Anti-Koopmanism

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Abstract

This article addresses several longstanding misconceptions concerning Koopman operators, including the existence of lattices of eigenfunctions, common eigenfunctions between Koopman operators, and boundedness and compactness of Koopman operators, among others. Counterexamples are provided for each misconception. This manuscript also proves that the Gaussian RBF's native space only supports bounded Koopman operator corresponding to affine dynamics, which shows that the assumption of boundedness is very limiting. A framework for DMD is presented that requires only densely defined Koopman operators over reproducing kernel Hilbert spaces, and the effectiveness of this approach is demonstrated through reconstruction examples.

1 Introduction

Dynamic mode decomposition (DMD) has been gaining traction as a model-free method of making short-run predictions for nonlinear dynamical systems using data obtained as snapshots of trajectories. DMD and its variant, extended DMD, have proven effective at extracting underlying governing principles for dynamical systems from data, and reconstruction methods using DMD allow for the modeling of nonlinear dynamical systems as a sum of exponential functions, which is analogous to models obtained for linear systems (Kutz et al., 2016).

DMD is closely connected to the Koopman operator corresponding to discrete time dynamical systems (Schmod, 2010). The Koopman Operator $\mathcal{K}_F$ over a Hilbert function space, H, is a composition operator corresponding to the discrete time dynamics, $F : \mathbb{R}^n \to \mathbb{R}^n$, acting on functions in the Hilbert space. Specifically, $\mathcal{K}_F g = g \circ F$. In the context of discrete time dynamical systems, F is the discrete time dynamics that maps the current state of the system to a future state $x_{i+1} = F(x_i)$. Frequently, the function $g \in H$ is referred to as an *observable*.

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DMD aims to obtain a finite rank representation of the Koopman operator by studying its action on the full state observable (i.e. the identity function) (Schmod, 2010). Koopman operators over reproducing kernel Hilbert spaces (RKHSs) were studied to take advantage of infinite dimensional feature spaces to extract more information from the snapshots of a system in Williams et al. (2015a). This perspective also enacts a dimensionality reduction by formulating the DMD method in a reproducing kernel Hilbert space (RKHS) framework and implicitly using the kernel trick to compute inner products in the high-dimensional space of observables. In (Williams et al., 2015b), it is shown that kernel-based DMD produces a collection of Koopman modes that agrees with other DMD results in the literature.

However, present in the literature are several misconceptions concerning Koopman operators and their properties (cf. Budišić et al. (2012); Kutz et al. (2016); Brunton and Kutz (2019)). These properties include boundedness, a lattice of eigenfunctions, common eigenfunctions, and many others. In many cases, each of these concepts arose from particular examples, where tools from ergodic theory or the study of Banach algebras allow for many of these ideas to work, but these concepts don't generally extend to a data driven context, where samples and particular Hilbert spaces are used in the execution of DMD methods. In particular, boundedness has been implicitly assumed, when there is no restriction on the selection of observables from a Hilbert space. Many of these misconceptions arise from an agnostic approach to the domain and codomain of Koopman operators, which ignores the structure of the underlying vector spaces that the operator is posed over. As properties of operators directly depend on their underlying spaces, this manuscript presents a thorough and transparent treatment of the Koopman operator as a densely defined operator over a RKHS, and several counterexamples are presented to dispel misconceptions. It should be emphasized, that even though these misconceptions are present in the literature, they have little impact on the practice of DMD, where there are a tremendous number of outstanding results present in the field. This manuscript is focused on a particular collection of misconceptions concerning the underlying operator theory.

The paper is organized as follows. Sections 2 and 3 provide a brief overview of reproducing kernel Hilbert spaces, and Koopman operators, respectively. Section 4 provide several counter examples to many of the misconceptions concerning Koopman operators in the field. Additionally, Section 4 proves that the only bounded Koopman operators over the Gaussian RBF's native space are those corresponding to affine dynamics. Section 5 details a DMD algorithm leveraging only the assumption that the Koopman operators are densely defined, and that they contain the kernel functions within their domain. A numerical example is provided in Section 6 and Section 7 concludes the paper.

2 Reproducing Kernel Hilbert Spaces

A Reproducing Kernel Hilbert Space (RKHS) H over a set X is a Hilbert space composed of functions from X to $\mathbb{C}$ such that for all $x \in X$ the evaluation functional $E_x f := f(x)$ is bounded. Therefore, for all $x \in X$ there exists a function $K_x \in H$ such that $f(x) = \langle f, K_x \rangle$ for all $f \in H$. The function K_x is the reproducing kernel function centered at x and the function $K : X \times X \to \mathbb{C}$ defined by $K(x, y) = \langle K_y, K_x \rangle$ is the unique kernel function corresponding to H (Aronszajn, 1950). Throughout most of this manuscript, the methods used will be restricted to RKHSs of real valued functions. However, for some specific examples in Section 4, it will be more convenient to employ RKHSs of complex valued functions.

