Lyapunov Equations with Non-Self-Adjoint Coefficients

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Model Reduction for Transport Dominated Phenomena

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Outline

We will survey a set of related problems that are motivated by the study of stability questions in fluid flows.

- Linear Stability Analysis, Transient Dynamics, Pseudospectra
  - Overview of linear stability analysis
  - When transient growth occurs and why it matters
  - Pseudospectral analysis for Differential Algebraic Equations

- Lyapunov Inverse Iteration for Bifurcation Detection
  - Algorithm for finding bifurcations points in linear ODEs/DAEs due to [Meerbergen, Spence 2010; Elman, Meerbergen, Spence, Wu 2012; Elman, Wu 2013]
  - Requires the solution of a Lyapunov equation at each iteration
  - Only possible at scale if Lyapunov solutions have low numerical rank
  - Existing bounds suggest these solutions will not have low rank

- Singular Values of Solutions of Lyapunov Equations
  - New analysis of Lyapunov solutions with nonnormal coefficients
  - Increasing departure from normality can give *faster* singular value decay
  - Interior eigenvalues of $(\mathbf{A} + \mathbf{A}^*)/2$ play a key role.

Linear Stability Analysis and Transients

Linear Stability Analysis for Dynamical Systems

Linear Stability Analysis

Consider the autonomous nonlinear system $\mathbf{u}'(t) = \mathbf{f}(\mathbf{u}(t))$.

- *Find a steady state* $\mathbf{u}_*$, *i.e.,* $\mathbf{f}(\mathbf{u}_*) = \mathbf{0}$.
- *Linearize* $\mathbf{f}$ *about this steady state and analyze small perturbations,* $\mathbf{u}(t) = \mathbf{u}_* + \mathbf{x}(t)$*:*

$$\begin{aligned} \mathbf{x}'(t) = \mathbf{u}'(t) &= \mathbf{f}(\mathbf{u}_* + \mathbf{x}(t)) \\ &= \mathbf{f}(\mathbf{u}_*) + \mathbf{A}\mathbf{x}(t) + O(\|\mathbf{x}(t)\|^2) \\ &= \mathbf{A}\mathbf{x}(t) + O(\|\mathbf{x}(t)\|^2). \end{aligned}$$

- *Ignore higher-order effects, and analyze the linear system* $\mathbf{x}'(t) = \mathbf{A}\mathbf{x}(t)$. *The steady state* $\mathbf{u}_*$ *is stable provided* $\mathbf{A}$ *is stable: i.e., all its eigenvalues are in the left half-plane.*

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But what if the small perturbation $\mathbf{x}(t)$ grows
by orders of magnitude before eventually decaying?

Example: A nonlinear heat equation

An example from [Zworski; Galkowski, 2012]:

For $x \in [-1, 1]$ and $t \geq 0$ with $u(-1, t) = u(1, t) = 0$, consider

$$u_t(x, t) = \nu u_{xx}(x, t)$$

with $\nu > 0$

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For $x \in [-1, 1]$ and $t \geq 0$ with $u(-1, t) = u(1, t) = 0$, consider

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The linearization L, an advection–diffusion operator,

$$Lu = \nu u_{xx} + \sqrt{\nu} u_x + \tfrac{1}{8} u$$

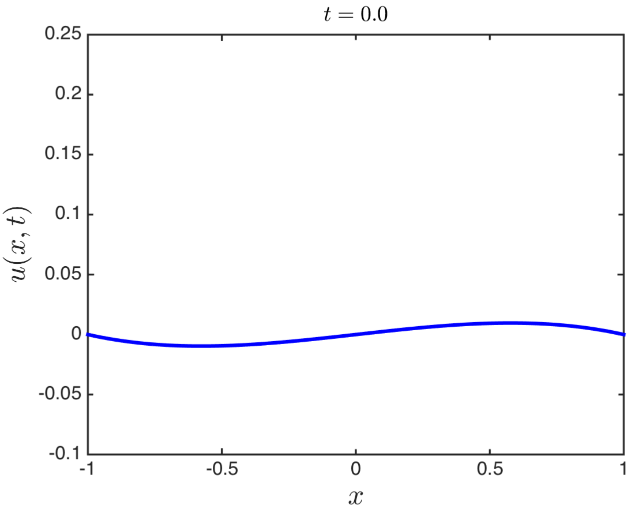
has eigenvalues and eigenfunctions

$$\lambda_n = -\frac{1}{8} - \frac{n^2 \pi^2 \nu}{4}, \qquad u_n(x) = e^{-x/(2\sqrt{\nu})} \sin(n\pi x/2);$$

see, e.g., [Reddy & Trefethen 1994].

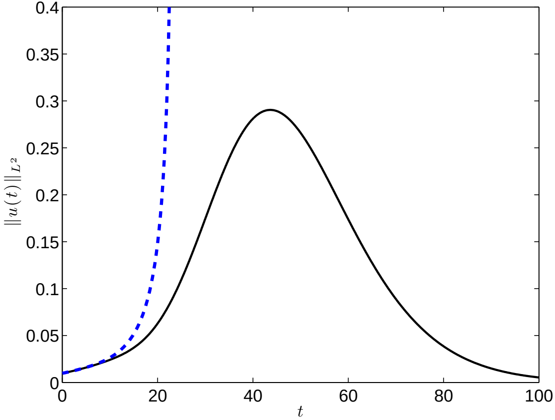
The linearized operator is stable for all $\nu > 0$, but has interesting transients . . . .

Evolution of a small initial condition



Nonlinear model (blue) and linearization (black)

Transient behavior



Linearized system (black) and nonlinear system (dashed blue)

Nonnormal growth feeds the nonlinear instability.

Transient behavior: reduction of the linearized model

The linearization L is stable. So too is any reasonable discretization $\mathbf{L}$.

What happens when we apply model reduction to the discretization, e.g., to create a surrogate in a design problem?

Apply Arnoldi moment-matching model reduction to the discretization $\mathbf{L}$ of order 100 to generate a $k = 10$ dimensional model $\mathbf{L}_{10} = \mathbf{V}_{10}^* \mathbf{L} \mathbf{V}_{10}$.
(This does not guarantee stability, but we will have $W(\mathbf{L}_{10}) \subseteq W(\mathbf{L})$.)

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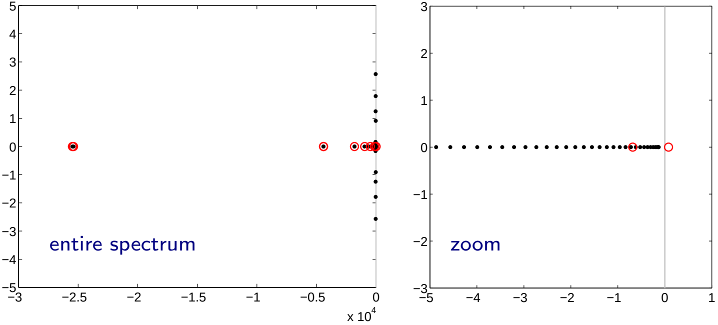
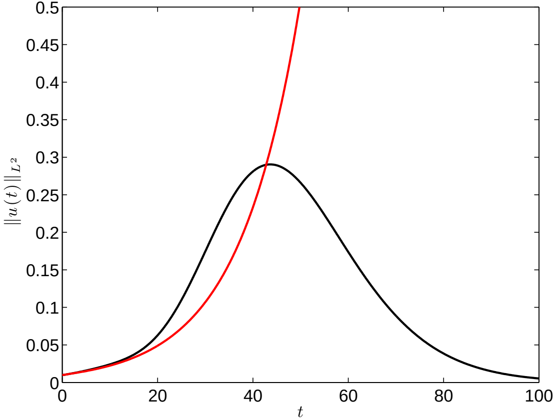


Spectral discretization, $n = 128$ (black) and Arnoldi reduction, $k = 10$ (red).
[Many Ritz values capture *spurious* eigenvalues of the discretization of the left.]

