Intrinsic and Extrinsic Approximation of Koopman Operators over Manifolds

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Abstract— This paper derives rates of convergence of certain approximations of the Koopman operators that are associated with discrete, deterministic, continuous semiflows on a complete metric space (X, d_X). Approximations are constructed in terms of reproducing kernel bases that are centered at samples taken along the system trajectory. It is proven that when the samples are dense in a certain type of smooth manifold $M \subseteq X$, the derived rates of convergence depend on the fill distance of samples along the trajectory in that manifold. Error bounds for projection-based and data-dependent approximations of the Koopman operator are derived in the paper. A discussion of how these bounds are realized in intrinsic and extrinsic approximation methods is given. Finally, a numerical example that illustrates qualitatively the convergence guarantees derived in the paper is given.

I. INTRODUCTION

Over the past decade an extensive literature has been archived on Koopman theory, and more generally on data-dependent approaches, for modeling various types of nonlinear systems. An idea of the breadth of applications of the theory can be gained by considering the work in [1], [2] for studies of molecular dynamics, or [3], [4] for applications to the study of fluid flows, or [5], [6] in the atmospheric sciences. A good account of the basics underlying Koopman theory can be found in texts like [7] or [8]. Recent notable references that feature some treatment of error estimates or convergence of Koopman operator approximations include [9], [10], [11], [12], [13]. The authors of [10] give an account of rates of approximation of certain Koopman operators in linear approximation spaces. This paper extends those results by relating the rates of approximation in terms of fill distances in manifolds.

The motivation for employing Koopman methods is now well-known: the theory provides an approach to the study of uncertain systems that makes extensive use of operator theory to enhance the understanding of the unknown dynamics. The theory is generally applicable to, indeed in a sense expressly designed for, the study of nonlinear systems. Koopman theory provides an elegant framework in which to carry out analysis of uncertain nonlinear dynamics as well as to develop data-driven algorithms for modeling and identification of such systems. To be sure, there are both theoretical and pragmatic reasons for the popularity of Koopman methods.

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As explained well in a number of other references such as [14], and in greater detail than is possible in this short conference paper, there is a fundamental trade-off in applying Koopman theory to a given nonlinear system. If we have a nonlinear system whose dynamics is poorly understood, Koopman theory *in principle* entails replacing the study of the system of interest, which is nonlinear and finite dimensional, with one that is linear and infinite dimensional. Since practical considerations dictate that finite dimensional representations are needed, questions regarding the convergence of approximations must be addressed in any full understanding of Koopman theory. Unfortunately, many of the finer points regarding the convergence of approximations of the Koopman operator are necessarily nuanced. The large number of explicitly cited papers above that have appeared over the past five years or so have carefully studied various questions related to convergence of Koopman approximations.

As motivation for this paper, it is useful to compare the state of the art in Koopman theory to that in the field of evolutionary partial differential equations (PDEs) or nonlinear regression. Several decades of research in these fields has resulted in a rich theory that relates rates of convergence of approximations to the choice of bases. Here, when we refer to rates of convergence we mean error bounds that are explicit in the dimension n of the space of approximants or the number of samples m, or both. As noted above, sufficient conditions that ensure convergence asymptotically as $n \to \infty$ or $m \to \infty$ are numerous in Koopman theory, whereas rates of convergence are far less common. There are many reasons for this. Approximations of the Koopman operator are typically generated using samples along the trajectory of an uncertain dynamical system, and consequently the domain over which approximations are to be constructed can be unknown *a priori*.

A. Summary of New Results

In this paper, a number of new results are derived that make precise the rates of convergence of approximations of some types of Koopman operators that are associated with deterministic flows on manifolds.

1) The Problem Setup and Formulation: We begin the analysis in this paper by assuming that we have discrete deterministic semiflow on a state space that is a complete metric space (X, d_X). Continuity of the semiflow is defined in terms of the metric d_X on the state space X. The continuous semiflow is induced by the autonomous recursion

$$\phi_{n+1} = f(\phi_n) \tag{1}$$

for some unknown function $f : X \to X$. Approximation results derived in this paper are stated for the Koopman operator $U_f g := g \circ f$. We let $\Omega_n := \{\xi_i \in X \mid 1 \leq i \leq n\}$ denote a finite set of observations of the state of the system, and the complete set of samples associated with some fixed initial condition is denoted $\Xi := \Xi(\phi_0) := \bigcup_{n \in \mathbb{N}} \Omega_n \subset \Gamma^+(\phi_0)$. Here $\Gamma^+(\phi_0) := \bigcup_{i \in \mathbb{Z}^+} \phi_i$ is the forward orbit through $\phi_0 \in X$. The samples Ξ are assumed to be dense in a limiting set Ω, which may coincide with the entire state space $\Omega = X$, or it can be a proper subset $\Omega \subset X$. One of the essential features of this paper is that the rates of convergence of approximations of the Koopman operator, which apply when it so happens that the limiting set Ω is a smooth manifold M, are given in terms of the fill distance $h_{\Omega_n, \Omega}$ of the finite collection of samples Ω_n in the limiting set Ω, $h_{\Omega_n, \Omega} := \sup_{x \in \Omega} \min_{\xi_i \in \Omega_n} d_X(x, \xi_i)$. Note that since we want $h_{\Omega_n, \Omega} \to 0$ as $n \to \infty$, it must be the case that the limiting set Ω is bounded in the analysis in this paper.

