

Approximation of Eigenvalues and Eigenvectors

In this chapter we deal with approximations of the eigenvalues and eigenvectors of a matrix $A \in \mathbb{C}^{n \times n}$. Two main classes of numerical methods exist to this purpose, *partial* methods, which compute the *extremal* eigenvalues of A (that is, those having maximum and minimum module), or *global* methods, which approximate the whole spectrum of A .

It is worth noting that methods which are introduced to solve the matrix eigenvalue problem are not necessarily suitable for calculating the matrix eigenvectors. For example, the *power method* (a partial method, see Section 5.3) provides an approximation to a *particular* eigenvalue/eigenvector pair.

The *QR method* (a global method, see Section 5.5) instead computes the real Schur form of A , a canonical form that displays *all* the eigenvalues of A but *not* its eigenvectors. These eigenvectors can be computed, starting from the real Schur form of A , with an extra amount of work, as described in Section 5.8.2.

Finally, some *ad hoc* methods for dealing effectively with the special case where A is a symmetric ($n \times n$) matrix are considered in Section 5.10.

5.1 Geometrical Location of the Eigenvalues

Since the eigenvalues of A are the roots of the characteristic polynomial $p_A(\lambda)$ (see Section 1.7), iterative methods must be used for their approximation when $n \geq 5$. Knowledge of eigenvalue location in the complex plane can thus be helpful in accelerating the convergence of the process.

A first estimate is provided by Theorem 1.4,

$$|\lambda| \leq \|A\|, \quad \forall \lambda \in \sigma(A), \quad (5.1)$$

for any consistent matrix norm $\|\cdot\|$. Inequality (5.1), which is often quite rough, states that *all* the eigenvalues of A are contained in a circle of radius $R_{\|A\|} = \|A\|$ centered at the origin of the Gauss plane.

Another result is obtained by extending Definition 1.23 to complex-valued matrices.

Theorem 5.1 *If $A \in \mathbb{C}^{n \times n}$, let*

$$H = (A + A^H) / 2 \quad \text{and} \quad iS = (A - A^H) / 2$$

be the hermitian and skew-hermitian parts of A , respectively, i being the imaginary unit. For any $\lambda \in \sigma(A)$

$$\lambda_{\min}(H) \leq \operatorname{Re}(\lambda) \leq \lambda_{\max}(H), \quad \lambda_{\min}(S) \leq \operatorname{Im}(\lambda) \leq \lambda_{\max}(S). \quad (5.2)$$

Proof. From the definition of H and S it follows that $A = H + iS$. Let $\mathbf{u} \in \mathbb{C}^n$, $\|\mathbf{u}\|_2 = 1$, be the eigenvector associated with the eigenvalue λ ; the Rayleigh quotient (introduced in Section 1.7) reads

$$\lambda = \mathbf{u}^H A \mathbf{u} = \mathbf{u}^H H \mathbf{u} + i \mathbf{u}^H S \mathbf{u}. \quad (5.3)$$

Notice that both H and S are hermitian matrices, whilst iS is skew-hermitian. Matrices H and S are thus unitarily similar to a real diagonal matrix (see Section 1.7), and therefore their eigenvalues are real. In such a case, (5.3) yields

$$\operatorname{Re}(\lambda) = \mathbf{u}^H H \mathbf{u}, \quad \operatorname{Im}(\lambda) = \mathbf{u}^H S \mathbf{u},$$

from which (5.2) follows. \diamond

An a priori bound for the eigenvalues of A is given by the following result.

Theorem 5.2 (of the Gershgorin circles) *Let $A \in \mathbb{C}^{n \times n}$. Then*

$$\sigma(A) \subseteq \mathcal{S}_{\mathcal{R}} = \bigcup_{i=1}^n \mathcal{R}_i, \quad \mathcal{R}_i = \{z \in \mathbb{C} : |z - a_{ii}| \leq \sum_{\substack{j=1 \\ j \neq i}}^n |a_{ij}|\}. \quad (5.4)$$

The sets \mathcal{R}_i are called Gershgorin circles.