Transient behavior: reduction of the linearized model



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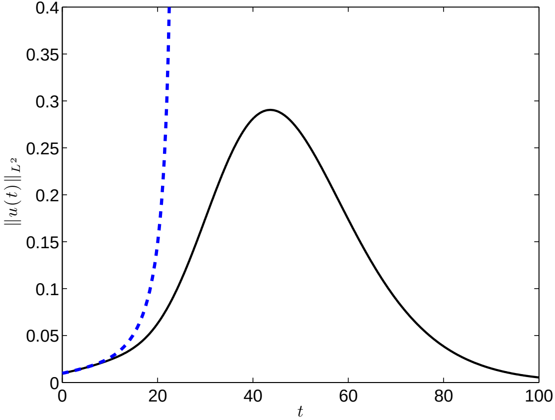
Transient behavior: nonlinear versus linear system



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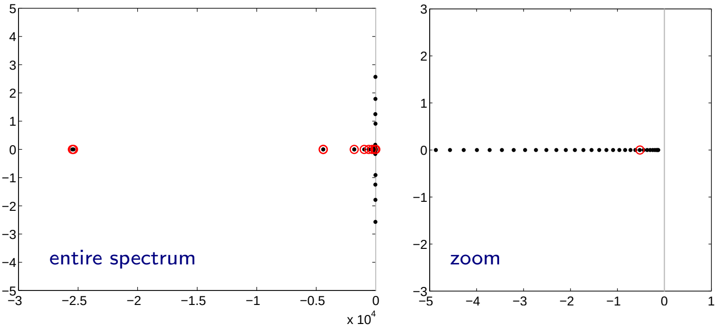
Transient behavior: stabilized reduction of the linearized model

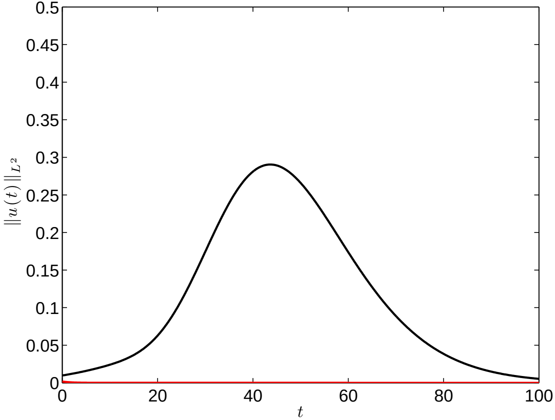
We can *restart* the Arnoldi reduction to preserve stability (now matches moments of a modified problem); [Grimme, Sorensen, Van Dooren 1994; Jaimoukha, Kasenally 1997]



Spectral discretization, $n = 128$ (black) and Arnoldi reduction, $k = 10$ (red) after a restart to remove the spurious eigenvalue.

[This effectively pushes Ritz values to the left.]

Transient behavior: stabilized reduction of the linearized model



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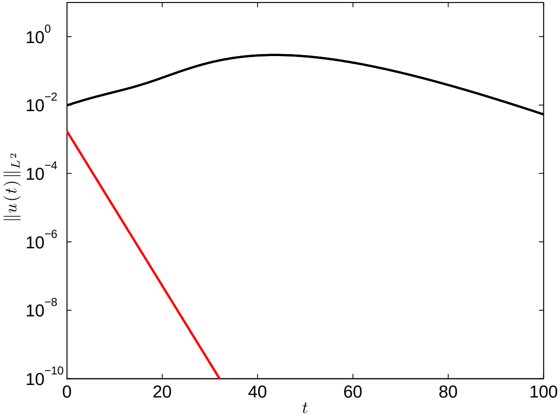

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MORAL. Beware of suppressing spurious instabilities: they can give rich insight into the original problem!

Tools for Understanding Transient Growth: Eigenvectors

If $\mathbf{A}$ is diagonalizable, $\mathbf{A} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^{-1}$, then one can bound the transient growth in $e^{t\mathbf{A}}$ using the *condition number of the eigenvector matrix*.

Example (Eigenvalue/Eigenvector Bound for Continuous-Time Systems)

$$\begin{aligned}
\|\mathbf{x}(t)\| = \|e^{t\mathbf{A}}\mathbf{x}(0)\| &\leq \|e^{t\mathbf{A}}\|\|\mathbf{x}(0)\| \\
&\leq \|\mathbf{V}e^{t\mathbf{\Lambda}}\mathbf{V}^{-1}\|\|\mathbf{x}(0)\| \\
&\leq \kappa(\mathbf{V}) \max_{\lambda\in\sigma(\mathbf{A})} |e^{t\lambda}|\|\mathbf{x}(0)\|,
\end{aligned}$$

where $\kappa(\mathbf{V}) := \|\mathbf{V}\|\|\mathbf{V}^{-1}\|$.

Tools for Understanding Transient Growth: Numerical Range

Definition (Numerical Range, a.k.a. Field of Values)

The *numerical range* of $\mathbf{A}$ is the set

$$W(\mathbf{A}) = \left\{ \frac{\mathbf{x}^*\mathbf{A}\mathbf{x}}{\mathbf{x}^*\mathbf{x}} : \|\mathbf{x}\| = 1 \right\}.$$

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\|\mathrm{e}^{t\mathbf{A}}\mathbf{x}_0\|\Big|_{t=0} &= \frac{\mathrm{d}}{\mathrm{d}t}\left(\mathbf{x}_0^*\mathrm{e}^{t\mathbf{A}^*}\mathrm{e}^{t\mathbf{A}}\mathbf{x}_0\right)^{1/2}\Big|_{t=0} \\ &= \frac{\mathrm{d}}{\mathrm{d}t}\left(\mathbf{x}_0^*(\mathbf{I}+t\mathbf{A}^*)(\mathbf{I}+t\mathbf{A})\mathbf{x}_0\right)^{1/2}\Big|_{t=0} = \frac{1}{\|\mathbf{x}_0\|}\mathbf{x}_0^*\left(\frac{\mathbf{A}+\mathbf{A}^*}{2}\right)\mathbf{x}_0 \end{aligned}$$

So, the rightmost point in $W(\mathbf{A})$ reveals the maximal slope of $\|\mathrm{e}^{t\mathbf{A}}\|$ at $t = 0$.

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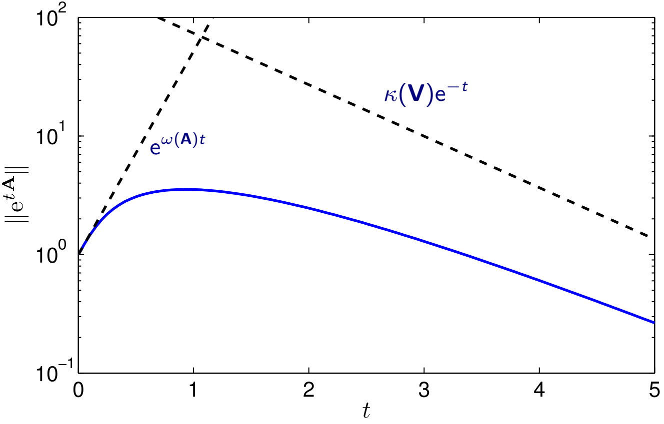
Definition (numerical abscissa)

The *numerical abscissa* is the rightmost in $W(\mathbf{A})$:

$$\omega(\mathbf{A}) := \max_{z \in W(\mathbf{A})} \operatorname{Re} z.$$

Initial Transient Growth via Numerical Abscissa

$$\mathbf{A} = \begin{bmatrix} -1.1 & 10 \\ 0 & -1 \end{bmatrix}.$$



Tools for Understanding Transient Growth: Pseudospectra

[Use the convention that if $\mathbf{A}$ does not have a bounded inverse, $\|\mathbf{A}^{-1}\| = \infty$.]

Theorem

The following three definitions of the ε-pseudospectrum are equivalent:

1. $\sigma_\varepsilon(\mathbf{A}) = \{z \in C : z \in \sigma(\mathbf{A} + \mathbf{E})$ *for some bounded* $\mathbf{E}$ *with* $\|\mathbf{E}\| < \varepsilon\}$;
2. $\sigma_\varepsilon(\mathbf{A}) = \{z \in C : \|(z - \mathbf{A})^{-1}\| > 1/\varepsilon\}$;
3. $\sigma_\varepsilon(\mathbf{A}) = \{z \in C : z \in \sigma(\mathbf{A})$ *or* $\|\mathbf{A}\mathbf{v} - z\mathbf{v}\| < \varepsilon$ *for some unit vector* $\mathbf{v}\}$.

See, e.g., [Trefethen, E. 2005].

