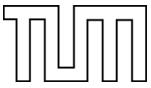

Technische Universität München

School of Computation, Information and Technology

Master's Thesis

Resolvent-based Methods for Robust Spectral Analysis in Dynamical Systems

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I assure the single handed composition of this master's thesis only supported by declared resources.

Garching,

Abstract

Koopmania

Contents

1 Introduction

Dynamical systems theory has seen many revolutions. One recent such revolution is to use operator theoretic tools to analyze the global behavior of chaotic systems. Concieved in the 1930's by Koopman and Von Neumann [11], the study of global dynamics under a mapping S is conducted by studying the action of the composition $\psi \circ S$ of S with an observable ψ. Observables which act as eigenvalues for the composition operator and its dual hold information on slowly decaying structures in phase space.

Currently the most popular method by far for analyzing composition operators (named Koopman operators) is dynamic mode decomposition (DMD). The past 2 decades have seen massive growth in this topic, and DMD has recieved many evolutions [5]. One primary concern of nearly all DMD methods is *spectral pollution*. The Koopman operator often has unfavorable spectral qualities such as continuous spectrum which are unstable, and are destroyed by finite approximation. The task presented in the present paper is to identify which candidate eigenvalues (computed e.g. by DMD) are approximations of eigenvalues of the true Koopman operator (or its adjoint), and which arise due to discretization.

2 Background

We consider a discrete dynamical system generated by a map $S : \Omega \to \Omega$ defined on a measure space $(\Omega, \mathcal{A}, dx)$ which is *nonsingular*, that is $\int_{S^{-1}(A)} dx = 0$ for any $A \in \mathcal{A}$ with $\int_A dx = 0$.

2.1 Koopman and Perron-Frobenius Operators

Koopman operator theory shifts the focus from dynamics of points in state space $\mathcal{X}$ to dynamics of observables $g : \Omega \to \mathbb{C}$. A state $x \in \Omega$ evolves by iteratively applying the map S, and similarly observables evolve under the action of the *Koopman operator*

$$\mathcal{K}g = g \circ S. \tag{2.1}$$

The primary benefit of this alternative viewpoint of dynamics is that $\mathcal{K}$ is *linear* and can therefore be analyzed using algebraic and functional analytic tools. However, the Koopman operator acts on function spaces which are typically infinite-dimensional. Even the Krylov space $\{g, \mathcal{K}g, \mathcal{K}^2 g, \ldots\}$ is generically infinite-dimensional: consider e.g. an indicator function $g = \mathbb{1}_{[0,1]}$ and a translation $S(x) = x - 1$.

It should be noted that until now we have not declared a function space to act as a domain for $\mathcal{K}$. This is because there are many potential domains for which $\mathcal{K}$ is not only well-defined, but has interesting properties worth studying. For the current section we consider $\mathcal{K} : L^\infty \to L^\infty$. On this space $\mathcal{K}$ is obviously bounded, in fact it is a contraction. However, that need not be the case for other spaces. Depending one the function space and in S, $\mathcal{K}$ may not even be bounded.

The Koopman operator tracks how observables evolve with S. There is however a dual viewpoint: that of *densities* and *pushforwards*. From the duality pairing

$$\langle f,\ \mathcal{K}g\rangle = \langle \mathcal{L}f,\ g\rangle \tag{2.2}$$

for $f \in L^1,\ g \in L^\infty$ we may deduce the form of an adjoint operator, known as the *transfer operator* or *Perron-Frobenius operator*. Consider an indicator $g = \mathbb{1}_A$ for an $A \in \mathcal{A}$ and let $f \geq 0$. The left hand side of 2.2 is

$$\int f(x)\, \mathbb{1}_A(S(x))\ dx = \int f(x)\, \mathbb{1}_{S^{-1}(A)}(x)\ dx = \int_{S^{-1}(A)} f(x)\ dx, \tag{2.3}$$

and the right hand side

$$\int \mathcal{L}f(x)\, \mathbb{1}_A(x)\ dx = \int_A \mathcal{L}f(x)\ dx. \tag{2.4}$$

Hence $\mathcal{L}f \in L^1$ should satisfy the equation

$$\int_A \mathcal{L}f(x)\ dx = \int_{S^{-1}(A)} f(x)\ dx. \tag{2.5}$$

A short exercise in measure theory shows that

$$A \mapsto \int_{S^{-1}(A)} f(x)\ dx \tag{2.6}$$

defines a finite absolutely continuous measure, and hence by the Radon-Nikodym theorem the measure has a unique density which by 2.5 is precisely $\mathcal{L}f$. For general $f \in L^1$ decompose $f = f^+ - f^-$ with $f^+, f^- \geq 0$ and set $\mathcal{L}f = \mathcal{L}f^+ - \mathcal{L}f^-$.

2.6 shows that $\mathcal{L}$ is precisely the action of the pushforward $S_\sharp\mu = \mu \circ S^{-1}$ for densities. This provides a useful intuition for the transfer operator: we move away from the viewpoint of single points $x \in \Omega$, and instead consider

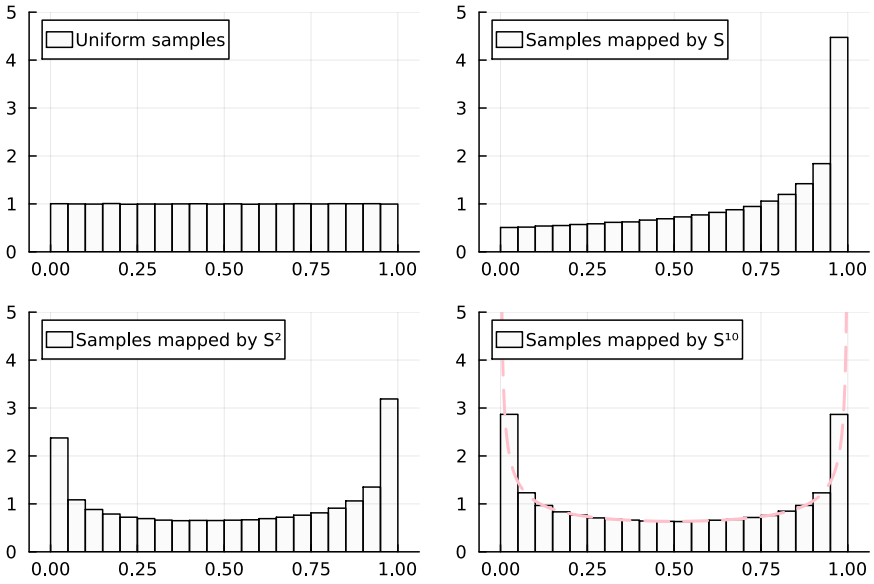

Figure 2.1: Illustration of the pushforward intuition of the Perron-Frobenius operator. Action of the $\mathcal{L}$ associated with the quadratic map $S : [0,1] \circlearrowleft$, $x \mapsto 4x(1-x)$. One million points are sampled uniformly in $[0,1]$ and mapped forward under S, S^2, and S^{10}. The respective distributions are shown in histograms.

distributions of point density. If x is chosen from a random distribution with density f, then the distribution of $S(x)$ has density $\mathcal{L}f$.

When S is a diffeomorphism, $\mathcal{L}$ has an explicit form.

Theorem 2.1. *Let S be a diffeomorphism. Then*

$$\mathcal{L}f = \frac{f \circ S^{-1}}{|\det D\, S^{-1}|} \tag{2.7}$$

In particular one sees that when S is a measure algebra isomorphism (that is, S and S^{-1} both preserve the measure) then the Koopman operator is unitary, i.e. $\mathcal{K}^*(= \mathcal{L}) = \mathcal{K}^{-1}$.

Proof. This follows from a change of variables $y = S(x)$

$$\int g \cdot \mathcal{L}f \, dx = \int \mathcal{K} \cdot f \, dx = \int f(y) \cdot g \circ S^{-1}(y) \left|\det D\, S(S^{-1}(y))\right| \, dy. \tag{2.8}$$

□

Corollary 2.2. *Assume S is a piecewise diffeomorphism, i.e. there exists a disjoint decomposition $\Omega = \biguplus_{l=1}^{n} U_l$ such that for each l, $S_l := S|_{U_l} : U_l \to V_l$*

is a diffeomorphism. Then

$$(\mathcal{L}f)(x) = \sum_{l=1}^{n} \frac{f \circ S_l^{-1}(x)}{\left|\det D\, S_l^{-1}(x)\right|} \mathbb{1}_{V_l}(x). \tag{2.9}$$

2.2 Spectral Properties

2.2.1 The Spectrum

We begin with abstract definitions for parts of the spectrum.

Definition 2.3. *Let $M : D(M) \to \mathcal{X}$ be a linear operator on a Banach space $(X, \|\cdot\|)$. The domain $D(M) \subset \mathcal{X}$ of M may be a dense subset of $\mathcal{X}$. M is called* closed *if: whenever $x_k \to x$ is a convergent sequence with Mx_k convergent, then $Mx_k \to Mx$.*

Closedness is weaker than continuity due to the extra assumption that Mx_k is convergent.

Definition 2.4. *The* spectrum *$\sigma(M)$ of a closed operator M is the set of numbers $\lambda \in \mathbb{C}$ for which $M - \lambda I$ does not have a bounded inverse. The complement $\rho(M) := \mathbb{C} \setminus \sigma(M)$ is called* resolvent set *and $(M - \lambda I)^{-1}$ is called the* resolvent*.*

Proposition 2.5. *The spectrum admits a disjoint decomposition*

$$\sigma(M) = \sigma_p(M) \uplus \sigma_c(M) \uplus \sigma_r(M) \tag{2.10}$$

into point-, continuous-, *and* residual-spectrum *with*

$$\sigma_p(M) = \{\lambda \in \mathbb{C} \mid M - \lambda I \text{ is not injective}\}, \tag{2.11}$$

$$\sigma_c(M) = \{\lambda \in \mathbb{C} \mid M - \lambda I \text{ is injective, but its range is a dense subset of } \mathcal{X}\}, \tag{2.12}$$

$$\sigma_r(M) = \{\lambda \in \mathbb{C} \mid M - \lambda I \text{ is injective, but does not have dense range}\}. \tag{2.13}$$

Remark. In some literature, 0 is never part of the spectrum. We do not take this approach.

An element $\lambda \in \sigma_p(M)$ is a *true* eigenvalue in the sense that there exists a vector $x \in \mathcal{X}$ such that $(M - \lambda I)x = 0$. The continuous spectrum has a similar characterization as the set of $\lambda \in \mathbb{C}$ for which $M_\lambda I$ is injective but *not* bounded from below, i.e. there exists a sequence $(x_k)_k$, $\|x_k\| = 1$, for which $(M - \lambda I)x_k \to 0$. Equivalently, $(M - \lambda I)^{-1}$ cannot be extended to a bounded linear operator, but is still a (densely defined) closed linear operator. (See the proof of theorem 2.18 for a proof of this characterization.)

One might ask why such detail is required in defining the spectrum. The answer lies in the subtle consequences of infinite-dimensionality. The following example from [9] shows the subtle interplay between residual spectrum and spectrum of the adjoint operator, all of which requires infinite-dimensionality.

