Pseudospectra and Nonnormal Dynamical Systems

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Overview of the Course

These lectures describe modern tools
for the spectral analysis of dynamical systems.
We shall cover a mix of theory, computation, and applications.

Lecture 1: Introduction to Nonnormality and Pseudospectra

Lecture 2: Functions of Matrices

Lecture 3: Toeplitz Matrices and Model Reduction

Lecture 4: Model Reduction, Numerical Algorithms, Differential Operators

Lecture 5: Discretization, Extensions, Applications

Outline for Today

Lecture 3: Functions of Matrices and Model Reduction

- Toeplitz matrices
- Model Reduction: Balanced Truncation
- Nonnormality and Lyapunov Equations
- Model Reduction: Moment Matching

3(a) Toeplitz Matrices

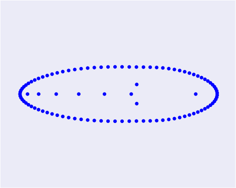
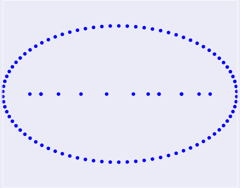
Pseudospectra

Recall the example that began our investigation of pseudospectra yesterday.

Example

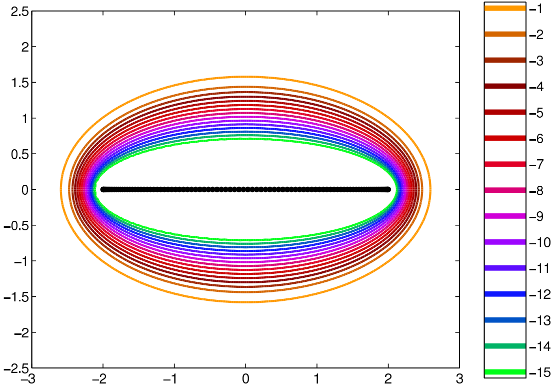
Compute eigenvalues of three similar 100×100 *matrices using MATLAB's* `eig`.

$$\begin{bmatrix} 0 & 1 & & \\ 1 & 0 & \ddots & \\ & \ddots & \ddots & 1 \\ & & 1 & 0 \end{bmatrix} \qquad \begin{bmatrix} 0 & 1/2 & & \\ 2 & 0 & \ddots & \\ & \ddots & \ddots & 1/2 \\ & & 2 & 0 \end{bmatrix} \qquad \begin{bmatrix} 0 & 1/3 & & \\ 3 & 0 & \ddots & \\ & \ddots & \ddots & 1/3 \\ & & 3 & 0 \end{bmatrix}$$

Toeplitz Matrices

Consider the pseudospectra of the 100×100 matrix in the middle of the last slide, $\mathbf{A} = \text{tridiag}(2, 0, 1/2)$.

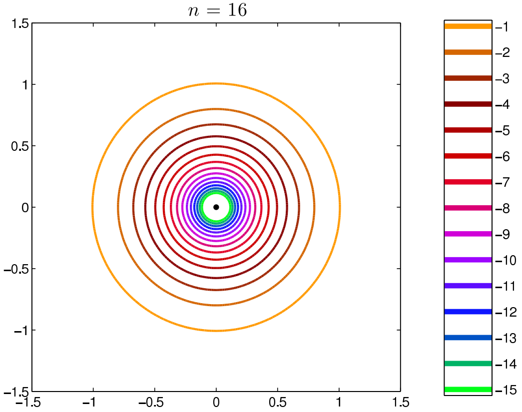


$\mathbf{A}$ is diagonalizable (it has distinct eigenvalues), but Bauer–Fike is useless here: $\kappa(\mathbf{V}) = 2^{99} \approx 6 \times 10^{29}$.

Jordan Blocks

We've already analyzed pseudospectra of Jordan blocks near λ for small $\varepsilon > 0$. Here we want to investigate the entire pseudospectrum for larger ε.

$$\mathbf{S}_n = \begin{bmatrix} 0 & 1 & & \\ & 0 & \ddots & \\ & & \ddots & 1 \\ & & & 0 \end{bmatrix}$$



Near the eigenvalue, the resolvent norm grows with dimension n; outside the unit disk, the resolvent norm does not seem to get big. We would like to prove this.

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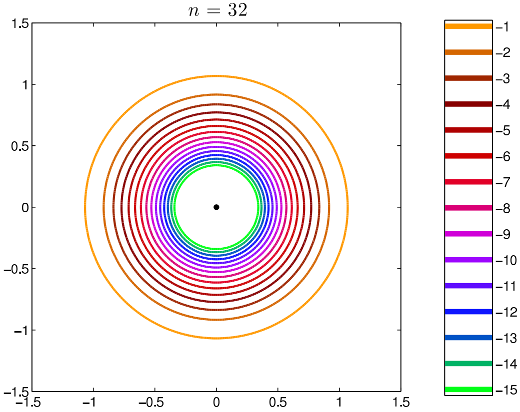

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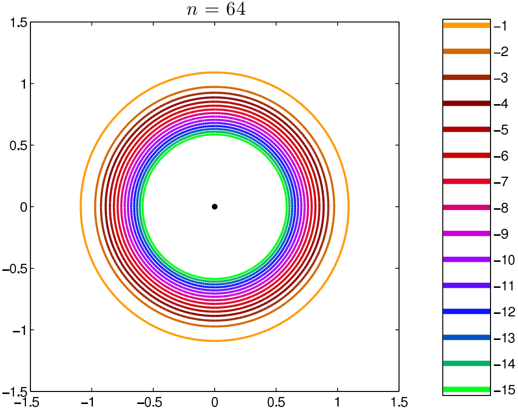

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Jordan Blocks/Shift Operator

Consider the generalization of the Jordan block to the domain

$$\ell^2(\mathbf{N}) = \{(x_1, x_2, \ldots) : \sum_{j=1}^{\infty} |x_j|^2 < \infty\}.$$

The shift operator $\mathbf{S}$ on $\ell^2(\mathbf{N})$ is defined as

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In particular,

$$\begin{aligned} \mathbf{S}(1, z, z^2, \ldots) &= (z, z^2, z^3, \ldots) \\ &= z(1, z, z^2, \ldots). \end{aligned}$$

So if $(1, z, z^2, \ldots) \in \ell^2(\mathbf{N})$, then $z \in \sigma(\mathbf{S})$.

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If $|z| < 1$, then

$$\sum_{j=1}^{\infty} |z^{j-1}|^2 = \frac{1}{1 - |z|^2} < \infty.$$

So,

$$\{z \in \mathbf{C} : |z| < 1\} \subseteq \sigma(\mathbf{S}).$$

Jordan Blocks/Shift Operator

$$\mathbf{S}(x_1, x_2, \dots) = (x_2, x_3, \dots).$$

We have seen that

$$\{z \in \mathbf{C} : |z| < 1\} \subseteq \sigma(\mathbf{S}).$$

Observe that

$$\|\mathbf{S}\| = \sup_{\|\mathbf{x}\|=1} \|\mathbf{Sx}\| = 1,$$

and so

$$\sigma(\mathbf{S}) \subseteq \{z \in \mathbf{C} : |z| \leq 1\}.$$

The spectrum is closed, so

$$\sigma(\mathbf{A}) = \{z \in \mathbf{C} : |z| \leq 1\}.$$

For any finite dimensional $n \times n$ Jordan block $\mathbf{S}_n$,

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So the $\mathbf{S}_n \to \mathbf{S}$ strongly, but there is a discontinuity in the spectrum:

$$\sigma(\mathbf{S}_n) \not\to \sigma(\mathbf{S}).$$

Pseudospectra of Jordan Blocks

Pseudospectra resolve this unpleasant discontinuity.