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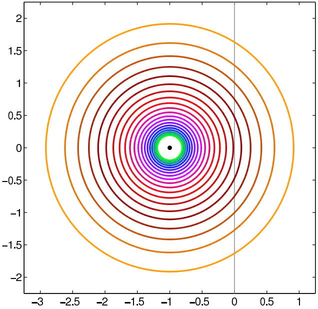
These different definitions are useful in different contexts:

1. interpreting numerically computed eigenvalues;
2. analyzing matrix behavior/functions of matrices;
   computing pseudospectra on a grid in $\mathbf{C}$;
3. proving bounds on a particular $\sigma_\varepsilon(\mathbf{A})$.

Example of Pseudospectra

$$\mathbf{A} = \begin{bmatrix} -1 & 2 & & & \\ & -1 & \ddots & & \\ & & \ddots & 2 & \\ & & & -1 & 2 \\ & & & & -1 \end{bmatrix} \in \mathbf{C}^{20\times 20}.$$

Pseudospectra of Toeplitz matrices have been deeply studied [Böttcher et al.].



$\sigma_\varepsilon(\mathbf{A})$ for $\varepsilon = 10^{-20}, 10^{-19}, \ldots, 10^{-1}$

Pseudospectral Bounds on the Matrix Exponential

We wish to use pseudospectra to bound $\|e^{t\mathbf{A}}\|$ (cf. Hille–Yosida theory).

Definition

The *ε-pseudospectral abscissa* is the supremum of the real parts of $z \in \sigma_\varepsilon(\mathbf{A})$:

$$\alpha_\varepsilon(\mathbf{A}) := \sup_{z \in \sigma_\varepsilon(\mathbf{A})} \operatorname{Re} z.$$

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Theorem (Upper and Lower Bounds on $\|e^{t\mathbf{A}}\|$)

For any $\mathbf{A} \in C^{n\times n}$ and $\varepsilon > 0$,

$$\|e^{t\mathbf{A}}\| \le \frac{L_\varepsilon}{2\pi\varepsilon} e^{t\alpha_\varepsilon(\mathbf{A})},$$

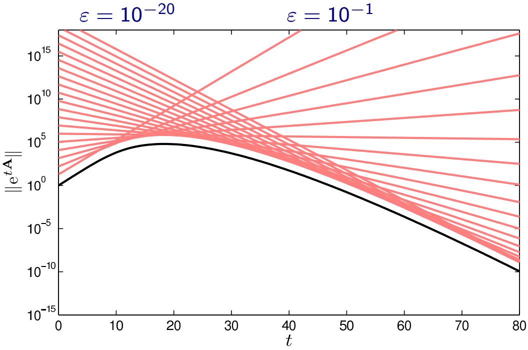
where L_ε denotes the contour length of the boundary of $\sigma_\varepsilon(\mathbf{A})$.

For stable $\mathbf{A}$ and any $\varepsilon > 0$,

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

Upper Bound on the Matrix Exponential from Pseudospectra

$$\mathbf{A} = \begin{bmatrix} -1 & 2 & & & \\ & -1 & \ddots & & \\ & & \ddots & 2 & \\ & & & -1 & 2 \\ & & & & -1 \end{bmatrix} \in \mathbf{C}^{20\times 20}.$$



Lower Bound on the Matrix Exponential from Pseudospectra

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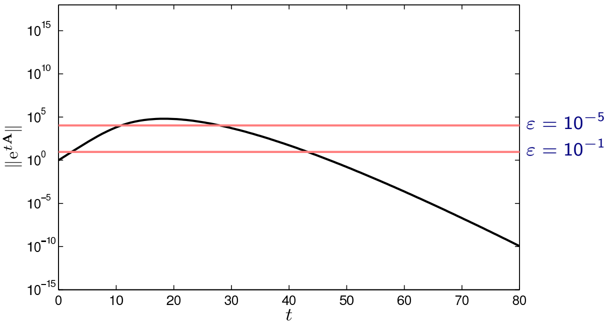
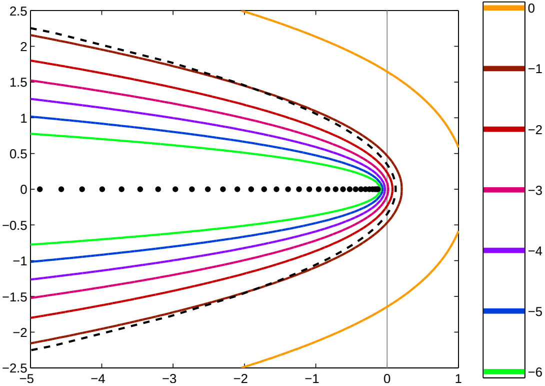


Nonnormality in the Linearized PDE Example



Spectrum, pseudospectra, and numerical range (L^2 norm, $\nu = 0.02$)

Transient growth can feed the nonlinearity; cf. [Trefethen, Trefethen, Reddy, Driscoll 1993], [Baggett, Driscoll, Trefehen 1995]

Interlude:
Pseudospectra for DAEs

Linear Stability Analysis for Fluid Flows

Pseudospectra/nornormality have provided a compelling tool for analyzing subcritical transition to turbulence in fluid flows, particularly for classical problems where the dynamics can be reduced to simple ODEs, e.g., Orr–Sommerfeld; e.g., [Butler, Farrell 1992], [Trefethen, Trefethen, Reddy, Driscoll 1993], [Reddy, Schmid, Henningson 1993], [Schmid, Henningson 2001].

More generally, for a given flow regime one needs to:

- Find a steady-state flow (Picard/Newton iterations).
- Linearize the flow about this steady-state to obtain

$$\begin{bmatrix} \mathbf{M} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{v}'(t) \\ \mathbf{p}'(t) \end{bmatrix} = \begin{bmatrix} \mathbf{F} & \mathbf{C}^* \\ \mathbf{C} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{v}(t) \\ \mathbf{p}(t) \end{bmatrix},$$

  which we write as $\mathbf{B}\mathbf{x}'(t) = \mathbf{A}\mathbf{x}(t)$.
- Analyze the spectral properties of the pencil $(\mathbf{A}, \mathbf{B})$.
- Need a generalization of pseudospectra for matrix pencils.
- For 2d examples we use the IFISS package [Elman, Silvester, Ramage].

See, e.g., [Gunzberger 1989].

Pseudospectra of Matrix Pencils

- Many definitions of pseudospectra of matrix pencils have been proposed: [Riedel 1994], [Ruhe 1995], [Frayssé, Gueury, Nicoud, Toumazou 1996], etc.
- Further generalizations (polynomial, delay, nonlinear EVPs): [Tisseur, Higham 2001], [Green, Wagenknecht 2006], [Bindel, Hood 2013].

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- Key: We use pseudospectra to analyze *dynamics*,
  rather than perturbations in eigenvalue computations.
- If $\mathbf{B}$ is invertible, the 'right' approach (cf. [Ruhe 1995]) considers

$$\mathbf{x}'(t) = \mathbf{B}^{-1}\mathbf{A}\mathbf{x}(t)$$

  and analyzes $\sigma_\varepsilon(\mathbf{B}^{-1}\mathbf{A})$ *in the correct physical norm*.

Pseudospectra of Matrix Pencils

- When **B** is singular, as it is when

$$\mathbf{B} = \begin{bmatrix} \mathbf{M} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}$$

  we must use tools from DAEs to understand transient dynamics [Cambpell, Meyer 1979], [Kunkel, Mehrmann 2006].

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- Simplest case: for invertible $\mathbf{A}$ we can write the Schur form

$$\mathbf{A}^{-1}\mathbf{B} = \begin{bmatrix} \mathbf{U}_1 & \mathbf{U}_2 \end{bmatrix} \begin{bmatrix} \mathbf{G} & \mathbf{S} \\ \mathbf{0} & \mathbf{N} \end{bmatrix} \begin{bmatrix} \mathbf{U}_1^* \\ \mathbf{U}_2^* \end{bmatrix}$$

  for $[\mathbf{U}_1\ \mathbf{U}_2]$ unitary, $\mathbf{G}$ invertible, and $\mathbf{N}$ nilpotent.

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- Then the dynamics evolve as

$$\mathbf{x}(t) = \mathbf{U}_1 e^{t\mathbf{G}^{-1}} \mathbf{U}_1^* \mathbf{x}(0)$$

  for initial conditions that satisfy the algebraic constraints, $\mathbf{x}(0) \in \text{Ran}(\mathbf{U}_1)$.