Proof. Let us decompose A as $A = D + E$, where D is the diagonal part of A , whilst $e_{ii} = 0$ for $i = 1, \dots, n$. For $\lambda \in \sigma(A)$ (with $\lambda \neq a_{ii}$, $i = 1, \dots, n$), let us introduce the matrix $B_\lambda = A - \lambda I = (D - \lambda I) + E$. Since B_λ is singular, there exists a non-null vector $\mathbf{x} \in \mathbb{C}^n$ such that $B_\lambda \mathbf{x} = \mathbf{0}$. This means that $((D - \lambda I) + E) \mathbf{x} = \mathbf{0}$, that is, passing to the $\|\cdot\|_\infty$ norm,

$$\mathbf{x} = -(D - \lambda I)^{-1} E \mathbf{x}, \quad \|\mathbf{x}\|_\infty \leq \|(D - \lambda I)^{-1} E\|_\infty \|\mathbf{x}\|_\infty,$$

and thus

$$1 \leq \|(D - \lambda I)^{-1} E\|_\infty = \sum_{j=1}^n \frac{|e_{kj}|}{|a_{kk} - \lambda|} = \sum_{\substack{j=1 \\ j \neq k}}^n \frac{|a_{kj}|}{|a_{kk} - \lambda|}, \quad (5.5)$$

for a certain k , $1 \leq k \leq n$. Inequality (5.5) implies $\lambda \in \mathcal{R}_k$ and thus (5.4). \diamond

The bounds (5.4) ensure that any eigenvalue of A lies within the union of the circles \mathcal{R}_i . Moreover, since A and A^T share the same spectrum, Theorem 5.2 also holds in the form

$$\sigma(A) \subseteq \mathcal{S}_C = \bigcup_{j=1}^n \mathcal{C}_j, \quad \mathcal{C}_j = \{z \in \mathbb{C} : |z - a_{jj}| \leq \sum_{\substack{i=1 \\ i \neq j}}^n |a_{ij}|\}. \quad (5.6)$$

The circles \mathcal{R}_i in the complex plane are called row circles, and \mathcal{C}_j column circles. The immediate consequence of (5.4) and (5.6) is the following.

Property 5.1 (First Gershgorin theorem) *For a given matrix $A \in \mathbb{C}^{n \times n}$,*

$$\forall \lambda \in \sigma(A), \quad \lambda \in \mathcal{S}_R \cap \mathcal{S}_C. \quad (5.7)$$

The following two location theorems can also be proved (see [Atk89], pp. 588-590 and [Hou75], pp. 66-67).

Property 5.2 (Second Gershgorin theorem) *Let*

$$\mathcal{S}_1 = \bigcup_{i=1}^m \mathcal{R}_i, \quad \mathcal{S}_2 = \bigcup_{i=m+1}^n \mathcal{R}_i.$$

If $\mathcal{S}_1 \cap \mathcal{S}_2 = \emptyset$, then \mathcal{S}_1 contains exactly m eigenvalues of A , each one being accounted for with its algebraic multiplicity, while the remaining eigenvalues are contained in \mathcal{S}_2 .

Remark 5.1 Properties 5.1 and 5.2 do not exclude the possibility that there exist circles containing no eigenvalues, as happens for the matrix in Exercise 1. ■

Definition 5.1 A matrix $A \in \mathbb{C}^{n \times n}$ is called *reducible* if there exists a permutation matrix P such that

$$PAP^T = \begin{bmatrix} B_{11} & B_{12} \\ 0 & B_{22} \end{bmatrix},$$

where B_{11} and B_{22} are square matrices; A is *irreducible* if it is not reducible. ■

To check if a matrix is reducible, the *oriented graph* of the matrix can be conveniently employed. Recall from Section 3.9 that the oriented graph of a real matrix A is obtained by joining n points (called vertices of the graph) P_1, \dots, P_n through a line oriented from P_i to P_j if the corresponding matrix entry $a_{ij} \neq 0$. An oriented graph is *strongly connected* if for any pair of distinct vertices P_i and P_j there exists an oriented path from P_i to P_j . The following result holds (see [Var62] for the proof).

