Pseudospectra

Seminar I - 1st year, 2nd cycle

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Outline

1. Introduction
2. Introduction to Pseudospectra
3. Pseudospectra and Its Properties
4. Pseudospectra and Stability Analysis
5. Transient Dynamics
6. Pseudospectra in Physics
7. Conclusion

Introduction

Eigenvalues and *eigenvectors* of *matrices* are one of the most successful tools for analyzing and understanding physical systems.

- Quantum mechanics: $\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle$
- Normal modes: $\ddot{x} = Ax$
- Sturm–Liouville: $\frac{\partial^2 u}{\partial t^2} = \Delta u$
- Diagonalization: $A = V\Lambda V^{-1}$
- $\mathrm{e}^{tA} = \sum_n \frac{t^n}{n!}\left(V\Lambda V^{-1}\right)^n = V\mathrm{e}^{t\Lambda}V^{-1}$

"They give a matrix personality".

Are eigenvalues always useful?

- Hermitian $A = A^*$, skew-Hermitian $A = -A^*$
- Unitary $AA^* = A^*A = I$
- Normal $AA^* - A^*A = 0$

However, caution is needed when a matrix lacks an *orthogonal* basis of eigenvectors $(AA^* - A^*A \neq 0)$

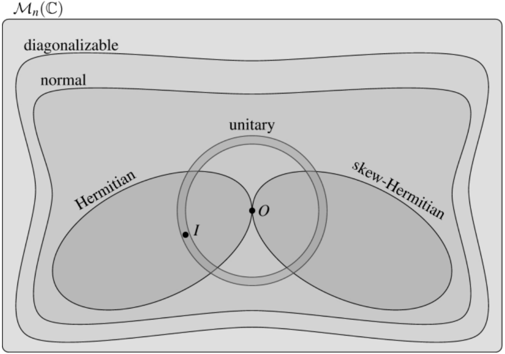
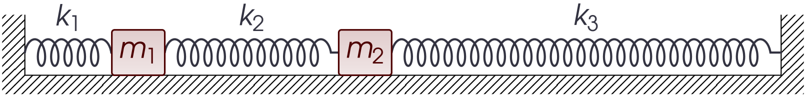


Figure: World of matrices as described in (1).



$$
\begin{aligned}
m_1\ddot{x}_1 &= -k_1x_1 - k_2(x_1 - x_2) \\
m_2\ddot{x}_2 &= -k_3x_2 + k_2(x_1 - x_2)
\end{aligned}
\tag{1}
$$

Matrix form of equation (1) : $\ddot{\mathbf{x}} = -K\mathbf{x}$, where $K = \begin{pmatrix} \frac{k_1+k_2}{m_1} & \frac{k_2}{m_1} \\ \frac{k_2}{m_2} & \frac{k_3}{m_2} \end{pmatrix}$

- Eigenvalue decomposition: $K = V\Lambda V^{-1}$
- Substitute into equation: $\ddot{\mathbf{x}} = -V\Lambda V^{-1}\mathbf{x}$
- Transform coordinates: $\mathbf{y} = V^{-1}\mathbf{x} \Rightarrow \ddot{\mathbf{y}} = -\Lambda\mathbf{y}$
- Normal modes: $\ddot{y}_i = -\lambda_i y_i \quad (i = 1, 2)$

Motivation: Toeplitz Matrices

Consider the following tridiagonal Toeplitz matrix and its symmetrized counterpart:

$$A = \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ \frac{1}{4} & 0 & 1 & \cdots & 0 \\ 0 & \frac{1}{4} & 0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 1 \\ 0 & \cdots & 0 & \frac{1}{4} & 0 \end{pmatrix}, \quad S = \begin{pmatrix} 0 & \frac{1}{2} & 0 & \cdots & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & \cdots & 0 \\ 0 & \frac{1}{2} & 0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \frac{1}{2} \\ 0 & \cdots & 0 & \frac{1}{2} & 0 \end{pmatrix}, \in \mathbb{C}^{N \times N}.$$

They are related by a similarity transformation,

$$S = DAD^{-1}, \quad D = \mathrm{diag}(2, 2^2, \ldots, 2^{N-1}, 2^N).$$

Spectral Properties

$$A = \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ \frac{1}{4} & 0 & 1 & \cdots & 0 \\ 0 & \frac{1}{4} & 0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 1 \\ 0 & \cdots & 0 & \frac{1}{4} & 0 \end{pmatrix}, \quad S = \begin{pmatrix} 0 & \frac{1}{2} & 0 & \cdots & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & \cdots & 0 \\ 0 & \frac{1}{2} & 0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \frac{1}{2} \\ 0 & \cdots & 0 & \frac{1}{2} & 0 \end{pmatrix}, \in \mathbb{C}^{N \times N}.$$