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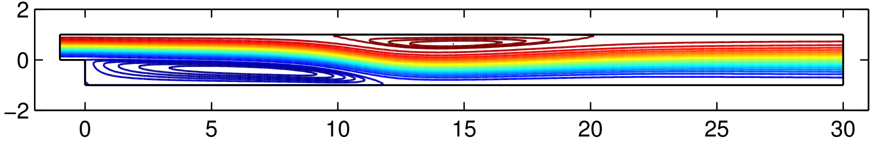
- *To understand the transient dynamics, study $\sigma_\varepsilon(\mathbf{G}^{-1})$ in the right norm.*

Pseudospectra for Flow over a Backward Facing Step



(viscosity $\nu = 1/600$)

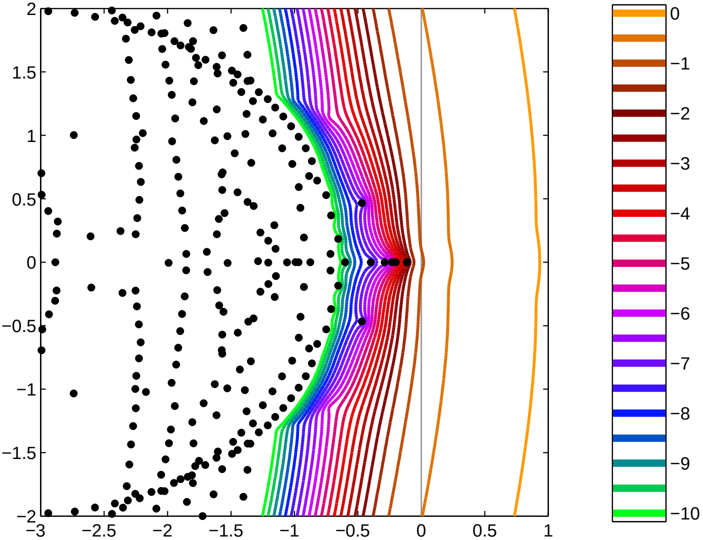
This is a notorious fluid stability problem; see [Gresho et al. 1993].

To compute pseudospectra $\sigma_\varepsilon(\mathbf{G}^{-1})$:

- Transform coordinates so the vector 2-norm approximates the energy norm for the PDE.
- Use the implicitly restarted Arnoldi algorithm (ARPACK/eigs) to compute the portion of $\mathbf{G}^{-1}$ active on the invariant subspace associated with the 1000 smallest magnitude eigenvalues.
- Numerous helpful tools are available: [Cliffe, Garratt, Spence 1994], [Stykel 2008], [Heinkenschloss, Sorensen, Sun 2008].

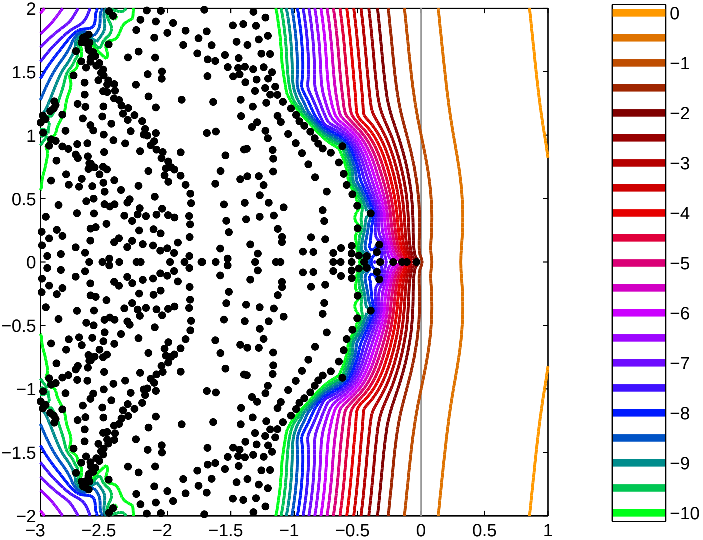
Pseudospectra for Flow over a Backward Facing Step

$\nu = 1/100$



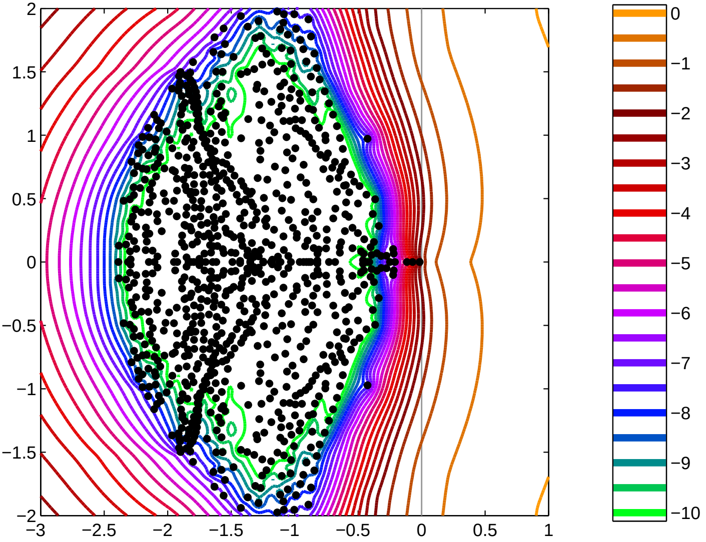
Pseudospectra for Flow over a Backward Facing Step

$\nu = 1/200$



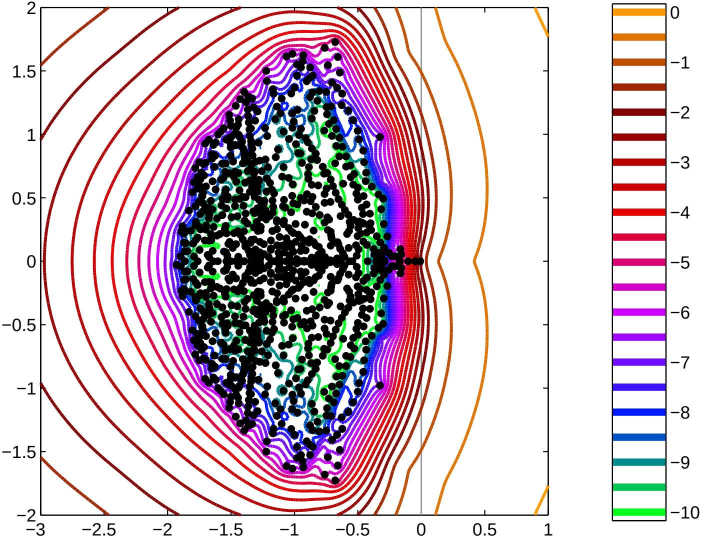
Pseudospectra for Flow over a Backward Facing Step

$\nu = 1/300$



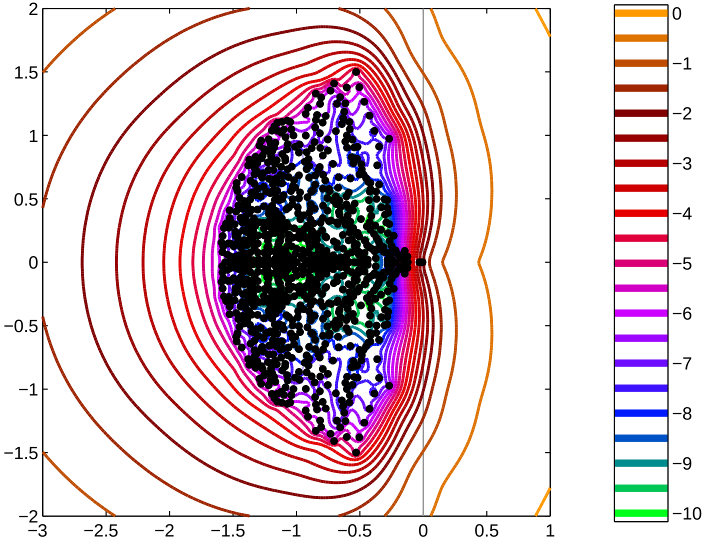
Pseudospectra for Flow over a Backward Facing Step