Recall the eigenvectors $(1, z, z^2, \ldots)$ for $\mathbf{S}$.

Truncate this vector to length n, and apply it to $\mathbf{S}_n$:

$$\begin{bmatrix} 0 & 1 & & & \\ & 0 & \ddots & & \\ & & \ddots & 1 & \\ & & & 0 & 1 \\ & & & & 0 \end{bmatrix} \begin{bmatrix} 1 \\ z \\ \vdots \\ z^{n-2} \\ z^{n-1} \end{bmatrix} = \begin{bmatrix} z \\ z^2 \\ \vdots \\ z^{n-1} \\ 0 \end{bmatrix}$$

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Hence, $\|\mathbf{S}_n\mathbf{x} - z\mathbf{x}\| = |z|^n$, so for all $\varepsilon > \dfrac{|z|^n}{\|\mathbf{x}\|} = |z|^n \dfrac{\sqrt{1-|z|^{2n}}}{\sqrt{1-|z|^2}}$,

$$z \in \sigma_\varepsilon(\mathbf{S}_n).$$

We conclude that for fixed $|z| < 1$, the resolvent norm $\|(z - \mathbf{S}_n)^{-1}\|$ grows *exponentially* with n.

Upper Triangular Toeplitz Matrices

Consider an upper triangular Toeplitz matrix giving the matrix with constant diagonals containing the Laurent coefficients:

$$\mathbf{A}_n = \begin{bmatrix} a_0 & a_1 & a_2 & \cdots & \\ & a_0 & \ddots & \ddots & \vdots \\ & & \ddots & a_1 & a_2 \\ & & & a_0 & a_1 \\ & & & & a_0 \end{bmatrix} \in \mathbf{C}^{n\times n}.$$

Definition (Symbol, Symbol Curve)

Toeplitz matrices are described by their *symbol* a with Taylor expansion

$$a(z) = \sum_{k=0}^{\infty} a_k z^k.$$

Call the image of the unit circle $\mathbf{T}$ under a the *symbol curve*, $a(\mathbf{T})$.

Pseudospectra of Upper Triangular Toeplitz Matrices

Apply the same approximate eigenvector we used for the Jordan block:

$$\begin{bmatrix} a_0 & a_1 & a_2 & \cdots & a_{n-1} \\ & a_0 & \ddots & \ddots & \vdots \\ & & \ddots & a_1 & a_2 \\ & & & a_0 & a_1 \\ & & & & a_0 \end{bmatrix} \begin{bmatrix} 1 \\ z \\ \vdots \\ z^{n-2} \\ z^{n-1} \end{bmatrix} = \begin{bmatrix} \sum_{k=0}^{n-1} a_k z^k \\ \sum_{k=0}^{n-1} a_k z^{k+1} \\ \vdots \\ a_0 z^{n-2} + a_1 z^{n-1} \\ a_0 z^{n-1} \end{bmatrix}.$$

If the matrix has fixed bandwidth $b \ll n$, (i.e., $a_k = 0$ for $k > b$), then

$$\begin{bmatrix} a_0 & \cdots & a_b & & \\ & a_0 & \ddots & \ddots & \\ & & \ddots & \ddots & a_b \\ & & & a_0 & \vdots \\ & & & & a_0 \end{bmatrix} \begin{bmatrix} 1 \\ z \\ \vdots \\ z^{n-2} \\ z^{n-1} \end{bmatrix} = \begin{bmatrix} \sum_{k=0}^{b} a_k z^k \\ \sum_{k=0}^{b} a_k z^{k+1} \\ \vdots \\ \sum_{k=0}^{b-1} a_k z^{k+n-b} \\ \vdots \\ a_0 z^{n-1} \end{bmatrix}.$$

Pseudospectra of Upper Triangular Toeplitz Matrices

$$\begin{bmatrix} a_0 & \cdots & a_b & & \\ & a_0 & \ddots & \ddots & \\ & & \ddots & \ddots & a_b \\ & & & a_0 & \vdots \\ & & & & a_0 \end{bmatrix} \begin{bmatrix} 1 \\ z \\ \vdots \\ z^{n-2} \\ z^{n-1} \end{bmatrix} = \begin{bmatrix} \sum_{k=0}^{b} a_k z^k \\ \sum_{k=0}^{b} a_k z^{k+1} \\ \vdots \\ \sum_{k=0}^{b-1} a_k z^{k+n-b} \\ \vdots \\ a_0 z^{n-1} \end{bmatrix}$$

$$= \sum_{k=0}^{b} a_k z^k \begin{bmatrix} 1 \\ z \\ \vdots \\ z^{n-2} \\ z^{n-1} \end{bmatrix} - \begin{bmatrix} 0 \\ \vdots \\ 0 \\ a_b z^n \\ \vdots \\ \sum_{k=1}^{b} a_k z^{n-1+k} \end{bmatrix}.$$

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Hence $\mathbf{A}_n\mathbf{x} - a(z)\mathbf{x}$ gets very small in size as $n \to \infty$.
In fact, this reveals the spectrum of the infinite Toeplitz operator on $\ell^2(\mathbf{N})\ldots.$

Spectrum of Toeplitz Operators on $\ell^2(\mathbb{Z})$

For the Toeplitz operator (semi-infinite matrix) $\mathbf{A}_\infty$ with the same symbol:

$$\begin{bmatrix} a_0 & \cdots & a_b & & & \\ & a_0 & \ddots & \ddots & & \\ & & \ddots & \ddots & a_b & \\ & & & a_0 & \ddots & \ddots \\ & & & & \ddots & \end{bmatrix} \begin{bmatrix} 1 \\ z \\ z^2 \\ \vdots \\ \vdots \end{bmatrix} = \begin{bmatrix} \sum_{k=0}^{b} a_k z^k \\ \sum_{k=0}^{b} a_k z^{k+1} \\ \sum_{k=0}^{b} a_k z^{k+2} \\ \vdots \\ \vdots \end{bmatrix} = a(z) \begin{bmatrix} 1 \\ z \\ z^2 \\ \vdots \\ \vdots \end{bmatrix}$$

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Thus $a(z) \in \sigma(\mathbf{A})$ for all $|z| < 1$. In fact, one can show that for this banded upper triangular symbol,

$$\sigma(\mathbf{A}_\infty) = \{a(z) : |z| \leq 1\}.$$

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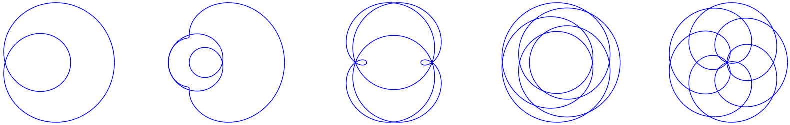
The calculation on the last slide guarantees that for any $\varepsilon > 0$, there exists $N > 0$ such that if $n > N$,

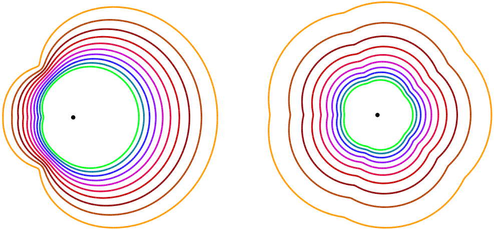
$$\sigma(\mathbf{A}_\infty) \subseteq \sigma_\varepsilon(\mathbf{A}_n).$$

Symbols of Upper Triangular Toeplitz Matrices

Symbol curves for banded upper triangular Toeplitz matrices.



