \infty$. Denote the $n \times n$ identity matrix by I. For an arbitrary $n \times n$ complex matrix Y, define $n \times n$ complex matrices R and S as $R := YA\tilde{X} - \tilde{D}$ and $S := Y\tilde{X} - I$, respectively. Then,

$$\min_{1 \le i \le n} |\lambda - \tilde{\lambda}_i| \le \varepsilon_{\mathrm{o}}, \quad \varepsilon_{\mathrm{o}} := \|R\| + \|A\| \|S\|.$$

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On the other hand, a theorem has been presented in [3] for enclosing all eigenvalues of the generalized eigenvalue problem

$$Ax = \lambda Bx, \qquad A, B \in \mathbb{C}^{n \times n}, \quad \lambda \in \mathbb{C}, \quad x \in \mathbb{C}^{n}.$$
 (2)

This theorem is also applicable even when *A* is not Hermitian. We can utilize this theorem for enclosing all eigenvalues in the standard eigenvalue problem (1) by substituting B = I into (2), where *I* is as in Theorem 1. Then, we obtain the following theorem ¹:

Theorem 2 (Miyajima [3]) Let λ , \tilde{D} , \tilde{X} , $\tilde{\lambda}_i$, $\|\cdot\|$, Y and S be defined as in Theorem 1. Define an $n \times n$ complex matrix T as $T := Y(A\tilde{X} - \tilde{X}\tilde{D})$. If $\|S\| < 1$. Then \tilde{X} and Y are nonsingular, and

$$\min_{1 \le i \le n} |\lambda - \tilde{\lambda}_i| \le \varepsilon_{\mathrm{m}}, \quad \varepsilon_{\mathrm{m}} := \frac{\|T\|}{1 - \|S\|}.$$

The purpose of this paper is to present a theorem showing that $\varepsilon_o \ge \varepsilon_m$ holds under an assumption. We discuss the validity of this assumption, and report some numerical results illustrating the presented theorem and showing that this assumption is satisfied in many cases.

2 Main Theorem

Let ε_0 and ε_m be defined as in Theorems 1 and 2, respectively. In this section, we establish Theorem 3 clarifying the relations between ε_0 and ε_m under an assumption.

Theorem 3 Let $\tilde{\lambda}_i$, $\|\cdot\|$ and ε_0 be defined as in Theorem 1, and let ε_m be defined as in Theorem 2. If $\max_{1 \le i \le n} |\tilde{\lambda}_i| + \varepsilon_0 \le \|A\|$, then $\varepsilon_0 \ge \varepsilon_m$.

Remark 1 Let $\tilde{\lambda}_j$ satisfy $|\tilde{\lambda}_j| = \max_{1 \le i \le n} |\tilde{\lambda}_i|$ and $\rho(A)$ denote the spectral radius of A. It is well known that $\rho(A) \le ||A||$ follows. Hence ||A|| is a "trivial" upper bound for $\rho(A)$ and overestimates $\rho(A)$ in general. In contrast, $|\tilde{\lambda}_j| + \varepsilon_0$ is generally a "nontrivial" upper bound and a tight estimation for $\rho(A)$ as long as $\tilde{\lambda}_j$ is good approximation and ε_0 is small compared with $|\tilde{\lambda}_j|$. Thus $|\tilde{\lambda}_j| + \varepsilon_0 \le ||A||$ holds in many cases when $\tilde{\lambda}_j$ and ε_0 are as such.

When A is Hermitian and $\|\cdot\|$ is the 2-norm, $|\tilde{\lambda}_j| + \varepsilon_0 \le ||A||$ does not hold even if $\tilde{\lambda}_j$ and ε_0 are as above, since $||A||_2 = \rho(A) \le |\tilde{\lambda}_j| + \varepsilon_0$, where the equality is given by Wilkinson and Weyl (see e.g. [11]). However some methods have been proposed in [4] and [5, Algorithm 3] for enclosing all eigenvalues of an Hermitian matrix², and are more efficient than those based on Theorems 1 and 2. Therefore the methods based on Theorems 1 and 2 are advantageous when they are not applied to an Hermitian matrix but to a general matrix. Moreover using the matrix 1-norm or ∞ -norm, it is disadvantageous in computational cost to compute verified upper bounds for the 2-norm has been proposed in [8], this method requires $\mathcal{O}(n^3)$ flops, while the computations for the verified upper bounds for the 1-norm and ∞ -norm require only $\mathcal{O}(n^2)$ flops. In fact, in [3, 5], the programs created for the methods based on Theorems 1 and 2 use the ∞ -norm.