$\nu = 1/400$



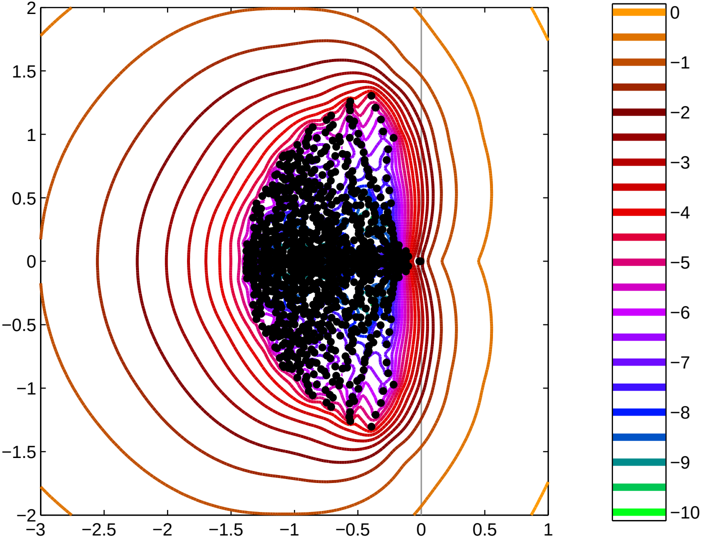
Pseudospectra for Flow over a Backward Facing Step

$\nu = 1/500$



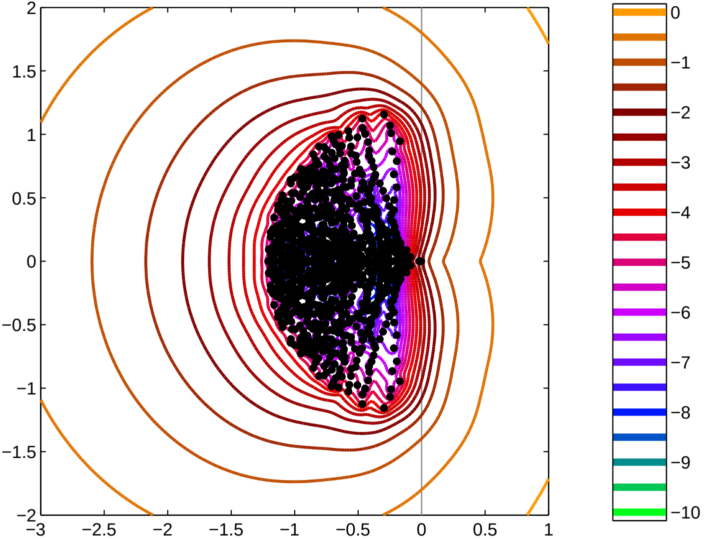
Pseudospectra for Flow over a Backward Facing Step

$\nu = 1/600$



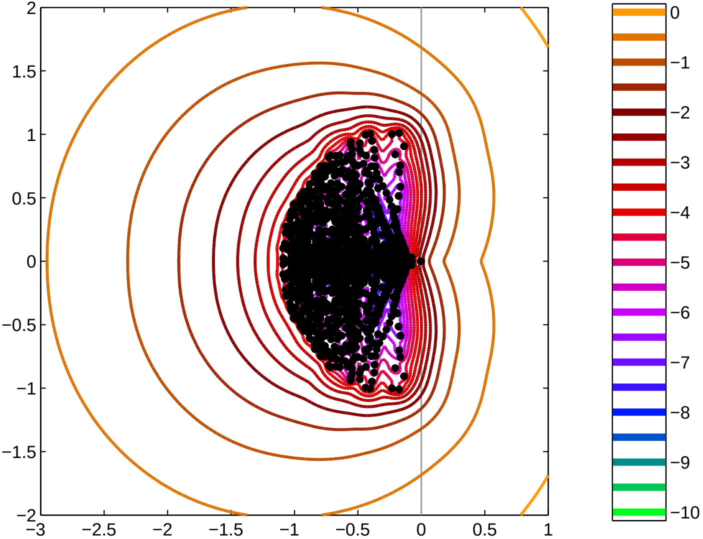
Pseudospectra for Flow over a Backward Facing Step

$\nu = 1/700$



Pseudospectra for Flow over a Backward Facing Step

$\nu = 1/800$



Singular Values of Solutions of Lyapunov Equations

Bifurcation Detection

Determine bifurcation points in the parameterized linearized system

$$\mathbf{x}'(t) = (\mathbf{A} - \omega\boldsymbol{\Delta})\mathbf{x}(t).$$

- Assume that $\mathbf{A}$ is stable.
- Find the smallest $|\omega|$ for which $\mathbf{A} - \omega\boldsymbol{\Delta}$ has an imaginary eigenvalue.

From classical bifurcation theory, this ω can be characterized as the smallest magnitude eigenvalue of the generalized eigenvalue problem

$$\mathbf{AX} + \mathbf{XA}^* = \omega(\boldsymbol{\Delta}\mathbf{X} + \mathbf{X}\boldsymbol{\Delta}^*)$$

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which can be written as

$$\mathcal{L}_{\mathbf{A}}\mathbf{X} = \omega\mathcal{L}_{\mathbf{\Delta}}\mathbf{X},$$

with the *Lyapunov operators* $\mathcal{L}_{\mathbf{A}}, \mathcal{L}_{\mathbf{\Delta}} : \mathbb{C}^{n\times n} \to \mathbb{C}^{n\times n}$ given by

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There are (at least) two problems with this approach for large n:

- Since $\mathcal{L}_{\mathbf{A}}$ is an $n^2 \times n^2$ matrix, this could take up to $O(n^6)$ operations;
- We might not even be able to store the dense 'eigenvector' $\mathbf{X}$.

Bifurcation Detection: Lyapunov Inverse Iteration

Find the smallest $|\omega|$ such that

$$\mathcal{L}_{\mathbf{A}}\mathbf{X} = \omega\mathcal{L}_{\mathbf{\Delta}}\mathbf{X},$$

for $\mathcal{L}_{\mathbf{A}}, \mathcal{L}_{\mathbf{\Delta}} : \mathbf{C}^{n\times n} \to \mathbf{C}^{n\times n}$ given by

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[Meerbergen, Spence, 2010] propose *Lyapunov inverse iteration* to find ω, which effectively applies $\mathcal{L}_{\mathbf{A}}^{-1}$ by solving a *Lyapunov equation* at each iteration.

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[Meerbergen, Spence, 2010] propose *Lyapunov inverse iteration* to find ω, which effectively applies $\mathcal{L}_{\mathbf{A}}^{-1}$ by solving a *Lyapunov equation* at each iteration.

- There exist good $O(n^3)$ methods for solving Lyapunov equations [Bartels, Stewart 1972], [Hammarling 1982].
- These methods still need to store the dense solution $\mathbf{X}$.
- When $\mathbf{A}$ is stable, $\mathbf{X}$ is (almost always) full rank.

We are particularly interested in bifurcation problems for nonlinear problems in fluid dynamics [Elman, Meerbergen, Spence, Wu, 2012; Elman, Wu, 2013].

Matrix Equations in Dynamical Systems

Many problems in model reduction, and control/dynamical systems in general, lead to matrix equations, the most common being the Lyapunov equation. (See the recent survey on linear matrix equations by [Simoncini].)

Assume that $\mathbf{A} \in \mathbb{C}^{n \times n}$ is stable: all eigenvalues have negative real part.

$$\mathbf{A}\,\mathbf{X} + \mathbf{X}\,\mathbf{A}^* = -\mathbf{B}\,\mathbf{B}^*$$

Given the $n \times n$ matrix $\mathbf{A}$ and the $n \times m$ matrix $\mathbf{B}$ $(m \ll n)$, solve for the square $n \times n$ matrix $\mathbf{X}$.