- $a(z) = z + 2z^2$
- $a(z) = z + 2z^2 + z^3 + z^5$
- $a(z) = z + z^3 - z^5$
- $a(z) = z^2 + 3z^5$
- $a(z) = z^2 + z^7$



General Toeplitz Matrices

More generally, the dense Toeplitz matrix

$$\mathbf{A}_n = \begin{bmatrix} a_0 & a_1 & a_2 & \cdots & \\ a_{-1} & a_0 & \ddots & \ddots & \vdots \\ a_{-2} & \ddots & \ddots & a_1 & a_2 \\ \vdots & \ddots & a_{-1} & a_0 & a_1 \\ & \cdots & a_{-2} & a_{-1} & a_0 \end{bmatrix} \in \mathbf{C}^{n \times n}$$

follows the same terminology.

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Call the image of the unit circle $\mathbf{T}$ under a the *symbol curve*, $a(\mathbf{T})$.

Spectrum of a General Toeplitz Operator

Theorem (Spectrum of a Toeplitz Operator)

Suppose the Toeplitz operator $\mathbf{A}_\infty : \ell^2(N) \to \ell^2(N)$ *has a symbol that is continuous. Then*

$$\sigma(\mathbf{A}_\infty) = a(\boldsymbol{T}) \cup \{\textit{all points } a(\boldsymbol{T}) \textit{ encloses with nonzero winding number}\}.$$

Due variously to: Wintner; Gohberg; Krein; Calderón, Spitzer, & Widom.

See Albrecht Böttcher and colleagues for many more details.

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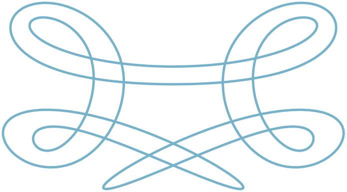

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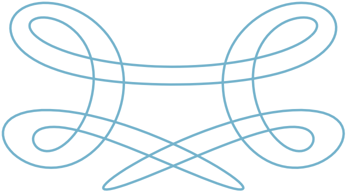

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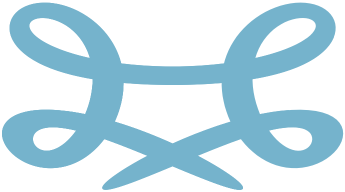

$\sigma(\mathbf{A}_\infty)$

Spectrum of a General Toeplitz Matrix

What can be said of the eigenvalues of a finite-dimensional Toeplitz matrix?

Theorem (Limiting Spectrum of Finite Toeplitz Matrices)

Consider the family of banded Toeplitz matrices $\{\mathbf{A}_n\}_{n \in N}$ with upper bandwidth b and lower bandwidth d. For any fixed $\lambda \in C$, label the roots $\zeta_1, \ldots, \zeta_{b+d}$ of the polynomial $z^d(a(z) - \lambda)$ by increasing modulus.

If $|\zeta_d| = |\zeta_{d+1}|$, then $\lambda \in \lim_{n \to \infty} \sigma(\mathbf{A}_n)$.

This result, proved by [Schmidt & Spitzer, 1960], shows that in general:

$$\lim_{n \to \infty} \sigma(\mathbf{A}_n) \neq \sigma(\mathbf{A}_\infty).$$

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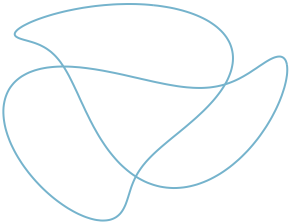

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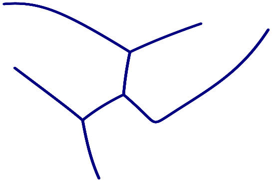
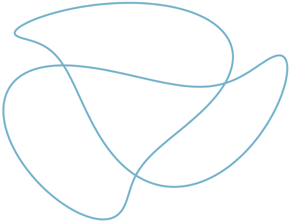


$\lim_{n\to\infty} \sigma(\mathbf{A}_n)$

Spectrum of a General Toeplitz Matrix: Example



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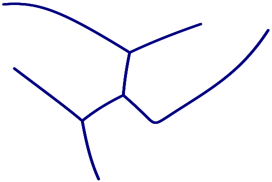

$\lim_{n \to \infty} \sigma(\mathbf{A}_n)$

$\sigma(\mathbf{A}_{50})$

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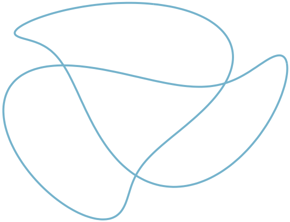
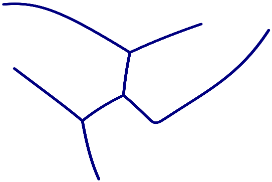
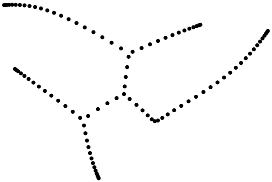


$a(\mathbb{T})$

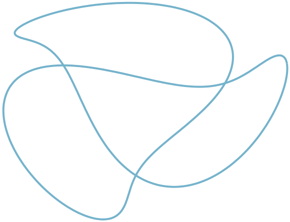


$\lim_{n\to\infty} \sigma(\mathbf{A}_n)$

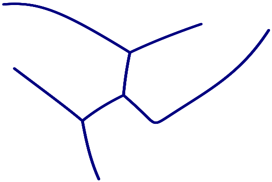


$\sigma(\mathbf{A}_{100})$

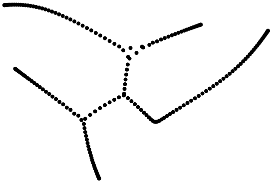
Spectrum of a General Toeplitz Matrix: Example



