5.3 Pseudospectra

We have seen that the eigenvalues of $\mathbf{A}$ reveal how $e^{t\mathbf{A}}$ behaves as $t \to \infty$, while the numerical range is a larger subset of $\mathbb{C}$ that illuminates the behavior of $e^{t\mathbf{A}}$ at $t = 0$. But how does $e^{t\mathbf{A}}$ behave between $t = 0$ and $t \to \infty$, what we call the *transient regime*?

To gain some insight into this question, we shall study series of sets that, in some sense, transition from $\sigma(\mathbf{A})$ at one extreme to $W(\mathbf{A})$ at the other. These sets are known as the *pseudospectra* of $\mathbf{A}$.

ε-pseudospectrum of $\mathbf{A} \in \mathbb{C}^{n\times n}$

Definition 5.1. *Given $\mathbf{A} \in \mathbb{C}^{n\times n}$ and $\varepsilon > 0$, the ε-pseudospectrum of $\mathbf{A}$ is the complex set*

$$\sigma_\varepsilon(\mathbf{A}) = \{z \in \mathbb{C} : \text{there exists } \mathbf{E} \in \mathbb{C}^{n\times n},\ \|\mathbf{E}\| < \varepsilon, \text{ such that } z \in \sigma(\mathbf{A}+\mathbf{E})\}. \quad (5.1)$$

A point $z \in \sigma_\varepsilon(\mathbf{A})$ is called an ε-pseudoeigenvalue of $\mathbf{A}$.

The ε-pseudospectrum can be equivalently defined as

$$\sigma_\varepsilon(\mathbf{A}) = \{z \in \mathbb{C} : \text{there exists } \mathbf{v} \in \mathbb{C}^{n},\ \|\mathbf{v}\| < 1, \text{ such that } \|\mathbf{A}\mathbf{v} - z\mathbf{v}\| < \varepsilon\}. \quad (5.2)$$

If $\mathbf{v} \in \mathbb{C}^n$ is a unit vector such that $\|\mathbf{A}\mathbf{v} - z\mathbf{v}\| < \varepsilon <$ then $\mathbf{v}$ is called an ε-pseudoeigenvector of $\mathbf{A}$ associated with the ε-pseudoeigenvalue z.

The ε-pseudospectrum can also be defined in terms of the resolvent:

$$\sigma_\varepsilon(\mathbf{A}) = \{z \in \mathbb{C} : \|(z\mathbf{I} - \mathbf{A})^{-1}\| > 1/\varepsilon\}, \quad (5.3)$$

with the convention that $\|(z\mathbf{I} - \mathbf{A})^{-1}\| = \infty$ when $z\mathbf{I} - \mathbf{A}$ is not invertible, i.e., when $z \in \sigma(\mathbf{A})$.

The ε-pseudospectrum has be re-invented a number of times for a variety of applications; it was popularized by the work on Trefethen beginning around 1990. See [TE05, chap. 6] for a discussion of this history; indeed, the book [TE05] serves as a source for the material here, and provides many more details for those interested in digging deeper.

The three equivalent definitions (5.1), (5.2), and (5.3) all prove useful in different settings. Many find (5.1) most intuitive; (5.2) is helpful when trying to prove bounds on $\sigma_\varepsilon(\mathbf{A})$ for a specific $\mathbf{A}$; (5.2) has rich connections to functions of matrices via the Dunford–Taylor integral (4.14), and also is the dominant approach used for computing pseudospectra. We shall take some time to prove the equivalence of these definitions.

Theorem 5.2. *The definitions (5.1), (5.2), and (5.3) are equivalent.*

Proof. We shall prove that (5.1) $\Longrightarrow$ (5.2) $\Longrightarrow$ (5.3) $\Longrightarrow$ (5.1), which permits us to go from any of the definitions to any of the others by cycling through these equivalences.