Reproducing kernels can be equivalently expressed as realizations of inner products of feature space mappings in $\ell^2(\mathbb{N})$. In particular, given an orthonormal basis for a RKHS, $\{e_m(\cdot)\}_{n=1}^{\infty} \subset H$, the kernel function may be expressed as $K(x, y) = \sum_{m=1}^{\infty} e_m(x)\overline{e_m(y)}$, where $\Psi(x) := (e_1(x), e_2(x), \ldots) \in \ell^2(\mathbb{N})$ is called a feature map. Equivalently, given a feature mapping $\Psi : X \to \ell^2(\mathbb{N})$, there is a RKHS whose kernel function is given as $K(x, y) = \langle \Psi(x), \Psi(y) \rangle_{\ell^2}$.

We will make repeated use of projections onto finite dimensional vector spaces arising from spans of collections of kernel functions centered at snapshots from a dynamical system. For a collection of centers $\{x_1, \ldots, x_m\}$ the projection of a function $g \in H$ onto $\alpha = \operatorname{span}\{K_{x_1}, \ldots, K_{x_m}\}$ is given as $\operatorname{argmin}_{h \in \alpha} \|h - g\|$, which can be resolved by expressing h as $h = \sum_{i=1}^{m} w_i K_{x_i}$, expanding $\| \sum_{i=1}^{m} w_i K_{x_i} - g \|^2$ via inner products, and finally setting the derivative with respect to

$w := (w_1, \ldots, w_m)^T \in \mathbb{R}^m$ to zero. This results in the following expression for the weights

$$\begin{pmatrix} w_1 \\ \vdots \\ w_m \end{pmatrix} = \begin{pmatrix} K(x_1, x_1) & \cdots & K(x_1, x_m) \\ \vdots & \ddots & \vdots \\ K(x_m, x_1) & \cdots & K(x_m, x_m) \end{pmatrix}^{-1} \begin{pmatrix} g(x_1) \\ \vdots \\ g(x_m) \end{pmatrix}$$

Hence, the projection is defined by $P_\alpha g := \sum_{i=1}^m w_i K_{x_i}$ where the weights are obtained as above.

3 Koopman Operators over RKHSs

Let H be a RKHS over $\mathbb{R}^n$. For a function $F : \mathbb{R}^n \to \mathbb{R}^n$ we define the Koopman Operator (sometimes called a composition operator), $\mathcal{K}_F : \mathcal{D}(\mathcal{K}_F) \to H$, as $\mathcal{K}_F g = g \circ F$ where $\mathcal{D}(\mathcal{K}_F) = \{g \in H : g \circ F \in H\}$. When $\mathcal{D}(\mathcal{K}_F)$ is dense in H, $\mathcal{K}_F$ is said to be densely defined. While not all densely defined Koopman operators over RKHSs are bounded, they are all closed operators.

Lemma 1. *Let $F : X \to X$ be the symbol for a Koopman operator over a RKHS H over a set X. $\mathcal{K}_F : \mathcal{D}(\mathcal{K}_F) \to H$ is a closed operator where $\mathcal{D}(\mathcal{K}_F)$ is given above.*

Proof. Suppose that $\{g_m\}_{m=1}^\infty \subset \mathcal{D}(\mathcal{K}_F)$ such that $g_m \to g \in H$ and $\mathcal{K}_F g_m \to h \in H$. To show that $\mathcal{K}_F$ is closed, we must show that $g \in \mathcal{D}(\mathcal{K}_F)$ and $\mathcal{K}_F g = h$. This amount to showing that $h = g \circ F$, by the definition of $\mathcal{D}(\mathcal{K}_F)$. Fix $x \in X$, then

$$\begin{aligned} h(x) = \langle h, K_x \rangle &= \lim_{m\to\infty} \langle \mathcal{K}_F g_m, K_x \rangle = \lim_{m\to\infty} g_m(F(x)) \\ &= \lim_{m\to\infty} \langle g_m, K_{F(x)} \rangle = \langle g, K_{F(x)} \rangle = g(F(x)). \end{aligned}$$

As x was an arbitrary point in X, $h = g(F(x))$ and the proof is complete. □

As Koopman operators are densely defined and closed over RKHSs, their adjoints are densely defined and closed as well (Pedersen, 2012). Given the kernel function centered at x, $\langle \mathcal{K}_F g, K_x \rangle = \langle g \circ F, K_x \rangle = g(F(x)) = \langle g, K_{F(x)} \rangle$. Thus, $K_x \in \mathcal{D}(\mathcal{K}_F^*)$ for all $x \in X$, and $\mathcal{K}_F^* k_x = k_{F(x)}$. Hence, each kernel function is in the domain of the adjoint of a densely defined Koopman operator.

4 Misconceptions Concerning Koopman Operators

There are several long standing misconceptions concerning Koopman operators and their properties. Many of these misconceptions go back as far as (Budišić et al., 2012) and still appear in recent textbooks and review papers (Kutz et al., 2016; Brunton and Kutz, 2019), and while they do not negatively impact the practical implementation of DMD and other Koopman based methods, they should be addressed. Most of these misconceptions and occasional errors stem from an agnostic treatment of the underlying vector spaces in which the Koopman operator acts. To wit, properties of the Koopman operator strongly depend on the selection of underlying vector space, and boundedness, compactness, eigenvalues, etc. change based on this selection. While Koopman operators were introduced by Koopman in 1931 in (Koopman, 1931) and then later picked up by the data science community in the early 2000s (e.g. (Mezić, 2005)), the study of composition operators and their properties continued in earnest througout the 20th century as composition operators (e.g. (Shapiro, 2012)). The extensive work on composition operators by the function theoretic operator theory community will help facilitate the discussion here.