$a(\mathbb{T})$

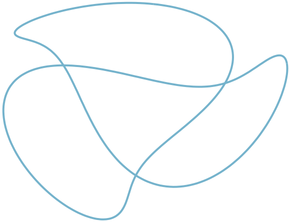


$\lim_{n\to\infty} \sigma(\mathbf{A}_n)$

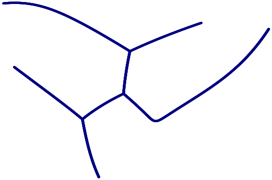


$\sigma(\mathbf{A}_{200})$

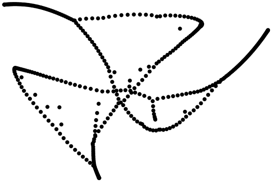
Spectrum of a General Toeplitz Matrix: Example



$a(\mathbb{T})$

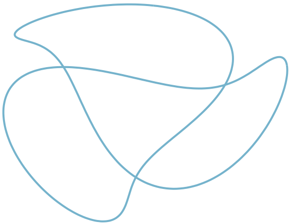


$\lim_{n\to\infty} \sigma(\mathbf{A}_n)$

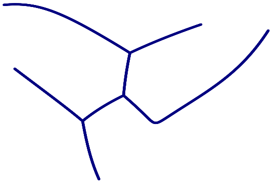


$\sigma(\mathbf{A}_{400})$

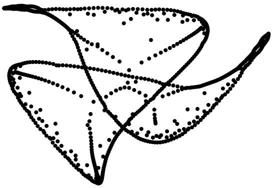
Spectrum of a General Toeplitz Matrix: Example



$a(\mathbb{T})$



$\lim_{n\to\infty} \sigma(\mathbf{A}_n)$



$\sigma(\mathbf{A}_{800})$

Pseudospectra of Toeplitz Matrices

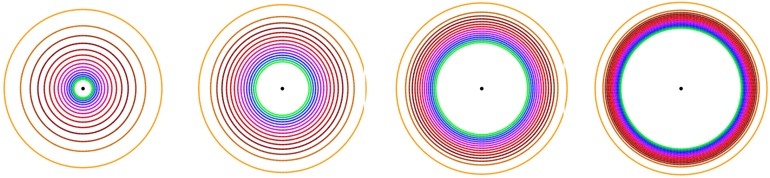
Theorem (Landau; Reichel and Trefethen; Böttcher)

Let $a(z) = \sum_{k=-M}^{M} a_k z^k$ be the symbol of a banded Toeplitz operator.

- *The pseudospectra of $\mathbf{A}_n$ converge to the pseudospectra of the Toeplitz operator on $\ell^2(\mathbf{N})$ as $n \to \infty$.*

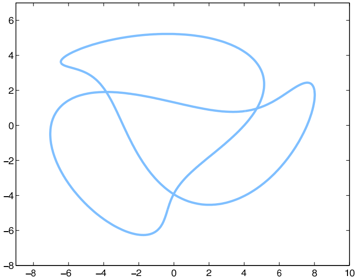
Let $z \in \boldsymbol{C}$ have nonzero winding number w.r.t. the symbol curve $a(\boldsymbol{T})$.

- *$\|(z - \mathbf{A}_n)^{-1}\|$ grows exponentially in n.*
- *For all $\varepsilon > 0$, $z \in \sigma_\varepsilon(\mathbf{A}_n)$ for all n sufficiently large.*

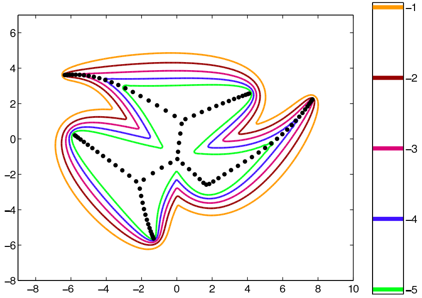


$n = 16$ $n = 32$ $n = 64$ $n = 128$

Pseudospectra of Toeplitz Matrices

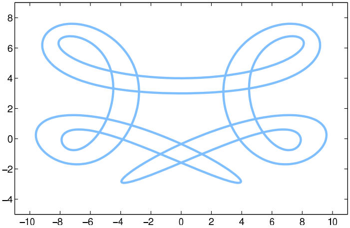


symbol curve

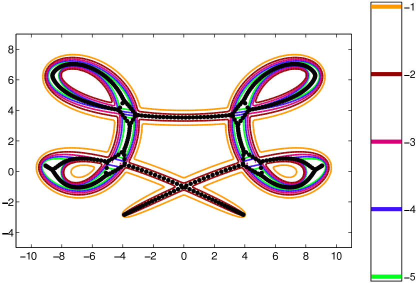


$\sigma_\varepsilon(\mathbf{A}_{100})$

Pseudospectra of Toeplitz Matrices



symbol curve



$\sigma_\varepsilon(\mathbf{A}_{500})$

Hermitian Toeplitz Matrices

We have seen “large” pseudospectra arise for generic Toeplitz matrices.

But what about Hermitian Toeplitz matrices?

For example, the matrix

$$\begin{bmatrix} 0 & 1 & & \\ 1 & 0 & \ddots & \\ & \ddots & \ddots & 1 \\ & & 1 & 0 \end{bmatrix}$$

has symbol $a(z) = z^{-1} + z$, so

$$a(e^{i\theta}) = e^{-i\theta} + e^{i\theta} = 2\cos(\theta) \in [-2, 2] \subset \mathbf{R}.$$

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In general, Hermitian symbols have $a_{-k} = \overline{a_k}$, so

$$\begin{aligned} a(e^{i\theta}) &= a_0 + \sum_{k=-\infty}^{-1} a_k e^{ik\theta} + \sum_{k=1}^{\infty} a_k e^{ik\theta} \\ &= a_0 + \sum_{k=1}^{\infty} \overline{a_k} e^{-ik\theta} + \sum_{k=1}^{\infty} a_k e^{ik\theta} = a_0 + \sum_{k=1}^{\infty} 2\mathrm{Re}(a_k e^{ik\theta}) \in \mathbf{R}. \end{aligned}$$

As $n \to \infty$, eigenvalues of $\mathbf{A}_n$ distribute according to Szegő's theorem.

Tridiagonal Toeplitz Matrices

Consider the case of a tridiagonal Toeplitz matrix,

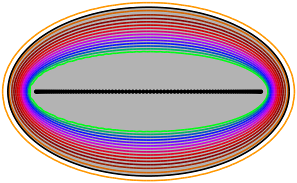
$$\mathbf{A}_n = \begin{bmatrix} \beta & \gamma & & \\ \alpha & \beta & \ddots & \\ & \ddots & \ddots & \gamma \\ & & \alpha & \beta \end{bmatrix} \in \mathbf{C}^{n\times n}$$