(5.1) $\Longrightarrow$ (5.2). Suppose $z \in \sigma_\varepsilon(\mathbf{A})$ by definition (5.1). Then there exists $\mathbf{E} \in \mathbb{C}^{n\times n}$ with $\|\mathbf{E}\| < \varepsilon$ such that $z \in \sigma(\mathbf{A}+\mathbf{E})$. Let $\mathbf{v} \in \mathbb{C}^n$ be a unit-length eigenvector of $\mathbf{A}+\mathbf{E}$ associated with z, so $(\mathbf{A}+\mathbf{E})\mathbf{v} = z\mathbf{v}$. Rearrange this to see that $\mathbf{A}\mathbf{v} - z\mathbf{v} = -\mathbf{E}\mathbf{v}$, which implies

$$\|\mathbf{A}\mathbf{v} - z\mathbf{v}\| = \|-\mathbf{E}\mathbf{v}\| \le \|\mathbf{E}\|\,\|\mathbf{v}\| = \|\mathbf{E}\| < \varepsilon.$$

Hence definition (5.1) implies (5.2).

(5.2) $\Longrightarrow$ (5.3). If $z \in \sigma_\varepsilon(\mathbf{A})$ by definition (5.2), then there exists some unit vector $\mathbf{v} \in \mathbb{C}^n$ such that $\|\mathbf{A}\mathbf{v} - z\mathbf{v}\| < \varepsilon$. Define $\mathbf{y} := z\mathbf{v} - \mathbf{A}\mathbf{v}$, so $\|\mathbf{y}\| < \varepsilon$. Since $1 = \|\mathbf{v}\|^2 = \mathbf{v}^*\mathbf{v}$,

$$z\mathbf{v} - \mathbf{A}\mathbf{v} = \mathbf{y} = \mathbf{y}\mathbf{v}^*\mathbf{v},$$

which can be rearranged to yield

$$(z\mathbf{I} - \mathbf{A} - \mathbf{y}\mathbf{v}^*)\mathbf{v} = \mathbf{0}.$$

This last equation implies that $\mathbf{v} \in \mathcal{N}(z\mathbf{I} - \mathbf{A} - \mathbf{y}\mathbf{v}^*)$, and since $z\mathbf{I} - \mathbf{A} - \mathbf{y}\mathbf{v}^*$ has a nontrivial null space, it must be rank-deficient:

$$\operatorname{rank}(z\mathbf{I} - \mathbf{A} - \mathbf{y}\mathbf{v}^*) < n.$$

Recall the link between singular values and optimal low-rank approximations from Theorem 3.7 and Corollary 3.8. Let $z\mathbf{I} - \mathbf{A}$ have the singular value decomposition

$$z\mathbf{I} - \mathbf{A} = \sum_{j=1}^{n} s_j \mathbf{u}_j \mathbf{v}_j^*.$$

Then, viewing $z\mathbf{I}-\mathbf{A}-\mathbf{y}\mathbf{v}^*$ as an approximation to $z\mathbf{I}-\mathbf{A}$ of rank less than n, we have

$$\begin{aligned} s_n = \min_{\mathrm{rank}(\mathbf{X})<n} \|(z\mathbf{I}-\mathbf{A})-\mathbf{X}\| &\le \|(z\mathbf{I}-\mathbf{A})-(z\mathbf{I}-\mathbf{A}-\mathbf{y}\mathbf{v}^*)\| \\ &= \|\mathbf{y}\mathbf{v}^*\| = \|\mathbf{y}\|\|\mathbf{v}\| = \|\mathbf{y}\| < \varepsilon. \end{aligned}$$

Now if $z\mathbf{I}-\mathbf{A}$ is singular (i.e., $s_n = 0$), then our convention gives $\infty = \|(z\mathbf{I}-\mathbf{A})^{-1}\| > 1/\varepsilon$. Otherwise, write

$$(z\mathbf{I}-\mathbf{A})^{-1} = \sum_{j=1}^{n} \frac{1}{s_j}\mathbf{v}_j\mathbf{u}_j^*,$$

showing that $(z\mathbf{I}-\mathbf{A})^{-1}$ has largest singular value $1/s_n$, and hence, since $s_n < \varepsilon$,

$$\|(z\mathbf{I}-\mathbf{A})^{-1}\| = \frac{1}{s_n} > \frac{1}{\varepsilon},$$

showing that definition (5.2) implies (5.3).