Realizations of approximations to the Koopman operator are built in this paper using finite dimensional spaces of approximants $H_{\Omega_n} := \operatorname{span}\{\mathfrak{K}_{X, \xi_i} \mid \xi_i \in \Omega_n\}$ with $\mathfrak{K}_{X, \xi_i}(\cdot) := \mathfrak{K}_X(\xi_i, \cdot)$ the basis function centered at the sample $\xi_i \in X$, where $\mathfrak{K}_X : X \times X \to \mathbb{R}$ is the kernel function that induces the native space of the reproducing kernel Hilbert space H_X.

2) Projection-Based Approximations: The first new result of the paper is stated in Theorem 2, and it applies when $\Omega = M$ is in fact a smooth, compact, connected, Riemannian manifold. In this case we select the native space H_M so that it is continuously embedded in a Sobolev space $W^{t,2}(M)$ of high enough order. This theorem gives sufficient conditions to ensure that the projection-based Koopman operator $U_f^n := (P_{\Omega_n}(\cdot)) \circ f$ satisfies a bound that has the form

$$\|U_f g - U_f^n g\|_{f^*(W^{s,2}(M))} \lesssim h_{\Omega_n, M}^{t-s} \|g\|_{W^{t,2}(M)} \tag{2}$$

for all g in the Sobolev space $W^{t,2}(M)$, provided that the limiting set Ω is in fact a smooth, connected, compact, Riemannian manifold $\Omega := M$. In this equation the error is measured in the pullback space $f^*(W^{s,2}(M))$, defined in Section II. The ranges for the smoothness indices t, s are dictated by the Sobolev embedding theorem and the "many zeros" theorem (Theorem 1) on manifolds. The bound in Equation 2 as of yet has no analog in the series of recent articles cited above for approximations of the Koopman operator.

3) Data-Dependent Approximations: The initial approximation $U_f^n(\cdot) := (P_{\Omega_n}(\cdot)) \circ f$ in Equation 2 uses the orthogonal projection operator $P_{\Omega_n} : H_M \to H_{\Omega_n}$, but this expression cannot be evaluated unless the function f is known. As shown in Section III, the operators $\mathfrak{U}_f^n$ can be constructed from the input-output samples $\{(\phi_i, y_i)\}_{1 \leq i \leq n} = \{(\phi_i, f(\phi_i))\}_{1 \leq i \leq n}$ along the discrete trajectory of the system in Equation 1. It is also worth noting that the realization of the coordinate representation of $\mathfrak{U}_f^n$ is closely related to the approximation of the Koopman operator that is defined

in terms of the Extended Dynamic Mode Decomposition (EDMD) algorithm [15], in the special case that the number of samples is equal to the dimension of the space of approximants. The definition above of $\mathfrak{U}_f^n$ makes sense only so long as $(P_{\Omega_n} g) \circ f \subseteq H_M$. Thus, a standing assumption in this case is that the pullback space $f^*(H_M) \subseteq H_M$. Since $(P_{\Omega_n} g) \circ f \in f^*(H_M)$, this structural assumption is enough to ensure that the data-driven operator $\mathfrak{U}_f^n$ is well-defined. Theorem 4 is representative of the type of bound that can be derived in this case. We have a pointwise error bound

$$|(U_f g)(x) - (\mathfrak{U}_f^n g)(x)| \leq C_M h_{\Omega_n, M}^{t-s} \|g\|_{W^{t,2}(M)}$$

for each $x \in M$ in terms of the fill distance of the samples Ω_n in the manifold M. Again, this result is novel among the articles in the recent literature on approximation of Koopman operators.

4) Intrinsic and Extrinsic Approximations: The representations of the approximations of the Koopman operator in this paper are explicit in terms of the kernel basis $\mathfrak{K}_{X, \xi_i}$ that is defined over the state space X, where $\mathfrak{K}_X : X \times X \to \mathbb{R}$ is the kernel that defines the reproducing kernel Hilbert (RKH) space H_X. In cases when the samples Ξ are dense in X, the kernel basis $\mathfrak{K}_{X, \xi_i}$ is defined from a kernel defined on all of X. A critical feature of the error bounds in the paper is that they are derived by assuming that the kernel induces a native space H_X that is embedded in or equivalent to a Sobolev space. In particular applications coming up with the needed closed form expressions for a kernel can sometimes be difficult. For this reason, we describe both intrinsic and extrinsic realizations of the approximation framework in this paper, which we describe next.