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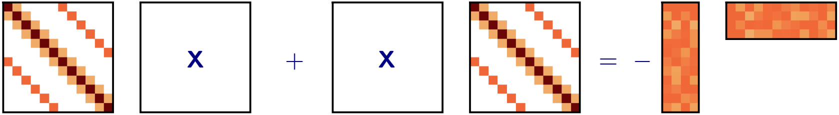

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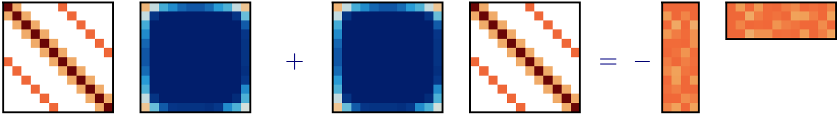

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- Under mild conditions (($\mathbf{A}, \mathbf{B}$) controllable), $\mathbf{X}$ is positive definite.
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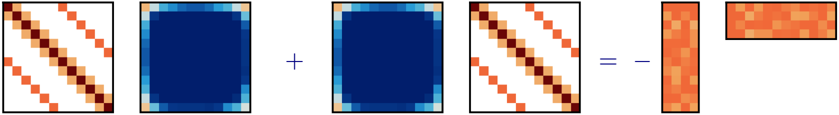

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- Under mild conditions ($(\mathbf{A}, \mathbf{B})$ controllable), $\mathbf{X}$ is positive definite.
- Typically $\mathbf{X}$ has n^2 nonzeros: cannot directly store $\mathbf{X}$ for large n.
- When m is small, *the singular values of* $\mathbf{X}$ *often decay quickly*, depending on eigenvalues of $\mathbf{A}$ (and related quantities) [Penzl 2000a, 2000b].

Low Rank Approximations from Iterative Methods

- How do spectral properties of $\mathbf{A}$ affect the singular values of $\mathbf{X}$?
- Iterative methods for solving the Lyapunov equation naturally construct low-rank approximations to $\mathbf{X}$. (Take $\operatorname{rank}(\mathbf{B}) = 1$ for simplicity.)

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- Galerkin Projection Methods
  [Saad 1990; Simoncini 2007; ...]

  - Let $\mathcal{K}_k \subseteq \mathbb{C}^n$ denote some k-dimensional subspace of $\mathbb{C}^n$
    e.g., a Krylov subspace, rational Krylov subspace, etc.
  - Construct a Hermitian (rank $\le k$) matrix $\mathbf{X}_k \in \mathbb{C}^{n\times n}$ such that

    $$\text{Ran}(\mathbf{X}_k) \subset \mathcal{K}_k.$$

    Equivalently,

    $$\mathbf{X}_k := \mathbf{Q}\mathbf{Y}_k\mathbf{Q}^* \in \{\mathbf{Q}\mathbf{Z}\mathbf{Q}^* : \mathbf{Z} \in \mathbb{C}^{k\times k}\},$$

    where the columns of $\mathbf{Q} \in \mathbb{C}^{n\times k}$ form an orthonormal basis for $\mathcal{K}_k$.
  - Impose a Galerkin condition in the inner product $\langle \mathbf{S}, \mathbf{T}\rangle = \text{tr}(\mathbf{T}^*\mathbf{S})$:

    $$0 = \langle \mathbf{A}\mathbf{X}_k + \mathbf{X}_k\mathbf{A}^* + \mathbf{B}\mathbf{B}^*, \mathbf{Q}\mathbf{Z}\mathbf{Q}^*\rangle,$$
  - which reduces to the $k \times k$ Lyapunov equation

    $$(\mathbf{Q}^*\mathbf{A}\mathbf{Q})\mathbf{Y}_k + \mathbf{Y}_k(\mathbf{Q}^*\mathbf{A}\mathbf{Q})^* = -(\mathbf{Q}^*\mathbf{B})(\mathbf{Q}^*\mathbf{B})^*.$$

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- Alternating Direction Implicit (ADI) Methods
  [Smith 1968; Wachspress 1988; Penzl 2000a; ...]
  - Set $\mathbf{X}_0 = \mathbf{0}$.
  - For $k = 0, 1, \ldots$, set

$$\mathbf{X}_{k+1} = \mathbf{A}_{\mu_k}\mathbf{X}_k\mathbf{A}_{\mu_k}^* + \mathbf{B}_{\mu_k}\mathbf{B}_{\mu_k}^*,$$

where

$$\mathbf{A}_{\mu_k} = (\mathbf{A} - \overline{\mu_k}\mathbf{I})^{-1}(\mathbf{A} + \mu_k\mathbf{I}), \qquad \mathbf{B}_{\mu_k} = \sqrt{2|\mu_k|}(\mathbf{A} - \overline{\mu_k}\mathbf{I})^{-1}\mathbf{B},$$

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    and the *shifts* $\{\mu_k\} \subset \mathbb{C}^+$ are chosen to optimize convergence.
  - Generally one wants $\{-\mu_k\} \in \mathbb{C}^-$ to cover the spectrum of $\mathbf{A}$.
  - Extensive theoretical/practical work is devoted to finding best shifts.
  - Favorable approximation properties of the shifts must be balanced against the cost of computing $(\mathbf{A} - \overline{\mu_k}\mathbf{I})^{-1}$ for many different μ_k values.

Bounds on Decay of Singular Values of $\mathbf{X}$

Denote the singular values of $\mathbf{X}$ by

$$s_1 \geq s_2 \geq \cdots \geq s_n > 0.$$

- Let $\mathbf{X}_k$ be a rank-k approximation to $\mathbf{X}_k$ (e.g., from Galerkin or ADI).
- Any bound on $\|\mathbf{X} - \mathbf{X}_k\|$ becomes a bound on s_{k+1} by the Schmidt–Mirsky–Eckart–Young theorem:

$$s_{k+1} \;=\; \min_{\text{rank}(\widehat{\mathbf{X}}) \leq k} \|\mathbf{X} - \widehat{\mathbf{X}}\| \;\leq\; \|\mathbf{X} - \mathbf{X}_k\|.$$

- Similarly, s_{k+1} bounds the best performance attainable by any iterative method that constructs a rank-k approximation $\mathbf{X}_k$. (This is helpful for understanding if subspaces/shifts are near-optimal.)

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- ADI Error Analysis. The error $\mathbf{E}_k = \mathbf{X} - \mathbf{X}_k$ satisfies

$$\mathbf{E}_k = \phi_k(\mathbf{A})\,\mathbf{X}\,(\phi_k(\mathbf{A}))^*, \qquad \phi_k(z) := \prod_{j=1}^{k} \frac{z + \mu_k}{z - \overline{\mu_k}}.$$

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- Hence we can bound the decay of the singular values of $\mathbf{X}$:

$$\frac{s_{k+1}}{s_1} \leq \frac{\|\mathbf{E}_k\|}{\|\mathbf{X}\|} \leq \|\phi_k(\mathbf{A})\|^2.$$

Bounds on Decay of Singular Values of X

Since

$$\frac{s_{k+1}}{s_1} \leq \frac{\|\mathbf{E}_k\|}{\|\mathbf{X}\|} \leq \|\phi_k(\mathbf{A})\|^2, \qquad \text{with} \qquad \phi_k(z) := \prod_{j=1}^{k} \frac{z+\mu_k}{z-\overline{\mu_k}},$$

one obtains a bound on singular value decay by bounding $\|\phi_k(\mathbf{A})\|$.

- Eigenvalues and eigenvectors. For diagonalizable $\mathbf{A} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^{-1}$,

  $$\|\phi_k(\mathbf{A})\| \leq \|\mathbf{V}\|\,\|\mathbf{V}^{-1}\| \max_{z\in\sigma(\mathbf{A})} \prod_{j=1}^{k} \frac{|z+\mu_k|}{|z-\overline{\mu_k}|},$$

  giving the bound

  $$\boxed{\frac{s_{k+1}}{s_1} \leq \|\mathbf{V}\|^2\,\|\mathbf{V}^{-1}\|^2 \max_{z\in\sigma(\mathbf{A})} \prod_{j=1}^{k} \frac{|z+\mu_k|^2}{|z-\overline{\mu_k}|^2},}$$

  which can be optimized over the shifts $\{\mu_1,\ldots,\mu_k\} \subset \mathbf{C}^+$
  [Levenberg & Reichel 1993; Penzl 2000b; Sorensen & Zhou 2002].

Bounds on Decay of Singular Values of X

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- Numerical range. Suppose the field of values

  $$W(\mathbf{A}) = \{\mathbf{v}^*\mathbf{A}\mathbf{v} : \|\mathbf{v}\| = 1\}$$

  is contained in the open left-half plane. Crouzeix's Theorem gives

  $$\|\phi_k(\mathbf{A})\| \le C \max_{z\in W(\mathbf{A})} \prod_{j=1}^{k} \frac{|z+\mu_k|}{|z-\overline{\mu_k}|},$$

  with Crouzeix's constant $C \in [2, 11.08]$. Thus

  $$\boxed{\frac{s_{k+1}}{s_1} \le C^2 \max_{z\in W(\mathbf{A})} \prod_{j=1}^{k} \frac{|z+\mu_k|^2}{|z-\overline{\mu_k}|^2}.}$$

Bounds on Decay of Singular Values of X

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one obtains a bound on singular value decay by bounding $\|\phi_k(\mathbf{A})\|$.

