An introduction to pseudospectra and application to validated computational dynamics

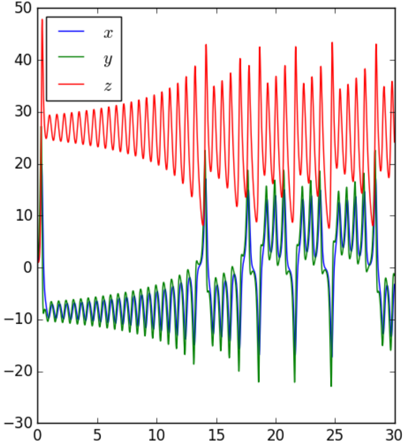
April Herwig

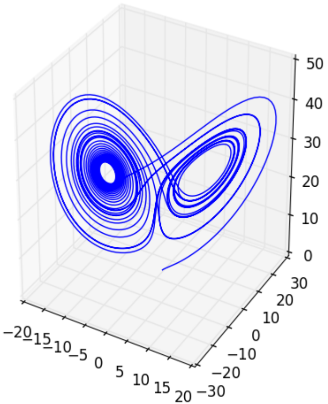
Department of Mathematics
Technical University of Munich

Contents

- Dynamical systems
- Definition (and equivalent formulations) of the ϵ-pseudospectrum $\sigma_\epsilon(M)$
- Theoretical results to gain some intuition
  - Geometry of $\sigma_\epsilon(M)$
  - Almost-invariant sets can be obtained from pseudoeigenvalues
- A note on backward-stability
- How to compute the pseudospectrum
  - General inner approximation
  - Specific methods for Perron-Frobenius / Koopman

Dynamical systems





Dynamical systems

- Discrete dynamical system generated by iteration of a continuous map $S : X \to X$
- Observables $\psi : X \to \mathbb{C}$ can be used to measure statistical behavior
- Evolution of observables is dictated by the operators

$$\begin{array}{cc} \text{Koopman} & \text{Perron-Frobenius} \\ K : L^2 \to L^2 & P : \mathcal{M} \to \mathcal{M} \\ f \mapsto f \circ S & \mu \mapsto \mu \circ S^{-1} \end{array}$$

- The spectrum of these operators describe macroscopic asymptotic statistics of the system

Petrov-Galerkin discretization of linear operators

- Given: bounded linear operator on a Banach space $M : \mathcal{X} \to \mathcal{X}$
- Approximation space $U = \{\varphi_i\}_{i=1}^n \subset \mathcal{X}$
- Trial space $V = \{\psi_j\}_{j=1}^m \subset \mathcal{X}^*$
- Representation matrix $A_{i,j} = \psi_j(M\varphi_i)$
- Examples:
  - EDMD: $U =$ Fourier / radial basis functions, $V =$ point evaluation functionals
  - Ulam's method: $U = V =$ characteristic functions
  - ...
- We now wish to compute eigenpairs of A

How 'well' does the spectrum of A reproduce the spectrum of M?

Pseudospectra

Definition 1. *[Trefethen, Landau, Varah, Godunov, Hinrichsen & Pritchard] The pseudospectrum of a closed linear operator $M : \mathcal{X} \to \mathcal{X}$ over a Banach space $\mathcal{X}$ is the set*

$$\sigma_\epsilon(M) = \bigcup_{\|E\|_{op} \leq \epsilon} \sigma(M + E) \tag{1}$$

228 L.N. Trefethen

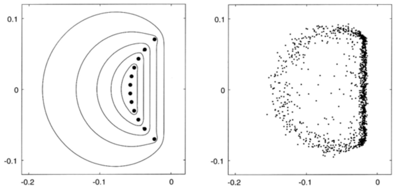


Fig. 2.2. Pseudospectra of a 12×12 Legendre spectral differentiation matrix. The left side shows the eigenvalues (solid dots) and the boundaries of the 2-norm ϵ-pseudospectra for $\epsilon = 10^{-3}, 10^{-4}, \ldots, 10^{-7}$ (from outer to inner). The right side shows 1200 of the 10^{-3}-pseudo-eigenvalues of A—specifically, a superposition of the eigenvalues of 100 randomly perturbed matrices $A + E$, where each E is a matrix with independent normally distributed complex entries of mean 0 scaled so that $\|E\| = 10^{-3}$. If all possible perturbations with $\|E\| = 10^{-3}$ were considered instead of just 100 of them, the dots on the right would exactly fill the outermost curve on the left.