with symbol

$$a(z) = \frac{\alpha}{z} + \beta + \gamma z.$$

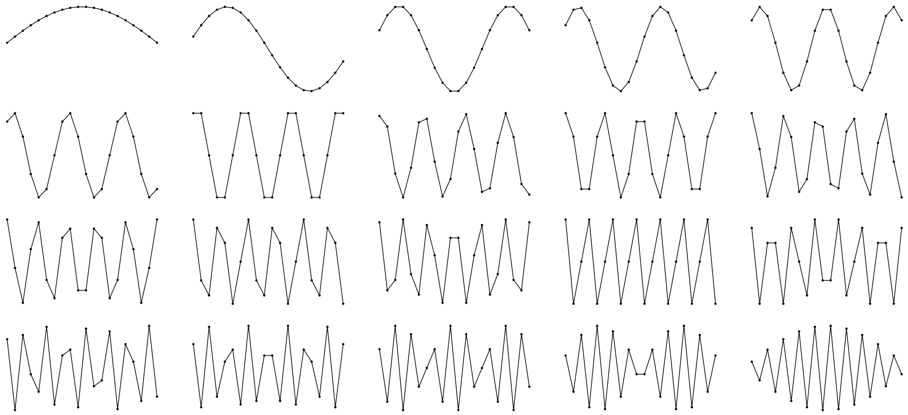
The symbol curve is the ellipse

$$a(\mathbf{T}) = \{z \in \mathbf{T} : \frac{\alpha}{z} + \beta + \gamma z\}.$$



Eigenvectors of Tridiagonal Toeplitz Matrices

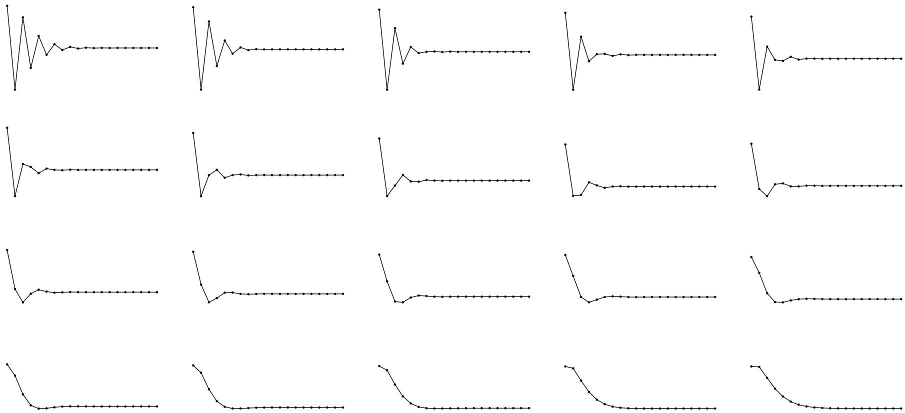
$$\mathbf{A} = \text{tridiag}(1, 0, 1),\ n = 20$$



Normal matrix: orthogonal eigenvectors

Eigenvectors of Tridiagonal Toeplitz Matrices

$$\mathbf{A} = \mathrm{tridiag}(2, 0, 1/2),\ n = 20$$



Nonnormal matrix: non-orthogonal eigenvectors

Circulant Matrices and Laurent Operators

In contrast, consider the *circulant matrix*

$$\mathbf{C}_n = \begin{bmatrix} a_0 & a_1 & \cdots & a_{-2} & a_{-1} \\ a_{-1} & a_0 & \ddots & \ddots & a_{-2} \\ \vdots & \ddots & \ddots & a_1 & \vdots \\ a_2 & \ddots & a_{-1} & a_0 & a_1 \\ a_1 & a_2 & \cdots & a_{-1} & a_0 \end{bmatrix} \in \mathbb{C}^{n\times n}$$

Circulant Matrices and Laurent Operators

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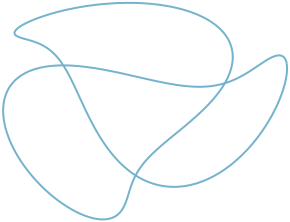
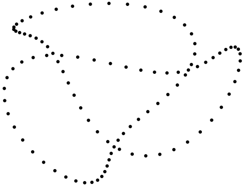
$$\mathbf{C}_n = \begin{bmatrix} a_0 & a_1 & \cdots & a_{-2} & a_{-1} \\ a_{-1} & a_0 & \ddots & \ddots & a_{-2} \\ \vdots & \ddots & \ddots & a_1 & \vdots \\ a_2 & \ddots & a_{-1} & a_0 & a_1 \\ a_1 & a_2 & \cdots & a_{-1} & a_0 \end{bmatrix} \in \mathbf{C}^{n\times n}$$

- $\mathbf{C}_n$ is *normal* for all symbols.
- $\mathbf{C}_n$ is diagonalized by the Discrete Fourier Transform matrix.
- $\sigma(\mathbf{C}_n) = \{a(z) : z \in \mathbf{T}_n\}$, where $\mathbf{T}_n := \{e^{2k\pi i/n}, k = 0, \ldots, n-1\}$: i.e., $\sigma(\mathbf{C}_n)$ comprises the image of the nth roots of unity under the symbol.
- Infinite dimensional generalization: Laurent operators $\mathbf{C}_\infty$ on $\ell^2(\mathbf{Z})$ (doubly-infinite matrices) with spectrum $\sigma(\mathbf{C}_\infty) = a(\mathbf{T})$.

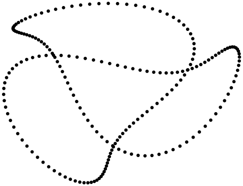
Circulant Matrix and Laurent Operators



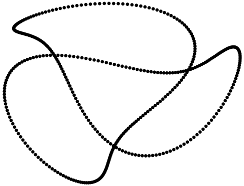
$\sigma(\mathbf{C}_\infty) = a(\mathbb{T})$



$\sigma(\mathbf{C}_{100})$



$\sigma(\mathbf{C}_{200})$



$\sigma(\mathbf{C}_{400})$

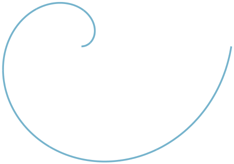
Piecewise Continuous Symbols

It is possible for the symbol

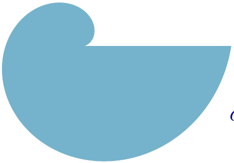
$$a(z) = \sum_{k=-\infty}^{\infty} a_k z^k$$

to, e.g., have a jump discontinuity. This compromises the exponential growth of the norm of the resolvent [Böttcher, E., Trefethen, 2002].

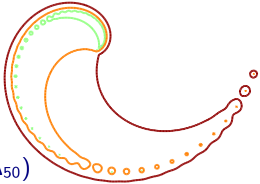
For example, take $a(e^{i\theta}) = \theta e^{i\theta}$, a symbol studied by [Basor & Morrison, 1994].



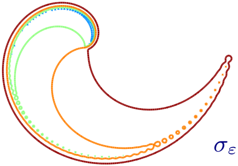
$a(\mathbf{T})$



$\sigma(\mathbf{A}_\infty)$



$\sigma_\varepsilon(\mathbf{A}_{50})$



$\sigma_\varepsilon(\mathbf{A}_{100})$

"Twisted" Toeplitz Matrices

A "twisted" Toeplitz matrix is a Toeplitz-like matrix with varying coefficients [Trefethen & Chapman, 2004].