- Pseudospectra. Suppose for some $\varepsilon > 0$ the ε-pseudospectrum

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

  is contained in the open left-half plane. Then

  $$\|\phi_k(\mathbf{A})\| \le \frac{L_\varepsilon}{2\pi\varepsilon} \max_{z\in\sigma_\varepsilon(\mathbf{A})} \prod_{j=1}^{k} \frac{|z+\mu_k|}{|z-\overline{\mu_k}|},$$

  where L_ε denotes the contour length of the boundary of $\sigma_\varepsilon(\mathbf{A})$. Thus

  $$\boxed{\frac{s_{k+1}}{s_1} \le \frac{L_\varepsilon^2}{4\pi^2\varepsilon^2} \max_{z\in\sigma_\varepsilon(\mathbf{A})} \prod_{j=1}^{k} \frac{|z+\mu_k|^2}{|z-\overline{\mu_k}|^2}}$$

  [Levenberg & Reichel 1993; Sabino 2006].

Nonnormality and Singular Values Decay Bounds

Consider this experiment:
Fix the spectrum $\sigma(\mathbf{A})$ but let *the departure of* $\mathbf{A}$ *from normality* increase.

- There are many essentially equivalent ways to measure departure from normality [Grone et al. 1987; Elsner & Paardekooper 1987].
- As the departure of $\mathbf{A}$ from normality increases, typically:
  - $\kappa(\mathbf{V})$ increases;
  - $W(\mathbf{A})$ gets larger;
  - $\sigma_\varepsilon(\mathbf{A})$ gets larger and/or $L_\varepsilon/(2\pi\varepsilon)$ increases.

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- All bounds described thus far predict slower decay of singular values of $\mathbf{X}$.

$$\frac{s_{k+1}}{s_1} \le \|\mathbf{V}\|^2 \, \|\mathbf{V}^{-1}\|^2 \max_{z\in\sigma(\mathbf{A})} \prod_{j=1}^{k} \frac{|z+\mu_k|^2}{|z-\overline{\mu_k}|^2}$$

$$\frac{s_{k+1}}{s_1} \le C^2 \max_{z\in W(\mathbf{A})} \prod_{j=1}^{k} \frac{|z+\mu_k|^2}{|z-\overline{\mu_k}|^2}$$

$$\frac{s_{k+1}}{s_1} \le \frac{L_\varepsilon^2}{4\pi^2\varepsilon^2} \max_{z\in\sigma_\varepsilon(\mathbf{A})} \prod_{j=1}^{k} \frac{|z+\mu_k|^2}{|z-\overline{\mu_k}|^2}$$

Nonnormality and Singular Values Decay Bounds

The same is true for bounds derived by entirely different methods.

- [Antoulas, Sorensen, Zhou, 2002] show (for $\text{rank}(\mathbf{B}) = 1$),

$$\frac{s_{k+1}}{s_1} \leq 2(n-k)^2 \|\mathbf{V}\|^2 \|\mathbf{V}^{-1}\|^2 \, \|\mathbf{A}\| \, \delta_{k+1},$$

  where

$$\delta_k = -\frac{1}{2\,\text{Re}\,\lambda_k} \prod_{j=1}^{k-1} \frac{|\lambda_k - \lambda_j|^2}{|\lambda_k + \overline{\lambda_j}|^2},$$

  with the eigenvalues $\lambda_1, \ldots, \lambda_n$ of $\mathbf{A}$ ordered to make $\delta_1 \geq \delta_2 \geq \cdots \geq \delta_n$.

- [Truhar & Veselić 2007] derive an alternative to this last bound that involves $\|\mathbf{V}\|^2 \|\widehat{\mathbf{b}}_j\|^2$, where $\widehat{\mathbf{b}}_j^*$ denotes the jth row of $\mathbf{V}^{-1}\mathbf{B}$.

- For the infinite dimensional case, [Grubisic & Kressner 2014] get a bound that involves $\|\mathbf{V}\|^2 \|\mathbf{V}^{-1}\|^2$, where $\mathbf{V}$ is the transformation that orthogonalizes a Riesz basis of eigenvectors.

- Error bounds for Galerkin projection typically involve some approximation problem on $W(\mathbf{A})$ that gets increasingly difficult as $W(A)$ gets larger; see, e.g., [Beckermann 2011; Druskin, Knizhnerman, Simoncini 2011].

An Example from Bifurcation Detection

An example from [Elman, Meerbergen, Spence, Wu, 2012; Elman, Wu, 2013]:

- 2d flow over an backward-facing step, viscosity $\nu = 1/400$, discretized using Q_2–Q_1 finite elements via IFISS [Elman, Silvester, Ramage].
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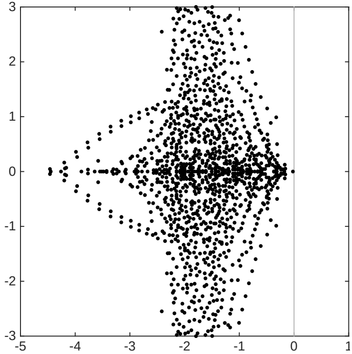

rightmost eigenvalues of **A**

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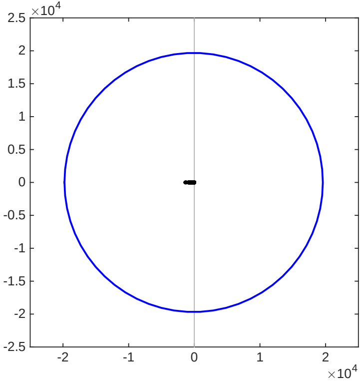

$W(\mathbf{A})$ and $\sigma(\mathbf{A})$

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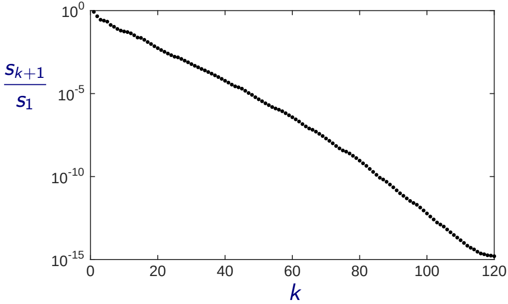
- The resulting matrix is *nondiagonalizable, and has a large numerical range, but the singular values still decay very rapidly.*



The Connection between $W(\mathbf{A})$ and $\frac{1}{2}(\mathbf{A}+\mathbf{A}^*)$

The *Hermitian part of* $\mathbf{A}$ is $\frac{1}{2}(\mathbf{A}+\mathbf{A}^*)$.

$$\begin{aligned} \text{eigenvalues of } \mathbf{A}: &\quad \lambda_1, \lambda_2, \ldots, \lambda_n \\ \text{eigenvalues of } \tfrac{1}{2}(\mathbf{A}+\mathbf{A}^*): &\quad \omega_n \le \omega_{n-1} \le \cdots \le \omega_1 \end{aligned}$$

Recall that the numerical range $W(\mathbf{A})$ is the set of all Rayleigh quotients:

$$W(\mathbf{A}) = \{\mathbf{v}^*\mathbf{A}\mathbf{v} : \|\mathbf{v}\| = 1\}.$$

Now if $z \in W(\mathbf{A})$, then

$$\operatorname{Re} z = \frac{z+z^*}{2} = \frac{\mathbf{v}^*\mathbf{A}\mathbf{v} + (\mathbf{v}^*\mathbf{A}^*\mathbf{v})^*}{2} = \mathbf{v}^*\Big(\frac{\mathbf{A}+\mathbf{A}^*}{2}\Big)\mathbf{v}.$$

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Hence the extreme eigenvalues of $\frac{1}{2}(\mathbf{A}+\mathbf{A}^*)$ *dictate the real extent of* $W(\mathbf{A})$*:*

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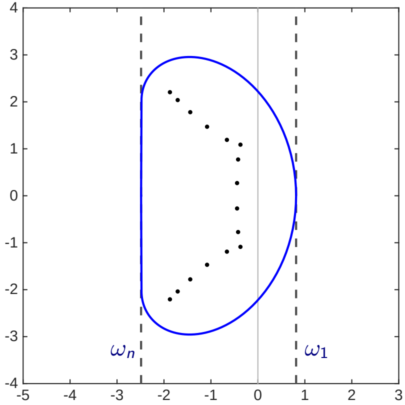

$W(\mathbf{A})$ computed with Higham's Test Matrix Toolbox

An Extreme Example Illuminates: No Decay

- What properties of **A** permit a solution **X** with no singular value decay?