4.1 Misconceptions concerning Sampling and Discretizations

4.1.1 Sampling and Data Science

Fundamental to any data science method is the collection and exploitation of samples. Machine learning techniques leverage samples to gain an approximation of a function. Sometimes these functions are classifiers, such as in support vector machines as in (Steinwart and Christmann, 2008), they can be continuous time signals as in (Higgins et al., 1996), and many other quantities (cf. (Hastie et al., 2009)). Sampling theory has a long history and are closely intertwined with RKHSs, where Shanon's sampling theory introduced in (Shannon, 1948) was placed on solid theoretical footing by

G. H. Hardy through the introduction of the Paley-Wiener space in (Hardy, 1941). What is important to note is that sampling theory requires that the underlying space where samples are being exploited is a function space. This requirement rules out the space $L^2(\mathbb{R}^n)$ as a domain of the Koopman operator for Dynamic Mode Decompositions as suggested by many sources such as (Kutz et al., 2016), (Klus et al., 2015), and (Takeishi et al., 2017), since $L^2(\mathbb{R}^n)$ is a space of *equivalence classes* of functions. Every two elements of $L^2(\mathbb{R}^n)$ are allowed to agree over any finite collection of samples, and thus samples have no meaning in $L^2(\mathbb{R}^n)$. Note that in (Takeishi et al., 2017), it is assumed that there is a finite dimensional invariant subspace for the Koopman operator, which changes the problem to a finite dimensional linear algebra problem, but at the cost of a very strong restriction on the Koopman operator.

4.1.2 Forward Invariant Dynamics

In applications, Koopman operators enter the theory of continuous time dynamics through a discretization of the continuous time dynamical system. That is, given the dynamical system $\dot{x} = f(x)$, the system is discretized through the selection of a fixed time-step, $\Delta t > 0$, as $x_{m+1} = x_m + \int_{t_m}^{t_m+\Delta t} f(x(t))dt$, where the right hand side plays the role of the discrete dynamics. However, for such a discretization to exist for arbitrarily large values of m, it is necessary that the dynamics be *forward invariant*.

For example, consider the one dimensional dynamics, $\dot{x} = 1 + x^2$. For fixed $0 < \Delta t < \pi/2$, the corresponding discrete time dynamics are given as $x_{m+1} = \tan(\arctan(x_m) + \Delta t)$. Setting $x_m = \tan(\pi/2 - \Delta t)$, it is clear that x_{m+1} is undefined. Consequently, the composition symbol, $F(x) = \tan(\arctan(x) + \Delta t)$ for the hypothetical Koopman operator, is not well defined over $\mathbb{R}^n$ for any selection of Δt.

The majority of papers dedicated to DMD leave this assumption unstated, such as (Li et al., 2017), and (Brunton et al., 2016), with (Bittracher et al., 2015) and (Mauroy and Mezić, 2016) being notable exceptions.

4.2 Properties of the Operators

In this section, we consider a single simple example. Consider the dynamical system $\dot{x} = \begin{pmatrix} x_2 & -x_1 \end{pmatrix}^T$, which corresponds to circular dynamics in the plane. For any fixed $\theta := \Delta t$, the discretization of this system yields the linear discrete dynamics $x_{m+1} = \begin{pmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{pmatrix} x_m$. That is, the discretization corresponding to a fixed time-step corresponds to a fixed rotation of $\mathbb{R}^2$. To simplify the presentation, we use $\mathbb{C}$ as a model for $\mathbb{R}^2$, where rotation of the complex plane reduces to multiplication by a unimodular constant, $z_{m+1} = e^{i\theta} z_m$. The corresponding discrete time dynamics will be written as $F_\theta(z) := e^{i\theta} z$.

As a function space for definition of the Koopman operator, this section will consider the classical Fock space consisting of entire functions for most of the counterexamples, which is used extensively in Quantum Mechanics (Hall, 2013) and it is a space where operators have been well studied (Zhu, 2012). The Fock space is given as

$$F^2(\mathbb{C}) := \left\{ f(z) = \sum_{m=0}^{\infty} a_m z^m : \sum_{m=0} |a_m|^2 m! < \infty \right\}.$$

The Fock space is a RKHS, with kernel function $K(z, w) = e^{\bar{w} z}$. Kernel function for the Fock space over $\mathbb{C}^n$ may be obtained through a product of single variable kernels as $K(z, w) = e^{w^* z} = e^{\bar{w}_1 z_1} \cdots e^{\bar{w}_n z_n}$.