They are related by a similarity transformation,

$$S = DAD^{-1}, \quad D = \operatorname{diag}(2, 2^2, \ldots, 2^{N-1}, 2^N).$$

The eigenvalues for both matrices are given by

$$\lambda_k(A) = \lambda_k(S) = \cos\left(\frac{k\pi}{N+1}\right), \quad 1 \leqslant k \leqslant N.$$

Perturbed Spectra

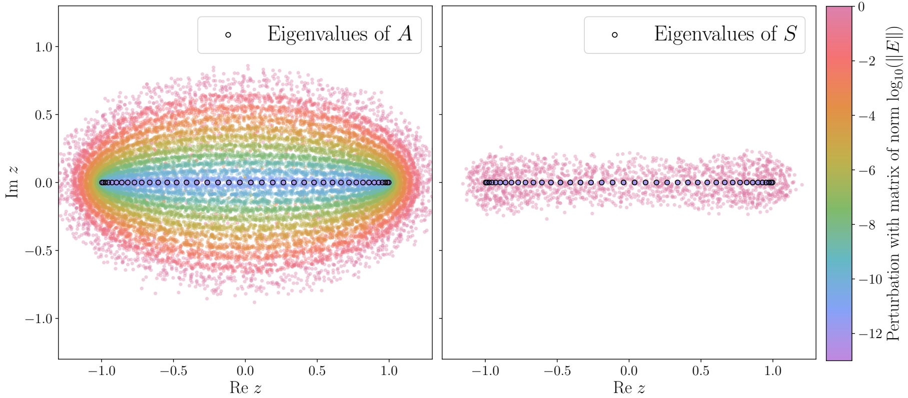


Figure: The spectra of the perturbed matrices $A + E \in \mathbb{C}^{40\times40}$ and $S + E \in \mathbb{C}^{40\times40}$, with E as the perturbation, are illustrated. Different colors represent varying magnitudes of the perturbation.

Definition of Pseudospectra

Theorem ([2])

Let $A \in \mathbb{C}^{n \times n}$ and $\varepsilon > 0$. The ε-pseudospectrum $\sigma_\varepsilon(A)$ is the set of $z \in \mathbb{C}$ such that one of the following holds:

1. $\|(zI - A)^{-1}\| > \varepsilon^{-1}$,
2. $z \in \sigma(A + E)$ *for some* E *with* $\|E\| < \varepsilon$,
3. $z \in \sigma(A)$ *or there exists a unit vector* u *with* $\|(zI - A)\mathbf{u}\| < \varepsilon$.

- $\varepsilon - \textit{pseudospectra}$ $\Leftrightarrow$ ε-perturbed operator.
- spectrum of a perturbed matrix $\Leftrightarrow$ norm of its resolvent.
- vector **u** - ε-*pseudoeigenvectors.*

Pseudospectra and Norms

- As ε varies, the ε-*pseudospectra* form a nested sequence.
- The intersection over all $\varepsilon > 0$ equals the *spectrum*: $\bigcap_{\varepsilon>0} \sigma_\varepsilon(A) = \sigma(A)$.

The *pseudospectra* depend on the choice of norm!

Since the matrices A and S are finite they can be regarded as a bounded operator, allowing us to use the operator norm:

$$\|A\| = \sup_{\|x\|=1} \|Ax\|.$$

For matrices it coincides with the largest singular value (SVD):