In all of the theorems developed in this paper, the limiting set Ω is assumed to be a smooth Riemannian manifold $M := \Omega$. In some cases the limiting set fills the entire state space $X = M = \Omega$, and in others it is a proper subset $M = \Omega \subset X$. When the limiting set $\Omega = M$ is in fact the entire state space X, it is possible to use an intrinsic approximation method since the manifold is known in this case. When we say that an approximation method is intrinsic, we mean that the kernel used in approximations is defined in terms of the intrinsic definition of the manifold M. For example, the kernel may be defined in terms of the eigenfunctions of a differential operator on the manifold. A fine analysis of rates of convergence for intrinsic approximations of functions are described in the set of papers [16], [17], [18]. However, coming up with the required closed form expressions is a nontrivial task for a general Riemannian manifold M and requires detailed knowledge of the form of the manifold M.

It is perhaps most usually the case in practical problems that the samples Ξ do not fill the entire state space X. Rather, the limiting set Ω in which the samples Ξ are dense is typically not known. In this case, even if the limiting set Ω is a nice smooth manifold, it is impossible to use a kernel basis $\mathfrak{K}_{M, \xi_i}$ that is defined intrinsically with respect to the manifold $M := \Omega$. In this latter case we employ an *extrinsic* approximation. A general study of extrinsic methods for approximation of functions can be found in [19]. We choose

a kernel $\mathfrak{K}_X$ that is well-defined and known on the large state space X, and we define a kernel on the manifold M by restriction. Even though the manifold M is not known, if we are given samples that reside on M, all the coordinate realizations of the approximations of the Koopman operator can still be computed. Moreover, the rates of approximation above can still be shown to hold when restricted to a regularly embedded submanifold $M \subset X$. Since the submanifold is a set of zero measure as a subset of X, there is some loss of regularity that reduces the guaranteed rate of convergence. We outline this analysis in Section IV.

II. CONSTRUCTIONS IN RKH SPACES

As mentioned in Section I, H_X is an RKH space of real-valued functions over X. In this section, we review relevant definitions and properties of the RKH space H_X, the restricted RKH space of functions over the manifold $M \subset X$ H_M, and the pullback space $f^*(H_M)$ where $f : M \to M$. This section also includes a brief discussion of the interpolation and the projection operators defined on RKH spaces.

A. RKH Space H_X and H_M of Functions

A symmetric, continuous, real valued function $\mathfrak{K}_X : X \times X \to \mathbb{R}$, is a reproducing kernel if it is a positive type function, i.e. for any finite collection of points $\{\xi_i\}_{1 \leq i \leq n} \subseteq X$, the Grammian $\mathbb{K}_{X,n} := [\mathfrak{K}_X(\xi_i, \xi_j)]$ is a positive semi-definite matrix. All such positive type functions induce an reproducing kernel Hilbert (RKH) space H_X that is defined as $H_X := \overline{\text{span}}\{\mathfrak{K}_{X,x} \mid x \in X\}$, where $\mathfrak{K}_{X,x}(\cdot)$ is the kernel centered at $x \in X$ and is equal to $\mathfrak{K}_X(x, \cdot)$. The inner product $(\cdot, \cdot)_{H_X}$ of the Hilbert space H_X is defined as $(\mathfrak{K}_{X,x}, \mathfrak{K}_{X,y})_{H_X} := \mathfrak{K}_X(x,y)$ for any two functions $\mathfrak{K}_{X,x}, \mathfrak{K}_{X,y} \in H_X$ and for all $x,y \in X$. It satisfies the reproducing property $(f, \mathfrak{K}_{X,x})_{H_X} = f(x)$ for all $f \in H_X$ and $x \in X$. Not all Hilbert spaces are RKH spaces. A necessary and sufficient condition for a Hilbert space to be an RKH space is the boundedness of the evaluation functional $\mathcal{E}_x : f \to f(x)$ for any $x \in X$. In our analysis, we assume that the evaluation functional is in fact uniformly bounded, i.e. there exists a constant $\bar{k}$ such that $\|\mathcal{E}_x\| \leq \bar{k}$ for all $x \in X$. This assumption guarantees that the RKH space is embedded into the space of continuous function $C(X)$, that is, $H_X \hookrightarrow C(X)$. If the manifold $M = X$, the RKH space $H_M = H_X$. However, when $M \subset X$ and the intrinsic structure of M is not exactly known, we define the space H_M by restricting the kernel $\mathfrak{K}_X$ to $M \times M$. The restriction of $\mathfrak{K}_X$, $\mathfrak{K}_M : M \times M \to \mathbb{R}$, is defined as $\mathfrak{K}_M(x,y) := \mathfrak{K}_X|_{M \times M}(x,y)$ for all $x,y \in M$. Naturally, we can define the space H_M using the kernel $\mathfrak{K}_M$ similar to the way we defined H_X. The space H_M is itself an RKH space and its inner product is defined in terms of the kernel $\mathfrak{K}_M$. Alternatively, if R_M represents the restriction operator to M, we can define H_M as $H_M = R_M(H_X) := \{R_M f | f \in H_X\}$.