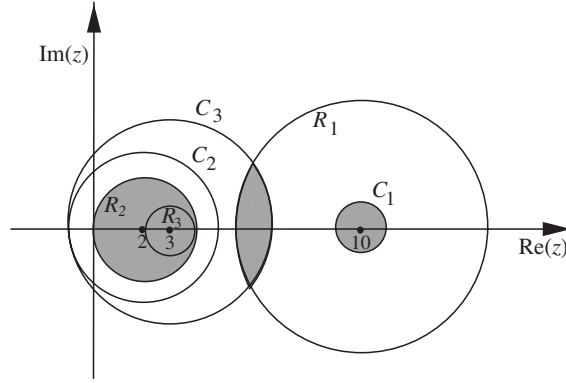


Fig. 5.1. Row and column circles for matrix A in Example 5.1

Property 5.3 *A matrix $A \in \mathbb{C}^{n \times n}$ is irreducible iff its oriented graph is strongly connected.*

Property 5.4 (Third Gershgorin theorem) *Let $A \in \mathbb{C}^{n \times n}$ be an irreducible matrix. An eigenvalue $\lambda \in \sigma(A)$ cannot lie on the boundary of $\mathcal{S}_{\mathcal{R}}$ unless it belongs to the boundary of every circle \mathcal{R}_i , for $i = 1, \dots, n$.*

Example 5.1 Let us consider the matrix

$$A = \begin{bmatrix} 10 & 2 & 3 \\ -1 & 2 & -1 \\ 0 & 1 & 3 \end{bmatrix},$$

whose spectrum is (to four significant figures) $\sigma(A) = \{9.687, 2.656 \pm i0.693\}$. The following values of the norm of A : $\|A\|_1 = 11$, $\|A\|_2 = 10.72$, $\|A\|_\infty = 15$ and $\|A\|_F = 11.36$ can be used in the estimate (5.1). Estimate (5.2) provides instead $1.96 \leq \operatorname{Re}(\lambda(A)) \leq 10.34$, $-2.34 \leq \operatorname{Im}(\lambda(A)) \leq 2.34$, while the row and column circles are given respectively by $\mathcal{R}_1 = \{|z| : |z - 10| \leq 5\}$, $\mathcal{R}_2 = \{|z| : |z - 2| \leq 2\}$, $\mathcal{R}_3 = \{|z| : |z - 3| \leq 1\}$ and $\mathcal{C}_1 = \{|z| : |z - 10| \leq 1\}$, $\mathcal{C}_2 = \{|z| : |z - 2| \leq 3\}$, $\mathcal{C}_3 = \{|z| : |z - 3| \leq 4\}$.

In Figure 5.1, for $i = 1, 2, 3$ the \mathcal{R}_i and \mathcal{C}_i circles and the intersection $\mathcal{S}_{\mathcal{R}} \cap \mathcal{S}_{\mathcal{C}}$ (shaded areas) are drawn. In agreement with Property 5.2, we notice that an eigenvalue is contained in \mathcal{C}_1 , which is disjoint from \mathcal{C}_2 and \mathcal{C}_3 , while the remaining eigenvalues, thanks to Property 5.1, lie within the set $\mathcal{R}_2 \cup \{\mathcal{C}_3 \cap \mathcal{R}_1\}$. •

5.2 Stability and Conditioning Analysis

In this section we introduce some a priori and a posteriori estimates that are relevant in the stability analysis of the matrix eigenvalue and eigenvector problem. The presentation follows the guidelines that have been traced in Chapter 2.