$$\|A\|_2 = \max_{z\in\sigma(AA^*)} \sqrt{|z|}.$$

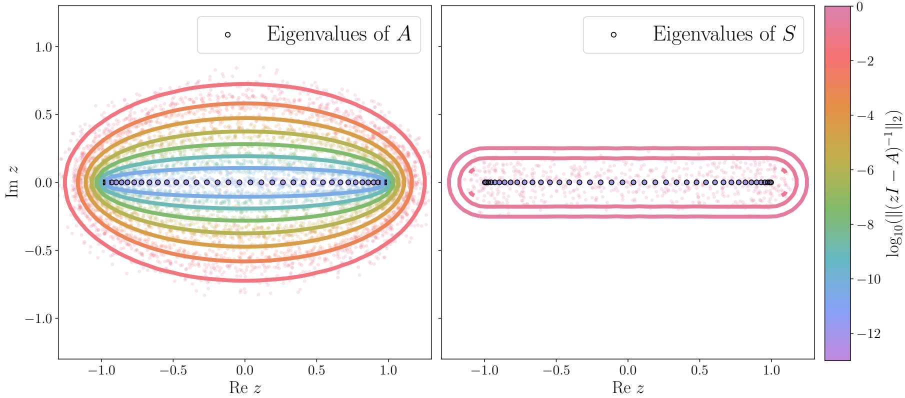


Figure: Comparison of pseudospectra computed via the resolvent norm (lines) and the spectra of the perturbed matrices A and S (dots). The solid curves represent the set of complex numbers z for which $\left\|(zI - A)^{-1}\right\| = \varepsilon$.

Bauer-Fike Theorem

Theorem (Bauer-Fike (2))

Let A be a diagonalizable matrix with $A = V\Lambda V^{-1}$. For any $\varepsilon > 0$, the ε-pseudospectrum satisfies

$$\{z \mid dist(\sigma(A), z) < \varepsilon\} \subseteq \sigma_\varepsilon(A) \subseteq \{z \mid dist(\sigma(A), z) < \kappa(V)\varepsilon\},$$

where $\kappa(V) = \|V\|\|V^{-1}\|$ is the condition number of the eigenvector matrix V.

- For normal matrices, $\kappa(V) = 1$; a perturbation E with $\|E\| < \varepsilon$ moves eigenvalues by at most ε.
- For non-normal matrices, $\kappa(V) \gg 1$, the same perturbation can displace eigenvalues by a maximum distance of $\kappa(V)\varepsilon$.

Effect of Matrix Dimension

Condition number for A is $\kappa(D) = 2^{N-1}$, which increases with the matrix dimension.

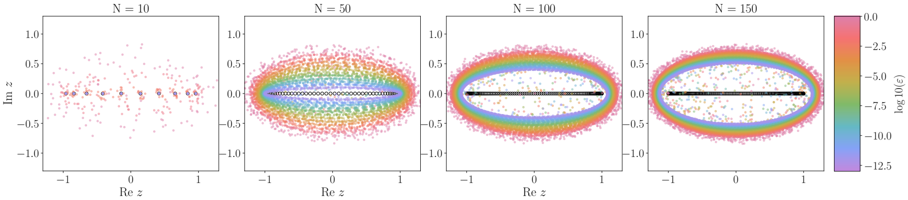


Figure: The impact of perturbations on the matrix A for different dimension N. As the dimension increases, the eigenvalues become increasingly sensitive to perturbations.

Connection to Stability

- Calculating eigenvalues and verifying that they lie on the left half-plane.

This criterion can be misleading for non-normal systems.

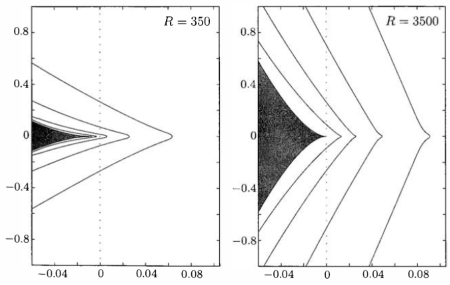


Figure: Spectra (shaded) and *pseudospectra* for plane Couette flow at two Reynolds numbers, from (3). Boundaries of ϵ-*pseudospectra* are shown, from right to left, for $\epsilon = 10^{-2}, 10^{-2.5}, 10^{-3}$, and $10^{-3.5}$. This flow is eigenvalue stable for all R, with the spectrum contained strictly inside the left half-plane, but it is unstable in practice for $R \gg 1000$.

Transient Dynamics

Consider the iteration $\mathbf{u}_{n+1} = A\mathbf{u}_n$ whose solution is $\mathbf{u}_n = A^n\mathbf{u}_0$.

Definitions

$$\rho(A) = \sup\{|z| : z \in \sigma(A)\} \quad (\textit{spectral} \text{ radius})$$

$$\rho_\varepsilon(A) = \sup\{|z| : z \in \sigma_\varepsilon(A)\} \quad (\varepsilon\textit{-pseudospectral} \text{ radius})$$

Theorem ((2))

Let $A \in B(H)$, where $B(H)$ denoting bounded operators. We have

$$\rho(A) = \lim_{n\to\infty} \|A^n\|^{1/n}. \tag{2}$$

We also have

$$\|A^n\| \geqslant \rho(A)^n \quad \textit{for all } n \geqslant 0. \tag{3}$$

However there is still an option that the value $\|A^n\|$ will grow large before decaying .