(5.3) $\Longrightarrow$ (5.1). Suppose $z \in \sigma_\varepsilon(\mathbf{A})$ by definition (5.3), so $\|(z\mathbf{I}-\mathbf{A})^{-1}\| > 1/\varepsilon$, and write the singular value decomposition of $z\mathbf{I}-\mathbf{A}$ as

$$z\mathbf{I}-\mathbf{A} = \sum_{j=1}^{n} s_j\mathbf{u}_j\mathbf{v}_j^*.$$

Since $\|(z\mathbf{I}-\mathbf{A})^{-1}\| > 1/\varepsilon$, we conclude that $s_n < \varepsilon$. Define

$$\mathbf{E} := s_n\mathbf{u}_n\mathbf{v}_n^*, \tag{5.4}$$

with $\|\mathbf{E}\| = s_n < \varepsilon$. Then

$$(z\mathbf{I}-\mathbf{A}-\mathbf{E})\mathbf{v}_n = \left(\sum_{j=1}^{n-1} s_j\mathbf{u}_j\mathbf{v}_j^*\right)\mathbf{v}_n = \sum_{j=1}^{n-1} s_j\mathbf{u}_j(\mathbf{v}_j^*\mathbf{v}_n) = \mathbf{0}$$

by the orthogonality of $\mathbf{v}_n$ with $\mathbf{v}_1, \ldots, \mathbf{v}_{n-1}$. Since $(z\mathbf{I}-\mathbf{A}-\mathbf{E})\mathbf{v}_n = \mathbf{0}$,

$$(\mathbf{A}+\mathbf{E})\mathbf{v}_n = z\mathbf{v}_n,$$

so $z \in \sigma(\mathbf{A}+\mathbf{E})$ with $\|\mathbf{E}\| < \varepsilon$. Thus we conclude not only that definition (5.3) implies (5.1), but we get the added insight that any $z \in \sigma_\varepsilon(\mathbf{A})$ can be realized as an eigenvalue of $\mathbf{A}+\mathbf{E}$ for some $\mathbf{E}$ of the form (5.4) *having rank one.* ■

5.4 Classic Eigenvalue Containment Theorems

Several classic results can be used to bound the eigenvalues of a matrix (and can often be adapted to bound the pseudospectra or numerical range). We begin with GERSCHGORIN's Theorem, a fascinating result that seems like it deserves a more complicated proof.

Gerschgorin's Theorem

Theorem 5.3. *For any* $\mathbf{A} \in \mathbb{C}^{n\times n}$*, define*

$$c_j := |a_{j,j}|, \qquad r_j := \sum_{\substack{k=1\\k\neq j}}^{n} |a_{j,k}|.$$

The eigenvalues of $\mathbf{A}$ *are contained within the union of* n *closed disks in the complex plane, each one centered at* c_j *having radius* r_j*:*

$$\sigma(\mathbf{A}) \subset \bigcup_{j=1}^{n} \{z \in \mathbb{C} : |z - c_j| \le r_j\}.$$

Moreover, if the union $\mathcal{D}$ *of* k *disks is disjoint from all the other disks, then* $\mathcal{D}$ *must contain exactly* k *eigenvalues of* $\mathbf{A}$*.*

Proof. Suppose $\lambda \in \sigma(\mathbf{A})$ and let $\mathbf{v} \in \mathbb{C}^n$ be a corresponding unit-length eigenvector:

$$\mathbf{A}\mathbf{v} = \lambda\mathbf{v}, \qquad \|\mathbf{v}\| = 1.$$

Pick $j \in \{1, \ldots, n\}$ such v_j is a largest-magnitude entry of $\mathbf{v}$:

$$|v_j| = \max_{1\le \ell\le n} |v_\ell|;$$

note that $|v_j| > 0$ since $\mathbf{v} \neq \mathbf{0}$. The jth row of the equation $\mathbf{A}\mathbf{v} = \lambda\mathbf{v}$,

$$\sum_{k=1}^{n} a_{j,k}v_k = \lambda v_j,$$

can be rearranged to give

$$\Big(a_{j,j} - \lambda\Big)v_j = -\sum_{\substack{k=1\\k\neq j}}^{n} a_{j,k}v_k.$$