For example, for $x_j = 2\pi j/n$, set

$$\mathbf{A}_n = \begin{bmatrix} x_1 & \frac{1}{2}x_1 & & \\ & x_2 & \ddots & \\ & & \ddots & \frac{1}{2}x_{n-1} \\ & & & x_n \end{bmatrix}.$$

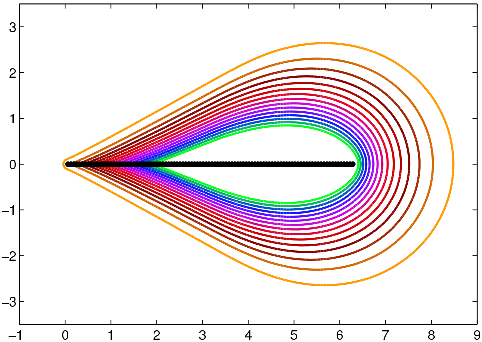
The "symbol" now depends on two variables: $a(x,z) = x + \frac{1}{2}xz$.

The pseudospectra resemble those of standard Toeplitz matrices, but the (pseudo)-eigenvectors have an entirely different character.

"Twisted" Toeplitz Matrices

For $x_j = 2\pi j/n$, set

$$\mathbf{A}_n = \begin{bmatrix} x_1 & \frac{1}{2}x_1 & & \\ & x_2 & \ddots & \\ & & \ddots & \frac{1}{2}x_{n-1} \\ & & & x_n \end{bmatrix}.$$

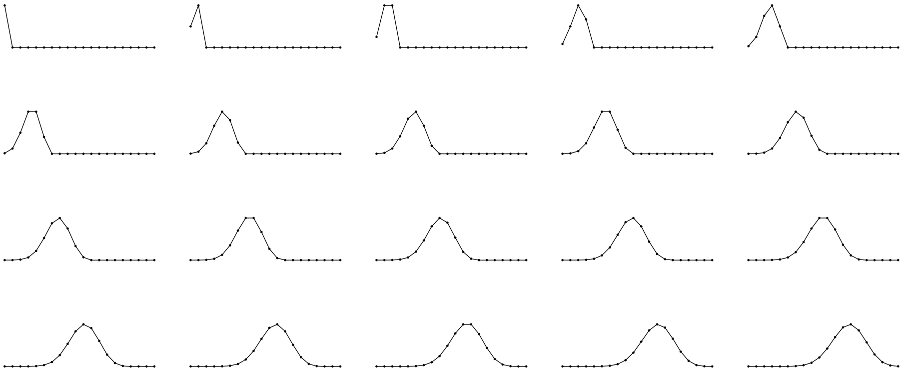


Pseudospectra of $\sigma_\varepsilon(\mathbf{A}_{100})$

Eigenvectors of a Twisted Toeplitz Matrix

Eigenvectors form *wave packets* for twisted Toeplitz matrices.

Pseudoeigenvectors for $z \in \sigma_\varepsilon(\mathbf{A})$ have a similar form.



Eigenvectors of $\mathbf{A}_{20}$ for $a(x,z) = x + \frac{1}{2}xz$

Looking Forward to Differential Operators

Where do Toeplitz (and twisted Toeplitz) matrices come from?

Numerous applications – be we will highlight just one of them: discretization of differential operators.

Consider the steady–state convection diffusion equation $Lu = f$, where

$$Lu = u'' + c\,u'$$

posed over for $x \in [0, 1]$ with $u(0) = u(1) = 0$.

- Fix a discretization parameter n
- Approximate the problem on a simple grid $\{x_j\}_{j=0}^{n+1}$ with spacing $h = 1/(n+1)$:
$$x_j = j\,h.$$
- Replace the first and second derivatives with second-order accurate formulas on the grid:

$$\begin{aligned} u'(x_j) &= \frac{u(x_{j+1}) - u(x_{j+1})}{2h} + \mathcal{O}(h^2) \\ u''(x_j) &= \frac{u(x_{j-1}) - 2u(x_j) + u(x_{j+1})}{h^2} + \mathcal{O}(h^2). \end{aligned}$$

Finite Difference Discretizations

Now let $u_j \approx u(x_j)$ with $u_0 = u_{n+1} = 0$, so that

$$\begin{aligned} u'(x_j) &\approx \frac{u_{j+1} - u_{j+1}}{2h} \\ u''(x_j) &\approx \frac{u_{j-1} - 2u_j + u_{j+1}}{h^2}. \end{aligned}$$

Approximate $Lu = f$, with

$$Lu = u'' + c\,u', \qquad u(0) = u(1) = 0,$$

via

$$\frac{1}{h^2}\begin{bmatrix} -2 & 1 + ch/2 & & \\ 1 - ch/2 & -2 & \ddots & \\ & \ddots & \ddots & 1 + ch/2 \\ & & 1 - ch/2 & -2 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{bmatrix} = \begin{bmatrix} f(x_1) \\ f(x_2) \\ \vdots \\ f(x_n) \end{bmatrix}.$$

Label these components: $\mathbf{A}_n \mathbf{u} = \mathbf{f}$.
$\mathbf{A}_n$ is Toeplitz for this constant-coefficient differential operator.

Finite Difference Discretizations

$$\mathbf{A}_n := \frac{1}{h^2}\begin{bmatrix} -2 & 1+ch/2 & & \\ 1-ch/2 & -2 & \ddots & \\ & \ddots & \ddots & 1+ch/2 \\ & & 1-ch/2 & -2 \end{bmatrix}$$

Notice that the symbol of $\mathbf{A}_n$ depends on n (recall $h = 1/(n+1)$):

$$a_n(z) = \left(\frac{1}{h^2} - \frac{c}{2h}\right) z^{-1} - \left(\frac{2}{h^2}\right) + \left(\frac{1}{h^2} + \frac{c}{2h}\right) z$$

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- For all n, the symbol curve $a_n(\mathbb{T})$ is an ellipse.

Finite Difference Discretizations

$$\mathbf{A}_n := \frac{1}{h^2}\begin{bmatrix} -2 & 1+ch/2 & & \\ 1-ch/2 & -2 & \ddots & \\ & \ddots & \ddots & 1+ch/2 \\ & & 1-ch/2 & -2 \end{bmatrix}$$

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- For all n, the symbol curve $a_n(\mathbb{T})$ is an ellipse.
- If $c = 0$ (no convection), then $a_n(\mathbb{T})$ is a real line segment: $\mathbf{A}_n$ and L are both self-adjoint, hence normal.
- If $c \neq 0$, the eigenvalues of $\mathbf{A}_n$ will be real, but the pseudospectra can be far from these eigenvalues.