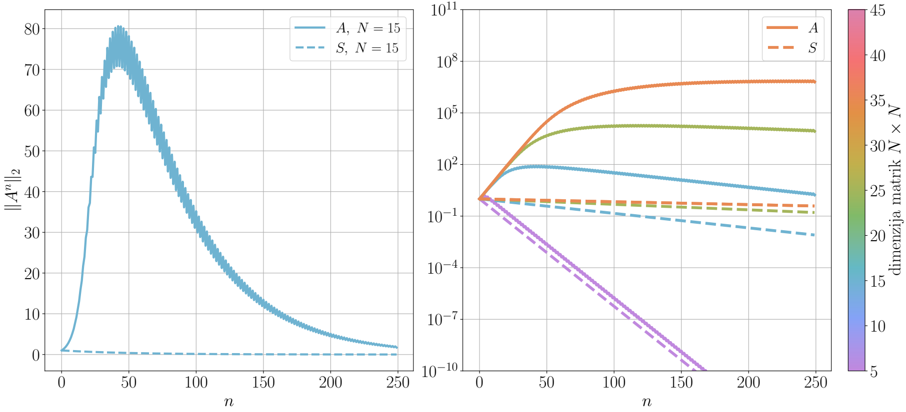


Figure: The figure illustrates the transient growth of A, despite all its eigenvalues being less than one. Although A and S share the same eigenvalues, for larger-dimensions $\sup_{n \geqslant 0} \|A^n\|$ appears to increase while $\|S^n\|$ stays bounded.

Psudospectral bounds

Theorem ((2))

Suppose $A \in \mathcal{B}(H)$. Then, for every $\varepsilon > 0$, we have the inequality

$$\sup_{n \geqslant 0} \|A^n\| \geqslant \frac{(\rho_\varepsilon(A) - 1)}{\varepsilon}. \tag{4}$$

This is where pseudospectra is useful. If $\rho_\varepsilon > 1 + \varepsilon$ for some ε, there must be transient growth. We define Kreiss constant as:

$\mathcal{K}(A) = \sup_{\varepsilon > 0} \frac{\rho_\varepsilon - 1}{\varepsilon}$

Theorem (Kreiss Matrix Theorem: (2))

For an $N \times N$ matrix,

$$\mathcal{K}(A) \leqslant \sup_{n \geqslant 0} \|A^n\| \leqslant eN\mathcal{K}(A). \tag{5}$$

Finite-Time Bound

Theorem ((2))

Suppose $A \in \mathcal{B}(H)$ *and for some* z *with* $\|z\| = r > 1$, $\|(zI - A)^{-1}\| = \frac{K}{r-1}$. *Then for any* $\tau > 0$,

$$\max_{0<n\leqslant\tau} \|A^n\| \geqslant r^\tau / \left(1 + \frac{r^\tau - 1}{rK - r + 1}\right). \tag{6}$$

If $\|A^\tau\| \leqslant M$ *for all* $\tau \geqslant 0$*,then for any* $\tau \geqslant 0$, *with* K *defined as before but now with* $r < 1$ *permitted and* $-\infty < K/M \leqslant 1$, *we have*

$$\|A^\tau\| \geqslant r^\tau - \frac{r^\tau - 1}{K/M} \tag{7}$$

Now if $r^\tau \ll rK$ there exist some n for which $\|A^n\|$ is approximately as big as r^τ, or bigger.