By the definition of j, $v_j \neq 0$ and $|v_j| \geq |v_k|$ for all $k = 1, \ldots, n$, so we can divide through by v_j to obtain

$$|a_{j,j} - \lambda| \;=\; \left|\sum_{\substack{k=1\\k\neq j}}^{n} a_{j,k}\frac{v_k}{v_j}\right| \;\leq\; \sum_{\substack{k=1\\k\neq j}}^{n} |a_{j,k}|\left|\frac{v_k}{v_j}\right| \;\leq\; \sum_{\substack{k=1\\k\neq j}}^{n} |a_{j,k}|,$$

which, using the definitions of c_j and r_j, is equivalent to

$$|\lambda - c_j| \leq r_j.$$

Hence every eigenvalue $\lambda \in \sigma(\mathbf{A})$ must fall inside at least one of the closed disks centered at c_j having radius r_j.

Notice a subtle point: *this result does not guarantee that each disk contains an eigenvalue of* $\mathbf{A}$; each eigenvalue must be contained in *some* disk, but it is possible that one disk contains multiple eigenvalues, while another disk contains none. The second part of the theorem illuminates this nuance, which is evident in the example in Figure 5.1.

Suppose the union $\mathcal{D}$ of k of these disks is disjoint from the other $n-k$ disks. Then $\mathcal{D}$ must contain exactly k eigenvalues of $\mathbf{A}$ (counting multiplicity). To see this, let $\mathcal{D} = \operatorname{diag}(a_{1,1}, \ldots, a_{n,n})$ and define $\mathbf{E} = \mathbf{A} - \mathbf{D}$. Now consider the family of matrices $\mathbf{A}_t := \mathbf{D} + t\mathbf{E}$ for $t \in [0,1]$. The Gerschgorin disks for $\mathbf{A}_t$ have the same centers $\{c_j\}$ for all t, but the corresponding radii are now scaled, $\{tr_j\}$.

When $t = 0$, $\mathbf{A}_0 = \mathbf{D}$ has eigenvalues

$$\sigma(\mathbf{D}) = \{a_{1,1}, \ldots, a_{n,n}\} = \{c_1, \ldots, c_n\},$$

and, by assumption, exactly k of these eigenvalues fall in $\mathcal{D}$. As t increases from $t = 0$, the jth disk increases in radius from 0 to r_j. Since the eigenvalues of $\sigma(\mathbf{A}_t)$ are continuous functions of t, the eigenvalues $\{\lambda_j(t)\}$ of $\mathbf{A}_t$ must trace out continuous curves that never stray beyond the union of the disks $\{z \in \mathbb{C} : |z - c_j| \leq tr_j\}$. Thus, the k eigenvalues of $\mathbf{D}$ that fall in $\mathcal{D}$ trace out curves $\{\lambda_j(t)\}$ as t increases from $t = 0$ to $t = 1$ that never leave $\mathcal{D}$. By the same reasoning, none of the eigenvalues of $\mathbf{D}$ that fall outside $\mathcal{D}$ can ever enter $\mathcal{D}$ as t increases from 0 to 1. (See Figure 5.2 for an illustration of this argument.) ■

The proof of the above result could just have easily used a *left eigenvector* of $\mathbf{A}$, in which case the disk radii would be given by the sum of the absolute values of the off-diagonal elements of each *column* of $\mathbf{A}$. When applying

Gerschgorin's Theorem in practice, one chooses to take radii from rows or columns depending on which version gives the smaller disks.

If is Hermitian, $\mathbf{A}^* = \mathbf{A}$, then we further know what $\sigma(\mathbf{A}) \subset \mathbb{R}$, so we can collapse the disks to Gerchgorin intervals by intersecting the disks with the real line.