Pseudospectra

Theorem 1. *[Trefethen] The following formulations are equivalent:*

(i)

$$\sigma_\epsilon(M) = \bigcup_{\|E\|_{op} \leq \epsilon} \sigma(M + E)\,, \tag{2}$$

(ii)

$$\sigma_\epsilon(M) = \left\{ z \in \mathbb{C} \mid \|(M - z)^{-1}\|_{op} \geq 1/\epsilon \right\}, \tag{3}$$

(iii)

$$\sigma_\epsilon(M) = \left\{ z \in \mathbb{C} \mid \inf_{\|v\|=1} \|(M - z)v\| \leq \epsilon \right\}, \tag{4}$$

(iv) *If* $\dim(\mathcal{X}) < \infty$ *is an inner product space,*

$$\sigma_\epsilon(M) = \{ z \in \mathbb{C} \mid s_{min} \leq \epsilon \}\,. \tag{5}$$

Theoretical results

Geometry of pseudospectra

Theorem 2. *[Trefethen]*

(i) *If M is normal, $\sigma_\epsilon(M) = \sigma(M) + B_\epsilon$ are ϵ-balls around the spectrum.*

(ii) $\bigcap_{\epsilon>0} \sigma_\epsilon(M) = \sigma(M)$ *and conversely* $\sigma_{\epsilon+\delta}(M) \supset \sigma_\epsilon + B_\delta$

Theoretical results

Almost invariant sets

Theorem 3. *[Dellnitz, Junge]*

From now on we assume that $\lambda \neq 1$ is an eigenvalue of P_ε with corresponding real valued eigenmeasure $\nu \in \mathcal{M}_{\mathbb{C}}$, that is,

$$P_\varepsilon \nu = \lambda \nu.$$

PROPOSITION 5.7 *Suppose that ν is scaled so that $|\nu| \in \mathcal{M}$, and let $A \subset X$ be a set with $\nu(A) = \frac{1}{2}$. Then*

$$\delta + \sigma = \lambda + 1, \tag{5.3}$$

if A is δ-almost invariant and $X - A$ is σ-almost invariant with respect to $|\nu|$.

Theorem 4. *Suppose ν is an ϵ-pseudoeigenmeasure for the ϵ-pseudoeigenvalue $0 < \lambda < 1$ of a Perron-Frobenius operator P. Suppose further that ν is scaled so $|\nu| \in \mathcal{M}$ and A is a set with $\nu(A) = 1/2$. Then*

$$\delta + \sigma = \lambda + 1 + const \cdot \epsilon \tag{6}$$

if A is δ-almost invariant and $X - A$ is σ-almost invariant with respect to $|\nu|$.

A note on backward-stability

Theorem 5. *Let (X, d) be a metric space with Borel measure. Let $S, \hat{S} : X \to X$ be two continuous functions with*

$$d^{\infty}_{ess}(S, \hat{S}) = \operatorname*{ess\,sup}_{x} \; d(\, S(x), \, \hat{S}(x) \,) > 0 \tag{7}$$

Then the induced Perron-Frobenius (pushforward) operators $P_S, P_{\hat{S}} : \mathcal{M} \to \mathcal{M}$ satisfy

$$\|P_S - P_{\hat{S}}\|_{op} \geq 2. \tag{8}$$

This remains true (under adjustment of the const 2) if $P_S, P_{\hat{S}}$ are induced by (sufficiently) small random perturbations in the sense of [Kifer].

Note that this does not contradict the continuous dependence of eigenvalues of P_S.

How to compute the pseudospectrum

General inner approximation

Lemma 1. *Let $M : \mathcal{X} \to \mathcal{X}$ be a closed linear operator, $(\Pi_d)_d$ be a collection of projections which converge pointwise to the identity* [1]*. Let*

$$(\lambda, x) \text{ be an } \epsilon\text{-pseudoeigenpair for } \Pi_d \, M \, \Pi_d. \tag{9}$$

Then for every δ there exists a $D = D(\delta, x)$ such that $\lambda \in \sigma_{\epsilon+\delta}(M)$ for all $d > D$.

Note that this does not necessarily imply that $\sigma_\epsilon(V_d M V_d) \nearrow \sigma_\epsilon(M)$ as $d \to \infty$.

[1] $V_d x \xrightarrow{d\to\infty} x \quad \forall x$

How to compute the pseudospectrum

EDMD [Williams, Kevrekidis, Rowley]

- Given:
  - quadrature scheme: weights $(w^i)_{i=1}^m$, nodes $(x^i)_{i=1}^m$
  - dictionary $(\psi_j)_{j=1}^N$ of L^2 observables, $span\{\psi_j\}_{j=1}^N \xrightarrow{N\to\infty} L^2$
- Data matrices:

$$\Psi_X = \Psi.(\mathbf{x}) = \begin{pmatrix} \psi_1(x^1) & \cdots & \psi_N(x^1) \\ \vdots & & \vdots \\ \psi_1(x^m) & \cdots & \psi_N(x^m) \end{pmatrix} \tag{10}$$

$$\tag{11}$$

$$\Psi_Y = (\Psi . \circ S).(\mathbf{x}) \tag{12}$$

How to compute the pseudospectrum

ResDMD [Colbrook, Townsend]

$$\begin{array}{ccccc} \text{Graham matrix} & & \text{EDMD matrix} & & \text{ResDMD matrix} \\ G = \Psi_X' W \Psi_X & & A = \Psi_X' W \Psi_Y & & L = \Psi_Y' W \Psi_Y \\ \downarrow & {\scriptstyle m\to\infty} & \downarrow & {\scriptstyle m\to\infty} & \downarrow \\ \langle \psi_i,\ \psi_j \rangle_{i,j} & & \langle \psi_i,\ K\psi_j \rangle_{i,j} & & \langle K\psi_i,\ K\psi_j \rangle_{i,j} \end{array} \tag{13}$$