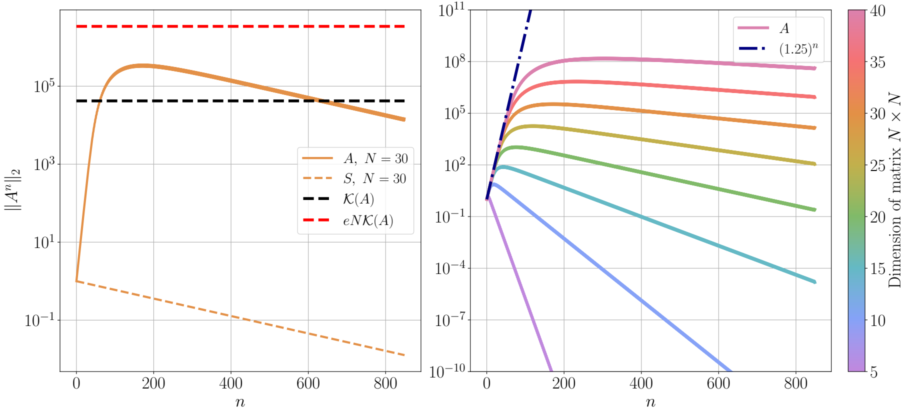


Figure: Figure shows lower and upper bounds determined by Kreiss matrix theorem (4) for the numerical example, the slope of $\|A^n\|$ for large n is the same as slope of $\|S^n\|$. The bound $(1.25)^n$ is inspired by equation (6) where r is boundary of *pseudospectrum* of infinite operator $\lim_{N\to\infty} A_N$ for more details refer to (2, chapter 4, theorem (29.24)).

Transient Dynamics: Continuous Case

- Consider the continuous-time evolution:

$$\frac{d\mathbf{u}}{dt} = A\mathbf{u}, \quad \mathbf{u}(t) = e^{At}\mathbf{u}(0).$$

- Define key quantities:

$$\alpha(A) = \sup\{\mathrm{Re}\, z : z \in \sigma(A)\},$$
$$\alpha_\varepsilon(A) = \sup\{\mathrm{Re}\, z : z \in \sigma_\varepsilon(A)\},$$
$$\omega(A) = \sup\{\mathrm{Re}\, z : z \in W(A)\}.$$

- These quantities characterize the long-time decay ($\alpha(A)$) and initial growth ($\omega(A)$) of the evolution.

Continuous-Time Theorems

Asymptotic Decay (2)

For $A \in B(H)$,

$$\alpha(A) = \lim_{t \to \infty} \frac{1}{t} \log \|e^{tA}\|$$

and

$$\|e^{tA}\| \geqslant e^{t\alpha(A)} \quad \text{for all } t \geqslant 0.$$

Initial Growth (2)

$$\omega(A) = \lim_{t \downarrow 0} \frac{1}{t} \log \|e^{tA}\| = \frac{d}{dt}\|e^{tA}\|\Big|_{t=0},$$

with the upper bound

$$\|e^{tA}\| \leqslant e^{t\omega(A)} \quad \text{for all } t \geqslant 0.$$

Pseudospectral Bounds in Continuous Time

Pseudospectral Lower Bound (2)

For all $\varepsilon > 0$,

$$\sup_{t \geqslant 0} \|e^{tA}\| \geqslant \frac{\alpha_\varepsilon(A)}{\varepsilon}.$$

- Define the continuous Kreiss constant:

$$\mathcal{K}(A) = \sup_{\varepsilon > 0} \frac{\alpha_\varepsilon(A)}{\varepsilon}.$$

- For an $N \times N$ matrix,

$$\mathcal{K}(A) \leqslant \sup_{t \geqslant 0} \|e^{tA}\| \leqslant eN\mathcal{K}(A).$$

Non-normality in Physics

- Open systems
- Linearized operators
- non-Hermitian $\mathcal{PT}$-quantum mechanics

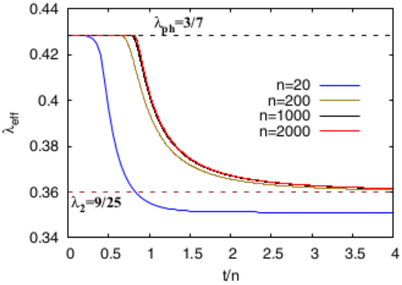


Figure: Effective purity decay rate $\lambda_{\mathrm{eff}} = \exp\left(\frac{I'}{I}\right)$, i.e., $I(t) = C\lambda_{\mathrm{eff}}^{t}$,for qutrits ($d = 3$). Figure and text are taken from article (4, Marko Žnidarič)