Example 2.6 (Shift operators on $\ell^2(\mathbb{N})$). The canonical right-shift operator

$$R : (a_1, a_2, \ldots) \mapsto (0, a_1, a_2, \ldots) \tag{2.14}$$

is adjoint to the left shift

$$L : (a_1, a_2, \ldots) \mapsto (a_2, a_3, \ldots). \tag{2.15}$$

We claim:

$$\sigma_p(L) = \{\lambda \in \mathbb{C} \mid |\lambda| < 1\} \qquad \sigma_p(R) = \emptyset \tag{2.16}$$
$$\sigma_c(L) = \{\lambda \in \mathbb{C} \mid |\lambda| = 1\} \qquad \sigma_c(R) = \{\lambda \in \mathbb{C} \mid |\lambda| = 1\} \tag{2.17}$$
$$\sigma_r(L) = \emptyset \qquad \sigma_r(R) = \{\lambda \in \mathbb{C} \mid |\lambda| < 1\}. \tag{2.18}$$

Indeed, to see 2.16 consider $|\lambda| < 1$, $a^\lambda = (\lambda, \lambda^2, \ldots)$. Then clearly $La^\lambda = \lambda a^\lambda$. On the other hand, suppose $Ra = \lambda a$ for some $a \neq 0$, $\lambda \in \mathbb{C}$. Then letting n be the first index such that $a_n \neq 0$, we must have $0 = a_{n-1} = (Ra)_n = \lambda a_n$ so $\lambda = 0$. But the kernel of R is clearly $\{0\}$.

To see 2.17, take $|\lambda| = 1$ and construct *approximate* (L, λ)-eigenvectors $v^n = (\lambda, \lambda^2, \ldots, \lambda^n, 0, \ldots)$. Then $(L - \lambda I)v^n = (0, \ldots, 0, \lambda^{n+1}, 0, \ldots)$ so $\|(L - \lambda I)v^n\| = 1$ but $\|v^n\| = \sqrt{n}$. It remains to show that λ is of continuous spectrum, as opposed to residual spectrum. Indeed, for any w such that for all $v \in \ell^2$, $0 = \langle (L - \lambda I)v, w\rangle = \langle v, (R - \bar{\lambda} I)w\rangle$ so that w is an eigenvector of R which by 2.16 is a contradiction. An entirely analogous argument shows that the circle is also continuous spectrum for R.

We now reverse the discussion to see that any $|\lambda| < 1$ is in the residual spectrum of R. For $v \in \ell^2$ and w a $\bar{\lambda}$-eigenvector of L we have $0 = \langle v, 0\rangle = \langle v, (L - \bar{\lambda} I)w\rangle = \langle (R - \lambda I)v, w\rangle$ so that the range of $R - \lambda I$ is orthogonal to w.

Finally, $\sigma(M)$ is bounded by $\|M\|$ for any operator M, and clearly $\|L\| = 1$. But $\sigma_p(L) \cup \sigma_c(L) = \{\lambda \in \mathbb{C} \mid |\lambda| \leq 1\}$ so $\sigma_r(L) = \emptyset$. Combined with the previous paragraph, this shows 2.18.

The example already suggests some important relationships regarding the spectrum of adjoint operators.

Theorem 2.7. *Let M be a densely defined closed linear operator on a Hilbert space.*

1. *$\lambda \in \sigma(M)$ iff $\bar{\lambda} \in \sigma(M^*)$.*
2. *If $\lambda \in \sigma_r(M)$, then $\bar{\lambda} \in \sigma_p(M^*)$.*
3. *Conversely, if $\lambda \in \sigma_p(M)$, then $\bar{\lambda} \in \sigma_p(M^*) \cup \sigma_r(M^*)$.*
4. *$\sigma_c(M) = \sigma_c(M^*)$.*

Proof.
1. Suppose $M - \lambda I$ has a bounded inverse B. Then $(M - \lambda I)B = B(M - \lambda I) = I$. Equivalently $B^*(M^* - \bar{\lambda} I) = (M^* - \bar{\lambda} I)B^* = I^* = I$.
2. The range of $M - \lambda I$ is not dense in $\mathcal{X}$. Hence there exists a $v \perp \mathrm{ran}(M - \lambda I)$. But this implies $v \in \ker(M^* - \bar{\lambda} I)$.
3. There exists a $v \in \ker(M - \lambda I)$ which implies $v \perp \mathrm{ran}(M^* - \bar{\lambda} I)$.
4. This follows from 1, 2, and 3.

□

2.2.2 Spectra of Koopman and Perron-Frobenius Operators

The Koopman and Perron-Frobenius operator spectrum holds information about the long-term mixing rates of structures in phase space. We write (with some abuse of notation) $\mathcal{L}|_{\mathcal{X}}$ and $\mathcal{K}|_{\mathcal{X}}$ to denote the Perron-Frobenius / Koopman operators acting on the domain $\mathcal{X}$.

Definition 2.8. *An eigenfunction f for $\mathcal{L}|_{L^1}$ with eigenvalue 1 is the density of a* (signed) invariant measure. *We say S* preserves the measure $f\,dx$.

The following are well-known facts about the Koopman and Perron-Frobenius operator. They can be found in many sources e.g. [13].

Theorem 2.9.
1. *If S is ergodic*[1]*, then there is at most one invariant density. Conversely, if there is a unique invariant density which is $(dx-)$almost everywhere positive, then S is ergodic.*
2. *If S is ergodic, then every eigenvalue of $\mathcal{K}|_{L^1}$ is simple.*
3. *Suppose S is invertible. Then S is weak-mixing iff 1 is the only eigenvalue of $\mathcal{K}|_{L^1}$.*

The following theorem is from [8].

[1] Ergodicity and mixing describe how obeservations become decorrelated over time. S is *ergodic* if for all $A, B \in \mathcal{A}$ we have $\frac{1}{n}\sum_{j=0}^{n-1} \int_{S^{-j}(A)\cap B} dx \to \int_A dx \int_B dx$ as $n \to \infty$. S is weak-mixing if we have $\frac{1}{n}\sum_{j=0}^{n-1} \left| \int_{S^{-j}(A)\cap B} dx - \int_A dx \int_B dx \right| \to 0$ as $n \to \infty$.

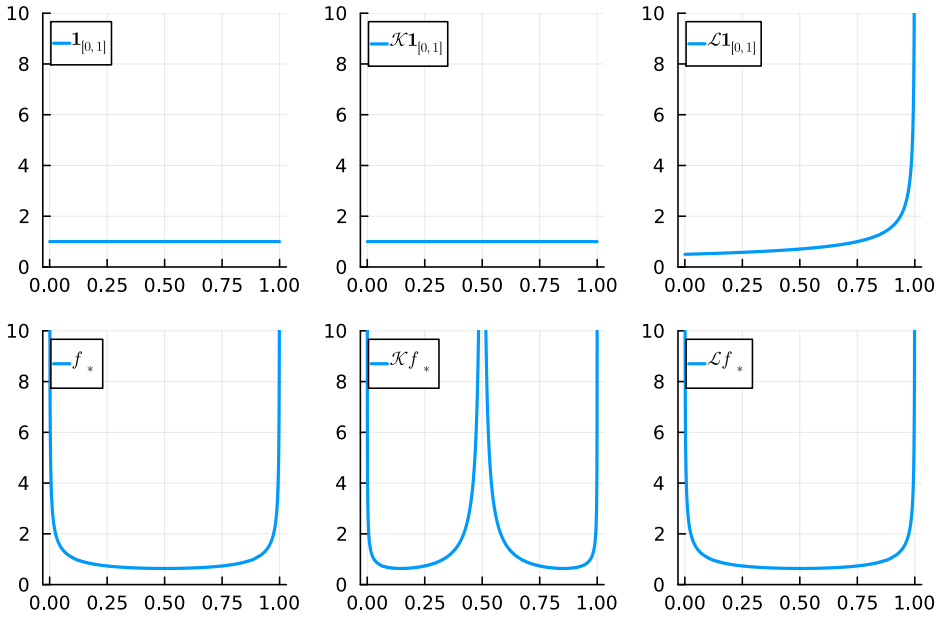

Figure 2.2: Actions of the Koopman and Perron-Frobenius operators associated with the quadratic map $S : [0,1] \circlearrowleft,\ x \mapsto 4x(1-x)$. The constant density $\mathbb{1}_{[0,1]}$ is fixed under $\mathcal{K}$ and the density $f_*(x) = \frac{1}{\pi\sqrt{x(1-x)}}$ is fixed under $\mathcal{L}$ (c.f. figure 2.1).

Definition 2.10. *A set $A \subset \Omega$ in phase space is called* δ-almost-invariant *if*

$$\int_{S^{-1}(A)\cap A} dx = (1-\delta) \cdot \int_A dx. \tag{2.19}$$

Theorem 2.11. *Let $\mathbb{R} \ni \lambda < 1$ be an eigenvalue corresponding to a real-valued normalized eigenfunction f of $\mathcal{L}|_{L^1}$. Let further $A \subset \Omega$ be such that $\int_A f\, dx = \frac{1}{2}$. Then*

$$\delta + \eta = \lambda + 1 \tag{2.20}$$

if A is δ-almost-invariant and $\Omega \setminus A$ is η-almost-invariant.

These are only a few interesting properties of the spectrum of these operators, but there are many more which can be studied.

2.3 Pseudospectra

The reader will have likely noticed the sensitivity required in understanding the spectrum for infinite-dimensional operators. In particular the spectral types can be unstable w.r.t. perturbations of the operator. For example, for any self-adjoint operator M (e.g. the generator for the Koopman semigroup in a

continuous-time dynamical system) there exists a compact operator E with arbitrarily small norm such that the perturbation $M + E$ has purely point spectrum.

The situation is even worse when one considers *perturbations of the dynamics* instead of perturbations of the Koopman / Perron-Frobenius operators. Consider a circle rotation $S : \mathbb{T} \to \mathbb{T}$, $e^{2\pi i\theta} \mapsto e^{2\pi i(\theta+\alpha)}$. We have $\sigma(\mathcal{L}|_{L^2}) = \sigma_p(\mathcal{L}|_{L^2}) = \alpha^{\mathbb{N}_0}$. If the rotation is rational then the spectrum is discrete, but if the rotation is irrational then the spectrum is dense in the unit circle.

In the present paper we tackle the instability problem for operator perturbations. One might wonder whether operators which are "close" (in some sense) also have spectra which are "close". Unfortunately, this is in general not true. Even in finite dimensions this breaks down, as the following example shows.

Example 2.12 ([18]). Let $\mathcal{X} = \mathbb{R}^n$ and let

$$M = \begin{bmatrix} 0 & 1 & & \\ & \ddots & \ddots & \\ & & & 1 \\ & & & 0 \end{bmatrix}. \tag{2.21}$$

M is nilpotent so $\sigma(M) = \{0\}$. However, for an arbitrarily small $\epsilon > 0$, the perturbation

$$M + E = \begin{bmatrix} 0 & 1 & & \\ & \ddots & \ddots & \\ & & & 1 \\ \epsilon & & & 0 \end{bmatrix}. \tag{2.22}$$

has characteristic polynomial $(-\lambda)^n - (-1)^n\epsilon$ so that $\sigma(M+E) = \{\lambda \in \mathbb{C} \mid \lambda^n = \epsilon\}$. For growing n, $\sigma(M + E)$ comes asymptotically close to filling the unit circle.

2.3.1 Definitions of the Pseudospectrum

Definition 2.13. *Let $M : D(M) \to \mathcal{X}$ be a closed linear operator. The* ϵ-pseudospectrum *of M is the smallest set in $\mathbb{C}$ which contains the spectrum of all perturbations of M with norm less than ϵ:*[2]

$$\sigma_\epsilon(M) = \bigcup_{\|E\|<\epsilon} \sigma(M + E). \tag{2.23}$$

Theorem 2.14. *We have the following equivalent formulation of the pseudospectrum:*

$$\sigma_\epsilon(M) = \left\{\lambda \in \mathbb{C} \mid \|(M - \lambda I)^{-1}\| > \frac{1}{\epsilon}\right\} \tag{2.24}$$

[2]Some authors will deine the pseudospectrum with "$\leq$" instead of "$<$". This makes $\sigma_\epsilon(M)$ a closed set, but breaks theorem 2.14.