¹The only case considered in [3] is when $\|\cdot\|$ is the ∞ -norm. However Theorem 2 follows for an arbitrary *p*-norm.

²The methods in [4] and [5, Algorithm 3] have been proposed for enclosing all eigenvalues of a real symmetric matrix. On the other hand, these methods can be extended for enclosing all eigenvalues of an Hermitian matrix.

Proof Let \tilde{D} , \tilde{X} , I, Y, R and S be defined as in Theorem 1. From ||S|| < 1, we obtain

$$\begin{aligned}
\varepsilon_{\rm m} &= \frac{\|YA\tilde{X} - \tilde{D} + \tilde{D} - Y\tilde{X}\tilde{D}\|}{1 - \|S\|} \\
&\leq \frac{\|YA\tilde{X} - \tilde{D}\| + \|\tilde{D} - Y\tilde{X}\tilde{D}\|}{1 - \|S\|} \\
&\leq \frac{\|R\| + \|I - Y\tilde{X}\|\|\tilde{D}\|}{1 - \|S\|} = \frac{\|R\| + \max_{1 \le i \le n} |\tilde{\lambda}_i| \|S\|}{1 - \|S\|} \\
&= \|R\| + \frac{(\max_{1 \le i \le n} |\tilde{\lambda}_i| + \|R\|)\|S\|}{1 - \|S\|} = \|R\| + \left(\|A\| - \frac{\|A\| - (\max_{1 \le i \le n} |\tilde{\lambda}_i| + \varepsilon_0)}{1 - \|S\|}\right) \|S\| \\
&= \varepsilon_0 - \frac{(\|A\| - (\max_{1 \le i \le n} |\tilde{\lambda}_i| + \varepsilon_0))\|S\|}{1 - \|S\|}.
\end{aligned}$$
(3)

The inequalities $\max_{1 \le i \le n} |\tilde{\lambda}_i| + \varepsilon_0 \le ||A||$ and ||S|| < 1 yield

$$\frac{\left(\|A\| - (\max_{1 \le i \le n} |\tilde{\lambda}_i| + \varepsilon_0)\right)\|S\|}{1 - \|S\|} \ge 0.$$

This and (3) prove the theorem.

3 Numerical Results

Let \tilde{D} , \tilde{X} , $\|\cdot\|$, Y, R, S and ε_0 be defined as in Theorem 1, and let ε_m be defined as in Theorem 2. In this section, we report some numerical results to illustrate Theorem 3 and to show that the assumption in Theorem 3 is satisfied in many cases. We used a computer with an Intel Xeon 2.66GHz Dual CPU, 4.00GB RAM and MATLAB 7.5 with Intel Math Kernel Library and IEEE 754 double precision. We applied the MATLAB function eig to obtain \tilde{D} and \tilde{X} .

We created Programs³ 1 and 2 for executing the methods based on Theorems 1 and 2, respectively, when $\|\cdot\|$ is ∞ -norm. For $F^{(c)}$, $F^{(r)} \in \mathbb{R}^{n \times n}$ where all elements of $F^{(r)}$ are nonnegative, the notation $\langle F^{(c)}, F^{(r)} \rangle$ denotes a matrix interval whose center and radius are $F^{(c)}$ and $F^{(r)}$, respectively. For $n \times n$ real matrices \underline{F} and \overline{F} with $\underline{F} \leq \overline{F}$, the notation $[\underline{F}, \overline{F}]$ denotes a matrix interval whose lower and upper bounds are \underline{F} and \overline{F} , respectively.

Program 1 This program computes a verified upper bound for $\min_{1 \le i \le n} |\lambda - \tilde{\lambda}|$ based on Theorem 1, when $\|\cdot\|$ is the ∞ -norm and \tilde{D} and \tilde{X} are given. The functions cerrt and cerrb return verified upper bounds for $\|R\|_{\infty}$ and $\|S\|_{\infty}$, respectively (see [5] for details). The INTLAB [6] function setround(+1) switches the rounding mode to upwards (towards ∞). The computational cost of this program is $72n^3$ flops.

function ε_0 = voeig $(A, \tilde{D}, \tilde{X})$ $Y = inv(\tilde{X});$ $r = cerrt(Y, A, \tilde{X}, \tilde{D});$ $s = cerrb(Y, \tilde{X}, eye(n));$ setround(+1); $\varepsilon_0 = r + norm(A, inf)*s;$