B. The Pullback RKH Spaces $\gamma^*(H_M)$ for $\gamma : S \to M$

The pullback space $\gamma^*(H_M)$ generated by the space of functions H_M and any mapping $\gamma : S \to \mathbb{R}$ is defined to be $\gamma^*(H_M) := \{g : S \to \mathbb{R} \mid g = h \circ \gamma, h \in H_M\}$ for any set S. By definition, the Koopman operator U_f maps an element of H_M to its pullback space $f^*(H_M)$. When H_M is a general normed vector space with the norm $\| \cdot \|_{H_M}$, the norm of the pullback space is defined as $\|g\|_{\gamma^*(H_M)} := \min\{\|h\|_{H_M} \mid g = h \circ \gamma, \ h \in H_M\}$. When H_M is an RKH space, which is what we assume in this paper, the pullback space $\gamma^*(H_M)$ is itself an RKH space with the kernel $\mathfrak{K}_{M,\gamma}$ defined as $\mathfrak{K}_{M,\gamma}(\tau, s) := \mathfrak{K}_M(\gamma(\tau), \gamma(s))$ for all $\tau, s \in S$. In other words, the kernel $\mathfrak{K}_{M,\gamma}$ generates the pullback space $\gamma^*(H_M)$, i.e. $\gamma^*(H_M) := \overline{\text{span}}\{\mathfrak{K}_{M,\gamma,s} \mid s \in S\}$ with $\mathfrak{K}_{M,\gamma,s} := \mathfrak{K}_M(\gamma(s), \gamma(\cdot))$ for each $s \in S$.

C. Interpolation and Projection

The space H_M discussed in the previous subsection is infinite-dimensional and the Koopman operator U_f maps this space to corresponding infinite-dimensional dimensional pullback space $f^*(H_M)$. We define the approximation of the Koopman operator in terms of a certain finite-dimensional subspace of H_M. Let $\Omega_n := \{\xi_1, \ldots, \xi_n\} \subseteq M$ be a set of n points, and let $H_{\Omega_n} := \text{span}\{\mathfrak{K}_{M,\xi_i} \mid \xi_i \in \Omega_n\}$ be the corresponding RKH space. We define the orthogonal projection operator $P_{\Omega_n} : H_M \to H_{\Omega_n}$ as the unique mapping that satisfies the identity $((I - P_{\Omega_n})h, g)_{H_M} = 0$ for all $g \in H_{\Omega_n}$ and $h \in H_M$. The projection operator decomposes the space H_M into $H_M = H_{\Omega_n} \oplus V_{\Omega_n}$, where $V_{\Omega_n} := \{f \in H_M \mid f|_{\Omega_n} = 0\}$. We define the interpolation operator $I_{\Omega_n} : H_M \to H_{\Omega_n}$ to be the unique operator that satisfies the interpolation conditions $(I_{\Omega_n} f)(\xi_i) = f(\xi_i)$ for all $\xi_i \in \Omega_n$ and $f \in H_M$. For RKH spaces, the interpolation operator is identical to the projection operator, in other words, $I_{\Omega_n} f = P_{\Omega_n} f$ for all $f \in H_M$.

D. Sobolev Spaces over Riemannian Manifolds M

Suppose we have a (smooth) Riemannian manifold M with metric g_p and inner product $(\cdot, \cdot)_{g_p}$ on the tangent space $T_p M$ at point $p \in M$. When r is an integer, the Sobolev space $W^{r,2}(\Omega)$ for a subset $\Omega \subseteq M$ contains all the functions in $L^2(\Omega)$ such that the norm induced by the inner product $(f,g)_{W^{k,2}(\Omega)} := \sum_{0 \leq j \leq r} \int_{\Omega} (\nabla^j f, \nabla^j g)_{g,p} d\mu(p)$ is bounded. In the above definition of the inner product, the term μ is the volume measure on the manifold M. Given a set of coordinates $(x^1, \ldots, x^d)$, the volume measure is $d\mu(x) := \sqrt{det(g)} dx^1 \ldots dx^d$. For $r > 0$, the Sobolev space $W^{r,2}(\Omega)$ is defined as an interpolation space between the integer order Sobolev space and $L^2(\Omega)$. A theorem we use to prove the results of this paper is a simplified version of the "many zeros" theorem [16], [17], [20] given below.