Closely related to the Fock space is the exponential dot product kernel, $e^{x^T y}$, where for a single variable, the exponential dot product kernel's native space may be obtained by restricting the Fock space to the reals, and then taking the real part of the restricted functions. Through a conjugation of the exponential dot product kernel, the Gaussian RBF may be obtained as $K_G(x, y) = e^{-\|x\|^2/2} e^{x^T y} e^{-\|y\|^2/2} = \exp\left(-\frac{\|x-y\|^2}{2}\right)$, and performing the same operation on the Fock space kernel over $\mathbb{C}^n$ yields $K_G(z, w) = e^{-z^2/2} e^{w^* z} e^{-\bar{w}^2/2} = \exp\left(-\frac{(z-\bar{w})^2}{2}\right)$, which is

the kernel corresponding to the complexified native space for the Gaussian radial basis function over $\mathbb{C}^n$ (cf. (Steinwart and Christmann, 2008)). This space may be expressed as

$$H_G^2(\mathbb{C}) = \left\{ g(z)e^{-z^2/2} : g \in F^2(\mathbb{C}^n) \right\},$$

and the native space corresponding to the Gaussian RBF can be obtained by taking the real parts of functions from H_G^2 and restricting to $\mathbb{R}^n$.

4.2.1 Lattice of Eigenfunctions

As presented in (Budišić et al., 2012), there is a misconception that the eigenfunctions for the Koopman operator form a lattice. That is if φ_1 and φ_2 are two eigenfunctions for the Koopman operator, then so is $\varphi_1 \cdot \varphi_2$. This assumes that the product of these eigenfunctions are also members of the underlying vector space. There are circumstances where this would hold, such as the space of continuous functions and other Banach algebras. For example, (Klus et al., 2015) discuss lattices of eigenfunctions for the setting of $L^1(\mathbb{R}^n)$, which is a Banach algebra, but that paper does not make a distinction when discussing $L^2(\mathbb{R}^n)$. However, Hilbert spaces are not generally Banach algebras, and since it is desirable to work over Hilbert spaces for properties such as best approximations, projections, and orthonormal bases among others (cf. (Folland, 1999)), it is important to demonstrate that this property of eigenfunctions of Koopman operators does not hold in general.

Setting $\theta = \pi$, the discrete dynamics corresponding to rotation by π in the complex plane becomes $z_{m+1} = e^{i\pi} z_m = -z_m$. That is the corresponding Koopman operator, $\mathcal{K}_{F_\pi} : F^2(\mathbb{C}) \to F^2(\mathbb{C})$, is given as $\mathcal{K}_{F_\pi} g(z) := g(-z)$. Hence, every even function is an eigenfunction for this Koopman operator with eigenvalue 1.

An important property of the Fock space should be noted. That is, given $g \in F^2(\mathbb{C})$, the function g exhibits a strict bound on its growth rate (cf. (Zhu, 2012)). To wit, $|g(z)| = |\langle g, K(\cdot, z)\rangle_{F^2(\mathbb{C})}| \leq \|g\|_{F^2(\mathbb{C})} \|K(\cdot, z)\|_{F^2(\mathbb{C})} = \|g\|_{F^2(\mathbb{C})} e^{\frac{|z|^2}{2}}$. That is, if a function is in the Fock space then the function is of order at most 2, and if the function is of order 2 it has type at most $1/2$ (cf. (Boas, 2011)). Conversely, if an entire function is of order less than 2, it is in the Fock space, and if it is of order 2 and type less than $1/2$, then it is also in the Fock space. While functions of order 2 and type $1/2$ can be in the Fock space, it does not hold for every such function. For example, $e^{z^2/2}$ is of order 2 and type $1/2$, but is not in the Fock space.

Thus, $\varphi(z) = e^{z^2/4}$ is an eigenfunction for $\mathcal{K}_{F_\pi}$ in the Fock space. However, $\varphi \cdot \varphi = e^{z^2/2}$ is not in the Fock space, and cannot be an eigenfunction for $\mathcal{K}_{F_\pi} : F^2(\mathbb{C}) \to F^2(\mathbb{C})$. *Hence, the eigenfunctions for $\mathcal{K}_{F_\pi}$ do not form a lattice.*

4.2.2 Common Eigenfunctions

The intuition behind the use of Koopman operators in the study of continuous time dynamical systems is that eigenfunctions for the Koopman operators should be "close" to that of the Koopman generator for small timesteps. Moreover, (Brunton and Kutz, 2019) (equation (7.64)) expresses strong operator topology limits of Koopman eigenfunctions as the time-step approaches zero. However, there is a missing parameter in these equations, where the eigenfunctions are not expressed with their step size dependence. The absence of step size dependence belies the assumption that the eigenfunctions are common between Koopman operators corresponding to different fixed step sizes.

To dispel this misconception, set $\theta = \pi/2$, which yields $F_{\pi/2}(z) = iz$. In this case, the polynomial $z^4 + z^8 \in F^2(\mathbb{C})$ is an eigenfunction for the Koopman operator corresponding to $\theta = \pi/2$ with eigenvalue 1. However, $z^2 + z^8$ is not an eigenfunction for $\mathcal{K}_{F_{\pi/3}}$, as $(e^{i\pi/3}z)^4 + (e^{i\pi/3}z)^8 = e^{i4\pi/3}z^4 + e^{i2\pi/3}z^8$, and the constants cannot be factored out of the polynomial as an eigenvalue.