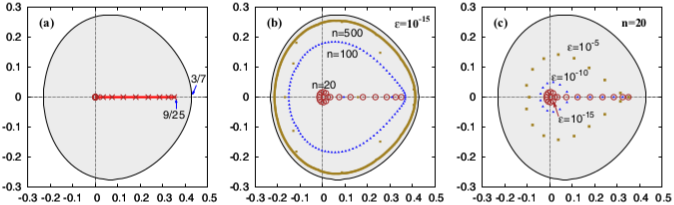
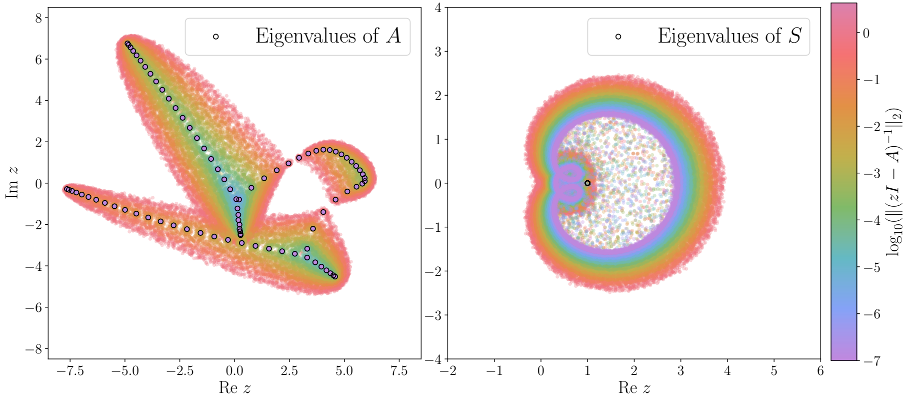


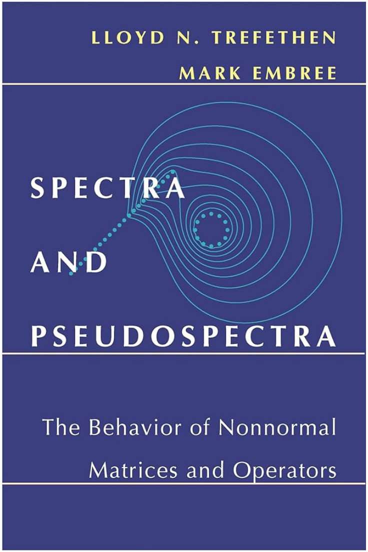
Figure: (a) Exact spectrum of the Toeplitz operator T_∞ (shaded oval) versus the spectrum of a finite large Toeplitz matrix T (red line) for $d = 3$. Red symbols indicate eigenvalues for $n = 20$ (crosses denote $\tilde{\lambda}_j$ and the circle represents $\lambda = 0$). (b) Pseudospectrum: Numerically computed spectrum of a single perturbed matrix $T + \varepsilon E$ (where E is a matrix of i.i.d. real Gaussian random numbers and $\varepsilon = 10^{-15}$) for $n = 20, 100, 500$ (represented by circles, triangles, and squares, respectively). (c) As the perturbation ε decreases at fixed $n = 20$, the spectrum of $T + \varepsilon E$ (points) converges toward that of the finite matrix T. Figure and text are taken from article (4, Marko Žnidarič)

Summary and Conclusions

- Eigenvalues alone can be misleading for non-normal operators.
- *Pseudospectra* provide quantitative bounds that capture transient dynamics.

Trefethen: "Anyone who plots eigenvalues of nonsymmetric /nonhermitian matrices operators in the complex plane should routinely include pseudospectra. This gives an instant check of whether the eigenvalues are likely to be meaningful. Some people do this. Most don't". (5).


Eigenvalues of A
Eigenvalues of S
Re z
Im z
$\log_{10}(\|(zI - A)^{-1}\|_2)$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References I

(1) Nathaniel Johnston. *Matrix Decompositions*, pages 167–295. Springer International Publishing, Cham, 2021. ISBN 978-3-030-52815-7. doi: 10.1007/978-3-030-52815-7_2. URL https://doi.org/10.1007/978-3-030-52815-7_2.

(2) Lloyd Trefethen and Mark Embree. *Spectra and Pseudospectra: The Behavior of Nonnormal Matrices and Operators*. 01 2005.

(3) Lloyd N. Trefethen, Anne E. Trefethen, Satish C. Reddy, and Tobin A. Driscoll. Hydrodynamic stability without eigenvalues. *Science*, 261(5121):578–584, 1993. doi: 10.1126/science.261.5121.578. URL https://www.science.org/doi/abs/10.1126/science.261.5121.578.

(4) Marko Žnidarič. Solvable non-hermitian skin effect in many-body unitary dynamics. *Phys. Rev. Res.*, 4:033041, Jul 2022. doi: 10.1103/PhysRevResearch.4.033041. URL https://link.aps.org/doi/10.1103/PhysRevResearch.4.033041.

References II

(5) Lloyd N. Trefethen. Lecture 2: Nonnormality and pseudospectra, 2018. https://people.maths.ox.ac.uk/trefethen/outline2.pdf.