Theorem 1: Suppose that M is a smooth d-dimensional manifold. Let $t \in \mathbb{R}$ with $t > d/2$, $s \in \mathbb{N}_0$ with $0 \leq s \leq \lceil t \rceil - 1$. Then there are constants $h_M, C_M > 0$ such that for all $\Omega_n \subset \Omega$ such that the fill distance $h_{\Omega_n,M} \leq h_M$ and for all $u \in W^{t,2}(M)$ that satisfies $u|_{\Omega_n} = 0$, we have

$$\|u\|_{W^{s,2}(M)} \leq C_M h_{\Omega_n,M}^{t-s} \|u\|_{W^{t,2}(M)}.$$

E. Relationships between RKH Spaces and Sobolev Spaces

In this paper, we derive the convergence results and approximation rates when the RKH space H_M is embedded

in a Sobolev space $W^{r,2}(M)$ for real $r > 0$. When the manifold M is a d-dimensional, connected, smooth, Riemannian manifold having a positive radius of injectivity and bounded geometry, by the Sobolev embedding theorem, we have $W^{r,2}(M) \overset{i}{\hookrightarrow} C(M)$ for $r > d/2$. When this is true, we have $|\mathcal{E}_x f| = |f(x)| \leq \|f\|_{C(M)} \leq C\|f\|_{W^{r,2}(M)}$. This shows that the evaluation functional is bounded, which in turn implies that $W^{r,2}(M)$ is a RKH space when $r > d/2$. A discussion of these results can be found in [16], [17], [18].

III. APPROXIMATIONS OF THE KOOPMAN OPERATOR U_f

This section presents the principal results of this paper. We present error rates for two different types of approximations of the Koopman operator U_f, (i) the projection-based approximation $U_f^n := U_f P_{\Omega_n}$, and (ii) the data-dependent approximation $\mathfrak{U}_f^n := P_{\Omega_n}((P_{\Omega_n} g) \circ f)$.

We define the first approximation of the Koopman operator U_f^n as $U_f^n g = (P_{\Omega_n} g) \circ f$, where $f : M \to M$. When the samples are dense in the manifold M, we can express this finite-dimensional approximation using the relation

$$(U_f^n g)(x) = \sum_{1 \leq i,j \leq n} \mathbb{K}_{M,j,i}^{-1}(\Omega_n) g(\xi_i) \mathfrak{K}_{M,\xi_j}(f(x))$$

for all $x \in M$ and $g \in H_M$. In the above identity, the term $\mathbb{K}_M^{-1}(\Omega_n)$ represents the inverse of the Grammian matrix $\mathbb{K}_M(\Omega_n) := [\mathfrak{K}_M(\xi_m, \xi_n)]$ associated with the finite sample set Ω_n. From the above expression, we note that this approximation of the Koopman operator can be computed only when the function f is explicitly known.

For the data-driven approximation, we use the second approximation of the Koopman operator $\mathfrak{U}_f^n$. In this paper, when constructing the operator $\mathfrak{U}_f^n$, we assume that (i) the samples Ξ are dense in the manifold M, and (ii) the pullback space $f^*(H_M)$ is a subset of the RKH space H_M. Note that the projection operator $P_{\Omega_n} : H_M \to H_M$. The definition of the approximated Koopman operator $\mathfrak{U}_f^n$ makes sense only when the second assumption mentioned above is valid. A coordinate representation of the data-dependent approximation is given by

$$\mathfrak{U}_f^n g := \sum_{1 \leq i,j \leq n} \mathbb{K}_{M,j,i}^{-1}(\Omega_n) h(\xi_i) \mathfrak{K}_{M,\xi_j},$$

where $h(\xi_i) := \sum_{1 \leq p,q \leq n} \mathbb{K}_{M,q,p}^{-1}(\Omega_n) g(\xi_p) \mathfrak{K}_{M,\xi_q}(f(\xi_i))$.

Theorem 2: Suppose that M is a d-dimensional, connected, compact, Riemannian manifold without boundary, let $\mathfrak{K}_M : M \times M \to \mathbb{R}$ be a positive definite kernel that induces a native space H_M, and suppose that H_M is equivalent to the Sobolev space $W^{t,2}(M)$ for some $t \in \mathbb{R}$ that satisfies $d/2 < s \leq \lceil t \rceil - 1$ for a given $s \in \mathbb{N}$. Then there are constants $C_M, h_M > 0$ such that for all $\Omega_n \subset \Omega$ that satisfy $h_{\Omega_n, \Omega} \leq h_M$, we have

$$\|U_f g - U_f^n g\|_{f^*(W^{s,2}(M))} \leq C_M h_{\Omega_n, M}^{t-s} \|g\|_{W^{t,2}(M)}$$

for $g \in W^{t,2}(M)$.