Now

$$\inf_{\|v\|_{L^2}=1} \|(K-\lambda)v\|^2 = \inf_{\|v\|_{L^2}=1} \langle Kv,\ Kv\rangle - \bar{\lambda}\,\langle v,\ Kv\rangle - \lambda\langle Kv,\ v\rangle + |\lambda|^2\langle v,\ v\rangle \tag{14}$$

$$= \lim_{N\to\infty} \lim_{m\to\infty} \inf_{\mathbf{v}' G \mathbf{v}=1} v'(\,L - \bar{\lambda}\,A - \lambda\,A' + |\lambda|^2\,G\,)v \tag{15}$$

How to compute the pseudospectrum

Residual Ulam

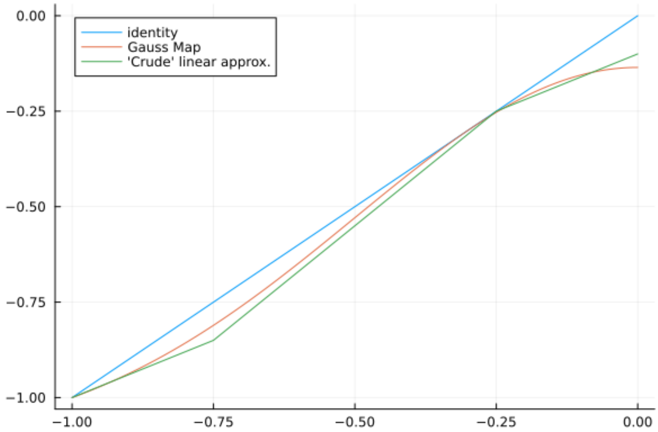
Theorem 6. *Let* $S : X \to X$ *be an a.e. diffeomorphism onto its image,* $P = P_S$ *the induced transfer operator. Consider a sequence of box partitions* $\mathcal{P} = \{A_1, \ldots, A_N\}$ *of the phase space* X *with* $\operatorname{diam}(\mathcal{P}) \to 0$*. Then*

$$\inf_{\|v\|_{L^2}=1} \|(P-\lambda)v\|^2 = \lim_{N\to\infty} \inf_{\mathbf{v}'G\mathbf{v}=1} v'(\,L - \bar{\lambda}\,A - \lambda\,A' + |\lambda|^2\,G\,)v \tag{16}$$

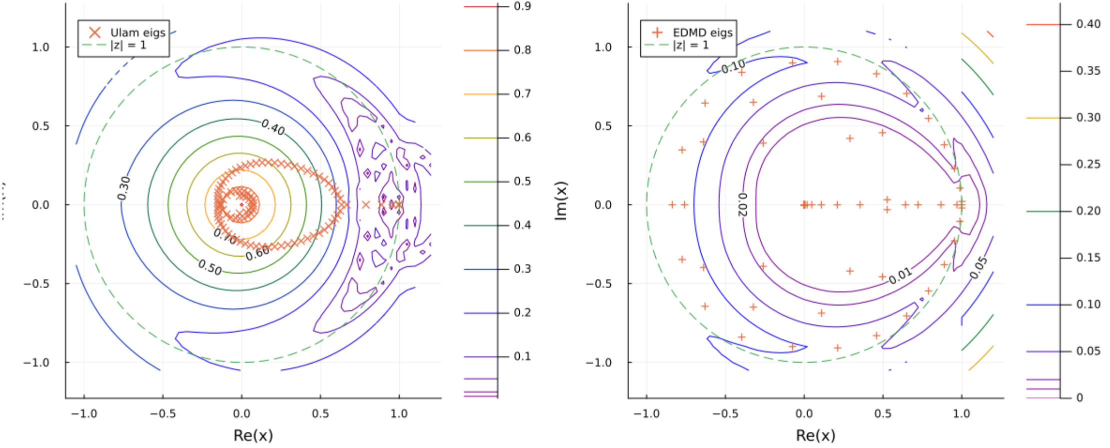
where

$$L_{i,j} = \int_{A_i \cap A_j} \frac{dx}{|\det DS(x)|}\,, \quad A_{i,j} = \underbrace{m(A_i \cap S^{-1}(A_j))}_{\textit{(scaled) Ulam matrix}}\,, \quad G_{i,j} = m(A_i \cap A_j). \tag{17}$$

Numerical results



Numerical results



Numerical results