Hence, since each Koopman operator obtained through a fixed time-step may produce a different collection of eigenfunctions, there is no way to distinguish which, if any, should correspond to eigenfunctions of the Koopman generator.

4.2.3 Boundedness of Koopman Operators

In many contexts it is tacitly assumed that Koopman operators are bounded. In particular, an unrestricted selection of observables in the study of the Koopman operator means that the Koopman

operator is frequently assumed to be defined over the entire Hilbert space. In this setting, the Koopman operator is an operator whose domain is the entire Hilbert space that is also closed. Hence, by the closed graph theorem (cf. (Folland, 1999)), such an operator must be bounded. The collection of finite rank operators is dense in the collection of bounded operators over a Hilbert space in the strong operator topology (SOT) (cf. (Pedersen, 2012)). This was used in the work (Korda and Mezić, 2018) where the DMD routine was demonstrated to converge to a bounded Koopman operator in SOT, and cited by (Li et al., 2017), among others.

In fact, SOT convergence does not in general lead to convergence of the eigenvalues as mentioned in (Korda and Mezić, 2018), and the finite rank approximations produced by DMD algorithms should converge to Koopman operators in the operator norm topology to preserve spectral convergence. Hence, it is implicitly assumed in the literature that the Koopman operators are compact in addition to being bounded. It isn't immediately clear when one can expect a continuous dynamical system to yield a compact Koopman operator through discretizations. For example, the Koopman operator corresponding to discretizations of the continuous time system $\dot{x} = 0$ is the identity operator, I, for any fixed timestep, and I is not compact over any infinite dimensional Hilbert space.

In addition, for any given RKHS, the collection of bounded Koopman operators is very small. In particular, it was demonstrated in (Carswell et al., 2003) that a Koopman operator over the Fock space is bounded only when the corresponding discrete dynamics are *affine*. It follows that the same result holds over the exponential dot product kernel's native space.

It may perhaps be less obvious that this extends to the Gaussian RBF's native space, and a proof of this is given here. As far as the authors are aware, this is the first time this result has appeared in the literature, and it demonstrates that even for popular selections of RKHSs, the collection of bounded Koopman operators is small.

Lemma 2. *If $\mathcal{K}_F$ is a bounded operator over the Gaussian RBF's native space, then F is a real analytic vector valued function over $\mathbb{R}^n$.*

Proof. If $\mathcal{K}_F$ is bounded, then $\mathcal{K}_F K_y(x) = K_y(F(x)) = \exp(-\|F(x) - y\|^2)$ is in the RBF's native space for each $y \in \mathbb{R}^n$. Since every function in the RBF's native space is real analytic, so is $K_y(F(x))$, and thus, the logarithm, $-\|F(x) - y\|^2 = -\|F(x)\|^2 + 2y^T F(x) - \|y\|^2$ is real analytic. This holds if $y = 0$, and hence $\|F(x)\|^2$ is real analytic. Thus, for every y, the quantity $y^T F(x)$ is real analytic. That each component of $F(x)$ is real analytic follows from the selection of y as the cardinal basis elements of $\mathbb{R}^n$, and this completes the proof. □

Lemma 3. *If F is a real analytic vector valued function that yields a bounded Koopman operator, $\mathcal{K}_F$, over a the Gaussian RBF's native space, then its extension to an entire function, $F : \mathbb{C}^n \to \mathbb{C}^n$ induces a bounded operator over $H_G(\mathbb{C}^n)$.*

Proof. Since an entire function on $\mathbb{C}^n$ is uniquely determined by its restriction to $\mathbb{R}^n$, it follows that the span of the complex valued Gaussian RBFs with centers in $\mathbb{R}^n$ is dense in H_G. Moreover, to demonstrate that $\mathcal{K}_F$ is bounded, it suffices to show that there is a constant C such that

$$C^2 K_G(z, w) - K_G(F(z), F(w)) \tag{1}$$

is a positive kernel. By the above remark, it suffices to show this for real $x, y \in \mathbb{R}^n$, but then this is equivalent to the statement that $\mathcal{K}_F$ is bounded over the Gaussian RBF's native space over $\mathbb{R}^n$. □

Theorem 1. *If $F : \mathbb{C}^n \to \mathbb{C}^n$ is an entire function, and $\mathcal{K}_F$ is bounded on H_G, then $F(z) = Az + b$ for a matrix $A \in \mathbb{C}^{n \times n}$ and vector $b \in \mathbb{C}^n$.*

Proof. If $\mathcal{K}_F$ is bounded, then it has a bounded adjoint, $\mathcal{K}_F^*$, which acts on the complex Gaussian as $\mathcal{K}_F^* K_G(\cdot, z) = K_G(\cdot, F(z))$. In particular, there is a constant $C > 0$ such that $\|K_G(\cdot, F(z))\|^2 \leq C^2 \|K_G(\cdot, z)\|^2$. Noting the identity $\|K_G(\cdot, z)\|^2 = \exp\left(2\sum_{j=1}^n (\mathcal{I}z_j)^2\right)$ and taking the logarithm, it follows that

$$\sum_{j=1}^n (\mathcal{I}F_j(z))^2 \leq \log(C^2) + \sum_{j=1}^n (\mathcal{I}z_j)^2 \leq \log(C^2) + \|z\|^2. \tag{2}$$