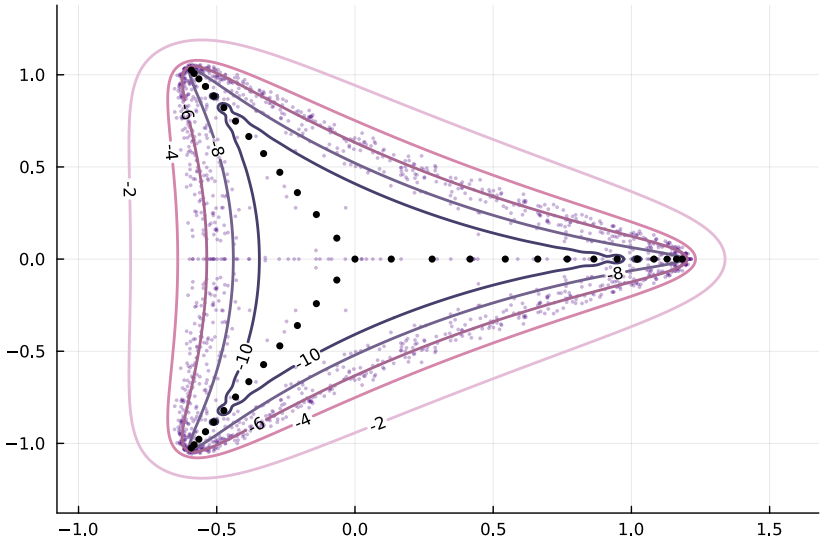

Figure 2.3: Pseudospectra for the 40×40 Toeplitz matrix T with 0 on the main diagonal, 1 on the first upper off-diagonal, and 1/4 on the second lower off-diagonal. Contour lines show the boundary of the ϵ-pseudospectrum for $\epsilon = 10^{-2}, 10^{-4}, 10^{-6}, 10^{-8}, 10^{-10}$. Black: Spectrum of T. Purple: Spectra of $T + E$ for 40 randomly sampled perturbations E with $\|E\| < 10^{-4}$.

where we use the convention that $\|(M-\lambda I)^{-1}\| = \infty$ *if* $M-\lambda I$ *is not invertible.*

Remark. While this result is practically pseudospectrum folklore, a correct proof in the general case of closed linear operators on Banach spaces is difficult to find. Virtually all sources which cite this result, cite an unpublished technical report by Chaitin-Chatelin and Harrabi [4]. The following proof is based on [2] and extended slightly from bounded operators to closed (potentially) unbounded operators.

Proof. We prove "$\subset$" by contraposition: assume $\|(M - \lambda I)^{-1}\| > \frac{1}{\epsilon}$ and let $\|E\| < \epsilon$. Then $\|(M - \lambda I)^{-1}E\| < 1$ and hence $I + (M - \lambda I)^{-1}E$ is invertible. This implies

$$M - \lambda I + E = (M - \lambda I)\left(I + (M - \lambda I)^{-1}E\right) \tag{2.25}$$

is invertible.

Conversely, we prove "$\supset$" by showing there exists an operator E with $\|E\| < \epsilon$ sich that $M - \lambda I + E$ is not invertible. Since $\|(M - \lambda I)^{-1}\| > \frac{1}{\epsilon}$ there exists a $u \in \mathcal{X}$ with $\|u\| = 1$ and $(M - \lambda I)^{-1}u = v \in D(M)$ with $\|v\| = \frac{1}{\delta} > \frac{1}{\epsilon}$.[3] The Hahn-Banach theorem provides a $v^* \in \mathcal{X}^*$ with $\|v^*\| = 1$ and $v^*v = \|v\| = \frac{1}{\delta}$.

[3] At this point we require the strict inequality. Otherwise, the existence of such a pair u, v is not guaranteed.

Set $E = -\delta uv^*$. Then $\|E\| = \delta < \epsilon$ and

$$Ev = -\delta uv^*v = -u = -(M - \lambda I)(M - \lambda I)^{-1}u = -(M - \lambda I)v. \tag{2.26}$$

Rearranging yields $(M + E - \lambda I)v = 0$. □

The proof of the above theorem also shows that one can consider only rank-one perturbations in 2.23:

Corollary 2.15. *We can restrict 2.23 to*

$$\sigma_\epsilon(M) = \bigcup_{\substack{\|E\|<\epsilon \\ rank\ E=1}} \sigma(M + E). \tag{2.27}$$

The following formulation of the pseudospectrum in the Hilbert space case will be the main tool we use in the section on numerical methods.

Definition 2.16. *The function*

$$\sigma_{\inf}(M) = \inf_{\|x\|=1} \|Mx\| \tag{2.28}$$

is known as the injection modulus.

Lemma 2.17. *Let $M : D(M) \to \mathcal{X}$ be a closed linear operator on a Hilbert space. If $\lambda \in \rho(M)$ then*

$$\sigma_{\inf}(M - \lambda I) = \sigma_{\inf}(M^* - \bar{\lambda} I), \tag{2.29}$$

but this is not *necessarily true if $\lambda \in \sigma(M)$.*

Proof. 2.29 for $\lambda \in \rho(M)$ follows from the fact that for bounded operators A we have $\|A\| = \|A^*\|$, applied to $A = (M - \lambda I)^{-1}$. To see that 2.29 does not hold for $\lambda \in \sigma(M)$, consider again the right shift from example 2.6. Clearly $\|Rx\| = \|x\|$ so R is bounded from below but 0 is part of the spectrum. □

Theorem 2.18. *For a Hilbert space operator M,*

$$\frac{1}{\|(M - \lambda I)^{-1}\|} = \min\left\{\sigma_{\inf}(M - \lambda I),\ \sigma_{\inf}(M^* - \bar{\lambda} I)\right\}. \tag{2.30}$$

where we use the convention that $1/\|(M - \lambda I)^{-1}\| = 0$ when $\lambda \in \sigma(M)$.

Proof. When $\lambda \in \sigma_p(M)$, then obviously $\sigma_{\inf}(M - \lambda I) = 0$. Due to theorem 2.7 part 2, $\lambda \in \sigma_r(M)$ has $\sigma_{\inf}(M^* - \bar{\lambda} I) = 0$. Finally, let $\lambda \in \sigma_c(M)$ so $M - \lambda I$ is injective. Assume $\sigma_{\inf}(M - \lambda I) > 0$. Then $(M - \lambda I)^{-1} : \mathrm{ran}(M - \lambda I) \to D(M)$ is bounded. But since $\mathrm{ran}(M - \lambda I) \subset \mathcal{X}$ is dense, $(M - \lambda I)^{-1}$ has a unique bounded extension to $\mathcal{X}$, a contradiction. □

Corollary 2.19. *In the Hilbert space setting, the psudospectrum can be formulated as:*

$$\sigma_\epsilon(M) = \{\lambda \in \mathbb{C} \mid \exists\, u \in \mathcal{X} : \|u\| = 1 \text{ and either } \|(M - \lambda I)u\| < \epsilon \text{ or } \left\|(M^* - \bar{\lambda} I)u\right\| < \epsilon\}. \quad (2.31)$$

In the general Banach space setting,

$$\sigma_\epsilon(M) = \sigma(M) \cup \{\lambda \in \mathbb{C} \mid \exists\, u \in \mathcal{X} : \|u\| = 1,\ \|(M - \lambda I)u\| < \epsilon\}. \quad (2.32)$$

One sees from the proofs of lemma 2.17 and theorem 2.18 that $\sigma(M)$ in equation 2.32 can be replaced with $\sigma_r(M)$. The residual spectrum causes many common and unintuitive issues in spectral theory. In the study of pseudospectra, this issue is alleviated in one of three ways: (1): consider only classes of operators which have no residual spectrum (e.g. finite-dimensional or compact operators), (2): compute a slightly different object known as the *approximate-point spectrum* (see below), (3): ignore the problem entirely and write proofs which are all slightly incorrect.

Definition 2.20. *The* approximate-point pseudospectrum *is the set of points for which there exists an* ϵ-approximate pseudoeigenvector

$$\sigma_{ap,\epsilon}(M) = \{\lambda \in \mathbb{C} \mid \exists\, u \in \mathcal{X} : \|u\| = 1,\ \|(M - \lambda I)u\| < \epsilon\}. \quad (2.33)$$

The $\epsilon \to 0$ *limit of such sets is the* approximate-point spectrum

$$\sigma_{ap}(M) = \bigcap_{\epsilon > 0} \sigma_{ap,\epsilon}(M) \quad (2.34)$$

$$= \left\{\lambda \in \mathbb{C} \mid \exists\, (u_k)_k : \|u_k\| = 1\ \forall\, k,\ \lim_{k\to\infty} \|(M - \lambda I)u_k\| = 0\right\}. \quad (2.35)$$

2.3.2 Properties

To gain some intuition for the pseudospectrum, we derive some properties for specific types of operators.

Definition 2.21. *An operator* M *on a Hilbert space is called* normal *if* $M^*M = MM^*$. *Special classes of normal operator include* unitary *operators* ($M^* = M^{-1}$) *and* self-adjoint *operators* ($M^* = M$).

Proposition 2.22. *For a normal operator* M, $\sigma_r(M) = \emptyset$.

Proof. Let $\lambda \in \sigma(M)$, $A = M - \lambda I$. If λ is not an eigenvalue then $\ker A = \{0\}$ and

$$\{0\} = \ker A = \ker A^* = (\mathrm{ran} A)^\perp \quad (2.36)$$

where for the second equality we used the normality. Hence $\mathrm{ran} A$ is dense. □

Lemma 2.23. *For a closed linear operator M we have*

$$dist(\lambda, \sigma(M)) \geq \frac{1}{\|(M - \lambda I)^{-1}\|}. \tag{2.37}$$

Moreover, if M is a normal operator on a Hilbert space, then we have equality.

Proof. Let $\eta \in \sigma(M)$. Denote $A = M - \lambda I$, $B = M - \eta I$. Then A is invertible and

$$B = A - (A - B) = A(I - A^{-1}(A - B)). \tag{2.38}$$

Now $\|A^{-1}(A - B)\| \leq \|A^{-1}\| \, |\lambda - \eta|$ so if $|\lambda - \eta| < \frac{1}{\|B^{-1}\|}$ then the right hand side of 2.38 is invertible, a contradiction to $\eta \in \sigma(M)$.

To prove equality in the case of normal operators requires some heavy machinery from operator theory, namely:

1. Every normal operator is unitarily similar to a multiplication operator on some semi-finite measure space (i.e. there exists a unitary U such that $M = U^{-1} M_a U$ where $(M_a f)(x) = a(x) f(x)$ is a multiplication operator).
2. For multiplication operators, equation 2.37 holds with equality.

These results can be found in many sources e.g. [17]. □

Theorem 2.24. *We have*

1. $\sigma_\delta(M) \subset \sigma_\epsilon(M)$ *whenever* $\delta \leq \epsilon$,
2. $\bigcap_{\epsilon > 0} \sigma_\epsilon(M) = \sigma(M)$,
3. $\sigma(M) + B_\epsilon \subset \sigma_\epsilon(M)$, *where* B_ϵ *is the ball with radius* ϵ *centered at* 0 *and* $+$ *refers to pointwise summation* $C + D = \{x + y \mid x \in C,\ y \in D\}$.
4. *When M is normal,* $\sigma(M) + B_\epsilon = \sigma_\epsilon(M)$.

Remark. Theorem 2.24 effectively says that the Pseudospectra are nested sets which grow *at least* as quickly as ϵ-balls around the spectrum.