Program 2 This program computes a verified upper bound for $\min_{1 \le i \le n} |\lambda - \tilde{\lambda}|$ based on Theorem 2, when $\|\cdot\|$ is ∞ -norm and \tilde{D} and \tilde{X} are given. The functions cerrb and setround(+1)

³Although a faster program than Program 2 is described in [3], we adopted Program 2 for fairness.

are defined as in Program 1. For $F, G \in \mathbb{C}^{n \times n}$, the function cprod returns $n \times n$ real matrices $\underline{H_r}, \overline{H_r}, \underline{H_i}$ and $\overline{H_i}$ satisfying $[\underline{H_r}, \overline{H_r}] + i * [\underline{H_i}, \overline{H_i}] \ni FG$, where $i = \sqrt{-1}$. For $\underline{F}, \overline{F} \in \mathbb{R}^{n \times n}$ with $\underline{F} \leq \overline{F}$, the function cr returns $n \times n$ real matrices $F^{(c)}$ and $F^{(r)}$ satisfying $\langle F^{(c)}, F^{(r)} \rangle \supseteq [\underline{F}, \overline{F}]$. For $F_r, G^{(c)}, G^{(r)} \in \mathbb{R}^{n \times n}$ where all elements of $G^{(r)}$ are nonnegative, the function iprod returns $n \times n$ real matrices \underline{H} and \overline{H} satisfying $[\underline{H}, \overline{H}] \supseteq Fr * \langle G^{(c)}, G^{(r)} \rangle$. See [5] for details of the functions cprod, cr and iprod. The INTLAB function setround (-1) switches the rounding mode to downwards (towards $-\infty$). The computational cost of this program is 72n³ flops.

 $\begin{array}{ll} \text{function } & \mathcal{E}_{\text{m}} = \text{vmeig}(A, \tilde{D}, \tilde{X}) \\ Y = \text{inv}(\tilde{X}); \\ s = \text{cerrb}(Y, \tilde{X}, \text{eye}(n)); \\ \text{if } s \geq 1; & \text{error}(\text{'Enclosure failed.'}); & \text{end}; \\ [\underline{B_r}, \underline{B_r}, \underline{B_i}, \overline{B_i}] = \text{cprod}(A, \tilde{X}); & [\underline{C_r}, \overline{C_r}, \underline{C_i}, \overline{C_i}] = \text{cprod}(-\tilde{X}, \tilde{D}); \\ \text{setround}(-1); & \underline{P_r} = \underline{B_r} + \underline{C_r}; & \overline{P_i} = \underline{B_i} + \underline{C_i}; \\ \text{setround}(+1); & \overline{P_r} = \overline{B_r} + \overline{C_r}; & \overline{P_i} = \overline{B_i} + \overline{C_i}; \\ [P_r^{(c)}, P_r^{(r)}] = \text{cr}(\underline{P_r}, \overline{P_r}); & [P_i^{(c)}, P_i^{(r)}] = \text{cr}(\underline{P_i}, \overline{P_i}); \\ Y_r = \text{real}(Y); & Y_i = \text{imag}(Y); \\ [\underline{Q_{rr}}, \overline{Q_{rr}}] = \text{iprod}(Y_r, P_r^{(c)}, P_r^{(r)}); & [\underline{Q_{ii}}, \overline{Q_{ii}}] = \text{iprod}(-Y_i, P_i^{(c)}, P_i^{(r)}); \\ \underline{Q_{ri}}, \overline{Q_{ri}}] = \text{iprod}(Y_r, P_i^{(c)}, P_i^{(r)}); & [\underline{Q_{ir}}, \overline{Q_{ir}}] = \text{iprod}(Y_i, P_r^{(c)}, P_r^{(r)}); \\ \text{setround}(-1); & \underline{T_r} = \underline{Q_{rr}} + \underline{Q_{ii}}; & \underline{T_i} = \underline{Q_{ri}} + \underline{Q_{ir}}; \\ \text{setround}(+1); & \overline{T_r} = \overline{Q_{rr}} + \underline{Q_{ii}}; & \overline{T_i} = \overline{Q_{ri}} + \underline{Q_{ir}}; \\ T_r = \text{max}(\text{abs}(\underline{T_r}), \text{abs}(\overline{T_r})); & T_i = \text{max}(\text{abs}(\underline{T_i}), \text{abs}(\overline{T_i})); \\ T = T_r + i*T_i; & t = \text{norm}(T, \text{inf}); \\ \mathcal{E}_m = t/(-(s-1)); \end{array} \right$

Let t_{λ} , $t_{\lambda x}$, t_0 and t_m be the computing time (sec) for obtaining \tilde{D} , \tilde{D} and \tilde{X} , for the methods based on Theorems 1 and 2, respectively. For nonsingular $M \in \mathbb{C}^{n \times n}$, define the condition number $\kappa(M) := \|M\|_2 \|M^{-1}\|_2$.