From this inequality, it follows that for each coordinate $j = 1, \ldots, n$, the harmonic function $v_j(z) = \mathcal{I}F_j(z)$ has linear growth. That is, there is a constant $\tilde{C}$ so that $|v_j(z)| \leq \tilde{C}(1 + \|z\|)$ for

all $z \in \mathbb{C}^n$. It follows (e.g. from the standard Cauchy estimates) that $v_j(z) = v_j(x + iy)$ must be an affine linear function of x and y, and therefore, so must its harmonic conjugate $u_j(z)$, and we conclude that $F(z) = Az + b$. □

Corollary 1. *If F is a real analytic vector valued function, and $\mathcal{K}_F$ is bounded on the Gaussian RBF's native space over $\mathbb{R}^n$, then F is affine.*

Hence, for the most commonly used kernel function in machine learning, the collection of bounded (and hence compact) Koopman operators over its native space is restricted to only those Koopman operators corresponding to affine dynamics. Each selection of RKHS and kernel function will yield a correspondingly small collection of bounded Koopman operators. It should be noted that Koopman operators were completely classified for over the classical sampling space, the Paley-Wiener space (Chacón and Giménez, 2007), as also being those that correspond to affine dynamics, and it is a simple exercise to show that the native space for the polynomial kernel also only admits bounded Koopman operator when the dynamics are affine.

Consequently, in most practical respects Koopman operators should not be assumed to be bounded, and certainly not compact.

5 Dynamic Mode Decomposition with Koopman Operators over RKHSs

As a product of its genesis in the machine learning community, many DMD procedures appeal to feature space, and this continues to hold in the current implementations of kernel-based extended DMD (Williams et al., 2015b), which casts the snapshots from a finite dimensional nonlinear system into an infinite feature space. The direct involvement of the feature space in the estimation of the Koopman operator leads to rather complicated numerical machinery. To avoid directly computing the infinite dimensional vectors that result, an involved collection of linear algebra techniques are leveraged to extract the Koopman modes. Here it is shown that this process may be simplified and that a procedure that directly involves the kernel functions centered at the snapshots simplifies the design of DMD algorithms. This approach keeps to the spirit of the "kernel trick," where feature vectors should never be directly evaluated and only accessed through evaluations of the kernel function itself.

Throughout this algorithm, a Koopman operator will be assumed to be densely defined, as Section 4 demonstrated that most Koopman operators cannot be expected to be bounded or compact. An additional assumption will be made that the kernel functions themselves reside in the domain of the Koopman operator. It was demonstrated in Section 3 that the kernels are always in the domain of the adjoint, and so alternatively, a finite rank representation may be derived for the adjoint operator without adding an assumption.

Moreover, for the sake of discussion, it is assumed that the Koopman operator is actually diagonalizable, which shouldn't generally be expected to hold. However, the finite rank representations leveraged here are almost always diagonalizable, since the set of non-diagonalizable matrices are of measure zero in the collection of all matrices. Moreover, for periodic data sets, the adjoint of the Koopman operator will be invariant on the span of the collection of kernel functions centered at the snapshots, and thus, the finite rank representations will be explicitly the adjoint of the Koopman operator on that subspace, which supports the assumption of the availability of eigendecompositions for the Koopman operator in the periodic or quasiperiodic settings.

For a given collection of snapshots $\{x_1, x_2, ..., x_m\}$[1], the goal is to determine a finite rank representation of $\mathcal{K}_F$ that is derived from the kernel functions centered at the snapshots. To express a finite rank representation, the ordered basis $\alpha = \{k_{x_1}, ..., k_{x_{m-1}}\}$ is leveraged. In particular, if P_α is the projection on to $\operatorname{span}(\alpha)$, the operator $P_\alpha \mathcal{K}_F$ maps $\operatorname{span}(\alpha)$ to itself, which enables the discussion of eigenfunctions and eigenvalues of $\mathcal{K}_F$ using only functions in $\operatorname{span}(\alpha)$.

Suppose that given a function $g \in \operatorname{span} \alpha$, with coefficients $a_1, ..., a_{m-1}$, the function $P_\alpha \mathcal{K}_F g$ can be expressed in the basis α using the coefficients $b_1, ..., b_{m-1}$. As a result, the operator $P_\alpha \mathcal{K}_F$ can be represented using a matrix that maps the vector $(a_1, ..., a_{m-1})^T$ to the vector $(b_1, ..., b_{m-1})^T$. In the following development, the finite rank representation of $P_\alpha \mathcal{K}_F$, expressed in a matrix form, is

[1]While availability of a time series of snapshots $\{x_1, x_2, ..., x_m\}$ such that $x_{i+1} = F(x_i)$ is a more typical use case, the developed method does not require such a time series. It can also be implemented using arbitrary snapshots $\{x_1, x_2, ..., x_m\}$ and $\{y_1, y_2, ..., y_m\}$ provided $y_i = F(x_i)$.

denoted by $[P_\alpha \mathcal{K}_F]_\alpha^\alpha$, where the notation $[\cdot]_\alpha^\alpha$ indicates that both the domain and range of $P_\alpha \mathcal{K}_F$ is restricted to $\mathrm{span}(\alpha)$.