Proof: Since $s > d/2$, the Sobolev embedding theorem implies that $W^{s,2}(M)$ is a RKH space, and therefore the pullback space $f^*(W^{s,2}(M))$ is a well-defined RKH space. By the definition of the pullback space we have

$$\|U_f g - U_f^n g\|_{f^*(W^{s,2}(M))} \leq \|U_f\| \|(I - P_{\Omega_n})g\|_{W^{s,2}(M)}.$$

By definition of the norm of the pullback space, we have $\|U_f g\|_{f^*(W^{s,2}(M))} \leq \|g\|_{W^{s,2}(M)}$, which implies that $\|U_f\| \leq 1$. Additionally, we know that $((I - P_{\Omega_n})g)|_{\Omega_n} = 0$ on Ω_n since the projection is identical to the interpolant over Ω_n. By the many zeros Theorem 1, we conclude that

$$\|U_f g - U_f^n g\|_{f^*(W^{s,2}(M))} \leq C_M h_{\Omega_n, M}^{t-s} \|g\|_{W^{t,2}(M)}.$$

∎

The bound above is stated in terms of the norm on the pullback space $f^*(H_M)$, which may seem rather abstract. The following theorem illustrates that such a bound naturally leads to a more intuitive pointwise bound.

Theorem 3: Suppose that the hypotheses of Theorem 2 hold. There are constants $C_M, h_M > 0$ such that for all $\Omega_n \subset \Omega$ that satisfy $h_{\Omega_n, \Omega} \leq h_M$, we have the pointwise bound

$$|(U_f g)(x) - (U_f^n g)(x)| \leq C_M h_{\Omega_n, M}^{t-s} \|g\|_{W^{t,2}(M)}$$

for all $g \in W^{t,2}(M)$ and $x \in M$.

Proof: First, we note that

$$|(U_f g)(x) - (U_f^n g)(x)| = |g(f(x)) - (P_{\Omega_n} g)(f(x))|$$
$$\leq \sup_{\eta \in M} |g(\eta) - (P_{\Omega_n} g)(\eta)| = \|(I - P_{\Omega_n})g\|_{C(M)}.$$

Since $s > d/2$, by the Sobolev embedding theorem, there exists a constant K such that $\|(I - P_{\Omega_n})g\|_{C(M)} \leq K\|(I - P_{\Omega_n})g\|_{W^{s,2}(M)}$. From Theorem 1, we can conclude that

$$|(U_f g)(x) - (U_f^n g)(x)| \leq C_M h_{\Omega_n, M}^{t-s} \|g\|_{W^{t,2}(M)}.$$

∎

The final, principal result of this paper uses the above to derive pointwise bounds for data-driven approximations of the Koopman operator.

Theorem 4: Suppose that the hypotheses of Theorem 2 holds. Furthermore, suppose that the mapping $f : M \to M$ is such that the pullback space $f^*(H_M) \hookrightarrow H_M$. Then there are constants $C_M, h_M > 0$ such that for all $\Omega_n \subset \Omega$ that satisfy $h_{\Omega_n, \Omega} \leq h_M$, we have the pointwise bound

$$|(U_f g)(x) - (\mathfrak{U}_f^n g)(x)| \leq C_M h_{\Omega_n, M}^{t-s} \|g\|_{W^{t,2}(M)}$$

for $g \in W^{t,2}(M)$ and $x \in M$.

Proof: Since $f^*(H_M) \subseteq H_M$, we know that $P_{\Omega_n} g \in H_M$ and $(P_{\Omega_n} g) \circ f \in f^*(H_M) \subset H_M$. By definition, we have

$$|(U_f g)(x) - (\mathfrak{U}_f^n g)(x)| \leq |(g \circ f)(x) - (P_{\Omega_n} g) \circ f)(x)|$$
$$+ |((I - P_{\Omega_n})((P_{\Omega_n} g) \circ f))(x)|.$$

Under the hypotheses of this theorem, we have $H_M \approx W^{t,2}(M) \hookrightarrow W^{s,2}(M) \hookrightarrow C(M)$. This implies that there

are positive constants K_1 and K_2 such that

$$|(U_f g)(x) - (\mathfrak{U}_f^n g)(x)| \leq \sup_{\eta \in M} |(((g - P_{\Omega_n}g) \circ f)(\eta)|$$
$$+ \sup_{\eta \in M} |((I - P_{\Omega_n})((P_{\Omega_n}g) \circ f))(\eta)|$$
$$\leq \|(I - P_{\Omega_n})g\|_{C(M)} + \|(I - P_{\Omega_n})((P_{\Omega_n}g) \circ f)\|_{C(M)}$$
$$\leq K_1 \|(I - P_{\Omega_n})g\|_{W^{s,2}(M)}$$
$$+ K_2 \|(I - P_{\Omega_n})((P_{\Omega_n}g) \circ f)\|_{W^{s,2}(M)}$$