3.1 Example 1

In this example, we observe the magnitudes of the error bounds and computing times for large n. Consider the case when $A \in \mathbb{C}^{n \times n}$ is generated by the MATLAB code $A = \operatorname{randn}(n) + i \times \operatorname{randn}(n)$; Then the real and the imaginary parts of the entries of A are normally distributed pseudo random numbers. Table 1 displays ε_0 , ε_m , $\max_{1 \le i \le n} |\tilde{\lambda}_i| + \varepsilon_0$ and ||A|| for various n. Table 2 shows t_λ , $t_{\lambda x}$, t_0 and t_m for various n. In Tables 1, 3 and 5, the computation of the absolute value and the addition in $\max_{1 \le i \le n} |\tilde{\lambda}_i| + \varepsilon_0$, and the computation of the norm $||A||_{\infty}$ are executed via floating point operations in rounding upwards and downwards mode, respectively.

Table 1: The quantities ε_0 , ε_m , max $|\tilde{\lambda}_i| + \varepsilon_0$ and ||A|| in Example 1, for the ∞ -norm

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n	Eo	$\epsilon_{\rm m}$	$\max \tilde{\lambda}_i + \varepsilon_{\mathrm{o}}$	$\ A\ $
1000	2.22e-07	8.24e-08	7.23e+01	1.92e+03
1500	2.19e-06	7.21e-07	1.27e+02	4.00e+03
2000	4.36e-06	1.50e-06	1.89e+02	6.96e+03
2500	2.23e-05	7.70e-06	2.61e+02	1.07e+04

n	t_{λ}	$t_{\lambda x}$	to	t _m
1000	2.76	5.27	12.9	13.1
1500	7.78	16.7	41.6	42.1
2000	17.4	39.6	95.8	96.9
2500	33.9	78.9	185	187

Table 2: Computing times (sec) in Example 1

It can be seen from Table 1 that $\max_{1 \le i \le n} |\tilde{\lambda}_i| + \varepsilon_0 < ||A||$ holds for all the cases in this example. Moreover $\varepsilon_0/\varepsilon_m \approx 2.88$. We can confirm from Table 2 that t_0 was approximately equal to t_m . This result coincides the fact that the computational cost of Program 1 is similar to that of Program 2. Computing times t_0 and t_m were larger than t_λ and $t_{\lambda x}$.

3.2 Example 2

In this example, we observe the magnitudes of the error bounds for matrices with ill-conditioned eigenvectors. Consider the case when $A \in \mathbb{C}^{n \times n}$ is generated by

A = gallery('chebspec', n, 0);

We used the Higham's test matrix chebspec [2]. Then A has ill-conditioned eigenvectors. Table 3 shows $\kappa(\tilde{X})$ and the other quantities as in Table 1 for various *n*, where $\kappa(\tilde{X})$ is an approximation obtained by the MATLAB function cond.

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n	$\kappa(ilde{X})$	$\epsilon_{\rm o}$	$\epsilon_{\rm m}$	$\max \tilde{\lambda}_i + \varepsilon_{\mathrm{o}}$	$\ A\ $
10	6.45e+14	2.30e+01	6.62e+00	2.32e+01	8.10e+01
15	8.19e+14	8.35e+01	2.90e+01	8.46e+01	1.96e+02
20	1.35e+14	2.61e+01	8.26e+00	2.93e+01	3.61e+02
25	2.63e+14	6.39e+01	1.78e+01	7.01e+01	5.76e+02

Table 3: The quantities $\kappa(\tilde{X})$, ε_0 , ε_m , max $|\tilde{\lambda}_i| + \varepsilon_0$ and ||A|| in Example 2 for ∞ -norm

We see from Table 3 that the relation between $\max_{1 \le i \le n} |\tilde{\lambda}_i| + \varepsilon_0$ and ||A|| is similar to that in Section 3.1. Moreover ε_0 and ε_m were larger than $\max_{1 \le i \le n} |\tilde{\lambda}_i|$.