Proof. 1 and 2 are consequences of the representation 2.23 of the pseudospectrum. 3 and 4 are consequences of lemma 2.23. □

Theorem 2.25. *The function which maps $(\epsilon, M) \mapsto \sigma_\epsilon(M)$ which sends an $\epsilon > 0$ and a bounded M acting on a Hilbert space $\mathcal{X}$ to the set $\sigma_\epsilon(M)$ is continuous using the metric*

$$d(\,(\epsilon_1, M_1),\ (\epsilon_2, M_2)\,) = |\epsilon_1 - \epsilon_2| + \|M_1 - M_2\| \tag{2.39}$$

in the domain and the Haussdorff metric in the codomain.

Remark. 1. The idea for the proof is taken from [7], though it originally included two errors: it does not take into account residual spectrum, and makes a bound which is unfortunately not correct. These issues can be lifted in the Hilbert space setting, so that the theorem is still correct as it is stated in [7].

2. If one replaces $\sigma_\epsilon(M)$ with $\sigma_{ap,\epsilon}(M)$ in theorem 2.25, then the proof in [7] is correct and even works for general Banach spaces. To the best of this author's knowledge, there is no published correct proof for the general Banach space setting with $\sigma_\epsilon(M)$, despite it being considered common knowledge in the study of pseudospectra.

Proof. Let (M,ϵ) and (M',ϵ') be such that $d\,(\,(M,\epsilon),\ (M',\epsilon')\,) < \delta$ for some $0 < \delta < \epsilon/2$. Without loss of generality let $\epsilon \leq \epsilon'$.

Let $\lambda \in \sigma_{\epsilon'}(M')$. By 2.31 there exists a normalized $v \in \mathcal{X}$ such that either $\|(M' - \lambda I)v\| < \epsilon'$ or $\left\|(M'^* - \bar{\lambda} I)v\right\| < \epsilon'$. Assume the former is true. It follows

$$\|(M - \lambda I)v\| \leq \|(M - M')v\| + \|(M' - \lambda I)v\| < \delta - |\epsilon - \epsilon'| + \epsilon' \leq \delta + \epsilon \quad (2.40)$$

where for the last inequality we used that $\epsilon \geq \epsilon' - |\epsilon' - \epsilon|$. By 2.31, $\lambda \in \sigma_{\epsilon+\delta}(M)$ and hence $\sigma_{\epsilon'}(M') \subset \sigma_{\epsilon+\delta}(M)$.

For the case that $\left\|(M'^* - \bar{\lambda} I)v\right\| < \epsilon'$, equation 2.40 can be done exactly the same with $\left\|(M^* - \bar{\lambda} I)v\right\|$ on the left hand side.

Now let $\lambda \in \sigma_{\epsilon-\delta}(M)$. Again this implies there exists a normalized $v \in \mathcal{X}$ such that either $\|(M - \lambda I)v\| < \epsilon - \delta$ or $\left\|(M^* - \bar{\lambda} I)v\right\| < \epsilon - \delta$. Assume again the former is true. Then

$$\|(M' - \lambda I)v\| \leq \|(M' - M)v\| + \|(M - \lambda I)v\| < \delta + \epsilon - \delta \leq \epsilon' \quad (2.41)$$

and hence $\lambda \in \sigma_{\epsilon'}(M')$ so that $\sigma_{\epsilon-\delta}(M) \subset \sigma_{\epsilon'}(M')$ (again the adjoint case can be done exactly the same with adjoints on the left hand side of the equation).

We now have $\sigma_{\epsilon-\delta}(M) \subset \sigma_{\epsilon'}(M') \subset \sigma_{\epsilon+\delta}(M)$ which implies for the Haussdorff distance between $\sigma_\epsilon(M)$ and $\sigma_{\epsilon'}(M')$,

$$\begin{aligned} &\mathcal{H}\,(\,\sigma_\epsilon(M),\ \sigma_{\epsilon'}(M')\,) && (2.42)\\ &\quad \leq \max\{\,\mathcal{H}\,(\,\sigma_\epsilon(M),\ \sigma_{\epsilon-\delta}(M)\,),\ \mathcal{H}\,(\,\sigma_\epsilon(M),\ \sigma_{\epsilon+\delta}(M)\,)\,\} && (2.43)\\ &\quad \leq \mathcal{H}\,(\,\sigma_{\epsilon-\delta}(M),\ \sigma_{\epsilon+\delta}(M)\,) && (2.44)\end{aligned}$$

so we must investigate the difference between $\sigma_{\epsilon-\delta}(M)$ and $\sigma_{\epsilon+\delta}(M)$. But

$$\sigma_{\epsilon+\delta}(M) \setminus \sigma_{\epsilon-\delta}(M) = \left\{\lambda \in \mathbb{C} \mid \frac{1}{\epsilon+\delta} < \left\|(M - \lambda I)^{-1}\right\| < \frac{1}{\epsilon-\delta}\right\} \quad (2.45)$$

which is just a difference of sublevel sets for the continuous function $\lambda \mapsto \|(M - \lambda I)^{-1}\|$. Hence 2.45 collapses continuously to $\emptyset$ as $\delta \to 0$, which implies 2.44 converges to 0 as $\delta \to 0$. □

We conclude the section on mathematical background by examining the interaction between an operator and finite rank approximations of it. The methods we will describe in the following section are special types of *finite-section methods*.

Theorem 2.26. *Let M be a closed linear operator and $(\Pi_n : \mathcal{X} \to V_n)_n$ be a collection of projections onto finite-dimensional subspaces V_n which converge pointwise to the identity. Let further (λ, c) be an ϵ-pseudoeigenpair of $\Pi_n M \Pi_n$. Then for every $\delta > 0$ there exists an $N = N(\delta, c)$ such that $\lambda \in \sigma_{\epsilon+\delta}(M)$ whenever $n > N$.*

However, this does not *necessarily imply $\sigma_\epsilon(\Pi_n M \Pi_n) \to \sigma_\epsilon(M)$ in the Hausdorff metric.*

Proof. Let N be such that of off-diagonal action of $(M - \lambda I)$ on c is bounded by δ, i.e. $\|(I - \Pi_N)(M - \lambda I)\Pi_N c\| < \delta$. Now the claim follows from the triangle inequality since

$$(M - \lambda I)c = (\Pi_N M \Pi_N - \lambda I)c + (I - \Pi_N)(M - \lambda I)\Pi_N c \tag{2.46}$$

and (by definition) $c = \Pi_N c$.

For the second claim of the theorem consider the *two-sided* left shift operator $L : \ell^2 \to \ell^2$ and let

$$\Pi_n : (\ldots, a_{-1}, a_0, a_1, \ldots) \mapsto (\ldots, 0, 0, a_{-n}, \ldots a_{-1}, a_0, a_1, \ldots, a_n, 0, 0, \ldots). \tag{2.47}$$

Then L is unitary and has spectrum on the (complex) unit circle $\mathbb{T}$, so $\sigma_\epsilon(L) = \mathbb{T} + B_\epsilon$. However, $\Pi_n L \Pi_n$ is nilpotent so $\sigma_\epsilon(\Pi_n L \Pi_n)$ always contains 0, which is not in $\mathbb{T} + B_\epsilon$ for any $\epsilon < 1$. □

With an understanding of the spectral properties of Koopman and Perron-Frobenius operators as well as the pseudospectrum, we are prepared to apply pseudospectral methods to some of the most common Koopman approximation methods, known under the umbrella term *dynamic mode decomposition*.

3 Numerical Methods

3.1 Petrov-Galerkin Methods

The original Ritz-Galerkin method is described as follows: we are given a PDE problem in its *weak formulation*:

$$\text{find } u \in \mathcal{X} \text{ such that } q(v, u) = \langle f, v \rangle \ \ \forall\, v \in \mathcal{W} \tag{3.1}$$

where q is some elliptic sesquilinear form, $f \in \mathcal{X}$ given, $\langle \cdot, \cdot \rangle$ some inner product, and $\mathcal{W}$ some *test set*. The form q is typically derived from some minimization problem for a functional representing energy.

The idea behind the Ritz-Galerkin method is to *solve 3.1 on a finite-dimensional subspace:* let $\mathcal{W} = \operatorname{span}\{\psi_1, \ldots, \psi_N\}$ be q-linearly independent.

Then writing

$$\Psi(x) = [\psi_1(x) \mid \ldots \mid \psi_N(x)], \tag{3.2}$$

we make the approximation $u \approx \Psi c_u$ and have $v = \Psi c_v$ for $c_u, c_v \in \mathbb{C}^N$. Now 3.1 reduces to

$$\text{find } c_u \in \mathbb{C}^N \text{ such that } q(\Psi c_v, \Psi c_u) = \langle f, \Psi c_v \rangle \ \ \forall\, c_v \in \mathbb{C}^N. \tag{3.3}$$

One quickly verifies that c_u is the unique solution to the matrix equation $Ax = b$ with

$$A_{ij} = q(\Psi e_i, \Psi e_j) = q(\psi_i, \psi_j), \quad b_i = \langle f, \Psi e_i \rangle = \langle f, \psi_i \rangle. \tag{3.4}$$

where $e_i \in \mathbb{C}^N$ is the i-th standard unit vector. A is known as the *stiffness matrix.*

One can extend the Ritz-Galerkin formulation by allowing the test space to differ from the basis space: keep $u \approx \Psi c_u$ but let $\mathcal{W} = \operatorname{span}\{\psi_1^*, \ldots, \psi_M^*\}$, then A and b become

$$A_{ij} = q(\psi_i^*, \psi_j), \quad b_i = \langle f, \psi_i^* \rangle. \tag{3.5}$$

In the regime $M > N$ this equation is *overdetermined* so it is solved in a least squares sense

$$\|Ax - b\|_2^2 = \min_{x \in \mathbb{C}^N} ! \tag{3.6}$$

where $\|\cdot\|_2$ is the vector ℓ^2 norm. This is known as the Petrov-Galerkin method.

One can extend the method further by asking that multiple solutions for multiple right hand sides $(f_j)_{j=1}^N$ are computed simultaneously, that is

$$\|AX - B\|_F^2 = \min_{X \in \mathbb{C}^{N \times N}} !, \quad B_{ij} = \langle f_j, \psi_i^* \rangle \tag{3.7}$$

where $\|\cdot\|_F$ denotes the Frobenius norm.

Numerically, 3.7 can be solved using the Moore-Penrose inverse

$$X = A^\dagger B. \tag{3.8}$$

An exercise in matrix calculus shows that the solution can also be written in the form

$$X = (A^* A)^{-1} A^* B. \tag{3.9}$$

Both forms will prove to be useful later.

3.2 Extended Dynamic Mode Decomposition (EDMD)

3.2.1 The Galerkin Ansatz

We apply the Petrov-Galerkin Ansatz to obtain a matrix approximation K for $\mathcal{K}|_{\mathcal{X}}$. Let $q(\cdot,\cdot) = \langle\cdot,\cdot\rangle$ and consider a linearly independent family of functions $\{\psi_1,\dots,\psi_N\} \subset \mathcal{X}$. Take delta distributions, that is $\langle\delta_x,\psi\rangle = \psi(x)$, for the test function(als): let $(w_i,x_i)_{i=1}^M$ represent a quadrature scheme and set $\psi_i^* = \sqrt{w_i}\delta_{x_i}$.