Consequently, the ith column of $[P_\alpha \mathcal{K}_F]_\alpha^\alpha$ may be determined through the examination of the action of the operator $P_\alpha \mathcal{K}_F$ on the basis function K_{x_i}, for $i = 1, \ldots, m-1$. Using the fact that $\mathcal{K}_F K_{x_i}(x) = K_{x_i}(F(x))$, $[P_\alpha \mathcal{K}_F]_\alpha^\alpha$ may be written as

$$[P_\alpha \mathcal{K}_F]_\alpha^\alpha = \begin{pmatrix} K(x_1, x_1) & \cdots & K(x_1, x_{m-1}) \\ \vdots & \ddots & \vdots \\ K(x_{m-1}, x_1) & \cdots & K(x_{m-1}, x_{m-1}) \end{pmatrix}^{-1} \begin{pmatrix} K(x_2, x_1) & \cdots & K(x_2, x_{m-1}) \\ \vdots & \ddots & \vdots \\ K(x_m, x_1) & \cdots & K(x_m, x_{m-1}) \end{pmatrix}.$$

It should be noted that this is precisely the pair of matrices examined in (Williams et al., 2015b) after the use of a truncated SVD.

The objective of DMD is to use the finite rank representation determined above to create a data driven model of the dynamical system. This makes use of a fundamental property of eigenfunctions of the Koopman operator. In particular, suppose that φ is an eigenfunction of $\mathcal{K}_F$ with eigenvalue λ. Evaluating the eigenfunction at a snapshot reveals $\varphi(x_{i+1}) = \varphi(F(x_i)) = \mathcal{K}_F \varphi(x_i) = \lambda \varphi(x_i)$. Hence, $\phi(x_{i+1}) = \lambda^i \phi(x_1)$. Now suppose that $\{\varphi_j\}_{j=1}^\infty$ is an eigenbasis for a diagonalizable Koopman operator, $\mathcal{K}_F$, corresponding to the eigenvalues $\{\lambda_j\}_{j=1}^\infty$. For a state $x \in \mathbb{R}^n$, let $(x)_d$ be the d-th component of x for $d = 1, \ldots, n$. If it is assumed that the mapping $x \mapsto (x)_d$ is in the RKHS (as it is when H is the native space for the exponential dot product space (Steinwart and Christmann, 2008)), then it may be expressed as $(x)_d = \lim_{M\to\infty} \sum_{j=1}^M (\xi_{j,M})_d \varphi_i(x)$ for some coefficients $\{(\xi_{j,M})_d\}_{j=1}^\infty$. Note that since the Koopman operator is not generally a normal operator, φ_i is not expected to be an orthonormal basis, and hence, there may be nonzero influences between the coefficients obtained by projection and this is expressed by the additional index M in $\xi_{j,M}$. *Hence, Koopman modes are not fixed quantities unless there is an orthonormal basis of eigenfunctions for the Koopman operator.* By stacking each $(x)_d$, the full state observable g_{id}, given by $g_{id}(x) = x$, is expressed as

$$g_{id}(x) = \lim_{M\to\infty} \sum_{j=1}^M \xi_{j,M} \varphi_j(x). \tag{3}$$

Hence, each snapshot may be reconstructed as

$$x_{i+1} = \lim_{M\to\infty} \sum_{j=1}^M \xi_{j,M} \lambda_j^i \varphi_j(x_1). \tag{4}$$

Since the Koopman operator is approximated here by a finite rank representation, perfect reproduction of g_{id} through a series of eigenfunctions is not possible. Instead, eigenfunctions determined through the finite rank representation are used to construct the approximation of g_{id}. In particular, the matrix $[P_\alpha \mathcal{K}_F]_\alpha^\alpha$ is the matrix representation of $P_\alpha \mathcal{K}_F$. If v_j is an eigenvector for the matrix $[P_\alpha \mathcal{K}_F]_\alpha^\alpha$ with eigenvalue λ_j, then

$$P_\alpha \mathcal{K}_F \left(\sum_{i=1}^{m-1} (v_j)_i K(x, x_i) \right) = \begin{pmatrix} K(x, x_1) \\ \vdots \\ K(x, x_{m-1}) \end{pmatrix}^T [P_\alpha \mathcal{K}_F]_\alpha^\alpha v_j = \lambda_j \sum_{i=1}^{m-1} (v_j)_i K(x, x_i).$$

That is, $\sum_{i=1}^{m-1} (v_j)_i K(x, x_i)$ is an eigenfunction of $P_\alpha \mathcal{K}_F$. The corresponding normalized eigenfunction is denoted by $\hat{\varphi}_j(x) := \frac{1}{\sqrt{v_j^T G v_j}} \sum_{i=1}^{m-1} (v_j)_i K(x, x_i)$, where $G = (K(x_i, x_\ell))_{i,\ell=1}^{m-1}$ is the Gram matrix associated with the snapshots and kernel function.