Example of Gerschgorin's Theorem.

Consider the non-Hermitian matrix

$$\mathbf{A} = \begin{bmatrix} -4 & 0 & 3 \\ 1 & 2 & -1 \\ 0 & 5 & 6 \end{bmatrix}. \tag{5.5}$$

The Gerschgorin disks have centers

$$c_1 = -4, \qquad c_2 = 2, \qquad c_3 = 6,$$

with corresponding radii

$$r_1 = 3, \qquad r_2 = 2, \qquad r_3 = 5.$$

Figure 5.1 shows these three disks in the complex plane. This example has been chosen to show a case where two disks overlap, but are disjoint from

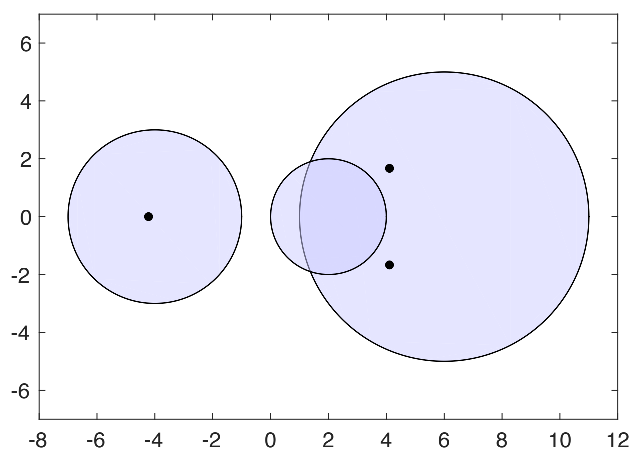

Figure 5.1. Gerschgorin disks for the 3×3 non-Hermitian matrix (5.5), with the three eigenvalues shown as black dots. Notice that two of the disks overlap, and one of those disks contains no eigenvalues.

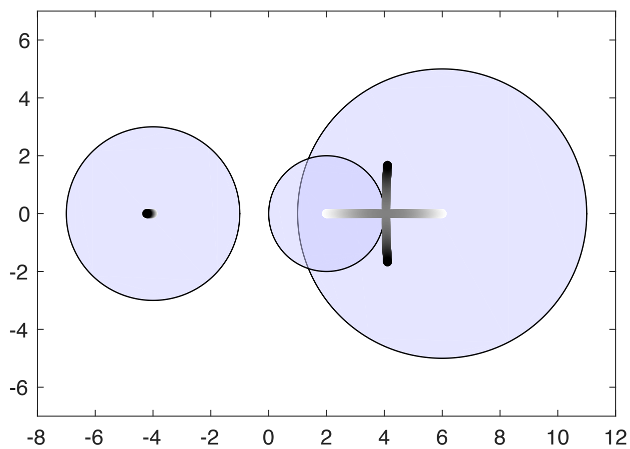

Figure 5.2. Repetition of Figure 5.1 for the 3×3 non-Hermitian matrix (5.5), but now showing eigenvalues of $\mathbf{A}_t = \mathbf{D} + t\mathbf{E}$ for $t \in [0, 1]$ tracing out curves that begin at the centers of the GERSCHGORIN disks for $t = 0$ (white dots) and end up at the eigenvalues of $\mathbf{A}$ at $t = 1$ (black dots). The eigenvalue in the disjoint disk centered at $c_1 = -4$ does not move much with t.

the third disk. As permitted by the theorem, a pair of eigenvalues fall in one of the overlapping disks, but none in the other of those disks.

Figure 5.2 illustrates the argument at the end of the proof of Theorem 5.3, showing the curves traced out by eigenvalues of $\mathbf{A}_t = \mathbf{D} + t\mathbf{E}$ as t goes from zero to one. One of these curves leaves the overlapping circle (centered at $c_2 = 2$), but none of the curves can exit the union of the GERSCHGORIN disks.

5.5 Spectral Variation for Hermitian, Normal Matrices

5.6 Illustration: Transient Energy Growth in Dynamical Systems

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