Finite Difference Discretizations

$$\mathbf{A}_n := \frac{1}{h^2}\begin{bmatrix} -2 & 1+ch/2 & & \\ 1-ch/2 & -2 & \ddots & \\ & \ddots & \ddots & 1+ch/2 \\ & & 1-ch/2 & -2 \end{bmatrix}$$

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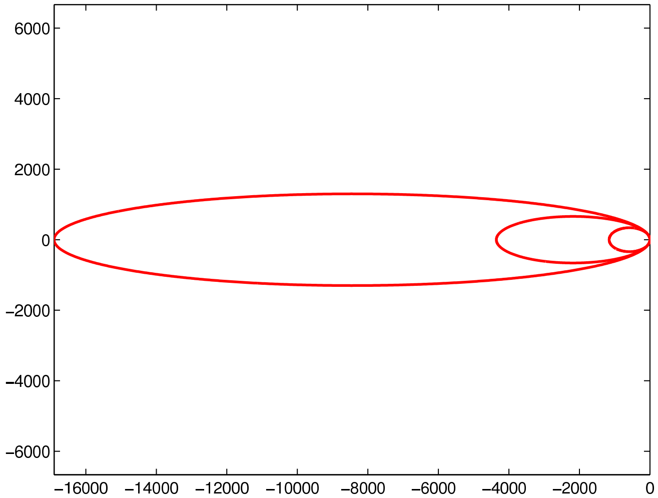
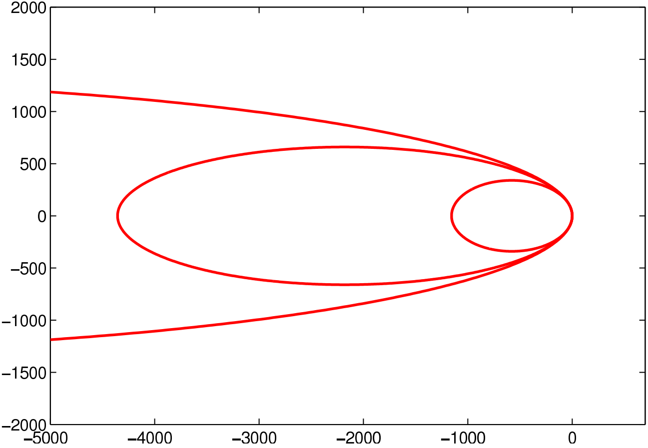
- If $c \neq 0$, the eigenvalues of $\mathbf{A}_n$ will be real, but the pseudospectra can be far from these eigenvalues.
- Rightmost part of $\sigma_\varepsilon(\mathbf{A}_n)$ approximates the corresponding part of $\sigma_\varepsilon(L)$.

Finite Differences: Symbol Curves



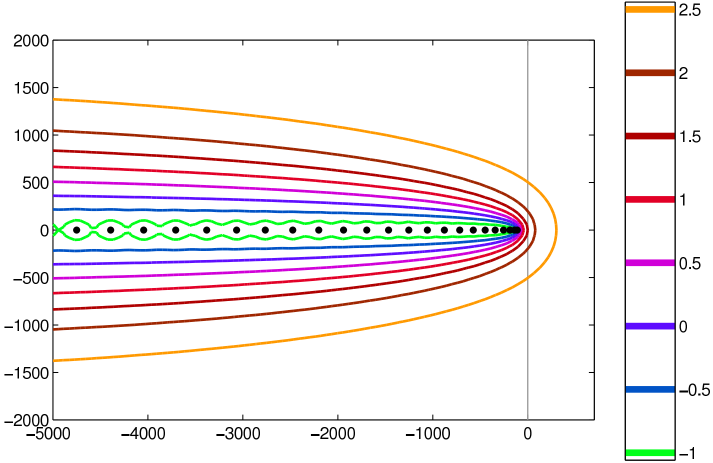
Symbol curves $a_n(\mathbf{T})$ for $n = 16, 32, 64$

Finite Differences: Symbol Curves



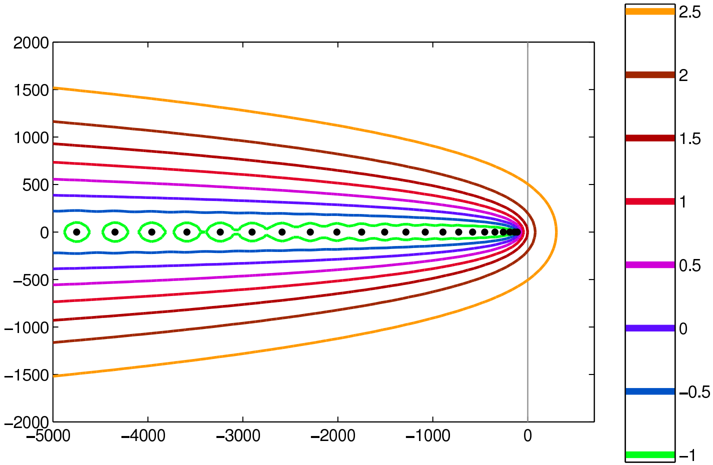
Symbol curves $a_n(\mathbf{T})$ for $n = 16, 32, 64$

Finite Differences: Approximate Pseudospectra



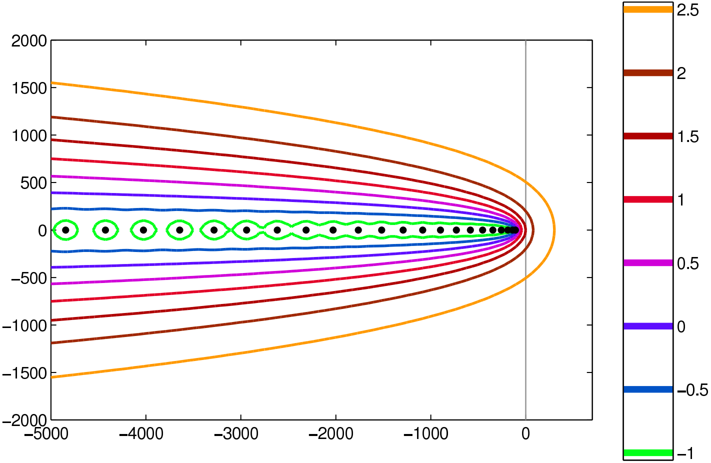
Rightmost part of $\sigma_\varepsilon(\mathbf{A}_n)$ for $n = 64$

Finite Differences: Approximate Pseudospectra



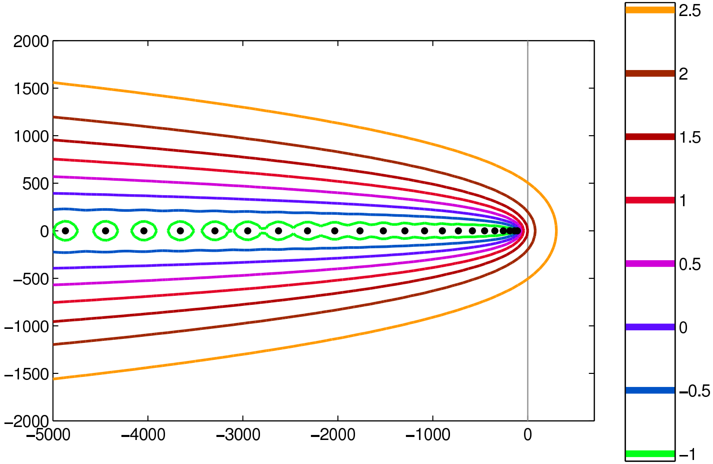
Rightmost part of $\sigma_\varepsilon(\mathbf{A}_n)$ for $n = 128$

Finite Differences: Approximate Pseudospectra



Rightmost part of $\sigma_\varepsilon(\mathbf{A}_n)$ for $n = 256$

Finite Differences: Approximate Pseudospectra



Rightmost part of $\sigma_\varepsilon(\mathbf{A}_n)$ for $n = 512$

3(b) Balanced Truncation Model Reduction

Balanced Truncation Model Reduction

Consider the single-input, single-output (SISO) linear dynamical system:

$$\begin{aligned} \dot{\mathbf{x}}(t) &= \mathbf{A}\mathbf{x}(t) + \mathbf{b}\,u(t) \\ y(t) &= \mathbf{c}\mathbf{x}(t), \end{aligned}$$

$\mathbf{A} \in \mathbb{C}^{n\times n}$, $\mathbf{b}, \mathbf{c}^{\mathsf{T}} \in \mathbb{C}^n$. We assume that $\mathbf{A}$ is stable: $\alpha(\mathbf{A}) < 0$.