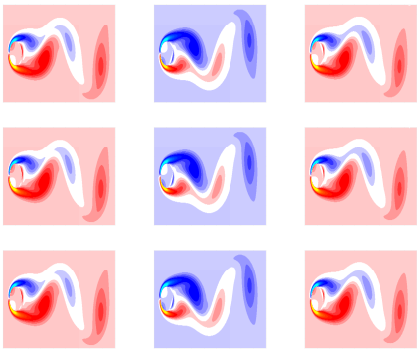
Using a finite rank representation of (3), it is easy to see that the d-th row of the matrix $\hat{\xi} := \begin{pmatrix} \hat{\xi}_1 & \ldots & \hat{\xi}_{m-1} \end{pmatrix}$ of Koopman modes is comprised of the components of $(x)_d$ along the (non-orthogonal) directions $\hat{\varphi}_j$. That is, $g_{id}(x_i) = x_i = \sum_{j=1}^{m-1} \xi_j \hat{\varphi}_j(x_i)$, which yields $\hat{\xi} = X \left(V^T G\right)^{-1}$, where $X := \begin{pmatrix} x_1 & \ldots & x_{m-1} \end{pmatrix}$ is the data matrix and

$$V := \begin{pmatrix} \frac{v_1}{\sqrt{v_1^T G v_1}} & \cdots & \frac{v_{m-1}}{\sqrt{v_{m-1}^T G v_{m-1}}} \end{pmatrix}$$

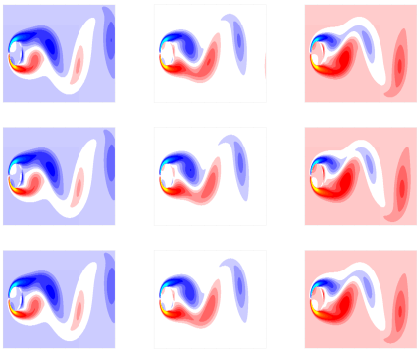
is the matrix of normalized eigenvectors of $[P_\alpha \mathcal{K}_F]_\alpha^\alpha$.

Using the approximate eigenfunctions, $\hat{\varphi}_j$, a data driven model for the system is obtained as

$$x_{i+1} \approx \sum_{j=1}^{m-1} \hat{\xi}_j \lambda_j^i \hat{\varphi}_j(x_1). \tag{5}$$



(a) This figure presents the reconstruction of the same time points using three different kernel functions. The first row contains the ground truth, the second leverages the Gaussian RBF kernel, and the third uses the exponential dot product kernel. The left column presents the reconstruction of the initial state, x_1. The middle column shows the reconstructions of the state, x_{15}, and the right column corresponds to the reconstruction of the state x_{30}. Note that each kernel generates nearly identical reconstructions of each state.



(b) This figure presents prediction of the same snapshots using three different kernel functions. The first row contains the ground truth, the second leverages the Gaussian RBF kernel, and the third uses the exponential dot product kernel. The left column presents the prediction of, x_{51}. The middle column shows the reconstructions of the state, x_{101}, and the right column corresponds to the reconstruction of the state x_{151}. Note that each kernel generates nearly identical prediction of the future states.

6 Numerical Example

The website accompanying the textbook (Kutz et al., 2016) provides several data sets that serve as benchmarks for spectral decomposition approaches to nonlinear modeling, which have been released to the public through their website at `http://www.dmdbook.com/`. This section utilizes the cylinder flow data set to demonstrate the results of the developed DMD method. The cylinder flow example is numerically generated, and the data provided corresponds to a planar steady state flow of the system. The data set consists of 151 snapshots, containing values of the vorticity of the flow at several mesh points in a plane, recorded every 0.02 seconds. In this demonstration, snapshots 1 through 30 are used as the input data, and snapshots 2 through 31 are used as output data, assuming that the ith and $(i+1)$th snapshots satisfy $x_{i+1} = F(x_i)$ for some unknown nonlinear function F.

The Koopman modes, eigenvalues, and eigenfunctions are then computed using the developed technique and snapshots 1 through 30 are reconstructed using (5). DMD is implemented using the exponential dot product kernel, $K(x,y) = \exp(\frac{1}{\mu} x^T y)$ (with $\mu = 500$), and the Gaussian RBF kernel, $K(x,y) = \exp\left(-\frac{1}{\mu}\|x-y\|_2^2\right)$ (with $\mu = 500$). Each of the kernels result in comparable reconstruction results that match with the input data as shown in Figure 1a.

To further demonstrate the accuracy of the obtained finite-dimensional representation of the Koopman operator, snapshots 32 through 151 are *predicted* using (5). As shown in Figure 1b, given the first 31 snapshots, the developed DMD technique is able to accurately predict the remaining 120 snapshots *without the knowledge of the underlying physics, F.*

7 Conclusion

This manuscript discusses several long standing misconceptions surrounding the Koopman operator, which includes notions of boundedness, eigenfunctions, the existence of a unique collection of

Koopman modes, and lattices of eigenfunctions. For each misconception, an example has been provided, where a major theoretical result was demonstrated that showed the Gaussian RBF's native space only supports bounded Koopman operators that correspond to affine dynamics. Moreover, this manuscript gives a kernel-based DMD algorithm that simplifies that of (Williams et al., 2015a).

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