We then solve the Galerkin equation 3.7 for $f_j = \mathcal{K}\psi_j$:

$$\left\|\sqrt{W}\Psi_X K - \sqrt{W}\Psi_Y\right\|_F^2 = \min_{K\in\mathbb{C}^{N\times N}}! \tag{3.10}$$

with $W = \mathrm{diag}(w_1,\dots,w_M)$ and

$$(\Psi_X)_{ij} = \langle\delta_{x_i},\psi_j\rangle = \psi_j(x_i), \quad (\Psi_Y)_{ij} = \langle\delta_{x_i},\mathcal{K}\psi_j\rangle = \psi_j(\,S(x_i)\,). \tag{3.11}$$

This results in the *EDMD matrix*

$$K = \Psi_X^\dagger\Psi_Y = (\Psi_X^* W\Psi_X)^{-1}(\Psi_X^* W\Psi_Y). \tag{3.12}$$

Inverting Ψ_X involves computing the Moore-Penrose inverse of an $N\times M$ matrix, whereas inverting $\Psi_X^*\Psi_X$ involves computing the inverse of a symmetric $N\times N$ matrix. Depending on the relationship between M and N in the particular usecase, either forumlation might be cheaper.

Another look at the second formulation of the EDMD matrix shows that

$$G_{ij} \coloneqq (\Psi_X^* W\Psi_X)_{ij} = \sum_{k=1}^M w_k\overline{\psi_i(x_k)}\psi_j(x_k) \xrightarrow{\mathrm{M}\to\infty} \langle\psi_i,\psi_j\rangle =: \mathbb{G}_{ij}, \tag{3.13}$$

$$A_{ij} \coloneqq (\Psi_X^* W\Psi_Y)_{ij} = \sum_{k=1}^M w_k\overline{\psi_i(x_k)}\psi_j(\,S(x_k)\,) \xrightarrow{\mathrm{M}\to\infty} \langle\psi_i,\mathcal{K}\psi_j\rangle =: \mathbb{A}_{ij}, \tag{3.14}$$

which can be computed with constant memory requirement.

3.2.2 Functional Minimization

TODO: replace P with Π We could have arrived at equation 3.10 completely differently: equation 3.10 is precisely a quadrature approximation of the functional least squares minimization:

$$\|\Psi K - \mathcal{K}\Psi\|_{\mathcal{X}^{1\times N}}^2 = \min_{K\in\mathbb{C}^{N\times N}}! \tag{3.15}$$

where $\mathcal{K}\Psi$ is understood elementwise and $\mathcal{X}^{1\times N}$ is the space of (row) vector-valued functions with each component in $\mathcal{X}$

$$\|[f_1 \mid \ldots \mid f_N]\|^2_{\mathcal{X}^{1\times N}} = \|f_1\|^2_{\mathcal{X}} + \ldots + \|f_N\|^2_{\mathcal{X}}\,. \tag{3.16}$$

Let us investigate $\Psi : \mathbb{C}^N \to \mathcal{X}$ a bit closer. Decompose the Hilbert space $\mathcal{X}$ into

$$\mathcal{X} = \operatorname{span}\{\psi_j\}_{j=1}^N \oplus \mathcal{V}, \quad \mathcal{V} = \left(\{\psi_j\}_{j=1}^N\right)^{\perp} \tag{3.17}$$

and let $\{\psi_j\}_{j=N+1}^{\infty}$ be a basis of $\mathcal{V}$.

A short calculation using the orthogonality of $\{\psi_j\}_{j=1}^N$ and $\{\psi_j\}_{j=N+1}^{\infty}$ shows that for $\phi \in \mathcal{X}$,

$$\langle \phi, \Psi c\rangle = \sum_{j=1}^{N} \langle \phi, \psi_j\rangle\, c_j. \tag{3.18}$$

Hence the adjoint quasi-matrix $\Psi^* : \mathcal{X} \to \mathbb{C}^N$ acts as

$$\Psi^*\phi = \begin{pmatrix} \langle \phi, \psi_1\rangle \\ \vdots \\ \langle \phi, \psi_1\rangle \end{pmatrix}. \tag{3.19}$$

Lemma 3.1. *For an arbitrary basis $\{\psi_j\}_{j=1}^N$, the orthogonal projector P onto the space spanned by the basis is*

$$P = \Psi(\Psi^*\Psi)^{-1}\Psi^*. \tag{3.20}$$

Proof. The solution of a linear least squares problem $\|Ax - b\| = \min!$ is the result of orthogonally projecting b onto the range of A, that is, $Ax = Pb$. From equation 3.9 we know $x = (A^*A)^{-1}A^*b$. Therefore $Pb = Ax = A(A^*A)^{-1}A^*b$. Since this holds for arbitrary b, the result is proven. □

Using equation 3.9 we see that in the infinite-data limit $M \to \infty$, K has the form

$$K = (\Psi^*\Psi)^{-1}\Psi^*(\mathcal{K}\Psi) \tag{3.21}$$

Inserting the definitions of Ψ and Ψ^* yields $K = \mathbb{G}^{-1}\mathbb{A}$ exactly as in equations 3.13 and 3.14.

If we view the result of applying K as in equation 3.21 to a vector c as an object in $\mathcal{X}$, that is, ΨKc, we see that

$$\Psi Kc = \Psi(\Psi^*\Psi)^{-1}\Psi^*(\mathcal{K}\Psi)c = P\mathcal{K}\Psi c = P\mathcal{K}P\Psi c. \tag{3.22}$$

Since this holds for arbitrary c we have proven that (when viewed as an operator on $\mathcal{X}$) K is precisely the action of $P\mathcal{K}P$, the finite section of $\mathcal{K}$ over $\operatorname{span}\{\psi_j\}_{j=1}^N$. In this way, EDMD can just as well be viewed as a finite section method.

Algorithm 1 Extended Dynamic Mode Decomposition (EDMD)

Require: Dictionary $\{\psi_j\}_{j=1}^{N}$, data points and weights $\{(w_i, x_i)\}_{i=1}^{M}$

1: Construct G, A as in 3.13, 3.14
2: Set $K = G^{-1}A$ (or $L = G^{-1}A^*$)
3: Compute an eigendecomposition $KV = V\Lambda$ (or $LV = V\Lambda$)
4: **return** Eigenvalues and eigenvectors Λ, V

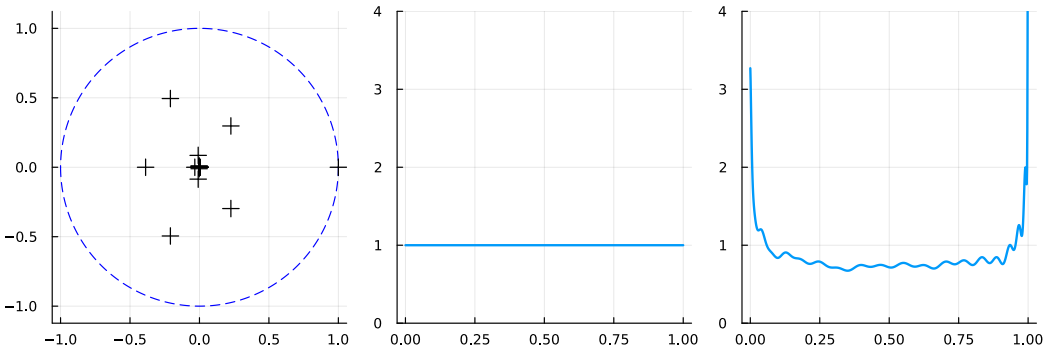

Figure 3.1: Algorithm 1 applied to the quadratic map (c.f. figure 2.1) performed with $M = 100$ Gauß-Legendre quadrature nodes and weights, and $N = 40$ Legendre polynomials transplanted to the interval $[0, 1]$. Left: spectrum of K. Middle: (normalized) eigenfunction of K for the eigenvalue $\lambda = 1$. Right: (normalized) eigenfunction of L for the eigenvalue $\lambda = 1$. Compare with figure 2.2.

3.2.3 EDMD for the Perron-Frobenius Operator

From equation 3.21, and noting the form of $\mathbb{A}$,

$$\langle \psi_i, \mathcal{L}\psi_j \rangle = \langle \mathcal{K}\psi_i, \psi_j \rangle = \overline{\langle \psi_j, \mathcal{K}\psi_i \rangle} = \overline{\mathbb{A}_{ji}} \tag{3.23}$$

yields an equivalent Galerkin method for $\mathcal{L}$:

$$L = (\Psi^*\Psi)^{-1}\Psi^*(\mathcal{L}\Psi) = \mathbb{G}^{-1}\mathbb{A}^* \tag{3.24}$$

or the finite analogue:

$$L = G^{-1}A^*. \tag{3.25}$$

3.3 Residual EDMD (ResDMD)

3.3.1 Validation of Koopman Eigenpairs

The formulation 3.22 shows that K (when viewed as a operator on $\mathcal{X}$) converges weakly to $\mathcal{K}$. However, from example 2.12 we know that the spectrum is already unstable for operators which are close in the *strong* operator topology, let alone in the *weak* topology. It is therefore entirely unclear *a priori* that the eigenvalues and eigenvectors of K actually represent eigenvalues and eigenfunctions of $\mathcal{K}$.

In the Perron-Frobenius operator community, a common solution to the mentioned issue is *stochastic smoothing*. Instead of considering a deterministic dynamical system generated by S, one consider a stochastic system: $x \in \Omega$ is assigned a *distribution* of possible image points instead of being assigned to the point $S(x)$. The resulting Markov process has an associated (stochastic) Perron-Frobenius operator which (under some conditions on the type of stochastic smoothing) is Hilbert-Schmidt on $L^2(\Omega)$. This way, the finite sections converge strongly to the (stochastic) Perron-Frobenius and (since it is Hilbert-Schmidt) so do the eigenvalues [8].

We take a different approach using the theory of pseudospectra. We wish to know which of our eigenvalues are *spurious*, that is, caused by the reduction to a finite section, and which eigenvalues are accurate. To determine this, we consider equation 2.31: if a sequence $(\lambda_N, c_N)_N$ of (normalized) eigenpairs for $K = K(\{\psi_j\}_{j=1}^N)$ converges to a true $\lambda \in \sigma(\mathcal{K})$ then we must have

$$\lim_{N\to\infty} \|(\mathcal{K} - \lambda_N I)\Psi c_N\|_{\mathcal{X}}^2 = 0 \tag{3.26}$$

(where $\Psi = \Psi_N$ is as in 3.2) or

$$\lim_{N\to\infty} \|(\mathcal{L} - \lambda_N I)\Psi c_N\|_{\mathcal{X}}^2 = 0. \tag{3.27}$$

Conversely, if neither of these tend to 0 as N grows, then we can rule out λ_N as a candidate eigenvalue.

From section 3.2.2 we know that the Galerkin equation 3.10 is a quadrature approximation of equation 3.15. Similarly, the *regression error*

$$\mathrm{res}_{N,M}(\lambda_N, c_N) \coloneqq \left\| \sqrt{W}(\Psi_Y - \lambda_N \Psi_X) c_N \right\|_2^2 \tag{3.28}$$

is precisely a quadrature approximation of equation 3.26.