We wish to reduce the dimension of the dynamical system by projecting onto well-chosen subspaces.

Balanced truncation: Change basis to match states that are easy to *reach* and easy to *observe*, then project onto that prominent subspace.

Controllability and Observability Gramians

To guage the *observability* of an initial state $\mathbf{x}_0 = \widehat{\mathbf{x}}$,
measure the energy in its output (when there is no input, $u = 0$):

$$y(t) = \mathbf{c}\mathrm{e}^{t\mathbf{A}}\widehat{\mathbf{x}}.$$

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$$\begin{aligned}\int_0^\infty |y(t)|^2\,\mathrm{d}t &= \int_0^\infty \widehat{\mathbf{x}}^*\mathrm{e}^{t\mathbf{A}^*}\mathbf{c}^*\mathbf{c}\mathrm{e}^{t\mathbf{A}}\widehat{\mathbf{x}}\,\mathrm{d}t \\ &= \widehat{\mathbf{x}}^*\Big(\int_0^\infty \mathrm{e}^{t\mathbf{A}^*}\mathbf{c}^*\mathbf{c}\mathrm{e}^{t\mathbf{A}}\,\mathrm{d}t\Big)\widehat{\mathbf{x}} =: \widehat{\mathbf{x}}^*\mathbf{Q}\widehat{\mathbf{x}}.\end{aligned}$$

Controllability and Observability Gramians

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Similarly, we measure the *controllability* by the total input energy required to steer $\mathbf{x}_0 = \mathbf{0}$ to a target state $\widehat{\mathbf{x}}$ as $t \to \infty$. The special form of u that drives the system to $\widehat{\mathbf{x}}$ with minimal energy satisfies

$$\int_0^\infty |u(t)|^2\,\mathrm{d}t = \widehat{\mathbf{x}}^*\Big(\int_0^\infty \mathrm{e}^{t\mathbf{A}}\mathbf{b}\mathbf{b}^*\mathrm{e}^{t\mathbf{A}^*}\,\mathrm{d}t\Big)^{-1}\widehat{\mathbf{x}} =: \widehat{\mathbf{x}}^*\mathbf{P}^{-1}\widehat{\mathbf{x}}.$$

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Thus we have the infinite controllability and observability gramians $\mathbf{P}$ and $\mathbf{Q}$:

$$\mathbf{P} := \int_0^\infty e^{t\mathbf{A}}\mathbf{b}\mathbf{b}^*e^{t\mathbf{A}^*}\,\mathrm{d}t, \qquad \mathbf{Q} := \int_0^\infty e^{t\mathbf{A}^*}\mathbf{c}^*\mathbf{c}\,e^{t\mathbf{A}}\,\mathrm{d}t.$$

See, e.g., [Antoulas, 2005].

Balanced Truncation Model Reduction

The gramians

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(Hermitian positive definite, for a controllable and observable stable system) can be determined by solving the Lyapunov equations – see the next lecture.

If $\mathbf{x}_0 = \mathbf{0}$, the minimum energy of u required to drive $\mathbf{x}$ to state $\widehat{\mathbf{x}}$ is

$$\widehat{\mathbf{x}}^*\mathbf{P}^{-1}\widehat{\mathbf{x}}.$$

Starting from $\mathbf{x}_0 = \widehat{\mathbf{x}}$ with $u(t) \equiv 0$, the energy of output y is

$$\widehat{\mathbf{x}}^*\mathbf{Q}\,\widehat{\mathbf{x}}.$$

$\widehat{\mathbf{x}}^*\mathbf{P}^{-1}\widehat{\mathbf{x}}$: $\widehat{\mathbf{x}}$ is *hard to reach* if it is rich in the lowest modes of $\mathbf{P}$.
$\widehat{\mathbf{x}}^*\mathbf{Q}\,\widehat{\mathbf{x}}$: $\widehat{\mathbf{x}}$ is *hard to observe* if it is rich in the lowest modes of $\mathbf{Q}$.

Balanced truncation transforms the state space coordinate system to make these two gramians the same, then it truncates the lowest modes.

Balanced Truncation Model Reduction

Consider a generic coordinate transformation, for $\mathbf{S}$ invertible:

$$\begin{aligned}(\mathbf{S}\mathbf{x})'(t) &= (\mathbf{S}\mathbf{A}\mathbf{S}^{-1})(\mathbf{S}\mathbf{x}(t)) + (\mathbf{S}\mathbf{b})u(t)\\ y(t) &= (\mathbf{c}\mathbf{S}^{-1})(\mathbf{S}\mathbf{x}(t)) + du(t), \qquad (\mathbf{S}\mathbf{x})(0) = \mathbf{S}\mathbf{x}_0.\end{aligned}$$

With this transformation, the controllability and observability gramians are

$$\widehat{\mathbf{P}} = \mathbf{S}\mathbf{P}\mathbf{S}^*, \qquad \widehat{\mathbf{Q}} = \mathbf{S}^{-*}\mathbf{Q}\mathbf{S}^{-1}.$$

For balancing, we seek $\mathbf{S}$ so that $\widehat{\mathbf{P}} = \widehat{\mathbf{Q}}$ are diagonal.

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Observation (How does nonnormality affect balancing?)

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- *The choice of internal coordinates will affect* $\mathbf{P}$, $\mathbf{Q}$, ...
- *but not the Hankel singular values:* $\widehat{\mathbf{P}}\widehat{\mathbf{Q}} = \mathbf{S}\mathbf{P}\mathbf{Q}\mathbf{S}^{-1}$,
- *and not the transfer function:*
$$(\mathbf{c}\mathbf{S}^{-1})(z - \mathbf{S}\mathbf{A}\mathbf{S}^{-1})^{-1}(\mathbf{S}\mathbf{b}) = d + \mathbf{c}(z - \mathbf{A})^{-1}\mathbf{b},$$
- *and not the system moments:*
$$(\mathbf{c}\mathbf{S}^{-1})(\mathbf{S}\mathbf{b}) = \mathbf{c}\mathbf{b}, \quad (\mathbf{c}\mathbf{S}^{-1})(\mathbf{S}\mathbf{A}\mathbf{S}^{-1})(\mathbf{S}\mathbf{b}) = \mathbf{c}\mathbf{A}\mathbf{b}, \quad \ldots.$$