Now we apply the many zeros Theorem 2 to each of the right hand side terms above. We know that $(I - P_{\Omega_n})g)|_{\Omega_n} = 0$, $(I - P_{\Omega_n})((P_{\Omega_n}g) \circ f))|_{\Omega_n} = 0$ since the projection operator P_{Ω_n} is identical to the interpolation operator on $\Omega_n \subset M$. By the many zeros theorem on the manifold M, we get

$$|(U_f g)(x) - (\mathfrak{U}_f^n g)(x)|$$
$$\leq C_1 h_{\Omega_n,M}^{t-s} \|g\|_{W^{t,2}(M)} + C_2 h_{\Omega_n,M}^{t-s} \|(P_{\Omega_n}g) \circ f\|_{W^{t,2}(M)}$$
$$\leq \max\{C_1, C_2\} h_{\Omega_n,M}^{t-s}(1+c)\|g\|_{W^{t,2}(M)},$$

where c is the constant of the embedding $f^*(H_M) \hookrightarrow H_M$. ∎

IV. NUMERICAL EXAMPLE AND CONCLUSIONS

In this section, we study the application of the derived bounds on rates of convergence to the classical model of a bouncing ball on a vibrating surface. The difference equation that defines the state trajectory is given by

$$\phi_{j+1} = \phi_j + \nu_j, \qquad \nu_{j+1} = \alpha\nu_j - \gamma\cos(\phi_j + \nu_j),$$

where ϕ and ν are the nondimensional impact time and the velocity after impact, respectively. The constants α and γ in the above equation represent the dissipation coefficient and force amplitude, respectively. We refer the reader to [21] for a more detailed discussion of this dynamical system. The red markers in Figure 1 show the state trajectory generated by this system when $\alpha = 1$ and $\gamma = 0.45$, $[\phi_0, \nu_0]^T = [0.1, 0]^T$ after 1024 iterations. The function $f : \mathbb{R}^2 \to \mathbb{R}^2$ in this case is given by $f([\phi_j, \nu_j]) \to [\phi_{j+1}, \nu_{j+1}]^T$. For purposes of illustration, we choose the observable function $g : \mathbb{R}^2 \to \mathbb{R}$ defined as $g([\phi, \nu]^T) = \phi + \nu$.

A. Challenges to Intrinsic Approximations

This example has been selected in part to emphasize some of the inherent difficulties when seeking to generate bounds on rates of approximation of Koopman operators by intrinsic methods. In view of Figure 1, it seems reasonable to believe that the samples Ξ are dense in a smooth, one-dimensional, regularly embedded submanifold M of $X := \mathbb{R}^2$. Even though this example is exceptionally straightforward, where the mapping $f : X \to X$ and the observable $g : X \to \mathbb{R}$ are known in closed form, it remains difficult to employ the bounds in Theorems 2 through 4 in an intrinsic approximation over M. To employ the results of these theorems, we would first need to define some Riemannian metric on M. Theoretically this is always possible if M is a smooth manifold. Subsequently we must define an appropriate kernel

$\mathfrak{K}_M : M \times M \to \mathbb{R}$ whose native space is equivalent to a Sobolev space. *In principle*, this too can be accomplished. For example, we can solve for the fundamental solution of a sufficiently high order of the Laplace-Beltrami operator over M, which could then be taken as the kernel of H_M. By definition we would obtain $H_M \approx W^{t,2}(M)$ for some $t > 0$, see [16] and the references therein for a general discussion. With such a definition of the kernel $\mathfrak{K}_M : M \times M \to \mathbb{R}$, the results of the theorems in this paper would then apply. However, even in this remarkably simple example, it is no simple feat to solve for the fundamental solution over M. Pragmatically speaking, we do not have a closed form expression for an atlas for M, and consequently we cannot solve the coordinate representations of the equation defining the fundamental solution. It would seem that constructing a kernel that is intrinsic to M would be prohibitively difficult in this case. We should note of course, that not all examples pose such problems for intrinsic approximations. If the samples Ξ of the semiflow are dense in some well-known manifold for which the solution of the Laplace-Beltrami operator equation is known, then the approximations and theorems in this paper are directly applicable.

B. Explicit Approximations

Fortunately, the theorems in this paper are easily applied for certain types of extrinsic approximations. We briefly outline the process. The Sobolev-Matern kernels $\mathfrak{K}_{X,\nu} : X \times X \to \mathbb{R}$ on $X = \mathbb{R}^2$ are known in closed form, and they induce a native space H_X that is contained in the Sobolev space $W^{\tau,2}(\mathbb{R}^p)$ for $\tau < 2\nu - p/2$. Note, the term ν is a positive parameter that defines a family of Sobolev-Matern kernels. By the trace theorem, the restriction $\mathfrak{K}_{M,\nu} := \mathfrak{K}_X|_M$ of the kernel $\mathfrak{K}_{X,\nu}$ induces a native space H_M over the manifold M that is contained in the Sobolev space $W^{t,2}(M)$, where $t < \tau - (p-d)/2$. In our example, a 1-dimensional manifold is contained in $\mathbb{R}^2$, and hence $p = 2$ and $d = 1$. Note that there is some loss of smoothness in restricting functions in $H_X \approx W^{\tau,2}(X)$ to the regularly embedded submanifold M in that $H_M \approx W^{t,2}(M)$.