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- No decay $\Longrightarrow$ $\mathbf{X}$ is a Hermitian matrix with $s_1 = \cdots = s_n$, i.e.,

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  for some real $\xi > 0$.
- Substituting this $\mathbf{X}$ into the Lyapunov equation $\mathbf{AX} + \mathbf{XA}^* = -\mathbf{BB}^*$,

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Worst case singular value decay $\iff$ $\mathrm{Re}\, W(\mathbf{A}) = [\omega_n, 0]$.

If $W(\mathbf{A})$ extends into the right-half plane, the singular values must decay.

Solvable Example: Jordan Block

An intriguing example from [Sabino 2006]:

$$\mathbf{A} = \begin{bmatrix} -1 & \alpha \\ 0 & -1 \end{bmatrix}, \qquad \mathbf{B} = \begin{bmatrix} t \\ 1 \end{bmatrix}.$$

Increasing α increases the distance of $\mathbf{A}$ from normality.

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The Lyapunov equation $\mathbf{AX} + \mathbf{XA}^* = -\mathbf{BB}^*$ has solution

$$\mathbf{X} = \frac{1}{4} \begin{bmatrix} 2t^2 + 2\alpha t + \alpha^2 & \alpha + 2t \\ \alpha + 2t & 2 \end{bmatrix}.$$

Maximizing over all $t \in \mathbb{R}$ gives the worst case singular value 'decay'

$$\frac{s_2}{s_1} = \frac{\operatorname{tr}(\mathbf{X}) - \sqrt{\operatorname{tr}(\mathbf{X})^2 - 4\det(\mathbf{X})}}{\operatorname{tr}(\mathbf{X}) + \sqrt{\operatorname{tr}(\mathbf{X})^2 - 4\det(\mathbf{X})}} = \begin{cases} \alpha^2/4, & 0 < \alpha \le 2; \\ 4/\alpha^2, & 2 \le \alpha. \end{cases}$$

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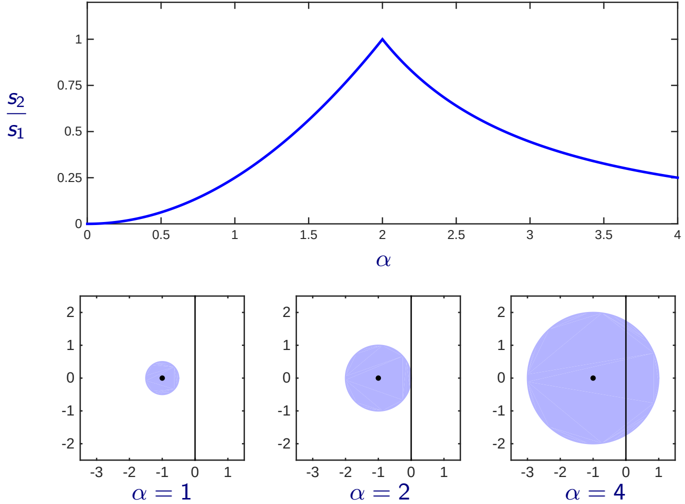

A More Nuanced Approach to Decay Bounds

We seek a different kind of decay bound that does a better job of handling matrices that are far from normal.

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If the singular values of **X** decay slowly, what must be true of **A**?

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&\leq \quad \max_{\|\mathbf{v}\|=1} \frac{\mathbf{v}^*(\mathbf{AE} + \mathbf{EA}^*)\mathbf{v}}{2} \\
&\leq \quad \tfrac{1}{2}\|\mathbf{AE} + \mathbf{EA}^*\|
\end{aligned}$$

A More Nuanced Approach to Decay Bounds, continued

In summary: for $\mathbf{X} = s_1(\mathbf{I} - \mathbf{E})$,

$$\begin{aligned}\omega_1 &\leq \tfrac{1}{2}\|\mathbf{AE} + \mathbf{EA}^*\| \\ &\leq \|\mathbf{A}\|\,\|\mathbf{E}\|.\end{aligned}$$

Thus we have bounded the relative size of the last singular value:

$$\boxed{\frac{s_n}{s_1} \leq 1 - \frac{\omega_1}{\|\mathbf{A}\|}.}$$

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In summary: for $\mathbf{X} = s_1(\mathbf{I} - \mathbf{E})$,

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Since $\mathbf{E} = \mathbf{E}^* = \mathbf{I} - \mathbf{X}/s_1$,

$$\text{eigenvalues of } \mathbf{E} \;=\; 1 - \frac{\text{eigenvalues of } \mathbf{X}}{s_1} \;=\; 1 - \frac{s_j}{s_1},$$

so

$$\|\mathbf{E}\| = 1 - \frac{s_n}{s_1}.$$

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A Family of Decay Bounds

We have only bounded s_n/s_1 here; more general bounds are possible.

Theorem. Suppose $\mathbf{A}$ is a stable matrix with $\mathbf{AX} + \mathbf{XA}^* = -\mathbf{BB}^*$.
Let $s_1 \ge s_2 \ge \cdots \ge s_n$ denote the singular values of of $\mathbf{X}$,
and $\omega_1 \ge \omega_2 \ge \cdots \ge \omega_n$ denote the eigenvalues of $\frac{1}{2}(\mathbf{A} + \mathbf{A}^*)$. Then

$$\boxed{\frac{s_k}{s_1} - 1 - \frac{\|\mathbf{B}\|^2}{2s_1\|\mathbf{A}\|} \;\le\; \frac{\omega_k}{\|\mathbf{A}\|} \;\le\; 1 - \frac{s_{n-k+1}}{s_1},}$$

which includes this bound on the trailing singular values,

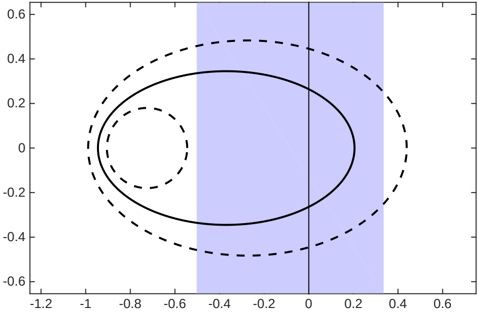
$$\boxed{\frac{s_{n-k+1}}{s_1} \;\le\; 1 - \frac{\omega_k}{\|\mathbf{A}\|},}$$

which gives *faster singular value decay as the departure of* $\mathbf{A}$ *from normality increases*. [Baker, E., Sabino, arXiv:1410.8741]

Possible and Impossible $W(\mathbf{A})$

Corollary.
$$-\frac{\|\mathbf{B}\|^2}{2s_1} \le \omega_1 \le \frac{s_1 - s_n}{s_1 + s_n}\|\mathbf{A}\|$$

Suppose that $\|\mathbf{A}\| = \|\mathbf{B}\| = s_1 = 1$ and $s_n = 1/2$.



Given this data, *the two dashed curves are not possible boundaries of $W(\mathbf{A})$*, while the solid curve could be the boundary of $W(\mathbf{A})$.

Summary

$$\boxed{\frac{s_{n-k+1}}{s_1} \le 1 - \frac{\omega_k}{\|\mathbf{A}\|}.}$$

- The bound *does not depend on* rank($\mathbf{B}$).
- The departure from normality (as reflected by $\omega_k > 0$) plays a very different role from the previously known bounds.
- The bound is not necessarily sharp. Take $\alpha \to \infty$ in the Jordan example:

  $$\|\mathbf{A}\| \sim \alpha, \qquad \omega_1(\mathbf{A}) = \frac{\alpha}{2} - 1,$$

  so

  $$\frac{s_n}{s_1} \to 0 \qquad \text{while} \qquad 1 - \frac{\omega_1}{\|\mathbf{A}\|} \sim \frac{1}{2}.$$

- There is more to understand about the solutions to Lyapunov (and Sylvester) equations with coefficients that are far from normal.
- The eigenvalues of $\frac{1}{2}(\mathbf{A} + \mathbf{A}^*)$ reveal a great deal! Cf. [Carden, E. 2012].