Theorem 3.2. *Let λ and $g = \Psi c$ be a candidate eigenpair for $\mathcal{K}$. Then*

$$\lim_{M\to\infty} res_{N,M}(\lambda, c) = \|(\mathcal{K} - \lambda I) g\|_{\mathcal{X}}^2 \tag{3.29}$$

Proof. Denote $J = \Psi_Y^* W \Psi_Y$ and observe that

$$\lim_{M\to\infty} J_{ij} = \langle \mathcal{K}\psi_i, \mathcal{K}\psi_j \rangle =: \mathbb{J}_{ij}. \tag{3.30}$$

Consider the action of Ψ on standard unit vectors:

$$\langle \Psi e_i, \Psi e_j \rangle = \langle \psi_i, \psi_j \rangle = \mathbb{G}_{ij} = e_i^* \mathbb{G} e_j. \tag{3.31}$$

Analogously $e_i^* \mathbb{A} e_j = \langle \psi_i, \mathcal{K}\psi_j \rangle$, $e_i^* \mathbb{J} e_j = \langle \mathcal{K}\psi_i, \mathcal{K}\psi_j \rangle$. Sesquilinearity of $\langle \cdot, \cdot \rangle$ yields

$$\langle g, g \rangle = c^* \mathbb{G} c, \quad \langle g, \mathcal{K} g \rangle = c^* \mathbb{A} c, \quad \langle \mathcal{K} g, \mathcal{K} g \rangle = c^* \mathbb{J} c. \tag{3.32}$$

The proof is now simply a calculation. Indeed,

$$\begin{aligned} &\left\| \sqrt{W}(\Psi_Y - \lambda \Psi_X) c \right\|_2^2 \\ &= \left((\Psi_Y - \lambda \Psi_X) c \right)^* W \left((\Psi_Y - \lambda \Psi_X) c \right) \\ &= c^* \left(\Psi_Y^* W \Psi_Y - \bar{\lambda} \Psi_X^* W \Psi_Y - \lambda \Psi_Y^* W \Psi_X + |\lambda|^2 \Psi_X^* W \Psi_X \right) c \\ &= c^* J c - \bar{\lambda}\, c^* A c - \lambda\, c^* A^* c + |\lambda|^2\, c^* G c. \end{aligned} \tag{3.33}$$

Taking the infinite-data limit,

$$\begin{aligned} &\lim_{M\to\infty} \left\| \sqrt{W}(\Psi_Y - \lambda \Psi_X) c \right\|_2^2 \\ &\qquad = c^* \mathbb{J} c - \bar{\lambda}\, c^* \mathbb{A} c - \lambda\, c^* \mathbb{A}^* c + |\lambda|^2\, c^* \mathbb{G} c \\ &\qquad = \langle \mathcal{K} g, \mathcal{K} g \rangle - \bar{\lambda} \langle g, \mathcal{K} g \rangle - \bar{\lambda} \langle \mathcal{K} g, g \rangle + |\lambda|^2 \langle g, g \rangle \\ &\qquad = \langle (\mathcal{K} - \lambda I) g, (\mathcal{K} - \lambda I) g \rangle \\ &\qquad = \|(\mathcal{K} - \lambda I) g\|_{\mathcal{X}}^2 . \end{aligned} \tag{3.34}$$

□

From the proof we also directly see the following corollaries.

Definition 3.3. *Let $M : \mathcal{X} \supset D(M) \to \mathcal{Y}$ be a closed linear operator and $V \subset \mathcal{X}$. We say that V forms a* core *of M if the closure*[4] *of $M|_V$ if M.*

Corollary 3.4. *Let $\lambda \in \mathbb{C}$, define*

$$res_{N,M}(\lambda) := \min_{c^*Gc=1} \left\| \sqrt{W}(\Psi_Y - \lambda\Psi_X)c \right\|_2. \tag{3.35}$$

Then

$$\lim_{M\to\infty} res_{N,M}(\lambda) = \min_{\substack{g\in span\{\psi_1,\ldots,\psi_N\} \\ \|g\|=1}} \|(\mathcal{K} - \lambda I)g\|_{\mathcal{X}}. \tag{3.36}$$

In particular this corollary implies that if we calculate some candidate eigenpairs, compute $\mathrm{res}_{N,M}$ for each one, and throw out eigenpairs which do not satisfy a threshhold $\mathrm{res}_{M,N}(\lambda, c) < \epsilon$, then the remaining candidate eignpairs really are close to eigenpairs of $\mathcal{K}$. This process is summarized in algorithm 2.

Corollary 3.5. *Let $\Lambda_M(\epsilon)$ denote the set of eigenvalues returned by algorithm 2. Then*

$$\limsup_{M\to\infty} \max_{\lambda\in\Lambda_M(\epsilon)} \left\|(\mathcal{K} - \lambda I)^{-1}\right\|^{-1} \leq \epsilon. \tag{3.37}$$

Finally, theorem 3.2 also provides a method to compute the ϵ-approximate point pseudospectrum of $\mathcal{K}$, summarized in algorithm 3.

Corollary 3.6. *Assume $span\{\psi_j\}_{j=1}^{\infty}$ forms a core of $\mathcal{K}$. Then*

$$\lim_{N\to\infty} \lim_{M\to\infty} res_{N,M}(\lambda) = \sigma_{\inf}(\mathcal{K} - \lambda I). \tag{3.38}$$

Moreover the outer limit $N \to \infty$ is monotonically decreasing so that

$$\sigma_{ap,\epsilon}(\mathcal{K}) = \bigcap_{N>0} \left\{ \lambda \in \mathbb{C} \mid \lim_{M\to\infty} res_{N,M}(\lambda) < \epsilon \right\}. \tag{3.39}$$

Proof. From 3.36 it is clear that $\lim_{M\to\infty} \mathrm{res}_{N,M}(\lambda) \geq \sigma_{\inf}(\mathcal{K} - \lambda I)$ and that $\mathrm{res}_{N,M}$ is decreasing with N. Let $\delta > 0$ be arbitrary and $g \in \mathcal{X}$ be such that $\|g\| = 1$ and $\|(\mathcal{K} - \lambda I)g\| < \sigma_{\inf}(\mathcal{K} - \lambda I) + \delta$. Since $\mathrm{span}\{\psi_j\}_{j=1}^{\infty}$ forms a core of $\mathcal{K}$, we can find an N and $\widehat{g} \in \mathrm{span}\{\psi_j\}_{j=1}^{N}$ such that $\|g - \widehat{g}\| < \delta$ and $\|(\mathcal{K} - \lambda I)\widehat{g}\| < \|(\mathcal{K} - \lambda I)g\| + \delta$. This implies $\|\widehat{g}\| > 1 - \delta$ and $\|(\mathcal{K} - \lambda I)\widehat{g}\| < (\sigma_{\inf}(\mathcal{K} - \lambda I) + 2\epsilon)/(1 - \epsilon)$. Since this holds for all $\epsilon > 0$, the claim is proven. In fact, the convergence is uniform on compact sets. □

The computation of $\mathrm{res}(\lambda)$ reduces to a generalized eigenvalue problem. Let

$$U\,(= U(\lambda)) = J - \bar{\lambda}A - \lambda A^* + |\lambda|^2 G. \tag{3.40}$$

[4] A linear operator $N : D(N) \to \mathcal{Y}$ which is *not* closed might only be so because the domain $D(N)$ might not be "large enough". If there exists an extension (i.e. $\bar{N} : D(\bar{N}) \to \mathcal{Y}$, $D(N) \subset D(\bar{N})$, $\bar{N}\big|_{D(N)} = N$) which is closed, then N is *closable* and the smallest such $\bar{N}$ is called the *closure* of N.

Then computing $\text{res}(\lambda)^2$ is equivalent to solving the minimization problem

$$\min_{c\in\mathbb{C}^N} c^*Uc \quad \text{such that} \quad c^*Gc = 1. \tag{3.41}$$

Let ξ be a Lagrange multiplier, that is, a necessary condition for s solution of 3.41 is

$$Uc - \xi Gc = 0 \tag{3.42}$$

since U and G are symmetric. Inserting such a c into the objective yields

$$c^*Uc = c^*\xi Gc = \xi \tag{3.43}$$

since $c^*Gc = 1$. Hence 3.41 is solved by computing the smallest generalized eigenvalue solution of 3.42 (symmetry of U and G guarantees that all such eigenvalues are real).

Algorithm 2 Verification of candidate eigenpairs for $\mathcal{K}$

Require: Dictionary $\{\psi_j\}_{j=1}^N$, data points and weights $\{(w_i, x_i)\}_{i=1}^M$, tolerance ϵ

1: Perform algorithm 1 to obtain G, A, $KV = V\Lambda$
2: Construct J as in 3.30
3: **for** each candidate eigenpair (λ, v) **do**
4: Compute $\text{res}_{N,M}(\lambda, v)$ as in 3.41
5: Throw out λ if $\text{res}_{N,M}(\lambda, v) \geq \epsilon$
6: **return** Verified Koopman (approximate-point) eigenvalues $\Lambda_M(\epsilon) = \{(\lambda, v) \mid \text{res}_{N,M}(\lambda, v) < \epsilon\}$

Algorithm 3 Residual EDMD to Compute $\sigma_{ap,\epsilon}(\mathcal{K})$

Require: Dictionary $\{\psi_j\}_{j=1}^N$, data points and weights $\{(w_i, x_i)\}_{i=1}^M$, grid $\{z_\nu\}_{\nu=1}^T \subset \mathbb{C}$, tolerance ϵ

1: Perform algorithm 1 to obtain G, A, K
2: Construct J as in 3.30
3: **for** z_ν **do**
4: Compute $\text{res}(z_\nu)$ as in 3.41
5: **return** $\{z_\nu \mid \text{res}(z_\nu) < \epsilon\}$ as an approximation for $\sigma_{ap,\epsilon}(\mathcal{K})$

3.3.2 A Naive Attempt at Duality

Algorithm 3 provides a way to compute the approximate-point pseudospectrum of the Koopman operator. In order to resolve the full pseudospectrum, one needs to compute $\sigma_{\text{inf}}(\mathcal{K} - \lambda I)$ *and* $\sigma_{\text{inf}}(\mathcal{L} - \bar{\lambda} I)$ for λ's of interest. One could hope to perform the calculations in 3.34 backwards using $\mathcal{L}$ instead of $\mathcal{K}$, but

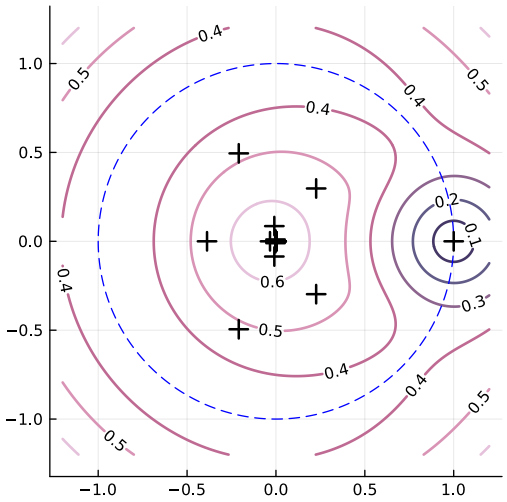

Figure 3.2: Algorithm 3 applied to the quadratic map (c.f. figure 2.1) performed with the same parameters as figure 3.1. Contours of $\lambda \mapsto \mathrm{res}(\lambda)$ are shown with the spectrum of K. The quadratic map is ergodic [16] which is verified by the residuals. The eigenvalues of K other than 1 are spurious.

quickly notices that the inner product $\langle \mathcal{L}g, \mathcal{L}g \rangle$ or $g = \Psi c$ is not computable using just the information at hand.

We instead try to follow the calculations forward. Starting with $L = G^{-1}A^*$ and $g = \Psi c$ we see that the analogous regression error for a candidate eigenpair can be written as

$$\left\| \left(\Psi_Y^* W \Psi_X - \lambda \Psi_X^* W \Psi_X \right) c \right\|_{\mathbb{C}^N}^2 = \left\| \left(\Psi_Y^* W - \lambda \Psi_X^* W \right) \Psi_X c \right\|_{\mathbb{C}^N}^2 . \tag{3.44}$$

Notice that $\Psi_X^* W$ is precisely a quadrature appoximation of Ψ^* from equation 3.19. $\Psi_X^* W$ takes an interpolation vector $f \in \mathbb{C}^M$ and approximates the integral with an interpolant function. Analogously we can deduce that $\Psi_Y^* W$ is a quadrature approximation of $(\mathcal{K}\Psi)^*$.