3.3 Example 3

In this example, we observe the magnitudes of the error bounds and computing times for matrices in the Matrix Market [1]. All the matrices in this example are real unsymmetric. Although these matrices are sparse, \tilde{X} is full. Hence the methods based on Theorems 1 and 2 are not applicable when *n* is large. Table 4 shows the names, *n*, $\kappa(A)$ and $\kappa(\tilde{X})$ of the matrices being used, where $\kappa(A)$ and $\kappa(\tilde{X})$ are approximations obtained by cond. Tables 5 and 6 display quantities as in Tables 1 and 2, respectively, for various matrices.

It can be seen from Table 5 that $\max_{1 \le i \le n} |\tilde{\lambda}_i| + \varepsilon_0 \le ||A||$ did not hold when the matrix was CDDE2, LOP163 and RW496. Nevertheless $\varepsilon_0 > \varepsilon_m$ held in LOP163 and RW496. These results show the existence of the case when $\varepsilon_0 \ge \varepsilon_m$ holds even if $\max_{1 \le i \le n} |\tilde{\lambda}_i| + \varepsilon_0 \le ||A||$ does not hold. In contrast, $\varepsilon_0 \ge \varepsilon_m$ did not follow in CDDE2. In this case, $\varepsilon_0 = 2.63 \times 10^1$ and $\max_{1 \le i \le n} |\tilde{\lambda}_i| = 5.73 \times 10^0$, i.e., ε_0 was larger than $\max_{1 \le i \le n} |\tilde{\lambda}_i|$. Similarly, relations regarding

Table 4. Floperties of matrices					
Name	n	$\kappa(A)$	$\kappa(\tilde{X})$		
CDDE2	961	1.29e+02	4.29e+23		
CRY2500	2500	4.35e+17	1.29e+08		
DW2048	2048	5.30e+03	6.35e+01		
LOP163	163	3.42e+07	6.32e+07		
OLM2000	2000	1.22e+07	8.11e+01		
QH1484	1484	5.58e+17	4.85e+08		
RDB2048L	2048	2.08e+03	9.38e+01		
RW496	496	1.14e+10	5.72e+10		
TOLS2000	2000	6.92e+06	5.19e+03		

Table 4: Properties of matrices

Table 5: The quantities ε_0 , ε_m , max $|\tilde{\lambda}_i| + \varepsilon_0$ and ||A|| in Example 3 for ∞ -norm

Name	Eo	$\epsilon_{\rm m}$	$\max \tilde{\lambda}_i + \varepsilon_{\mathrm{o}}$	$\ A\ $
CDDE2	2.63e+01	3.80e+02	3.20e+01	9.09e+00
CRY2500	5.68e–04	4.31e-05	9.56e+03	1.08e+04
DW2048	1.39e-11	3.94e-12	9.79e-01	1.00e+00
LOP163	6.36e-08	2.46e-08	1.01e+00	1.00e+00
OLM2000	1.61e-06	1.02e-07	4.07e+04	4.06e+05
QH1484	1.10e+08	5.62e+04	6.68e+11	1.27e+16
RDB2048L	3.93e-09	5.24e-10	7.31e+01	7.91e+01
RW496	4.03e-04	8.32e-06	1.01e+00	1.00e+00
TOLS2000	2.84e-06	1.31e-07	2.45e+03	5.96e+06

 ε_{o} , ε_{m} , $\max_{1 \le i \le n} |\tilde{\lambda}_{i}| + \varepsilon_{o}$ and ||A|| corresponding to Sections 3.1 and 3.2 can be confirmed except in the above cases. Table 6 showed the similar tendencies to Table 2.

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Name	t_{λ}	$t_{\lambda x}$	to	t _m
CDDE2	3.38	5.96	10.6	10.8
CRY2500	29.1	66.7	165	166
DW2048	29.7	66.7	95.4	96.0
LOP163	0.03	0.05	0.08	0.07
OLM2000	13.5	33.7	85.6	86.4
QH1484	5.49	11.6	36.0	36.5
RDB2048L	28.1	62.0	95.4	96.3
RW496	0.52	0.79	1.58	1.63
TOLS2000	3.28	14.9	84.9	85.7

Table 6: Computing times (sec) in Example 3

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