In this simulation, we use the Sobolev-Matern kernel $\mathfrak{K}_{X,\nu=5/2}$, which has the form $\mathfrak{K}_{X,\nu=5/2}(x,y) = \mathcal{K}(\|x-y\|)$, where $\mathcal{K}(r) := \left(1 + \frac{\sqrt{5}r}{l} + \frac{5r^2}{3l^2}\right)\exp\left(-\frac{\sqrt{5}r}{l}\right)$. The term l is a positive parameter, and we obtained the numerical results of this paper with $l = 1e - 1$. Note that the above kernel is defined over $X = \mathbb{R}^2$ and its RKH space is contained in $W^{\tau,2}(\mathbb{R}^2)$, where $\tau < 4$.

The pointwise error $|U_f(x) - U_f^n(x)|$ in $\mathbb{R}^2$ for $n = 768$ is shown in Figure 1. The kernels for this simulation were centered at the first 768 data points generated by the dynamical system. As expected, the error is minimized over the manifold. The error plots for the data driven approximation of the Koopman operator is similar.

Figure 2 shows how the C^∞-norm error $\|U_f - U_f^n\|_\infty$ varies as the fill distance h is decreased. Since the manifold M is not explicitly defined, we use the Euclidean metric, which is equivalent to the intrinsic metric of M, to calculate the fill distance h. Since we are plotting the variables on a
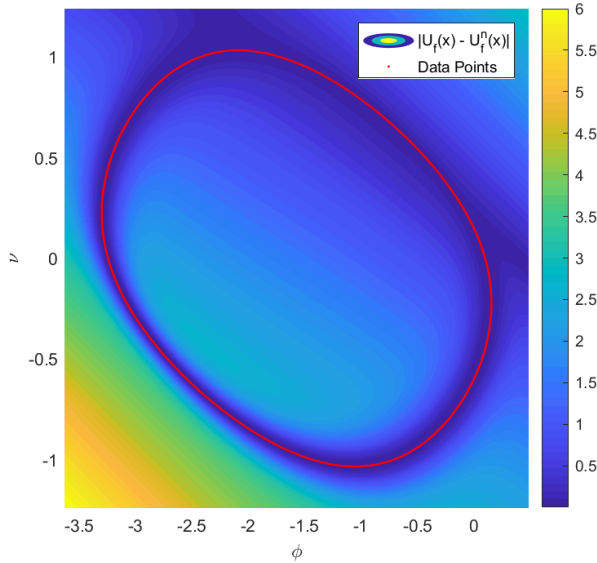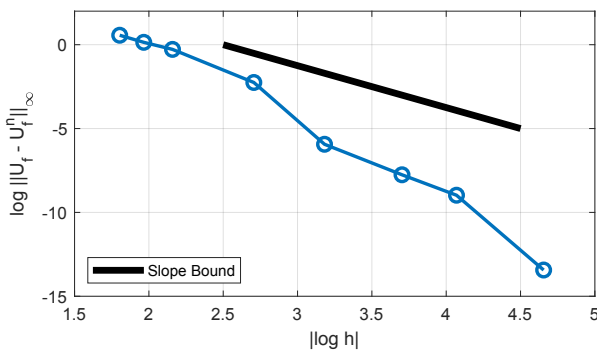
Fig. 1: Error Contour, U_f^n Approximation

Fig. 2: C^∞-norm Error, U_f^n Approximation

Fig. 3: C^∞-norm Error, $\mathfrak{U}_f^n$ Approximation ($\mathfrak{U}_f^n \equiv U_{d,f}^n$)

log scale, the slope of the error lines should be less than or equal to $t - s < 2.5$. Note, the constant $t < 3.5$ is defined by the choice of the kernel and the constant s satisfies $d/2 = 0.5 < s = 1 \leq \lceil 3.5 \rceil - 1$. Figure 3 shows the equivalent plot for the data-driven Koopman approximation. From these plots, it is clear that the error decays at a rate higher than the worst-case theoretical bound of $t - s < 2.5$.

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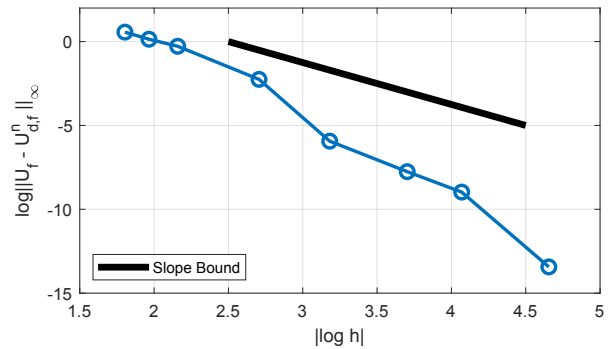[4] H. Zhang, C. W. Rowley, E. A. Deem, and L. N. Cattafesta, "Online Dynamic Mode Decomposition for Time-Varying Systems," *SIAM Journal on Applied Dynamical Systems*, vol. 18, no. 3, pp. 1586–1609, 2019.

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