Assuming that $\{\psi_j\}_{j=1}^N$ is an orthonormal family, taking the infinite data limit

yields

$$\begin{aligned}
&\lim_{M\to\infty} \left\|\left(\Psi_Y^* W - \lambda \Psi_X^* W\right) \Psi_X c\right\|_{\mathbb{C}^N}^2 \\
&\quad = \left\|\left((\mathcal{K}\Psi)^* - \lambda \Psi^*\right) g\right\|_{\mathbb{C}^N}^2 \\
&\quad = \left\| \begin{pmatrix} \langle\, (\mathcal{K} - \lambda I)\psi_1, g \,\rangle \\ \vdots \\ \langle\, (\mathcal{K} - \lambda I)\psi_N, g \,\rangle \end{pmatrix} \right\|_{\mathbb{C}^N}^2 \\
&\quad = \sum_{j=1}^{N} \left|\langle\, (\mathcal{K} - \lambda I)\psi_j, g \,\rangle\right|^2 \\
&\quad = \sum_{j=1}^{N} \left|\left\langle\, \psi_j, (\mathcal{L} - \bar{\lambda} I) g \,\right\rangle\right|^2 \\
&\quad = \left\|(P\mathcal{L}P - \bar{\lambda} I) g\right\|_{\mathcal{X}}^2
\end{aligned} \tag{3.45}$$

where P is the orthogonal projector onto span $\{\psi_j\}_{j=1}^N$. By the Galerkin property we know that L encodes precisely the action of $P\mathcal{L}P$. Hence,

$$\left\|(P\mathcal{L}P - \bar{\lambda} I) g\right\|_{\mathcal{X}}^2 = \left\|(L - \bar{\lambda} I) c\right\|_{\mathbb{C}^N}^2 \tag{3.46}$$

and so the least-squares Ansatz computes the pseudospectrum of L which by theorem 2.26 cannot be used analogously to algorithm 3 to compute $\sigma_{ap,\epsilon}(\mathcal{L})$. We would need to send $N \to \infty$ first, which would cause the equation $L = G^{-1}A^*$ to break.

While we will not use this immediately, we still expand the first line of 3.45 since we will see it again later.

$$\begin{aligned}
&\left\|\left(\Psi_Y^* W - \lambda \Psi_X^* W\right) \Psi_X c\right\|_{\mathbb{C}^N}^2 \\
&= \left\| \left(\Psi_Y^* \sqrt{W} - \lambda \Psi_X^* \sqrt{W}\right) \sqrt{W} \Psi_X c \right\|_{\mathbb{C}^N}^2 \\
&= \left(\sqrt{W}\Psi_X c\right)^* \sqrt{W} \left(\Psi_Y \Psi_Y^* - \bar{\lambda} \Psi_X \Psi_Y^* - \lambda \Psi_Y \Psi_X^* \right. \\
&\qquad\qquad \left. + |\lambda|^2 \Psi_X \Psi_X^*\right) \sqrt{W} \left(\sqrt{W}\Psi_X c\right)
\end{aligned} \tag{3.47}$$

3.4 kernel EDMD (kEDMD)

3.4.1 The Kernel Trick

TODO: replace c with v when M-dimensional The choice of dictionary $\{\psi_j\}_{j=1}^N$ naturally has massive impacts on the accuracy of the above methods. We will see later in section 4 that a poorly chosen dictionary can cause catastrophic results. This is because even though there may be many ways to (in the limit $N \to \infty$) form a basis of $\mathcal{X}$, any practical calculation will necessarily have a

finite cut-off. So the challenge becomes finding efficient ways to increase N without needing to perform $O(N^2)$ quadrature problems.

One method which is enormously popular in machine learning [1, 3, 10, 14] is the so-called *kernel trick*. Consider the function $k : \mathbb{C}^2 \times \mathbb{C}^2 \to \mathbb{C},\ (w, z) \mapsto (1 + w^* z)^2$. We can write this as

$$\begin{aligned} k(w,z) &= (1 + \bar{w_1} z_1 + \bar{w_2} z_2)^2 \\ &= (1 + 2\bar{w_1} z_1 + 2\bar{w_2} z_2 + 2\bar{w_1}\bar{w_2} z_1 z_2 + \bar{w_1}^2 z_1^2 + \bar{w_2}^2 z_2^2) \\ &= \langle \Psi(z), \Psi(w) \rangle_{\mathbb{C}^6} \ \ (= \Psi(z)\Psi(w)^*) \end{aligned} \tag{3.48}$$

for the basis

$$\Psi(x) = \left[1 \ \middle|\ \sqrt{2}x_1 \ \middle|\ \sqrt{2}x_2 \ \middle|\ \sqrt{2}x_1 x_2 \ \middle|\ x_1^2 \ \middle|\ x_2^2 \right]. \tag{3.49}$$

While the result is the same, computation of $(1+w^*z)^2$ requires only 5 floating-point operations, whereas $\Psi(z)\Psi(w)^*$ requires 23. More generally, any such relation $k(w, z) = \Psi(z)\Psi(w)^*$ is called a kernel trick.

Definition 3.7. *A function $\Psi : \Omega \to \mathcal{Y}$ with $k(w, z) = \langle \Psi(z), \Psi(w) \rangle_{\mathcal{Y}}$ is known in machine learning literature as a* feature map*.*

One sees that when $k(x, \cdot)$ is an element of some Hilbert space $\mathcal{Y}$, then an obvious kernel is given by $\Psi(x) = k(x, \cdot)$.[5] Another obvious kernel is given by a basis: letting $\Psi(x) = [\psi_1(x) \mid \ldots \mid \psi_N(x)]$ as before, $k(w, z) = \Psi(z)\Psi(w)^*$ is also a kernel.

Entire books are written on such kernels [15] and their properties. Common kernels include:

Example 3.8. The polynomial kernel $k : \mathbb{C}^d \times \mathbb{C}^d \to \mathbb{C},\ (w, z) \mapsto (1 + w^* z/c^2)^\alpha$ feature map is given by all (multivariate) polynomials up to degree α. Note that computing $k(w, z)$ requires only $O(d)$ operations, but computing $\Psi(z)\Psi(w)^*$ requires superexponentially (in α) many combinations.

Example 3.9. The Gaußian kernel $k(w, z) = \exp\left(-\frac{\|w-z\|^2}{c^2}\right)$ has a feature map which is infinite-dimensional. Indeed, consider (for notational simplicity) $w, z \in \mathbb{R}$:

$$\begin{aligned} k(w,z) &= \exp\left(-\frac{|w|^2}{c^2}\right) \cdot \exp\left(\frac{2\,w \cdot z}{c^2}\right) \cdot \exp\left(-\frac{|z|^2}{c^2}\right) \\ &= \exp\left(-\frac{|w|^2}{c^2}\right) \cdot \left(\sum_{k=0}^{\infty} \frac{1}{k!} \left(\frac{2}{c^2}\right)^k (w \cdot z)^k \right) \cdot \exp\left(-\frac{|z|^2}{c^2}\right) \end{aligned} \tag{3.50}$$

[5] In fact, when Ψ also satisfies the *reproducing property*, that $\langle \Psi(x), f \rangle = f(x)$ for all $f \in \mathcal{Y}$, then $\mathcal{Y}$ is known as *Reprodung Kernel Hilbert Space* and indeed span $\{k(x, \cdot) \mid x \in \Omega\}$ beomces dense in $\mathcal{Y}$.

so that

$$\Psi(x) = \exp\left(-\frac{|x|^2}{c^2}\right)\left[1 \;\middle|\; \frac{\sqrt{2}}{c}x \;\middle|\; \frac{1}{\sqrt{2!}}\left(\frac{\sqrt{2}}{c}x\right)^2 \;\middle|\; \dots\right]. \tag{3.51}$$

When $w, z \in \mathbb{C}$ then the middle term in 3.50 changes from $w \cdot z$ to $\bar{w} \cdot z + \bar{z} \cdot w$, and in higher dimensions this extends to all pairwise combinations of the components of w and z. We note (and will use later) that in the specific case $\mathcal{X} = L^2(\mathbb{T})$ where $\mathbb{T}$ is the (complex) unit circle, Ψ generates an orthogonal basis of $\mathcal{X}$, namely the Fourier basis.

3.4.2 Application to EDMD

Let k be a kernel with associated feature map Ψ that is rescaled such that

$$\Psi(x_j)\Psi(x_i)^* = \frac{k(x_i, x_j)}{\sqrt{w_i w_j}} \quad \text{for all } 1 \le i, j \le M. \tag{3.52}$$

In most cases $w_i = 1/M$ for all i so that the kernel is just scaled by a constant factor $1/M$.

Notice that

$$G = \Psi_X^* W \Psi_X = \sum_{i=1}^{M} w_i \, \Psi(x_i)^* \Psi(x_i), \quad A = \Psi_X^* W \Psi_Y = \sum_{i=1}^{M} w_i \, \Psi(x_i)^* \Psi(S(x_i)). \tag{3.53}$$

Each summand is a rank one matrix. This is not in a form where one could use the kernel trick, since we have summands of the form $\Psi(x_i)^*\Psi(x_i)$ instead of $\Psi(x_i)\Psi(x_i)^*$. However, if we reverse the order of multiplication in $\Psi_X^* W \Psi_X = (\sqrt{W}\Psi_X)^*(\sqrt{W}\Psi_X)$ then

$$\widehat{G} = \sqrt{W}\Psi_X\Psi_X^*\sqrt{W} = \left(\sqrt{w_j w_i}\Psi(x_j)\Psi(x_i)^* \right)_{i,j=1}^{M} = \left(k(x_i, x_j) \right)_{i,j=1}^{M}. \tag{3.54}$$

Analogously

$$\widehat{A} = \sqrt{W}\Psi_Y\Psi_X^*\sqrt{W} = \left(k(S(x_i), x_j) \right)_{i,j=1}^{M}. \tag{3.55}$$

We would now like to exploit the form of $K = \Psi_X^\dagger \Psi_Y$ to use these "flipped" matrices. The key to do so will be a (compact) singular value decomposition

$$\sqrt{W}\Psi_X = Q\Sigma Z^* \tag{3.56}$$

where $r = \min\{M, N\}$, $\Sigma \in \mathbb{R}_{\ge 0}^{r \times r}$ is a nonnegative diagonal matrix, and $Q \in \mathbb{C}^{M \times r}$ and $Z \in \mathbb{C}^{N \times r}$ are semi-unitary[6].

[6] A tall martrix $M \in \mathbb{C}^{q \times r}$, $q \ge r$, is semi-unitary if the columns form an orthonormal family.

Theorem 3.10 ([20]). *Let*

$$\widehat{K} \coloneqq \left(\Sigma^\dagger Q^*\right) \widehat{A} \left(Q\Sigma^\dagger\right). \tag{3.57}$$

Then (λ, c) (for $\lambda \neq 0$) is an eigenpair of $\widehat{K}$ iff (λ, Zc) is an eigenpair of K. Moreover, the eigenmodes $g = \Psi \cdot (Zc)$ can be evaluated at the data points x_i, $i = 1, \dots M$.

One should take a moment to consider that the second statement made in the theorem seems highly nontrivial. Often, the feature map is only given implicitly - one knows there exists such a Ψ, but does not have an explicit form. Even worse, the matrix Z is completely unatainable from just $\widehat{G}$ and $\widehat{A}$.

The benefit of using $\widehat{K}$ is that it can be computed in $O(M^2)$ time, *independent of N*. All that is required is an eigendecomposition for $\widehat{G}$ since by definition

$$\widehat{G} = Q\Sigma^2 Q^*. \tag{3.58}$$

Proof. Notice

$$Z\widehat{K}Z^* = \Psi_X^\dagger \sqrt{W}^{-1} \sqrt{W} \Psi_Y \Psi_X^* \sqrt{W} \sqrt{W}^{-1} {\Psi_X^*}^\dagger = K P_{\operatorname{ran} \Psi_X^* \sqrt{W}} \tag{3.59}$$

where $P_{\operatorname{ran}\Psi_X^*}$ is the orthogonal projection onto the range of Ψ_X^*. But since $\Psi_X^* \sqrt{W} = Z\Sigma Q^*$, this is equivalent to

$$\widehat{K} = Z^* K Z \tag{3.60}$$

which immediately proves the first claim of the theorem. Now to evaluate $g = \Psi \cdot (Zc)$ at each x_i, $i = 1, \dots, M$, observe that $\Psi_X \cdot (Zc) = Q\Sigma c$. □

Algorithm 4 Kernel EDMD

Require: kernel $k : \Omega \times \Omega \to \mathbb{C}$, data points and weights $\{(w_i, x_i)\}_{i=1}^M$, compression factor $r \leq M$

1: Construct $\widehat{G}$, $\widehat{A}$ as in 3.54, 3.55
2: Compute an eigendecomposition $\widehat{G} = Q\Sigma^2 Q^*$
3: Let $\widehat{\Sigma} = \Sigma[1:r, 1:r]$, $\widehat{Q} = Q[:, 1:r]$ be the r largest eigenvalues and corresponding eigenvectors
4: Construct $\widehat{K} = \left(\widehat{\Sigma}^\dagger \widehat{Q}^*\right) \widehat{A} \left(\widehat{Q}\widehat{\Sigma}^\dagger\right)$
5: Compute an eigendecomposition $\widehat{K}V = V\Lambda$
6: **return** Eigenvalues and eigenvectors Λ, V

3.5 kernel ResDMD (kResDMD)

3.5.1 Associating a Residual to $\widehat{K}$

We set out again to deduce which candidate eigenvalues produced by algorithm 4 are spurious, and which are accurate. Theorem 3.10 suggests that we could potentially compute $\|(\mathcal{K}-\lambda I)g\|$ by using the altered features $g = \Psi \cdot (Zc)$ the same way as in theorem 3.2. However, this is not effective in the regime $M \leq N$ (remember that the benefit of kernel methods was the ability to cheaply crank N up).

Proposition 3.11 ([6]). *Suppose $M \leq N$ and $\sqrt{W}\Psi_X \in \mathbb{C}^{M\times N}$ has full rank. Then for any eigenpair (λ, c) of $\widehat{K}$, the residual*

$$res_{N,M}(\lambda, Zc) = 0. \tag{3.61}$$

Proof. Write

$$\sqrt{W}(\Psi_Y - \lambda\Psi_X)(Zc) = \sqrt{W}\Psi_Y Zc - \lambda Q\Sigma c = \sqrt{W}\Psi_Y\Psi_X^*\sqrt{W}Q\Sigma^\dagger c - \lambda Q\Sigma c. \tag{3.62}$$

Since $\sqrt{W}\Psi_X$ has full rank, the singular value matrix Σ in $\sqrt{W}\Psi_X = Q\Sigma Z^*$ is invertible, and so $\sqrt{W}\Psi_Y\Psi_X^*\sqrt{W}Q\Sigma^\dagger = Q\Sigma\widehat{K}$. Inserting, we see

$$\sqrt{W}(\Psi_Y - \lambda\Psi_X)(Zc) = Q\Sigma(\widehat{K} - \lambda I)c = 0. \tag{3.63}$$

□

The proposition suggests that we are suffering from *overfitting* of the snapshot data. We therefore require a different way to associate a residual to the eigenpair.

Recall from equation 3.28 that $\text{res}_{N,M}$ has an alternative represtnation as a regression error. We could analogously ask if $\widehat{K}$ is the solution of a different regression problem.

Let

$$\widehat{\Psi_X} = \left(\sqrt{W}\Psi_X\right)^* Q\Sigma^\dagger = Z, \quad \widehat{\Psi_Y} = \left(\sqrt{W}\Psi_Y\right)^* Q\Sigma^\dagger. \tag{3.64}$$

Then we have

$$\widehat{\Psi_X}^\dagger\widehat{\Psi_Y} = Z^*\left(\sqrt{W}\Psi_Y\right)^* Q\Sigma^\dagger = \left(\Sigma^\dagger Q^*\right)\left(\sqrt{W}\Psi_X\Psi_Y^*\sqrt{W}\right)\left(Q\Sigma^\dagger\right) = \widehat{K}^*. \tag{3.65}$$

Hence $\widehat{K}^*$ is precisely the solution to the least squares problem

$$\min_{B\in\mathbb{C}^{M\times M}} \left\|\widehat{\Psi_Y} - \widehat{\Psi_X}B\right\|. \tag{3.66}$$

This means that for a candidate eigenpair (λ, c) of $\widehat{K}^*$, the regression error is given by

$$\widehat{\text{res}}_{N,M}(\lambda, c) = \left\|\left(\widehat{\Psi_Y} - \lambda\widehat{\Psi_X}\right)c\right\|. \tag{3.67}$$

To provide a computable formulation we write

$$\widehat{\mathrm{res}}_{N,M}(\lambda, c)^2 = \left\| \left(\Psi_Y^* - \lambda \Psi_X^*\right) \sqrt{W} \left(Q\Sigma^\dagger c\right) \right\|^2 \tag{3.68}$$

which, after expanding the squared norm as in equation 3.33, can be written as

$$c^* \left(\Sigma^\dagger Q^*\right) \left(\sqrt{W}\Psi_Y \Psi_Y^* \sqrt{W} - \bar{\lambda}\widehat{A} - \bar{\lambda}\widehat{A}^* + |\lambda|^2 \widehat{G} \right) \left(Q\Sigma^\dagger\right) c. \tag{3.69}$$

Notice $\left(\Sigma^\dagger Q^*\right) \widehat{G} \left(Q\Sigma^\dagger\right) = I$ and $\left(\Sigma^\dagger Q^*\right) \widehat{A} \left(Q\Sigma^\dagger\right) = \widehat{K}$. Finally, letting

$$\widehat{J} = \sqrt{W}\Psi_Y \Psi_Y^* \sqrt{W} = \left(\, k(S(x_i), S(x_j)) \, \right)_{i,j=1}^M \tag{3.70}$$

we have that

$$\widehat{\mathrm{res}}_{N,M}(\lambda, c)^2 = c^* \left(\left(\Sigma^\dagger Q^*\right) \widehat{J} \left(Q\Sigma^\dagger\right) - \bar{\lambda}\widehat{K} - \lambda \widehat{K}^* + |\lambda|^2 I \right) c. \tag{3.71}$$

At this point it is unclear whether $\widehat{\mathrm{res}}$ has any physical meaning. It is an error metric for some arbitrary seeming least squares regression problem with matrices $\widehat{\Psi_X}$ and $\widehat{\Psi_Y}$ which do not have a clear interpretation. The current state of research in this kernelized method stops here.

However, the fact that the *adjoint* $\widehat{K}^*$ solves the least squares problem, should give the reader a suspicion that the least squares problem might have more to do with the Perron-Frobenius operator than with the Koopman operator.

Algorithm 5 Kernel ResDMD

Require: kernel $k : \Omega \times \Omega \to \mathbb{C}$, data points and weights $\{(w_i, x_i)\}_{i=1}^M$, compression factor $r \leq M$, grid $\{z_\nu\}_{\nu=1}^T \subset \mathbb{C}$, tolerance ϵ

1: Construct $\widehat{G}$, $\widehat{A}$ as in 3.54, 3.55
2: Compute an eigendecomposition $\widehat{G} = Q\Sigma^2 Q^*$
3: Let $\widehat{\Sigma}$, $\widehat{Q}$ be as in agorithm 4
4: Construct $\widehat{K}$, $\widehat{J}$ as in 3.57, 3.70 (with $\widehat{Q}$ and $\widehat{\Sigma}$)
5: **for** z_ν **do**
6: Compute $\widehat{\mathrm{res}}(z_\nu) := \min_{\|c\|=1} \widehat{\mathrm{res}}(z_\nu, c)$, which is equivalent to finding the smallest eigenvalue of the matrix in 3.71
7: **return** $\{z_\nu \mid \widehat{\mathrm{res}}(z_\nu) < \epsilon\}$

3.5.2 The Perron-Frobenius Connection

It is worth reexamining equation 3.60. Returning for a moment to the case $N \leq M$ we have

$$\begin{aligned} \widehat{K}^* &= Z^* K^* Z \\ &= Z^* A^* G^{-1} Z \\ &= Z^* G G^{-1} A^* G^{-1} Z \\ &= (Z^* G)\, P \left(G^{-1} Z\right) \\ &= \left(\Sigma^2 Z^*\right) P \left(\Sigma^2 Z^*\right)^\dagger \end{aligned} \tag{3.72}$$

where we used that G is symmetric and (when $N \leq M$) invertible. While this may not be true in $N \geq M$, there still is one connection: compare equations 3.47 and 3.69. One sees that up to conjugation of λ and multiplication of a factor $\Sigma^2 Z^*$ they coincide exactly.

Since Q and Z are both finite-dimensional isometries, they do not affect the minimal value of 3.47 or 3.69. In the regime $N \leq M$, $G = Z\Sigma^2 Z^*$, Σ^2 holds the norm of the features after being linearly combined into an $\mathcal{X}$-orthogonal basis. Hence $Q\Sigma^\dagger$ in

$$\widehat{\mathrm{res}}_{N,M}(\lambda)^2 = \min_{\|c\|=1} c^* \left(\Sigma^\dagger Q^*\right) \left(\widehat{J} - \bar{\lambda}\widehat{A} - \lambda\widehat{A}^* + |\lambda|^2 \widehat{G}\right) \left(Q\Sigma^\dagger\right) c \tag{3.73}$$

serves the same purpose as the stiffness matrix G in

$$\widetilde{\mathrm{res}}_{N,M}(\lambda)^2 := \min_{c^* G c = 1} (\Psi_X c)^* \left(\widehat{J} - \lambda\widehat{A} - \bar{\lambda}\widehat{A}^* + |\lambda|^2 \widehat{G}\right) (\Psi_X c)\,. \tag{3.74}$$

In particular we see

$$\widehat{\mathrm{res}}_{N,M}(\lambda) = \widetilde{\mathrm{res}}_{N,M}(\bar{\lambda}) \tag{3.75}$$

so that algorithm 5 computes precisely the pseudospectrum of $P\mathcal{L}P$ as in 3.46.

So what happens in the regime $N \geq M$? In this regime, $L = G^{-1}A^*$ breaks down since $\Psi_X^\dagger = \left(\Psi_X^* \Psi_X\right)^{-1} \Psi_X^*$ no longer holds (rather, $\Psi_X^\dagger = \Psi_X^* \left(\Psi_X \Psi_X^*\right)^{-1}$). Nonetheless, $\widehat{\mathrm{res}}$ is still well-defined, it just loses its physical meaning.

4 Benchmark Examples

Having studied the current most popular Koopman operator approximation scheme in theory, it is time to set it in practice. Figures 2.1, 2.2, 3.1, 3.2 already show convincing results. We continue with three more results, showing both advantages and disadvantages of dynamic mode decompositions.

4.0.1 Duffing Oscillator

4.0.2 Alanine Dipeptide Molecule

4.0.3 Blaschke Products

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